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.
Topological 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.

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

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

Topological Superconductivity

Proximity induced topological superconductivity
Majorana bound states, quantum information

Many real materials and experiments

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

Tantalizing recent experimental progress
Topological Band Theory

Lecture #1: Topology and Band Theory

Lecture #2: Topological Insulators in 2 and 3 dimensions
   Topological Semimetals

Lecture #3: Topological Superconductivity
   Majorana Fermions
   Topological quantum computation

General References:

“Colloquium: Topological Insulators”
M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. 82, 3045 (2010)

“Topological Band Theory and the Z2 Invariant,”
C. L. Kane in “Topological insulators”
Topology and 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
   - Bulk-Boundary correspondence
   - Weyl semimetal
   - Higher dimensions
   - Topological Defects
The Insulating State

atomic insulator

atomic energy levels

The Integer Quantum Hall State

2D Cyclotron Motion, $\sigma_{xy} = e^2/h$

Landau levels

What’s the difference? Distinguished by Topological Invariant
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

$$\kappa = \frac{1}{r_1 r_2}$$

$$\kappa = \frac{1}{r^2} > 0$$

$$\kappa = 0$$

$$\kappa < 0$$

Gauss Bonnet Theorem: $$\int_S \kappa dA = 4\pi (1 - g)$$

Band Theory of Solids

Bloch Theorem:

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

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

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

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 \( C \)

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

Berry curvature:

\[ F = \nabla_k \times A \]

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

Famous example: eigenstates of 2 level Hamiltonian

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

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

\[ \gamma_C = \frac{1}{2} \text{(Solid Angle swept out by } \hat{d}(k) \text{)} \]
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 = \( S^1 \)
Circumstantial evidence #1:

The polarization and the Berry phase share the same ambiguity:

They are both only defined modulo an integer.

- 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
Circumstantial evidence #2: \[ r \sim i \nabla_k \]

\[
\begin{align*}
P &= e \oint_{BZ} \frac{dk}{2\pi} \langle u(k) | r | u(k) \rangle \\
&= \frac{ie}{2\pi} \oint_{BZ} \langle u(k) | \nabla_k | u(k) \rangle
\end{align*}
\]

A slightly more rigorous argument:

Construct Localized Wannier Orbitals:

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

Wannier states are gauge dependent, but for a sufficiently smooth gauge, they are localized states associated with a Bravais Lattice point \( R \)

\[
P = e \langle \varphi(R) | r - R | \varphi(R) \rangle \\
= \frac{ie}{2\pi} \oint_{BZ} \langle u(k) | \nabla_k | u(k) \rangle
\]
Su Schrieffer Heeger Model

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

\[ \delta t > 0 \]

\[ \delta t < 0 \]

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

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

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

\[ d_z(k) = 0 \]

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:

\[
H \sigma_z |\psi_E\rangle = -E \sigma_z |\psi_E\rangle \quad \Rightarrow \quad \sigma_z |\psi_E\rangle = |\psi_{-E}\rangle
\]

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

An interface between different topological states has topologically protected midgap states

\[ \delta t > 0 \quad \delta t < 0 \]

Low energy continuum theory:
For small \( \delta t \) focus on low energy states with \( k \sim \pi / a \)

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

Massive 1+1 D Dirac Hamiltonian

\[ v_F = ta \quad m = 2\delta t \]

"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)

\[ m > 0 \quad \text{Domain wall bound state } \psi_0 \]

\[ m < 0 \quad \text{E}_{\text{gap}} = 2|m| \]

\[ \psi_0(x) = e^{-\int_{0}^{x} m(x') dx' / v_F} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \]
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.

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

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

\[ n = \frac{1}{2\pi} \int_{T^2} F dk dt \]

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.

\[ n = \frac{1}{4\pi} \int_{T^2} dkdtd \mathbf{d} \cdot (\partial_t \hat{\mathbf{d}} \times \partial_k \hat{\mathbf{d}}) \]
Integer Quantum Hall Effect: Laughlin Argument

Adiabatically thread a quantum of magnetic flux through cylinder.

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

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

\[ \Delta Q = \int_0^T \sigma_{xy} \frac{d\Phi}{dt} dt = \sigma_{xy} \frac{h}{e} \]

Just like a Thouless pump:

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

\[ \Delta Q = ne \rightarrow \sigma_{xy} = \frac{n e^2}{h} \]
View cylinder as 1D system with subbands labeled by \( k_y^m(\Phi) = \frac{1}{R} \left( m + \frac{\Phi}{\phi_0} \right) \)

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

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
TKNN Invariant

For a 2D band structure, define  \( A(\mathbf{k}) = -i \langle u(\mathbf{k}) | \nabla_{\mathbf{k}} | u(\mathbf{k}) \rangle \)

\[
n = \frac{1}{2\pi} \oint_{C_1} A \cdot d\mathbf{k} - \frac{1}{2\pi} \oint_{C_2} A \cdot d\mathbf{k} \in \mathbb{Z}
\]

\[
= \frac{1}{2\pi} \int_{BZ} d^2k F(\mathbf{k})
\]

Physical meaning: Hall conductivity  \( \sigma_{xy} = n \frac{e^2}{h} \)

Laughlin Argument: Thread magnetic flux \( \phi_0 = h/e \) through a 1D cylinder

Polarization changes by \( \sigma_{xy} \phi_0 \)

\( \Phi \propto k_y \)  \( \Delta P = ne \)
Graphene

Two band model \( H = -t \sum_{<ij>} C_{Ai}^{\dagger} C_{Bj} \)

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

\[
E(k) = \pm |\mathbf{d}(k)|
\]

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

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

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

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

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

Break P or T symmetry: \[ H(\pm \mathbf{K} + \mathbf{q}) = v \mathbf{q} \cdot \mathbf{\sigma} + m_{\pm} \sigma_z \]

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

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

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

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

\[ \psi_0(x) \sim e^{i k y y} e^{-\int m(x')dx'/v_F} \]

\[ E_0(k_y) = v_F k_y \]

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

$N_R$ ($N_L$) = # 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
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

\[ H(k_0 + q) = \mathbf{v}(q_x \sigma_x + q_y \sigma_y + q_z \sigma_z) \]
\[ (\text{or } \mathbf{v}_{ia} q_i \sigma_a \text{ with } \det[\mathbf{v}_{ia}] > 0) \]

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

Surface BZ

$k_z$, $k_y$, $k_x$

$n_1=n_2=0$

$n_0=1$

$E_F$, $k_z=k_1$, $k_2$

$E_F$, $k_z=k_0$
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

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

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

Boundary states : 3+1D Chiral Dirac fermions

Higher Dimensions : “Bott periodicity”  

$d \rightarrow d+2$

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>no symmetry</td>
<td>0</td>
<td>Z</td>
<td>0</td>
<td>Z</td>
<td>0</td>
<td>Z</td>
<td>0</td>
<td>Z</td>
</tr>
<tr>
<td>chiral symmetry</td>
<td>Z</td>
<td>0</td>
<td>Z</td>
<td>0</td>
<td>Z</td>
<td>0</td>
<td>Z</td>
<td>0</td>
</tr>
</tbody>
</table>

Zhang, Hu ‘01
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

\[ n = \frac{1}{2\pi} \mathbf{G}_c \cdot \mathbf{B} \]

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

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