Topological Insulators and Superconductors

Lecture #1: Topology and Band Theory
Lecture #2: Topological Insulators in 2 and 3 dimensions
Lecture #3: Topological Superconductors, Majorana Fermions and Topological quantum computation

General References:

M.Z. Hasan and C.L. Kane, RMP in press, arXiv:1002.3895

My collaborators:

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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
   - Bulk-Boundary correspondence
   - Higher dimensions
   - Topological Defects
The Insulating State

Characterized by energy gap: absence of low energy electronic excitations

Covalent Insulator
e.g. intrinsic semiconductor

Atomic Insulator
e.g. solid Ar

The vacuum

Covalent Insulator Diagram

Atomic Insulator Diagram

The vacuum Diagram

Silicon Diagram

E\text{\textit{g}}_\text{\textsubscript{\textit{a}}} \sim 1\text{ eV}

E\text{\textit{g}}_\text{\textsubscript{\textit{a}}} \sim 10\text{ eV}

E\text{\textit{g}}_\text{\textsubscript{\textit{a}}} = 2\text{ m}_e\text{c}^2
\sim 10^6\text{ eV}
The Integer Quantum Hall State

2D Cyclotron Motion, Landau Levels

Energy gap, but NOT an insulator

Quantized Hall conductivity:

\[ J_y = \sigma_{xy} E_x \]

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

Integer accurate to \(10^{-9}\)
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, \( g = \# \text{holes} \)

\( g=0 \) \hspace{1cm} \( g=1 \)

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

\[ \kappa = \frac{1}{r_1 r_2} \]

Gauss Bonnet Theorem:

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

Band Theory of Solids

Bloch Theorem:
Lattice translation symmetry
\[ T(R) |\psi\rangle = e^{ik \cdot R} |\psi\rangle \quad \Rightarrow \quad |\psi\rangle = e^{i k \cdot r} |u(k)\rangle \]

Bloch Hamiltonian
\[ H(k) = e^{-i k \cdot r} e^{i k \cdot r} \quad H(k) |u_n(k)\rangle = E_n(k) |u_n(k)\rangle \]

\( k \in \text{Brillouin Zone} \)
\( = \text{Torus, } T^d \)

Band Structure:
A mapping \( k \mapsto H(k) \)
(or equivalently to \( E_n(k) \) and \( |u_n(k)\rangle \) )

Topological Equivalence: adiabatic continuity
Band structures are equivalent if they can be continuously deformed into one another without closing the energy gap
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 \( C \)

\[ \gamma_C = \oint_C A \cdot d\mathbf{k} \]

Berry curvature:

\[ F = \nabla_k \times A \]

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

Famous example: eigenstates of 2 level Hamiltonian

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

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

\[ \gamma_C = \frac{1}{2} \left( \text{Solid Angle swept out by } \hat{\mathbf{d}}(k) \right) \]
Electric Polarization

\[ P = \frac{\text{dipole moment}}{\text{length}} \quad \nabla \cdot P = \rho_b \]

1D insulator

\[ Q = P \mod e \]

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

\[ Q = P \mod e \]

Polarization as a Berry phase:

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

P is not gauge invariant under “large” gauge transformations. This reflects the end charge ambiguity

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

Changes in \( P \), due to adiabatic variation are well defined and gauge invariant

\[ \Delta P = P_{\lambda=1} - P_{\lambda=0} = \frac{e}{2\pi} \oint_C A \, dk = \frac{e}{2\pi} \int_S \mathbf{F} \, dk \, d\lambda \]

gauge invariant Berry curvature
Su Schrieffer-Heeger Model

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

\( \delta t > 0 \)

\[ H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \hat{\mathbf{\sigma}} \]

\[ d_x(\mathbf{k}) = (t + \delta t) + (t - \delta t) \cos k a \]

\[ d_y(\mathbf{k}) = (t - \delta t) \sin k a \]

\[ d_z(\mathbf{k}) = 0 \]

Provided symmetry requires \( d_z(\mathbf{k}) = 0 \), the states with \( \delta t > 0 \) and \( \delta t < 0 \) are topologically distinct. Without the extra symmetry, all 1D band structures are topologically equivalent.

Peierl's instability → \( \delta t \)

\[ \text{Gap } 4|\delta t| \]

\[ P = 0 \] \( \delta t > 0 \) : Berry phase 0

\[ P = e/2 \] \( \delta t < 0 \) : Berry phase \( \pi \)
Domain Wall States

An interface between different topological states has topologically protected midgap states

Low energy continuum theory:
For small $\delta t$ focus on low energy states with $k \sim \frac{\pi}{a}$

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

Massive 1+1 D Dirac Hamiltonian

$$E(q) = \pm \sqrt{(\nu_F q)^2 + m^2}$$

“Chiral” Symmetry:
$$\{\sigma_z, H\} = 0 \rightarrow \sigma_z |\psi_E\rangle = |\psi_{-E}\rangle$$

Any eigenstate at $+E$ has a partner at $-E$

Zero mode: topologically protected eigenstate at $E=0$
(Jackiw and Rebbi 76, Su Schrieffer, Heeger 79)

$$m > 0$$

Domain wall bound state $|\psi_0\rangle$

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

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

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

\[
n = \frac{1}{2\pi} \int_{t=0}^{T} \int A(k) dk dt\]

\[
n = \frac{1}{4\pi} \int_{t=0}^{T} dk dt \hat{\mathbf{d}} \cdot \left( \partial_k \hat{\mathbf{d}} \times \partial_t \hat{\mathbf{d}} \right)
\]
Integer Quantum Hall Effect: Laughlin Argument

Adiabatically thread a quantum of magnetic flux through cylinder.

\[ E = \frac{1}{2\pi R} \frac{d\Phi}{dt} \]

\[ I = 2\pi R \sigma_{xy} E \]

\[ \Delta Q = \int_{0}^{T} \sigma_{xy} \frac{d\Phi}{dt} dt = \sigma_{xy} \frac{h}{e} \]

Just like a Thouless pump:

\[ H(T) = U^\dagger H(0)U \]

\[ \Delta Q = ne \quad \rightarrow \quad \sigma_{xy} = \frac{n e^2}{h} \]
TKNN Invariant

Thouless, Kohmoto, Nightingale and den Nijs 82

View cylinder as 1D system with subbands labeled by

\[ k_y^m(\Phi) = \frac{1}{R} \left( m + \frac{\Phi}{\phi_0} \right) \]

\[ \Delta Q = \sum_m \frac{e}{2\pi} \int_0^{\phi_0} d\Phi \int dk_x F(k_x, k_y^m(\Phi)) = ne \]

TKNN number = Chern number

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

\[ n = \frac{1}{2\pi} \int_{BZ} d^2k F(k) = \frac{1}{2\pi} \oint_C A \cdot dk \]

Distinguishes topologically distinct 2D band structures. Analogous to Gauss-Bonnet thm.

Alternative calculation: compute \( \sigma_{xy} \) via Kubo formula
Two band model \[ H = -t \sum_{<ij>} C_{Ai}^\dagger C_{Bj} \]

\[
H(k) = d(k) \cdot \vec{\sigma} \\
E(k) = \pm |d(k)|
\]

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

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

\[
H(\pm K + q) = \nabla \cdot \vec{\sigma} \cdot q \quad \text{Massless Dirac Hamiltonian}
\]

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

Break P or T symmetry:

$$H(\pm K + q) = v q \sigma + m_\pm \sigma_z$$

$$E(q) = \pm \sqrt{v^2 |q|^2 + m_\pm^2}$$

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

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
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

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

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

\[ E_0(k_y) = v_F k_y \]

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 cannot exist in a purely 1D system.

Chiral Dirac Fermions

\(|t|=1\)

Disorder
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
Generalizations

Higher Dimensions: "Bott periodicity" \( d \rightarrow d+2 \)

\[ d=4 : \text{4 dimensional generalization of IQHE} \]

Zhang, Hu ‘01

\[ \mathbf{A}_{ij} = \langle u_i(k) | \nabla_k | u_j(k) \rangle \cdot dk \]

Non-Abelian Berry connection 1-form

\[ \mathbf{F} = d\mathbf{A} + \mathbf{A} \wedge \mathbf{A} \]

Non-Abelian Berry curvature 2-form

\[ n = \frac{1}{8\pi^2} \int_T \text{Tr}[\mathbf{F} \wedge \mathbf{F}] \in \mathbb{Z} \]

2nd Chern number = integral of 4-form over 4D BZ

Boundary states: 3+1D Chiral Dirac fermions

Higher Dimensions:

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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:
\[ n \text{ specifies the number of chiral Dirac fermion modes bound to defect line} \]

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?

Burgers' vector