Berry Phases, Anomalous Hall Effect, and spin-Hall effect

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An overview of novel Hall effect phenomena driven by Berry phase mechanisms rather than the Lorentz force
Hall Effect

\[ J^a = \sigma \_D^b E^b + \sigma \_H^a E^b \]

(electric) Current density

- Hall effect is the non-dissipative component of a current that flows in response to an electric field
- Present when the conduction occurs in the presence of broken time-reversal symmetry
- Can be an intrinsic property of a “clean” conducting medium
- Usual effect is when T-breaking is due to a uniform magnetic field (Lorentz Force)

Hall

Non-dissipative
\( E \cdot \vec{J}_H = 0 \)
\( \sigma \_H^a \) antisymmetric

\[
\begin{array}{cccc}
\vec{J} & \sigma \_D & \vec{E} & \vec{B} \\
\text{Time-reversal} & \text{odd} & \text{odd} & \text{even} & \text{odd} \\
\text{Spatial inversion} & \text{odd} & \text{even} & \text{odd} & \text{even} \\
\end{array}
\]

\[
\sigma \_H^a = \frac{n e}{B^2} \\
\text{electron density}
\]
Conventional Hall effect in metals

- If there is a magnetic field $\overrightarrow{B} \perp$ to the current density $\overrightarrow{J} = ne \overrightarrow{v}$, there must be a Hall field

$$\overrightarrow{E}_H = -u_B \times \overrightarrow{B}$$

- To balance it in steady state, so

$$P_{xy} = R_0 B^2, \quad R = \frac{1}{ne}$$

- But in ferromagnets, one often sees

$$P_{xy} \sim P_{xy}^0 + R_0 B^2$$

- Intercept $\to B \to 0$!

- Field strong enough to align domains $\to B^2$
Dissipationless Anomalous Hall Current in the Ferromagnetic Spinel CuCr$_2$Se$_{4-x}$Br$_x$.

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example of a very large AHE
- There is apparently a $\vec{B}$-independent force $1$ to the drift velocity (dissipationless) that is being balanced by the Hall field.

- $P_{xy} \propto M^2$ magnetization (aligned in 2-direction)

- What non-Lorentz force is deflecting The electrons

- Is it INTRINSIC or EXTRINSIC?
  (a property of the "clean" material, or of impurities and disorder?)
It is now clear that both extrinsic and intrinsic regimes of the anomalous Hall effect (AHE) occur.

INTRINSIC:
(dominate at intermediate temperature)

{ Karplus- Luttinger Formula
  "anomalous velocity", Berry Phases.

EXTRINSIC
(dominate at low temperatures)

{ Skew Scattering
  Side-Jump Scattering

All these effects are absent in "naive" (Stoner) theories of ferromagnets that ignore spin-orbit coupling effects.
• The Hall effect requires \underline{Broken time-reversal}

\underline{Symmetry}

\[ E_a = P_{ab} J^b \]

\[ J^a = \sigma^{ab} E_b \]

\[ \sigma_{ab} = \left( \frac{\partial J^a}{\partial E_b} - \frac{\partial J^b}{\partial E_a} \right) \right|_{E=0} \]

<table>
<thead>
<tr>
<th>E</th>
<th>B</th>
<th>M</th>
<th>J</th>
<th>\sigma_{ab}</th>
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<tbody>
<tr>
<td><strong>Time reversal</strong></td>
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<td><strong>Spatial inversion</strong></td>
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\[ \sigma_{ab} = 0 \quad \text{if Time-reversal symmetry is present.} \]
"Spin-Hall effect.\) (unbroken T-reversal sym.)

\[ M_a = \mathbf{f}_a^b \mathbf{J}^b \]

Magnetization \quad current

T-reversal

odd \quad even \quad odd

an electric current could have a \"Spin-Hall\" effect where a magnetization is generated by a current, even if time-reversal is unbroken, \(\text{but only as a consequence of spin-orbit coupling}\).

- Can the non-Lorentz forces responsible for AHE also give a SHE?
• Rather than \( \rho_{ab} \), focus on \( \sigma_{ab} \), given by Kubo formula

\[ J^a = \sigma_{ab} E_b. \]

• Strøda formula. (V. Fundamental!)

\[ \sigma_{ab} = \lim_{E \to 0} \left( \frac{\partial J^a}{\partial E_b} - \frac{\partial J^b}{\partial E_a} \right) = \epsilon^{abc} \frac{\partial f}{\partial B_c} \]

Dissipationless antisymmetric part of conductivity tensor

• This will allow \( \sigma_{ab} \) to be investigated by looking at response of conduction electron density to changes in (uniform) magnetic flux.
example \ Free electron gas (Drude model)

\[ \sigma_{xy} = \frac{ne}{B^2} \]

\[ \rho = ne = \sigma_{xy} B^2 \]

\[ \sigma_{xy} = \frac{\rho}{B^2} \]

example \ Integer quantum Hall effect (2D)

Landau levels, \( \varepsilon_n = (n+\frac{1}{2}) \frac{eB^2}{m} \).

\( \omega = \varepsilon_n A = \frac{e^2}{h} B \times \tau \xrightarrow{\text{number of filled levels}} \text{integer} \)
• General (Fractional) QHE:

\[ \sigma_{xy}^H = \nu \frac{e^2}{h} \]
\[ \nu = \frac{p}{q} \text{ rational} \]

For non-interacting electrons, WITH NO STATES (IN BULK) AT FERMI ENERGY,

\[ [\mathbb{R}^2] \rightarrow \sigma_{xy}^H = \nu \frac{e^2}{h} \quad \nu = \text{integer} \quad \text{2D} \]

• Generalization to 3D, no states at Fermi level (in bulk), periodic system, non-interacting electrons.

\[ [\mathbb{R}^3] \rightarrow \sigma_{ab}^H = \frac{1}{2\pi} \frac{e^2}{h} \epsilon_{abc} G_c \quad \text{3D} \]

\[ \text{a reciprocal vector} \]

(3D (integer) quantized Hall effect)

\[ \text{periodic array of 2D (I)QHE planes} \]
\[ G = \frac{2\pi}{d} \text{ reciprocal vector} \]
\[ H = \left( \frac{\vec{p} - e\vec{A}}{2m} \right)^2 + V(x) \]

- Translationaly invariant in y-direction.
- Apply periodic boundary conditions.
  \[ \vec{A} = B x \hat{y} \]
  \[ \psi(x, y + L_y) = \psi(x, y) \]

\[ \phi_y = \frac{2\pi m^*}{e B} = e B \xi_n \]

- Gapless excitations localized at edge.

\[ \psi_y = \frac{\partial \psi}{\partial \phi_y} \]  one-way motion

- "Spectral flow" to change number of states below Fermi level (occupied states) as \( B^2 \) changes.
(Integer) quantum Hall effect \( \nu = 1/2 \)

 Bulk region with quantized

\[ \sigma_{xy} = \nu e^2 / h \]

region with

\[ \sigma_{xy} = 0 \]


\[ l \]


gapless "chiral" edge states, with group velocities in same direction, (fixed by sign of \( \nu \))
* From the 2D Free electron Landau level model ($B \neq 0$) we see that $\sigma_{xy}$ is quantized, with chiral edge states needed for "spectral flow" as $B$ changes, if the "bulk" region is gapped (no bulk states at Fermi level).

* What about the "anomalous" case with $B = 0$ (no Landau levels, just Bloch states to give a gap at the Fermi level)?

Same principles work, but effect derives from **non-Lorentz force**! (Berry phases)
Classic Berry Phase:

$|\hat{\Omega}\rangle$ spin aligned along $\hat{z}$ axis
so $\hat{z} \cdot \hat{S} |\hat{\Omega}\rangle = \hat{S} |\hat{\Omega}\rangle$

$\hat{\Omega}$ evolves around closed path $\Pi$

$|\hat{\Omega}\rangle \rightarrow e^{i \chi_{\Pi}} |\hat{\Omega}\rangle$

$e^{i \chi_{\Pi}} = e^{i \text{solid angle}}$

Solid angle subtended by path $\Pi$
(defined modulo $4\pi$)
Berry curvature due to spin rotations:

- $g$-dependent spin direction: $\hat{\Omega}(g)$

\[
\mathcal{F}_{\mu \nu}(g) = \frac{S}{4\pi} \hat{\Omega}(g) \cdot \partial_\mu \hat{\Omega}(g) \times \partial_\nu \hat{\Omega}(g)
\]

- The Berry phase accumulated as a spin-$S$ rotates is $S$ times the solid angle enclosed by the path of its direction $\Omega$ on the unit sphere.

- (Here “$g$” is position on the Fermi surface, $S = \frac{1}{2}$)
geometry of a manifold of quantum states

\[ |\Psi(g)\rangle = \sum_i \Psi_i(g) |i\rangle \]

continuous family of states parameterized by \(d\) real parameters

\[ \{g^\mu, \mu \in 1, 2, \ldots d\} \]

- Berry gauge ambiguity: nothing physical changes if we make a \(g\)-dependent gauge change

\[ |\Psi(g)\rangle \rightarrow e^{i\chi(g)} |\Psi(g)\rangle \]
\[ |\Psi(g)\rangle = \sum_i \Psi_i(g) |i\rangle \]

\[ |\partial_\mu \Psi(g)\rangle \equiv \sum_i \frac{\partial}{\partial g_\mu} \Psi_i(g) |i\rangle \]

\[ A_\mu(g) = -i \langle \Psi(g) | \partial_\mu \Psi(g) \rangle \]

\[ |D_\mu \Psi\rangle \equiv |\partial_\mu \Psi\rangle - i A_\mu |\Psi\rangle \]

**significance of covariant derivative:**

- Transform the same way with a gauge change
- Transform the same way with a gauge change

\[ \langle \Psi(g) | D_\mu \Psi(g) \rangle = 0 \]

**gauge-invariant relation (parallel transport)**
• a generic quantum state on a manifold induces both a **Riemannian metric** and a **$U(1)$ gauge field** (the “Berry connection”) ("unitary" case)

\[
\langle D_\mu \Psi(g) \mid D_\nu \Psi(g) \rangle \neq G_{\mu \nu}(g) + i F_{\mu \nu}(g)
\]

(Hermitian)

covariant derivative

(Hermitian)

(antisymmetric)

\[
\langle D_\mu \Psi_{\sigma}(g) \mid D_\nu \Psi_{\sigma'}(g) \rangle = G_{\mu \nu}(g) \delta_{\sigma \sigma'} + i F_{\alpha \mu \nu}(g) \sigma^a_{\sigma \sigma'}
\]

(antisymmetric)

$symplectic$ case

(antisymmetric)

(antisymmetric)

$\sigma_{\sigma \sigma'}$

Pauli matrix

$\delta_{\sigma \sigma'}$

non-Abelian Berry curvature

(antisymmetric)

non-Abelian Berry curvature

$\delta_{\sigma \sigma'}$

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Unitary case:
Berry phase and Chern invariant:

• For a closed path $\Gamma$ on the manifold:
  \[ e^{i \phi(\Gamma)} = \exp i \oint_{\Gamma} A_\mu dg^\mu \]
  geometrical U(1) Berry phase factor

• For a closed 2-surface $\Sigma$ on the manifold:
  \[ \frac{1}{2\pi} \int_{\Sigma} dg^\mu \wedge dg^\nu F_{\mu\nu} = C_1(\Sigma) \]
  topological (1st) Chern class integer invariant

(These are the analogs of the Bohm-Aharonov phase and the Dirac monopole quantization)
Orthogonal case:

- Vanishing Berry curvature
  \[ \mathcal{F}_{\mu \nu} = 0 \]

- Berry phase factor:
  \[ \eta(\Gamma) = \exp i \int_{\Gamma} A_\mu dg^\mu = \pm 1 \]

  topological \( \mathbb{Z}(2) \)
  Berry phase factor
Examples of manifolds of states:

- bands of Bloch states (manifold = Brillouin zone)
- Fermi liquid quasiparticles (manifold = Fermi surface in 2D or 3D)
- eigenstates of a family of non-degenerate Hamiltonians (manifold = parameter space of Hamiltonians)
- Coherent states (spin coherent states, Landau level “guiding center” coherent states, etc.)
Application to Bloch states

\[ \psi_{R,i}(k) = e^{ik \cdot (R + r_i)} u_i(k) \]

- amplitude for a particle to be on i’th site at position \( R + r_i \) in unit cell \( R \). Note that the Bloch factor depends on the assumed relative location of site \( i \) in the unit cell.

- Manifold is the Brillouin zone \( k \mod G \). Berry connection is

\[ A^a(k) = -i \sum_i u_i^*(k) \nabla_k^a u_i(k) \]

- “mean position of particle relative to unit cell” \( r^a = -i \nabla_k^a - A^a(k) \)

\[ [r^a, r^b] = iF^{ab}(k) \]

non-commuting coordinates!
Semiclassical dynamics of Bloch electrons

Motion of the center of a wavepacket of band-n electrons centered at $k$ in reciprocal space and $r$ in real space:

$$\begin{align*}
\hbar \frac{d k_a}{d t} &= e E_a + e F_{ab} \frac{d r^b}{d t} \\
\hbar \frac{d r^a}{d t} &= \nabla_k \varepsilon_n(k) + \hbar \mathcal{F}^{ab}_n(k) \frac{d k_b}{d t}
\end{align*}$$

(Sundaram and Niu 1999)

write magnetic flux density as an antisymmetric tensor

$$F_{ab}(r) = \varepsilon_{abc} B^c(r)$$

Karplus and Luttinger 1954

Note the “anomalous velocity” term! (in addition to the group velocity)

- The Berry curvature acts in $k$-space like a magnetic flux density acts in real space.

- Covariant notation $k^a, r^a$ is used here to emphasize the duality between $k$-space and $r$-space, and expose metric dependence or independence ($a \in \{x,y,z\}$).
A useful way to write the semiclassical dynamics:

\[
\frac{\hbar}{i} \begin{pmatrix}
\begin{align*}
\epsilon_{abc} B^c(r) \\
\frac{e}{\hbar} F_{ab}(r) \\
\delta^a_b \\
-\delta^b_a \mathcal{F}^{ab}(k)
\end{align*}
\end{pmatrix} \begin{pmatrix}
\begin{align*}
d \left( \begin{array}{c}
k^b \\
r^b
\end{array} \right)
\end{align*}
\end{pmatrix} = \begin{pmatrix}
\nabla_a V(r) \\
\nabla_k^a \epsilon_n(k)
\end{pmatrix}
\]

commutators of variables
(symplectic form, Poisson brackets)

\[
\begin{pmatrix}
\begin{align*}
[k^a, k^b] & [k^a, r^b] \\
r^a, k^b & [r^a, r^b]
\end{align*}
\end{pmatrix}
\]

\[
H(r, k) = \epsilon_n(k) + V(r)
\]

determinant (Jacobian) of the symplectic form:

\[
\det | \ldots | = 1 + \epsilon_{abc} \mathcal{F}^{ab}(k) \left( \frac{e B^c(r)}{\hbar} \right)
\]

modifies phase space volume integral (will use later)
Streda formula

• the Hall conductance (linear response of transverse electric current density to electric field) also describes linear response of electron density \( n \) to magnetic flux density

\[ \sigma_{ab}^H = \frac{e^2}{\hbar} \epsilon_{abc} \frac{K_c}{2\pi} \]

\[ \frac{\partial n}{\partial B} \bigg|_{\mu, T=0} = \frac{e}{\hbar} \frac{K}{2\pi} \]

• Xiao, Shi and Niu (2005) note that

\[ n = \int d^3k \left( 1 + \epsilon_{abc} \frac{eB^a}{\hbar} \mathcal{F}^{bc} \right) n(k) \]

modified k-space density of states
Current flow as a Bloch wavepacket is accelerated

If the Bloch vector $k$ (and thus the periodic factor in the Bloch state) is changing with time, the current is the sum of a group-velocity term (motion of the envelope of the wave packet of Bloch states) and an “anomalous” term (motion of the $k$-dependent charge distribution inside the unit cell).

If both inversion and time-reversal symmetry are present, the charge distribution in the unit cell remains inversion symmetric as $k$ changes, and the anomalous velocity term vanishes.
The DC conductivity tensor can be divided into a symmetric Ohmic (dissipative) part and an antisymmetric non-dissipative Hall part:

$$\sigma^{ab} = \sigma^{ab}_{\text{Ohm}} + \sigma^{ab}_{\text{Hall}}$$

In the limit $T \rightarrow 0$, there are a number of exact statements that can be made about the DC Hall conductivity of a translationally-invariant system.

For non-interacting Bloch electrons, the Kubo formula gives an intrinsic Hall conductivity (in both 2D and 3D)

$$\sigma^{ab}_{\text{Hall}} = \frac{e^2}{\hbar} \frac{1}{V_D} \sum_{n\mathbf{k}} \mathcal{F}^{ab}_{n}(\mathbf{k}) \Theta(\varepsilon_F - \varepsilon_n(\mathbf{k}))$$

This is given in terms of the total Berry curvature of occupied states with band index $n$ and Bloch vector $\mathbf{k}$.
• The Karplus-Luttinger formula expresses a transport property (the intrinsic Hall conductivity) as an integral over all occupied states.

• But this contradicts the fundamental idea that transport theory as $T \to 0$ only involves states at the Fermi level.

• Formula can be integrated by parts to get an expression determined completely at the Fermi level.
2D case: “Bohm-Aharonov in k-space”

\[
\sigma_{xy} = \frac{e^2}{\hbar} \frac{1}{(2\pi)^2} \int d^2k \ (\nabla_k \times A(k)) \ n(k)
\]

\[
\sigma_{xy} = \frac{e^2}{\hbar} \frac{1}{(2\pi)^2} \int_{FS} A(k) \cdot dk
\]

\[
\sigma_{xy} = \frac{e^2}{\hbar} \left( \frac{\Phi_{\text{Berry}}^F}{2\pi} \right)
\]

- The Berry phase for moving a quasiparticle around the Fermi surface is only defined modulo $2\pi$:

- Only the non-quantized part of the Hall conductivity is defined by the Fermi surface!
• what about the “missing” quantized part of the formula?

• This is determined by properties of edge states at the Fermi level, rather than bulk Fermi surface states, and is the only contribution if there is no Fermi surface in the interior (bulk) region.
non-quantized part of 3D case can also be expressed as a Fermi surface integral

- **There is a separate contribution to the Hall conductivity from each distinct Fermi surface manifold.**

- Intersections with the Brillouin-zone boundary need to be taken into account.

\[
\text{"Anomalous Hall vector":} \quad K = \sum_{\alpha} K_{\alpha} \pmod{G} \quad K_{\alpha} = \frac{1}{2\pi} \left( \int d^2 \mathcal{F} k_F + \sum_{i=1}^{d_{\alpha}} G_i \oint_{\Gamma_{i\alpha}} dA \right)
\]

This is ambiguous up to a reciprocal vector, which is a non-FLT quantized Hall edge-state contribution.
Physical origin of Berry curvature in Ferromagnetic bands

• In a naive Stoner-type theory (neglecting spin-orbit coupling) of ferromagnetic metals, the bands are “exchange-split” into bands of “majority” and “minority” spin carriers.

• In this picture, the majority and minority spin Fermi surfaces are independent, and can intersect:

\[ \uparrow \text{and } \downarrow \text{Fermi surfaces intersect} \]

\[ \text{without spin-orbit coupling} \]

even though weak, SOC dominates near “avoided intersections” of the Fermi surface, where it causes rapid variation of quasiparticle spin with \( k_F \)
cond-mat/0307337


Only when the Fermi surface lies in a spin-orbit induced gap is there a large contribution. This can be seen in Fig. 3 where the Berry curvature along lines in k-space is compared with energy bands near $E_F$ and in Fig. 4 where it is compared with the intersection of the Fermi surface with the central (010) plane in the Brillouin zone.

This calculation sampled ALL states below the Fermi level (unnecessary work!) but shows how avoided Fermi surface intersections provide the dominant contributions to the KL formula.

FIG. 4: (010) plane Fermi-surface (solid lines) and Berry curvature $-\Omega^z(k)$ (color map). $-\Omega_z$ is in atomic units.
2D “graphene” bandstructure

two distinct “Dirac points” (at corners of hexagonal Brillouin zone)

Breaking either inversion (I) or time-reversal (T) symmetry opens a “mass gap” at Dirac points.

Break only T: \( m_A = m_B \)

**same sign** Berry curvature near A and B points

Break only I: \( m_A = -m_B \)

**opposite sign** Berry curvature near A and B points
**2D zero-field Quantized Hall Effect**


- **2D quantized Hall effect**: $\sigma_{xy} = \nu e^2/h$. In the absence of interactions between the particles, $\nu$ must be an integer. There are no current-carrying states at the Fermi level in the interior of a QHE system (all such states are localized on its edge).

- The 2D integer QHE does NOT require Landau levels, and can occur if time-reversal symmetry is broken even if there is no net magnetic flux through the unit cell of a periodic system. (This was first demonstrated in an explicit “graphene” model shown at the right.).

- Electronic states are “simple” Bloch states! (real first-neighbor hopping $t_1$, complex second-neighbor hopping $t_2 e^{i\phi}$, alternating onsite potential $M$.)

---

**FIG. 1.** The honeycomb-net model (“2D graphite”) showing nearest-neighbor bonds (solid lines) and second-neighbor bonds (dashed lines). Open and solid points, respectively, mark the $A$ and $B$ sublattice sites. The Wigner-Seitz unit cell is conveniently centered on the point of sixfold rotation symmetry (marked “*”) and is then bounded by the hexagon of nearest-neighbor bonds. Arrows on second-neighbor bonds mark the directions of positive phase hopping in the state with broken time-reversal invariance.

**FIG. 2.** Phase diagram of the spinless electron model with $|t_2/t_1| < \frac{1}{2}$. Zero-field quantum Hall effect phases ($\nu = \pm 1$, where $\sigma_{xy} = ve^2/h$) occur if $|M/t_2| < 3\sqrt{3}|\sin \phi|$. This figure assumes that $t_2$ is positive; if it is negative, $\nu$ changes sign. At the phase boundaries separating the anomalous and normal ($\nu = 0$) semiconductor phases, the low-energy excitations of the model simulate undoubled massless chiral relativistic fermions.
Graphene model with second neighbor hopping is very useful!

- Quantum Hall effect with simple Bloch states
- Used for anomalous Hall effect studies (Nagaosa), add disorder etc.
- used for testing/developing fundamental band-structure formulas for orbital magnetization (Vanderbilt)
- Quantum Spin Hall effect (Kane and Mele)
- Analog system for photonic edge states (Haldane and Raghu)
Zero field (Anomalous) Integer QHE

Graphene model

![Graphene model diagram]

2 atoms (orbitals) per unit cell

Tight binding (nearest neighbor hopping)

\[ H = \sum_{<ij>} t (c_i^+ c_j + c_j^+ c_i) \]

\[ H = H^* \quad \text{(time reversal symmetry)} \]

+ spatial inversion sym
2 Dirac points
(at $k_0$, $-k_0 \mod G$)
in Brillouin zone
(Zone corners,
3 fold symmetry points)

• Time-reversal sym:
  $F(k) = -F(-k)$
• Spatial Inversion
  $F(k) = F(-k)$

So $F(k) = 0$ No Berry curvature
(Orthogonal case)

→ allows Dirac points (can find a degeneracy
by varying two parameters = $k_x$, $k_y$ in 2D)
For the "orthogonal" case,

There is a \( \mathbb{Z}_2 \) topological invariant

\[ e^{i \gamma_n \phi_{\text{B}} \Delta} = \pm 1 = \gamma_n \text{ Berry phase factor} \]

In \( k \)-space

- \( \gamma_n = -1 \)
- Get a \(-1\) Berry phase factor
- If contour \( \Gamma \) in \( k \)-space encircles an (odd number of) Dirac points

Many interesting consequences in graphene theory
Near a Dirac point

\[
H = V_0 \left( \sigma^x p^x + \sigma^y p^y \right) + \Delta \sigma^z
\]

Mass gap

\[
\mathcal{E}(p) = \pm \sqrt{V_0^2 p^2 + \Delta^2}
\]

\[\Delta = 0\]

\[\Delta \neq 0\]

What happens in a magnetic field?

\[\vec{p} \rightarrow \vec{p} - e \vec{A}\]
Semiclassical quantization in a magnetic field

\[ p_x \rightarrow \Pi_x = p_x - ieAx \frac{\hbar}{m} \]

\[ [\Pi_x, \Pi_y] = \hbar eB \]

**Dirac case**

\[ E(k) = \pm \sqrt{|kv_k|} \]

\[ \Pi k_n^2 = \frac{2\pi}{\hbar^2} |n| |v_k| \]

\( n = 0, 1, 2, \ldots \)

Area of \( k \)-space orbit

**Semiclassical quantization**

\[ k_n = \frac{2\pi}{\hbar} (n + \frac{1}{2}) \]

\( n = 0, 1, 2 \ldots \)

Because of extra \(-1\) Berry phase for orbits around \( k = 0 \) Dirac point!
The -1 Berry phase at the Dirac point gives a zero-mode Landau level.

\[ E_n = \text{sgn}(n) \frac{\hbar v_D \sqrt{|n|}}{\ell} \propto \sqrt{|B|} \]

\[ \ell = \frac{\hbar}{eB} \]

What happens when a mass gap \( \Delta \) is opened?
\[ H = Vq (|x| \sigma_x + |y| \sigma_y) + \Delta \sigma_z \]

\( \Delta < 0 \)

\( \Delta = 0 \)

\( \Delta > 0 \)

Zero mode sticks to lower band for \( \Delta > 0 \), upper band for \( \Delta < 0 \).
In the graphene model, a gap $\Delta$ is opened up by:

(a) Breaking time reversal
(b) Breaking spatial inversion.

If only (a) or (b) (not both) occur, the $E(k) = E(-k)$ symmetry is maintained. Both Dirac points have same $|\Delta|$

- (a) Time reversal breaking
  $\Delta_A = \Delta_B$

- (b) Inversion symmetry breaking
  $\Delta_A = -\Delta_B$. 
Breaking
Inversion breaks
A site $\neq$ B site
symmetry.

$V_A \neq V_B$.

\[ T\text{-breaking} \]

Second neighbor hopping, which is complex

\[ e^{i\phi} \quad \rightarrow \quad \begin{array}{c}
\uparrow \\
0 \\
\downarrow \\
\end{array} \quad \left\downarrow e^{-i\phi} \right.

\[ t_2 (e^{i\phi}c_1^\dagger c_1 + e^{-i\phi} c_1^\dagger c_2) \]

$e^{i\phi} \neq e^{-i\phi}$ \neq \pm 1.
If both $T$ and $I$ are broken, the gaps at each Dirac point can vary independently.

\[ \sigma^y_H = -\frac{e^2}{\hbar} \]

\[ \sigma^x_H = \frac{e^2}{\hbar} \]

\[ \nu = -1 \quad \text{QHE} \]

\[ \nu = +1 \quad \text{QHE} \]
Edge states

Zig-zag edge

$\Delta = 0$ graphene has an edge state

# of zero modes of 
Bipartite lattice =
# of "A" sites - # of "B" sites
Armchair edge

No A-B site imbalance
(no zero mode in graphene)

Both Dirac points have same $k_{11}$

$T$ breaking must give chiral edge state
Berry curvature, and Chern number

\[ \int d^2_k F_n(k) = 2\pi C_1 \]

Integer, (first Chern class)
(analog of Dirac monopole
(quantization)

\( (k\text{-space analog of } B) \)

\( k\text{-space} \)

\( \text{Dirac points} \)

\( \text{Chem } \pm 1, 0 \)

\( \text{Th fumbling } \uparrow \text{ I breaking} \)

Berry curvature is only large near The (gapped) dirac points for small \( \Delta \)
- Immediately a 2D dirac point mass gap opens, (T or I breaking)
  There is a total $\pm \pi$ "Berry flux"
  near the point in the upper band,
  and $\pm \pi$ in the lower band.

- Anomalous Hall effect (with T-breaking gap)
What about spin. (Kane + Mele)

\[ H' = \sum_\sigma i \gamma \sigma \left( C_{1\sigma}^+ C_{2\sigma} - C_{2\sigma}^+ C_{1\sigma} \right) \]

Second neighbor spin-orbit coupling of this type is allowed by symmetry.

No net QHE, but a \text{spin-QHE}

\[ \gamma_{\text{tot}} = \gamma_\uparrow + \gamma_\downarrow \]

\[ \sigma_{xy}^{\text{xy}} = \frac{e^2}{h} \left( \frac{1}{\text{up-spin}} - \frac{1}{\text{down-spin}} \right) = 0. \]
apply a magnetic field

both \( \uparrow \)  
both \( \downarrow \)

(1) \( 2 \uparrow, 2 \downarrow \)
(2) \( 1 \uparrow \leftrightarrow 1 \downarrow \)
(3) \( 1 \uparrow \leftarrow 1 \downarrow \) \( 2 \uparrow, 2 \downarrow \).

edge states

where \( \uparrow \) and \( \downarrow \) are separately conserved,
what happens when "Rashba" SOC terms mix \( \uparrow \) and \( \downarrow \)?

Protected by Kramer's...
Quantum Spin-Hall effect

(C. Kane, E. Mele)
(C. Kane, F. H.)

- Unbroken Time-reversal Symmetry

\[ H = H_0^{\text{graphene}} + \sum_{\langle ij \rangle} \gamma \left( C_{ij}^+ C_{ij} \uparrow - C_{ij}^+ C_{ij} \downarrow \right) \]
\[ \text{second neighbors} \]

- Spin $\uparrow$ and Spin $\downarrow$ separately conserved

- $\sigma_{xy}^H = \left( \frac{e^2}{h} \text{sgn} (\theta) - \frac{e^2}{h} \text{sgn} (\theta) \right) = 0 \quad \text{No QHE}$

But \[ \frac{\partial}{\partial B} \left( n_{\uparrow} - n_{\downarrow} \right) = \frac{e}{h} \]
In real spin orbit coupling, ↑ and ↓ are not conserved, especially if the 2D system is not on a 3D mirror plane (Rashba).

* if processes allow $\uparrow \rightarrow \downarrow$, do we get $\begin{array}{c} \text{??} \\ \text{??} \end{array}$?

No, Kramers degeneracy forbids it.
Kramers

one-electron states of spin-$\frac{1}{2}$ particles are always doubled at T-symmetry is present in time-reversal-related pairs

\[(k^\uparrow, -k^\downarrow)\]

not allowed because doublet is split
$\mathbb{Z}_2$ invariant

- two branches of edge states

\[ \rightarrow \text{ allowed} \]

Three branches

\[ \rightarrow \text{ no gap} \]

# of edge states is protected modulo 2.
Is there a quantized (as opposed to "quantum")
Spin Hall effect?

- NO, because spin is no longer a good quantum
  number when SOC is present.

- Naive model has separate Spin^↑ and Spin^↓
  Chern numbers: \( C_\sigma = \sigma C \quad \sigma = \pm 1 \)
  \( C \mod 2 = (-1)^C \) is preserved when
  more general SOC is included.
what is the $\mathbb{Z}_2$ analog of the Chem number? (2D band)

- Simplest case, when both T-reversal, and Inversion sym. are present (Kane+Fu)

- States at $\bar{k} = (0, 0), (0, \pi), (\pi, 0), \text{and} (\pi, \pi)$ are Kramers doublets which are also parity eigenstates. (All bands are doubly degenerate at all $\bar{k}$)

- $\gamma = \prod_{\bar{k} \in \{\text{occupied bands}\}} \text{sign} \left( \text{In}_n(k_\bar{\omega}) \right) = \pm 1$

- If there is a gap at the Fermi level for all $\bar{k}$, $\gamma = \pm 1$ if there is no Spin-Orbit-Coupling.
$\mathcal{T}$ and Inversion symmetry present.

- $\mathcal{E}_0$

- $k^*$

$\text{Dirac point}$

$[\pm k^*] \rightarrow$ Invariant point.

- must be a parity doublet
  (4-fold degenerate)
Bulk Band Structure

![Graph showing the band structure of HgTe and Hg$_{0.32}$Cd$_{0.68}$Te with energy levels labeled as $\Gamma_6$, $\Gamma_8$, and $\Gamma_7$ and a vertical band offset (VBO) indicated.](image)
Quantum Well Sub-bands

Let us focus on E1(s-wave), H1(p-wave) bands close to crossing point.

$d < d_c$

normal

$d > d_c$

inverted
3D system

\[ Y = \prod_{k \in k^*} \text{In}(k) = \pm 1 \]

All 2D surface bands (any facet) have

\[ \prod e^{i\phi} = -1 \]

Can’t avoid fermi surface of at least one dirac point on any facet!
Topological invariants of Bloch bands:

- cannot change unless the energy gap between bands closes and reopens:
- The integer “Chern number” (First Chern Class) classifies Bloch bands with broken time-reversal symmetry:
- If there is a gap at the Fermi energy, a non-zero total Chern number of 2D bands below the Fermi energy implies that:

  There is an (integer) quantum Hall effect

  There are gapless chiral edge states at the edge of the system.
Bands with both time-reversal and spatial-inversion symmetry:

• Bands are doubly-degenerate at generic points in the Brillouin zone

• Bands at special k-points where \(2k_j = G\) are classified by inversion symmetry \(I_i(k_j) = +1\) or \(-1\) about inversion center \(i\) in the real-space unit cell.

• In 2D (3D) there are 4 (8) special k-points and 4 (8) distinct inversion centers; the product over all bands below the Fermi energy is

\[
\eta_0 = \prod_j I_i(k_j) = \pm 1
\]

Fu and Kane, 2006

• In 2D and above this is independent of which inversion center \(i\) is chosen

This is clearly a “topological invariant”, but Kane and Fu’s recent (2006) result shows the not-so-obvious fact that it must have the value \(+1\) in the absence of spin-orbit coupling.
\( \eta_0 \) is a topological invariant because it cannot change without the gap closing.

At special k-points, it is possible to “fine-tune” bands with opposite inversion quantum numbers to have an “accidental degeneracy” by varying a single parameter.
• example (with no spin-orbit coupling)

\[ H = \frac{p^2}{2m} + V_0 \sum_{i=1}^{6} e^{iG_i \cdot r} \]

\( V_0 < 0 \)  
lowest band  
has \( \eta_0 = +1 \)

\( V_0 > 0 \)  
lowest band  
has \( \eta_0 = -1 \)  
but no gap!
Topology of 2D bands with time-reversal symmetry

A 2D band with no SOC is topologically a 2-Torus (genus-1 2-manifold)

A 2D band with SOC (and no inversion symmetry) is topologically two 2-tori, punctured and joined at the four T-reversal-invariant k-points to make a genus-5 two manifold, (on which every point has a Kramers-conjugate antipode)
basic idea

• If the genus-5 2-manifold is sliced into the upper band and and the lower band, it falls apart into two 2-Tori, each with four “punctures”.

• The edges of the punctures are the 1-manifolds defined by the limit of the Bloch states at the T-invariant k-points, as a function of the direction they are approached from in the upper or lower band.

• There is no relation in general between these four punctures (except possible point-group symmetry on square and hexagonal Bravais lattices).

• Instead, divide the genus-5 manifold into two Kramers-conjugate 2-tori with four punctures. In this case the punctures come in Kramers-conjugate pairs...
Matched pairs of punctures on a Kramers-divided double-band.

- no pairs of points on this manifold are Kramers conjugates
- For each pair of “puncture boundaries”, one is open, one is closed.
- The puncture boundaries are topologically non-trivial paths on the uncut genus-5 manifold.
• On an unpunctured 2-manifold $\mathcal{M}$

$$\int_{\mathcal{M}} d^2 F = 2\pi \times \text{integer} \quad e^{i \int_{\mathcal{M}} d^2 F} = 1$$

• On a punctured 2-manifold with puncture boundaries $\partial \mathcal{M}_i$

$$e^{i \int_{\mathcal{M}} d^2 F} = \prod_i e^{i \phi_B(\partial M_i)}$$

integral of Berry curvature over manifold

product of Berry phases around the puncture edges

This is just Stokes theorem, exponentiated
• In general, no topological Chern invariant survives on a punctured manifold.

• Here, each member of a pair of Kramers-conjugate puncture boundaries has the same Berry phase factor!

\[ e^{i \int_{\mathcal{M}} d^2 F} = \left( \prod_i e^{i \phi_B (\partial M_i)} \right)^2 \]

Now take the square root:

\[ e^{i \frac{1}{2} \int_{\mathcal{M}} d^2 F} = \eta_0 \prod_i e^{i \phi_B (\partial M_i)} \]

The $\mathbb{Z}_2$ invariant, $\pm 1$
To conclude:

- Limit when Inversion symmetry is restored connects this to Kane and Fu’s Inversion-symmetric result.
- 3D follows (recover Moore and Balents’ result)
- Does this have a many body generalisation, like Chern number? Problem: notion of dividing the band into Kramers conjugate halves is fundamentally a one-particle band structure property.
- “Z2” is a rule for predicting edge states at interfaces: no special bulk properties of “topological insulators”?.