Topological Metals and Surface Fermi Arcs

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- A concise tour of the topology and geometry of Bloch-state Berry curvature, to define “Topological metals” and their surface Fermi arcs.

This talk is online at:
http://wwwphy.princeton.edu/~haldane/research.html
see also arXiv:1403.0577
Topologically non-trivial bulk phases commonly have robust edge states on their boundaries with topologically-trivial regions such as the vacuum.

* The time-reversal-invariant (TRI) combination of two conjugate copies of this model was the model in which Kane and Mele (2005) discovered the $Z_2$ Kramers-protected invariant of the TRI topological insulators.
- Projection of the 2D graphene band-structure into the 1D surface Brillouin zone of the zigzag edge

- Dirac points at corners of 2D BZ remain gapless provided both time-reversal and 2D inversion symmetry are unbroken

Edge state connects projected gapless Dirac points
• gapless graphene “zig-zag” edge modes

Broken inversion

Broken time-reversal (Chern insulator)
• recently a new type of unusual topological surface state was found in models of “Weyl semimetals” (3D analogs of graphene)


• I will put these “Fermi arcs” in the wider context of “topological metals” (Weyl semimetals are just a special limit of these), and relate them to the Fermi-surface expression for the Anomalous Hall Effect (FDMH, 2004).

• The arcs also play an important role in (eliminating) the proposed “Chiral Magnetic Effect” (CME) in these materials

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• What is a (3D) “topological metal”?

It is a metal where there are two or more disconnected sheets of the (spin-split) Fermi surface with a non-zero Chern number*

*(Note that the sum of the Fermi-surface Chern numbers is always 0 to satisfy gauge invariance)

• This requires spin-orbit coupling; either time-reversal or spatial inversion symmetry must also be broken
• Fermi arcs on a 2D surface of 3D metal with outward normal $n$:

The Fermi arc in the surface partial-band

Region of the BZ where the surface partial-band exists

Projection of a bulk Fermi surface with Chern number $+1$

Projection of a bulk Fermi surface with Chern number $-1$
Anatomy of the unusual 2D surface “partial bands” supporting “Fermi arcs”

Surface state exists in only part of surface Brillouin zone (surface BZ).

Contours of constant energy \( E(\mathbf{k}_\parallel) \)

\[ \kappa = 0 \]

Contours of constant evanescent inverse decay length \( \kappa(\mathbf{k}_\parallel) \)

Exponential decay into bulk

\[ |\Psi|^2 \]

\[ \Psi(\mathbf{r}) \propto \exp \left( \kappa(\mathbf{k}_\parallel) \mathbf{n} \cdot \mathbf{r} \right) \]
I will now take a rapid trip though the geometry and topology of Bloch-state Berry curvature to show where these results come from.
• Geometry and topology were first connected by the Gauss-Bonnet theorem:

$$\int d^2 x \ (\text{intrinsic curvature})$$

2D surface

local geometry

$$\int d^2 x \frac{1}{R^2} = 4\pi \times 1$$

seems trivial for a sphere, but still true for any genus-0 closed surface

Euler characteristic or (1 - genus)

global topology

• Integers

• Invariant under smooth local deformations of the surface

genus 0

genus 1

genus 2
• This remarkable relation evolved through mathematical abstraction to the Chern classes, in particular

\[ \int_{\mathcal{M}_2} d\mu^\mu \wedge d\mu^\nu \mathcal{F}_{\mu\nu}(\mathbf{x}) = 2\pi C_1 \]

integral over a closed orientable 2-manifold

“Chern number”

first Chern class (an integer) replaces Euler’s characteristic

Berry curvature

\[ \left\langle \frac{\partial \Psi(\mathbf{x})}{\partial x^\mu} \right| \frac{\partial \Psi(\mathbf{x})}{\partial x^\nu} \right\rangle - \left\langle \frac{\partial \Psi(\mathbf{x})}{\partial x^\nu} \right| \frac{\partial \Psi(\mathbf{x})}{\partial x^\mu} \right\rangle = i \mathcal{F}_{\mu\nu}(\mathbf{x}) \]

\[ \mathcal{F}_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \]

quantum state that depends on a set of continuous parameters \( \mathbf{x} \)

mathematically, this is a “U(1) fiber bundle”

\[ e^{i \oint_\Gamma d\mu A_\mu} = e^{i \Phi} \]

Berry phase of boundary
• on a 2-d manifold $\mathcal{M}$ with boundaries $\partial\mathcal{M}_i$

\[
\exp \left( i \int_{\mathcal{M}} F_{\mu\nu} dx^\mu \wedge dx^\nu \right) = \prod_i \exp i \int_{\partial\mathcal{M}_i} A_\mu dx^\mu
\]

Integrated Berry curvature ("flux") in interior

Product of Berry phase factors on boundaries

"punctures"

Stokes theorem
The first Chern invariant.

- for a compact 2d manifold with no boundaries

\[ \exp \left( i \int_{\mathcal{M}} F_{\mu\nu} \, dx^\mu \wedge dx^\nu \right) = 1 \]

can take logarithm

\[ \int_{\mathcal{M}} F_{\mu\nu} \, dx^\mu \wedge dx^\nu \equiv \int_{\mathcal{M}} d^2 x F = 2\pi C_1 \]

**Berry curvature**

\[ \int \mathcal{M} F_{\mu\nu} \, dx^\mu \wedge dx^\nu \equiv \int \mathcal{M} d^2 x F = 2\pi C_1 \]

integer “Chern number”

“first Chern class” topological invariant

- This topological invariant is central to systems with broken time-reversal symmetry (quantum Hall effect, Thouless et al. TKNN 1983, Simon 1983)
The compact 2D manifold of the first Chern class is now a frequent ingredient in modern physics, and can occur in many different ways:

- Parameter space is unit sphere
- Quantum spin
- Chern number = 2S

Berry phase:

\[ e^{i \hat{\Omega}} = e^{i S \omega} \]

solid angle enclosed is ambiguous modulo \( \frac{4\pi}{4\pi} \)
so 2S must be an integer

Electronic or photonic Bloch states in 2D Brillouin zone:

manifold is 2-torus
The quantum state must be non-degenerate, so for the 2D bandstructure with spin-orbit coupling, either time-reversal or spatial inversion symmetry must be broken to get Berry curvature.

\[ \mathcal{F}_n(k) = \mathcal{F}_n(-k) \]

inversion

\[ \mathcal{F}_n(k) = -\mathcal{F}_n(-k) \]

Time-reversal

The Chern number vanishes unless time-reversal symmetry is broken
• Though it’s not relevant for this talk, the recent “topological insulator” revolution started in 2005 when Kane and Mele discovered a new \( \mathbb{Z}_2 \) (as opposed to \( \mathbb{U}(1) \)) invariant in time-reversal-invariant 2D electronic bands with Kramers degeneracy.

• They first discovered the new invariant in systems with broken spatial inversion symmetry, when it can also be derived from the Berry curvature.
An explicitly gauge-invariant rederivation of the Kane-Mele $\mathbb{Z}_2$ invariant

- If inversion symmetry is absent, 2D bands with SOC split except at the four points where the Bloch vector is $1/2 \times$ a reciprocal vector. The generic single genus-1 band becomes a pair of bands joined to form a genus-5 manifold.

- This manifold can be cut into two Kramers conjugate parts, each is a torus with two pairs of matched punctures. In each pair, one puncture boundary is open one is closed.
• on a punctured 2-manifold

\[ \exp i \int d^2 k \, \mathcal{F}^{12}(k) = \prod_i e^{i\phi_i} \]

product of Berry phase-factors of puncture boundaries

• in T-invariant electronic half-bands with SOC, punctures come in Kramers pairs:

\[ \frac{2n}{i=1} e^{i\phi_i} = \left( \prod_{i=1}^n e^{i\phi_i} \right)^2 \]

a perfect square, so we can take a square root!
• If inversion symmetry is present, the bands are unsplit and doubly-degenerate at all points in k-space, so the Berry curvature is undefined.

• For that case, Fu and Kane found a beautiful formula

\[ \prod \prod I_{n,k^*} = \pm 1 = \text{the } \mathbb{Z}_2 \text{ invariant} \]

occupied bands
T+I-invariant k-points

Inversion quantum number \( \pm 1 \)

(this changes sign at band-inversion transitions, as stressed by Bernevig, Hughes and Zhang)
• It may be useful to point out that the Berry curvature in k-space associated with Bloch states is slightly non-standard:

$$|\Psi_n(k, \{r_i\})\rangle = U(-k; \{r_i\})|k, n\rangle \quad U(k) = \sum_i e^{ik \cdot r_i} |i\rangle \langle i|$$

• The states from which the Berry curvature is obtained are not eigenstates of the Hamiltonian, but

A periodic state that depends on the spatial embedding as well as $k$

The Bloch eigenstate, which is quasiperiodic, and independent of spatial embedding

Information on the embedding in Euclidean space

a basis of localized orbitals
• This extra feature becomes very clear in tight-binding models:

- the Bloch Hamiltonian only “knows” about the “hopping matrix elements” between orbitals, but not how the orbitals are embedded in space.

- the Berry curvature in k-space of \( |\Psi(k, \{r_i\})\) “knows” about the relative spatial locations of the orbitals, and allows the effect of perturbation by uniform electric and magnetic fields to be described.

- the Topological invariants themselves do not depend on the geometry of the embedding.
Semiclassical motion of a Bloch electron in weak quasi-uniform applied electromagnetic fields

\[ H = \varepsilon_n(k) - e\phi(r) \]

\[ F_{ab}(r) \equiv \varepsilon_{abc}B^c(r) \]

\[ E_a(r) = -\nabla_a \phi(r) \]

\[ \hbar \frac{d{\bf k}_a}{dt} = -e \left( \nabla_a \phi(r) + F_{ab}(r) \frac{d{r}^a}{dt} \right) \]

\[ \frac{d{r}^a}{dt} = \frac{1}{\hbar} \nabla^a \varepsilon_n(k) + \mathcal{F}_{ab}^{kn}(k) \frac{d{k}_b}{dt} \]

Lorentz force

\[ \text{group velocity} \quad + \quad \text{“anomalous velocity”} \]

- Karplus and Luttinger (1954), Sundaram and Niu (1999)
The Karplus-Luttinger formula for the intrinsic band-structure component of the anomalous Hall effect of a 3D ferromagnetic metal is equivalent to

\[ \sigma_{H}^{ab} = \frac{e^2}{h} \left( \frac{1}{2\pi} \sum_{n} \int_{BZ} d^3k \mathcal{F}_{n}^{ab}(k)n_n(k) \right) \]

This is just the sum of the Berry curvature over all the occupied electron states in the band-structure, rediscovered by TKNN in the QHE.

Only topological if all bands are completely filled or completely empty
The Karplus-Luttinger formula is somewhat strange because it relates a conductivity to properties of all occupied states, while on fundamental grounds this should be determined only at the Fermi level!

It can be reexpressed as a Fermi-level result (FDMH 2004)

As a 3D bulk formula, the topological part is fixed by the completely filled bands, while the residual geometric part is fixed at the Fermi level!

\[
\sigma_{H}^{ab} = \frac{e^2}{\hbar} \frac{1}{2\pi} \epsilon^{abc} K_c
\]

Topological part:
Kohmoto, Halperin and Wu

\[
K = \nu G
\]

In fact the bulk 3D topological part is also fixed at the Fermi level, as it can be reexpressed in terms of 2D surface states at the Fermi level which the topology gives rise to!

\[
G = \frac{2\pi n}{d}
\]
3D Metals

- The Fermi surface of a 3D metal is a 2D manifold on which the Fermi liquid quasiparticles are defined.

- Assume spin-orbit coupling + EITHER broken time-reversal symmetry OR broken spatial inversion symmetry causes spin-splitting of the Fermi surface, so the quasiparticles have no spin degeneracy.

- Then the quasiparticle defines a Berry connection on the Fermi surface.

- In Fermi-liquid theory, the infinite-lifetime quasiparticles at the Fermi surface are the only non-topological feature of Bloch band theory that remains unchanged in the presence of interactions!
Fermi surface of Cu

necks in [111] directions

Topological picture

Cu Fermi surface: has genus 4

\[ \Delta G = [111] \]
\[ \Delta G = [\bar{1}11] \]
\[ \Delta G = [11\bar{1}] \]
\[ \Delta G = [\bar{1}\bar{1}1] \]

Brillouin zone boundary inscribed on Fermi surface

reduced \( k \) jumps by \(-\Delta G\) when the BZ boundary is crossed in this sense
Topological Metals

• The Fermi surface of 3D metals can break up into topologically-disconnected sheets.

• A sheet of the Fermi surface of a 3D metal with spin-orbital coupling can have a non-zero Chern number.

• Sum of Chern numbers of all Fermi surface sheets must vanish.

Weyl points are monopole sources/sinks of Berry curvature flux.
The residual geometric part of the AHE formula is given as a “k-space dipole moment of Berry curvature on the Fermi surface” (FDMH 2004)

\[ K = G + \frac{1}{2\pi} \left( \sum_\alpha \int_{FS_\alpha} k_{F\alpha} F_\alpha dA + \sum_{\alpha,i} (\Delta G_i) \int_{\Gamma_{\alpha,i}} A^\mu d\kappa_{\mu} \right) \]

- label of distinct sheets of Fermi surface
- Berry phase for going around inscribed BZ Boundary \( i \), with k-discontinuity \( \Delta G_i \)
- gauge invariance (electric charge conservation) requires that this formula is invariant under the simultaneous displacement of all sheets of the Fermi surface by the same shift \( k_{F\alpha} \rightarrow k_{F\alpha} + \Delta k \)

\[ \sum_\alpha \int_{FS_\alpha} F_\alpha dA = 0 \]

- total Chern number must vanish
\[ K = G + \frac{1}{2\pi} \left( \sum_{\alpha} \int_{FS_{\alpha}} k_{F\alpha} F_{\alpha} dA + \sum_{\alpha,i} (\Delta G_i) \int_{\Gamma_{\alpha,i}} A^\mu d\kappa_\mu \right) \]

- "Dipole moment of Fermi-Surface Berry curvature in the Brillouin zone"

- "gauge invariance"

\[ k_{F} \rightarrow k_{F} + eA/\hbar \]

\[ K \rightarrow K + \frac{1}{2\pi} \sum_{\alpha} \int_{FS_{\alpha}} F dA \]

sum of Chern numbers must vanish

BZ boundary term ensures these two choices of BZ give same \( K \)
• However, in the case of topological metals, there is an ambiguity in the “BZ Berry dipole moment”

Dipoles differ by reciprocal vector G depending on choice of BZ
\[ K = G + \frac{1}{2\pi} \left( \sum_{\alpha} \int_{FS_{\alpha}} k_{F\alpha} F_{\alpha} dA + \sum_{\alpha,i} (\Delta G_i) \int_{\Gamma_{\alpha,i}} A^\mu d\kappa_\mu \right) \]

- If all the Fermi surface sheets have Chern number 0, the formula is invariant under individual (different) displacements of each sheet:
  \[ k_{F\alpha} \mapsto k_{F\alpha} + \Delta k_\alpha \]

- In this case, if only infinitesimal-momentum-transfer scattering events are allowed, there is no equilibration between disconnected Fermi-surface sheets, and **there is a separately-conserved quasiparticle charge for each topologically-trivial sheet.**
• scattering with infinitesimal momentum transfer \( q \) does not transfer quasiparticles between disconnected topologically-trivial (Chern number 0) Fermi surface sheets

\[
| \min k_{F1} - k_{F2} \ mod \ G | \gg \max |q|
\]

• displacement (generalized gauge transformation) of a subset of Fermi-surface sheets only conserves the AHE formula \textit{if they have total Chern number 0}
• As a bandstructure is adabatically varied, a single Fermi surface sheet may split up into two apparently disjoint topological Fermi surface sheets

- The “memory” that they used to be connected is imprinted in a surface “Fermi arc” that connects them on any surface where their projection into the surface BZ is disjoint

- These surface Fermi arcs prevent any difference of the chemical potentials of the two topological Fermi surface sheets
A Fermi Arc surface state exists to show the correct dipole!!

FDMH arXiv:1401.0529

number of outward arcs minus number of inward arcs = bulk Chern number!
• Bulk Fermi surface defines non-quantized geometric term

• inspection of edge states fixes quantized topological terms

• There are now two classes of chiral edge-state Fermi arcs:

[Diagram showing two classes of Fermi arcs:
- Open arc from 3D topological metal
- Closed arc (loop) from 3D stack of 2D IQHE plane edge states]

Maintains equality of the two Fermi energies
In the CME (Chiral Magnetic Effect), it is suggested that applying $E$ parallel to $B$ in clean systems could increase the Fermi level at one Weyl point, and decrease it at the other!

This picture appears to have missed the Fermi arcs on the faces of the metal that provide a return path, and keep the levels equilibrated!

Landau levels of a pair of Weil points

bulk spectral flow occurs if there is an electric field parallel to $B$!

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conclusions

• Have succeeded in applying the adjective “topological” to yet another state of matter: \textit{metals}

• Probably should be classified as SPT (Symmetry-Protected Topological state) where $S = U(1)$ charge conservation and lattice translation symmetry.

• Open surface Fermi arcs connecting topologically-non-trivial projected bulk Fermi surfaces are the latest exotic consequences of quantum topology.
simple toy model for Fermi arcs

\[ H = \sum_{n=1}^{\infty} (-1)^n V c_n^\dagger c_n + \sum_{n=1}^{\infty} (t_1 c_{2n-1}^\dagger + t_2 c_{2n+1}^\dagger) c_{2n} + H.c. \]

- band gap opens when \( V \neq 0 \) or \( |t_1| \neq |t_2| \)
- for \( t_2 > 0 \), gap is \( E < \sqrt{V^2 + (t_1 - t_2)^2} \)
- edge state at \( E = V \) for \( |t_1| < t_2 \)

- to model surface bands, make \( V, t_1 \) and \( t_2 \) depend on \((k_x, k_y)\)

\( (V, t_1, t_2) = (k_y, |k|, 1) \)

surface mode with \( E = k_y \) when \( |k| < 1 \)