Topological Insulators in 2D and 3D

I. Introduction
   - Graphene
   - 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
Energy gaps in graphene:

\[ H = v_F \sigma \cdot p + V \]

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

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)

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

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: $|\text{Haldane}|^2$ (conserves $S_z$)

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

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
Time Reversal Symmetry: \([H, \Theta] = 0\)

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

Spin ½: \(\Theta\begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = \begin{pmatrix} \psi_\downarrow^* \\ -\psi_\uparrow^* \end{pmatrix}\)
\(\Theta^2 = -1\)

Kramers’ Theorem: for spin ½ all eigenstates are at least 2 fold degenerate

Proof: for a non degenerate eigenstate

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

Consequences for edge states:

States at “time reversal invariant momenta” \(k^* = 0\) and \(k^* = \pi/a\) (=\(-\pi/a\)) 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 $\mathbb{Z}_2$ 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 $\mathbb{Z}_2$ topological invariant ($\nu = 0, 1$)

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

$\nu = 0$: Conventional Insulator

$\nu = 1$: Topological Insulator

Even number of bands crossing Fermi energy

Odd number of bands crossing Fermi energy

Kramers degenerate at time reversal invariant momenta $k^* = -k^* + G$
Physical Meaning of $Z_2$ Invariant

Sensitivity to boundary conditions in a multiply connected geometry

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

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

$\Delta Q = N\ e$

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 $\mathbb{Z}_2$ invariant

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

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

- 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
V is easier to determine if there is extra symmetry:

1. $S_z$ conserved: independent spin Chern integers:

   $$ n_{\uparrow} = - n_{\downarrow} \quad \text{(due to time reversal)} $$

   **Quantum spin Hall Effect:**

   $$ \nu = n_{\uparrow,\downarrow} \mod 2 $$

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.
Quantum Spin Hall Effect in HgTe quantum wells

Theory: Bernevig, Hughes and Zhang, Science ‘06

Hg$_x$Cd$_{1-x}$Te

\( d < 6.3 \text{ nm} : \text{Normal band order} \)
\( d > 6.3 \text{ nm} : \text{Inverted band order} \)

Conventional Insulator
\[ \prod \xi_{2n}(\Lambda_a) = +1 \]

Quantum spin Hall Insulator with topological edge states
\[ \prod \xi_{2n}(\Lambda_a) = -1 \]

\[ \Gamma_6 \sim s \]
\[ \Gamma_8 \sim p \]

Band inversion transition:
Switch parity at \( k=0 \)

\[ E_{\text{gap}} \sim 10 \text{ meV} \]
Experiments on HgCdTe quantum wells

Expt: König, Wiedmann, Brune, Roth, Buhmann, Molenkamp, Qi, Zhang  Science 2007

Measured conductance $2e^2/h$ independent of $W$ for short samples ($L < L_{\text{in}}$)

$d < 6.3 \text{ nm}$

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<th>Band Order</th>
<th>Insulator Type</th>
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<td>Normal</td>
<td>Conventional</td>
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$d > 6.3 \text{ nm}$

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<tr>
<td>Inverted</td>
<td>QSH</td>
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Landauer Conductance $G = 2e^2/h$

$T = 30 \text{ mK}$

$G = 0.01 \frac{e^2}{h}$

$G = 0.3 \frac{e^2}{h}$

$G = 2\frac{e^2}{h}$
3D Topological Insulators

There are 4 surface Dirac Points due to Kramers degeneracy

$E_k = \Lambda a k = \Lambda b$

Surface Brillouin Zone

$\nu_0 = 0$: 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

\[ (-1)^\nu = \prod_{a=1}^{4} \delta(L_a) \]

\[ \delta(L_a) = \frac{\text{Pf}[w(L_a)]}{\sqrt{\det[w(L_a)]}} \]

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

Weak Topological Invariants (vector):

\[ (-1)^{\nu_i} = \prod_{a=1}^{4} \delta(L_a) \quad \text{plane} \]

\[ G_v = \frac{2\pi}{a} \left( \nu_1, \nu_2, \nu_3 \right) \]

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

Strong Topological Invariant (scalar)

\[ (-1)^{\nu_o} = \prod_{a=1}^{8} \delta(L_a) \]
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

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

$n$ 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:

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

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

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

Gauge invariant up to an even integer.
Predict Bi$_{1-x}$Sb$_x$ is a strong topological insulator: (1 ; 111).
**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 $M$

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**Bi$_2$Se$_3$**

**ARPES Experiment:** Y. Xia et al., Nature Phys. (2009).


- $\nu_0; (\nu_1, \nu_2, \nu_3) = 1;(000)$: 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; 1/4 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

Exotic States when broken symmetry leads to surface energy gap:
- Quantum Hall state, topological magnetoelectric effect
  Fu, Kane ‘07; Qi, Hughes, Zhang ‘08, Essin, Moore, Vanderbilt ‘09
- Superconducting state
  Fu, Kane ‘08
**Surface Quantum Hall Effect**

**Orbital QHE:**  
$E=0$ Landau Level for Dirac fermions. “Fractional” IQHE

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

**Anomalous QHE:**  
Induce a surface gap by depositing magnetic material

\[ H_0 = \psi^\dagger \left( -i\tau \tilde{\nabla} - \mu + \Delta_M \sigma_z \right) \psi \]

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

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

**Chiral Edge State at Domain Wall:**  
\[ \Delta_M \leftrightarrow -\Delta_M \]
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.

- \( \Delta L = \alpha E \cdot B \)
- \( \alpha = \theta \frac{e^2}{2\pi h} \)
- TR sym.: \( \theta = 0 \) or \( \pi \) mod \( 2\pi \)

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<tr>
<th>( \Delta L )</th>
<th>formula</th>
<th>“uncertainty quantum”</th>
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<tbody>
<tr>
<td>( P \cdot E )</td>
<td>( \frac{e}{2\pi} \int_{BZ} \text{Tr}[A] )</td>
<td>( e ) (extra end electron)</td>
</tr>
<tr>
<td>( \alpha E \cdot B )</td>
<td>( \frac{e^2}{4\pi^2h} \int_{BZ} \text{Tr}[A \wedge dA + \frac{2}{3} A \wedge A \wedge A] )</td>
<td>( e^2 / h ) (extra surface quantum Hall layer)</td>
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