Topological Insulators: Some Basic Concepts

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References for This Lecture

Charlie Kane’s “pedagogical lectures” (highly recommended):

http://www.physics.upenn.edu/~kane/

My course notes:

http://www.physique.usherbrooke.ca/pages/en/node/8291

…and references therein
Introduction
Insulators (before 1980)

In insulators, an energy gap separates empty and filled electronic states at \( T=0 \).
(In contrast, metals have partially filled bands at \( T=0 \))

**Examples:**
Covalent insulators (e.g. GaAs),
atomic insulators (e.g. solid Ar),
vacuum.

Due to the energy gap, insulators do not conduct electricity under weak, time-independent electric fields.

This talk is about gapped systems that *do* conduct electricity.
Insulators (after 1980)

Quantum Hall insulator

In spite of bulk energy gap, the edges are metallic.
Metallic edge states are robust.
Hall conductivity is perfectly quantized.

Why is the quantization independent of sample details?

Why can some gapped systems conduct whereas other do not?
Insulators (after 2005)

Quantum Spin Hall insulator

Spin-up electrons

Spin-down electrons

Made possible by spin-orbit coupling

Metallic edge states are robust under non-magnetic perturbations

CdTe  HgTe  CdTe
Insulators (after 2007)

3D Time-reversal invariant topological insulators

BiSb, BiTe, BiSe…

Strong spin-orbit coupling

Surface states:

Massless Dirac fermions

Dirac cones robust under non-magnetic perturbations
Band Theory
Elements of Traditional Band Theory

Non-interacting electrons moving in a perfectly periodic array of atoms

\[ H |\Psi_{kn}\rangle = E_{kn} |\Psi_{kn}\rangle \]

**Eigenstate**

**Hamiltonian**

**Eigen-energy**

Energies and wave functions have the periodicity of the reciprocal lattice.

**Bloch’s theorem:**

\[ |\Psi_{kn}\rangle = e^{i\mathbf{k} \cdot \mathbf{r}} |u_{kn}\rangle \]

**Periodic part**

**Bloch Hamiltonian:**

\[ h(k) = e^{-i\mathbf{k} \cdot \mathbf{r}} H e^{i\mathbf{k} \cdot \mathbf{r}} \]

\[ h(k) |u_{kn}\rangle = E_{kn} |u_{kn}\rangle \]

**Crystal momentum** \( k \) is a good quantum number

\( n \) is the **band** label

1st Brillouin zone (BZ)
Elements of Topological Band Theory

**Berry phase:** [M. Berry, 1983]

Consider a Hamiltonian that depends on an external (vector) parameter $\mathbf{R}$.

\[ H(\mathbf{R}) \]

Imagine that $\mathbf{R}$ changes in time adiabatically.

What is the time evolution of the wave function?

Initial state: $|\psi(t = 0)\rangle = |n, \mathbf{R}(0)\rangle$

State at time $t$: $|\psi(t)\rangle = e^{i\theta(t)}|n, \mathbf{R}(t)\rangle$ (adiabaticity)

\[ \theta(t) = \frac{1}{\hbar} \int_0^t dt' E_n(\mathbf{R}(t')) - i \int_C d\mathbf{R} \cdot \langle n\mathbf{R}| \frac{d}{d\mathbf{R}} |n, \mathbf{R}\rangle \]

Dynamical phase.  

Berry phase (Geometrical phase)
Elements of Topological Band Theory

Berry connection: \[ A_n(R) = i \langle n, R| \nabla_R |n, R \rangle \]

Berry phase: \[ \gamma_n = \int_C A_n(R) \cdot dR \]

Reminiscent of phase of a particle in an EM field.

*The Berry connection is analogue to a vector potential.*

Thus, it is not gauge-invariant unless \( C \) is a closed loop.

Stokes’ theorem: \[ \oint_C A_n(R) \cdot dR = \int_S dS \cdot [\nabla_R \times A_n(R)] \]

Berry curvature: \[ F_n(R) = \nabla_R \times A_n(R) \]

*The Berry curvature is analogue to a magnetic field.*

Thus, it is gauge-invariant.
Elements of Topological Band Theory

Chern number:
Consider a closed surface $S$, such as

$$n_{\text{Chern}} = \frac{1}{2\pi} \oint_S \mathbf{F}_n(\mathbf{R}) \cdot d\mathbf{S}$$

The Chern number is an integer. It is also a topological invariant, i.e. independent of the details of the Hamiltonian.

Analogies:

**Electric field**  
**Gauss’ Law:**  
$$\oint_S \epsilon \mathbf{E} \cdot d\mathbf{S} = e \times \text{integer}$$

**Gaussian curvature**  
**Gauss-Bonnet theorem:**  
$$\frac{1}{4\pi} \oint_S \kappa \ dS = 1 - g$$  
“Genus” = number of holes
Elements of Topological Band Theory

Example: two-level system (e.g. spin 1/2 particle in a magnetic field)

\[ h(d) = d \cdot \sigma \]

Vector \( d \) plays the role of parameter \( R \)

Eigenstates: \( |\pm\rangle \) \quad Eigenvalues: \( E_{\pm} = \pm |d| \)

Berry curvature: \( F_{\pm} = \pm \frac{d}{2d^3} \)

Field of a monopole located at band degeneracy points.

\( \text{Berry phase} = \frac{1}{2} \) (solid angle subtended by \( C \))

Chern number=monopole charge inside closed surface
Band Topology in 1D
Electric Polarization of a 1D Insulator

Electric polarization = dipole moment per unit volume.

Polarization charge \( \rho = -\partial_x P \)

Polarization current \( \mathbf{j} = \partial \mathbf{P} / \partial t \)

Electrical polarization defined only modulo \( e \times \) integer
Relation between electric polarization and Berry phase

[Resta & Vanderbilt, 1994]

\[ P = \frac{e}{2\pi} \sum_{n \in \text{occ}} \int_{BZ} A_n(k) \, dk \]

Berry connection. \( k \) plays the role of \( R \)

\[ A_n(k) = i \langle u_{kn} | \frac{\partial}{\partial k} | u_{kn} \rangle \]

Berry phase defined modulo \( 2\pi \rightarrow P \) defined modulo \( e \times \text{integer} \)

Link between quantum mechanics and classical electrostatics.
Thouless Charge Pump (1983)

1D insulator under a **time-periodic perturbation**.

**Bloch Hamiltonian:**

\[ h(k, t) = h(k, t + \tau) \]

What is the charge pumped in one cycle of the external perturbation?

\[ Q = \int_0^\tau dt \frac{\partial P}{\partial t} = P(t = \tau) - P(t = 0) \equiv \Delta P \]

\[ \Delta P = \frac{e}{2\pi} \sum_{n \in \text{occ}} \oint_C A_n(R) \cdot dR \]
1D lattice, spinless electrons, half filling.

\[
h(k) = d_x(k)\sigma^x + d_y(k)\sigma^y
\]

How does \(d\) change as \(k\) runs from \(-\pi/a\) to \(\pi/a\) ?

Topological quantum phase transition.

Symmetry-protected topological phases.
Emergence of Dirac Fermions at low energies:

$$k = \pi/a - q$$

$$qa \ll 1$$

$$h(q) \simeq m\sigma^x + vq\sigma^y$$

1D Dirac Hamiltonian

$$m \equiv 2\delta t$$

Dirac mass

$$\nu \equiv at$$

Velocity of Dirac fermion
Emergence of zero modes at “domain walls”

\[ h(z) \simeq m(z)\sigma^x - iv\sigma^y \partial_z \]

Jackiw-Rebbi zero mode: localized at domain wall, decay length \( v/m_0 \)

Insensitive to details of the Hamiltonian.

This result can be generalized to 2 and 3 dimensions.
Band Topology in 2D
Quantum Hall Insulator

\[ H = \frac{1}{2m} \left[ p_x^2 + \left( p_y - \frac{eB}{c} x \right)^2 \right] \]

(Landau gauge)

\( p_y \) is a good quantum number.

In the \( x \)-direction, a harmonic oscillator with frequency \( \omega_c \) centered at \( c p_y / (eB) \)

\[ E_n = \omega_c (n + 1/2) \]

\( \omega_c = eB / (mc) \)
The Hall conductivity of a 2D band insulator is always quantized

\[ j = e \sum_{k_n} \langle \psi_{k_n} | v | \psi_{k_n} \rangle f_{k_n} \]

Electric current in a crystal.
Vanishes in equilibrium.

An applied electric field can induce a current in two ways:

(i) By changing the population of the states: \( \delta f_{k_n} \)

(ii) By changing the eigenstates: \( \delta | \psi_{k_n} \rangle \)

\[ \sigma_{xy} = \frac{e^2}{h} \sum_{n \in \text{occ}} \frac{1}{2\pi} \int_{S} dS \cdot F_n(k) \]

Chern number

Chern number vanishes in presence of time-reversal symmetry
Edge states in quantum Hall insulators:

Assume infinite length along $y$, finite length along $x$.

LLs bend near sample edge. Fermi level intersects LLs at the edge.

$\# \text{ of edge states at the Fermi level} = \# \text{ of occupied bulk LLs} = \text{total Chern number of occupied LLs}$

Electrons on same edge move along the same direction.

Electrons on opposite edges move along the opposite directions.

Robustness against backscattering
Inversion and time reversal symmetry require 2D Dirac points at zeros in Berry's phase. Two band model

\[ E_H(q) = \pm \frac{\hbar v}{2m} q^2 \]

Novoselov et al. '05 around Dirac point

\[ k = \pm \frac{\hbar v}{m} q \]

Graphene Massless Dirac Hamiltonian

\[ H = \left( \begin{array}{cc} 0 & d(k) \sigma_z \\ \sigma_z d^T(k) & 0 \end{array} \right) \]

One orbital per site
Two atoms per unit cell (A and B)
No spin (for now)

A/B pseudospin

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

Emergence of massless Dirac fermions at low energies:

K/K' pseudospin

\[ h(q) = \nu \tau^z \sigma_x q_x + \nu \sigma^y q_y \]

Momentum measured from Dirac node

Due to time-reversal symmetry and inversion symmetry, \( d_z = 0 \)
How to make spinless graphene insulating

\[ h(q) = \nu \tau^z \sigma^x q_x + \nu \sigma^y q_y + d_z(q) \sigma^z \]

Need to break either time-reversal symmetry or inversion symmetry

(i) Break inversion symmetry

\[ d_z(q) = m_S \]

Semenoff insulator (1984)

(ii) Break time-reversal symmetry

\[ d_z(q) = m_H \tau^z \]

Haldane insulator (1988) [a.k.a. Chern insulator]
Chern number in spinless graphene

“Partial” Chern number for Dirac fermion at $K$:

$$n_K = \frac{1}{2} \text{sgn}(v_K^x v_K^y m_K)$$

(similarly for $K'$)

Total Chern # of a band:

$$n_{\text{Chern}} = n_K + n_{K'}$$

Semenoff insulator:

$$m_K = m_{K'}$$

$\text{Trivial insulator}$

$\text{Topological insulator}$

Haldane/Chern insulator:

$$m_K = -m_{K'}$$

$$n_{\text{Chern}} = \text{sgn}(m_H)$$
Edge states

\[ m(z) \]

Chern insulator

Vacuum

\[ m_K \]

\[ m_{K'} \]

Propagating mode localized along edge

\[ K' \]

\[ K \]

Quantum Hall effect without magnetic field (1988)

\[ \sigma_{xy} = \frac{e^2}{h} \text{sgn}(m_H) \]
Kane-Mele model (2005)

One orbital per site
Two atoms per unit cell (A and B)
Include spin

Low-energy effective Hamiltonian:

\[ h(q) = v_x \tau^z \sigma^x q_x + v_y \sigma^y q_y + \lambda_{so} \tau^z \sigma^z s^z \]

Opens a gap at \( K \) and \( K' \) without breaking any symmetries

\( s^z \) is conserved.

Spin-degenerate energy spectrum.
Two copies of a Haldane/Chern insulator

\[ h(\mathbf{q}) = v_x \tau^z \sigma^x q_x + v_y \sigma^y q_y + \lambda_{so} \tau^z \sigma^z s^z \]

**Spin-up electrons:**
Haldane/Chern insulator with mass \( m_H = +\lambda_{so} \)

**Spin-down electrons:**
Haldane/Chern insulator with mass \( m_H = -\lambda_{so} \)

Total Chern number: \( n_\uparrow + n_\downarrow = 0 \)

"Spin Chern number": \( n_\uparrow - n_\downarrow = 2 \text{sgn}(\lambda_{so}) \)
**Spin-Hall conductivity:**

\[
\sigma_{xy}^s = \sigma_{xy}^\uparrow - \sigma_{xy}^\downarrow = (n^\uparrow - n^\downarrow) \frac{e^2}{h}
\]

Quantum spin-Hall insulator

**Edge states**

Time-reversal symmetry $\Rightarrow$

(i) spin-up and spin-down edge states counter-propagate.

(ii) edge states are degenerate at $k=0$ (Kramer’s degeneracy).
Practical issue: $\lambda_{so} < 1\text{mK}$

Alternative systems: HgTe/CdTe, InAs/GaSb, silicene,…

Fundamental issue: In general spin is not conserved along any direction

One can no longer think of two decoupled copies of a Chern insulator. Likewise, the spin-Chern number is ill-defined.

However, the Kane-Mele edges states remain robust so long as the bulk gap does not close. Symmetry-protected topological phase.

A (non-Chern) topological invariant is responsible for this robustness. This is the $\mathbb{Z}_2$ invariant. Its inception and development in 2D and 3D crystals (2005-2007) have led to an explosion of research in topological insulators.
Topological invariants in interacting systems

So far, we have discussed the band topology in terms of the single-particle wave functions.

How to capture the band topology of interacting systems beyond the mean field approximation?

**Topological Hamiltonian**

Full Green’s function (zero Matsubara frequency)

Electron self-energy (zero Matsubara frequency)

Non-interacting Hamiltonian

Use the eigenstates of $h_{\text{eff}}(\mathbf{k})$ to calculate the Chern number and $Z_2$ invariant in interacting systems.