

Berry Curvature and the Z_2 Topological Invariants of Spin-Orbit-Coupled Bloch Bands

F. D. M. Haldane, Princeton University

- Z_2 invariance with inversion symmetry
- Z_2 invariant without inversion symmetry,
and Berry curvature
- conclusions

Supported in part by NSF MRSEC DMR-0213706 at Princeton Center for Complex Materials

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.

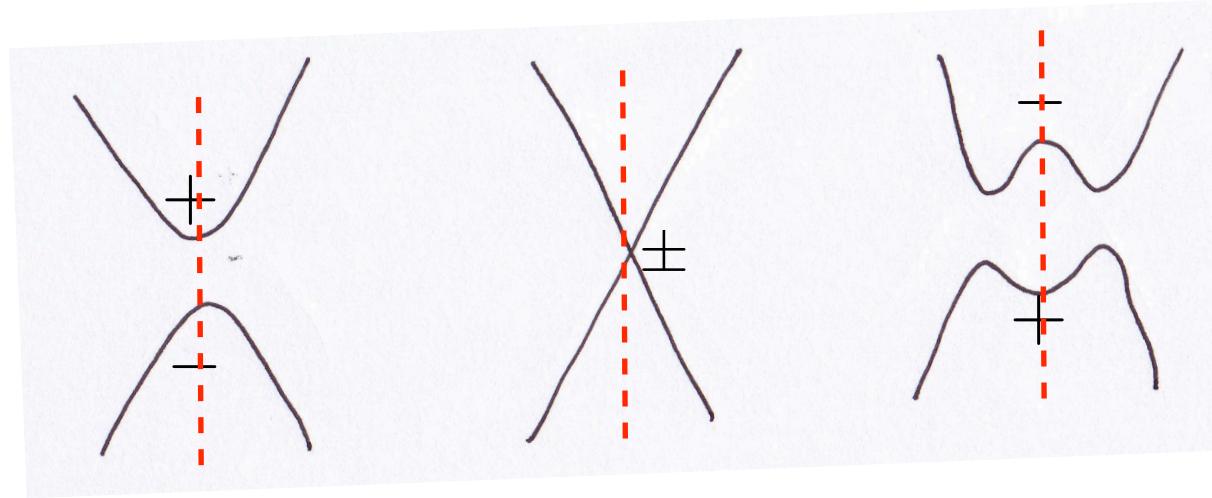
Bands with both time-reversal and spatial-inversion symmetry:

- Bands are doubly-degenerate at generic points in the Brillouin zone
- Bands at special \mathbf{k} -points where $2\mathbf{k}_j = \mathbf{G}$ are classified by **inversion symmetry** $I_i(\mathbf{k}_j) = +1$ or -1 about inversion center i in the real-space unit cell.
- In 2D (3D) there are 4 (8) special \mathbf{k} -points and 4 (8) distinct inversion centers; the product over all bands below the Fermi energy is

$$\eta_0 = \prod_j I_i(\mathbf{k}_j) = \pm 1 \quad \text{Fu and Kane, 2006}$$

- 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.



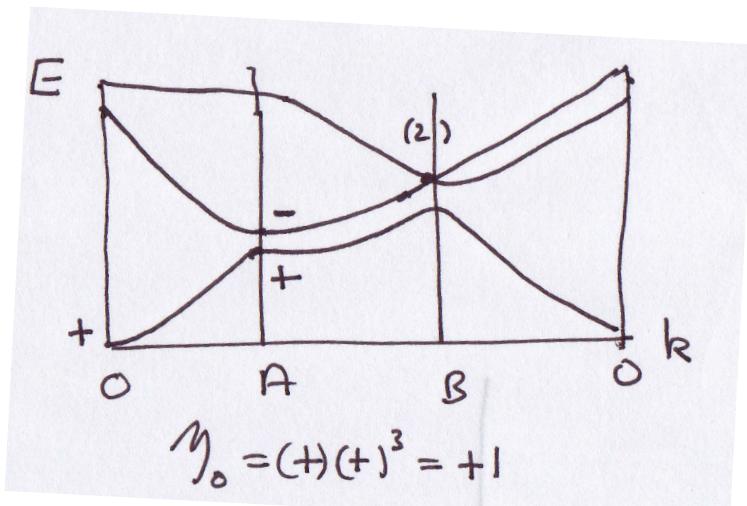
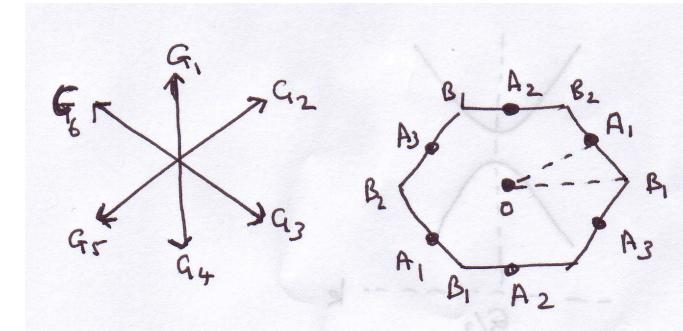
η_0 is a topological invariant because it cannot change without the gap closing

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.

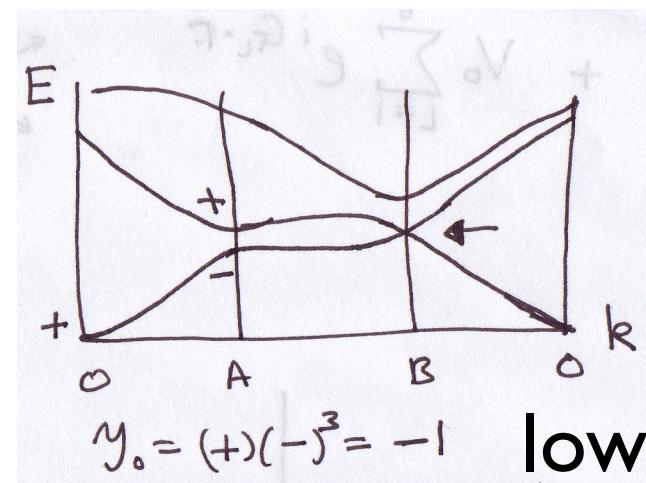
Disclaimer: my abstract **incorrectly** suggests doubt about Kane and Fu's result that η_0 is the Z_2 "spin-Hall" invariant

- The "counter example" (with no spin-orbit coupling) that failed:

$$H = \frac{p^2}{2m} + V_0 \sum_{i=1}^6 e^{i\mathbf{G}_i \cdot \mathbf{r}}$$



$V_0 < 0$ lowest band
has $\eta_0 = +1$



$V_0 > 0$ lowest band
has $\eta_0 = -1$
but no gap!

Berry curvature and the Z2 invariant when inversion symmetry is broken.

- Kane and Mele gave a formulation in terms of the zeroes of a “Pfaffian matrix”
- Kane and Fu gave a formulation in terms of what they identify as a Berry curvature of a determinant of occupied bands
- I will now give a formulation in terms of the Berry curvature structure of individual Bloch states, using the Berry curvature as defined by their semiclassical dynamics.

- Key point: these expressions are not **definitions** of the topological invariant, which fundamentally measures whether an even or an odd number of Dirac points have crossed the Fermi level as the band structure has evolved from one with no spin-orbit coupling.
- Instead, they are **sum rules** involving the Berry curvature (or Pfaffian zeroes)
- Indeed, the invariant is a property of the Hamiltonian alone, while the Berry curvature depends on **extra information about its embedding in Euclidean space**.

$c_{R\alpha}^\dagger$ ← Local basis: orbital α in unit cell R

$$H^0 = \sum_{R,\alpha; R'\alpha'} h_{\alpha\alpha'}(R - R') c_{R\alpha}^\dagger c_{R'\alpha'}$$

$$|\Psi_n(\mathbf{k})\rangle = \sum_{R\alpha} u_{n\alpha}(\mathbf{k}) e^{i\mathbf{k}\cdot(R + \mathbf{r}_\alpha)} |R\alpha\rangle$$

Hamiltonian and Bloch states depend on the matrix-elements $h_{\alpha\alpha'}(R)$

Bloch states and Berry curvature also depend on the positions r_α in the unit cell.

- varying the nominal orbital positions in the unit cell without changing the matrix elements changes the Berry curvature, **but does not affect the topological invariants.**
- The Berry curvature **of Bloch states** physically represents part of their linear response to **uniform** electromagnetic fields (which cannot be included in a periodic time-independent Hamiltonian)

$$A_n^a(\mathbf{k}) = -i \langle \Psi_n(\mathbf{k}) | \frac{\partial}{\partial k_a} \Psi_n(\mathbf{k}) \rangle$$

“Berry connection”: k-space analog of the magnetic vector potential.

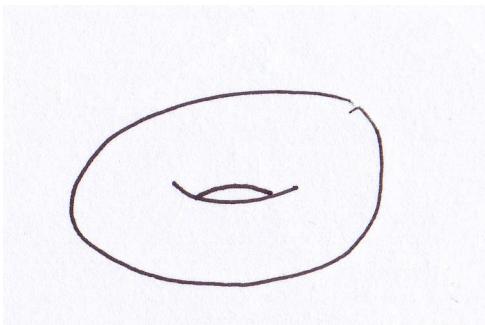
$$F_n^{ab}(\mathbf{k}) = \frac{\partial}{\partial k_a} A_n^b(\mathbf{k}) - \frac{\partial}{\partial k_b} A_n^a.$$

“Berry curvature”: k-space analog of magnetic flux density (gauge invariant)

The “anomalous velocity” term in the semiclassical dynamics is

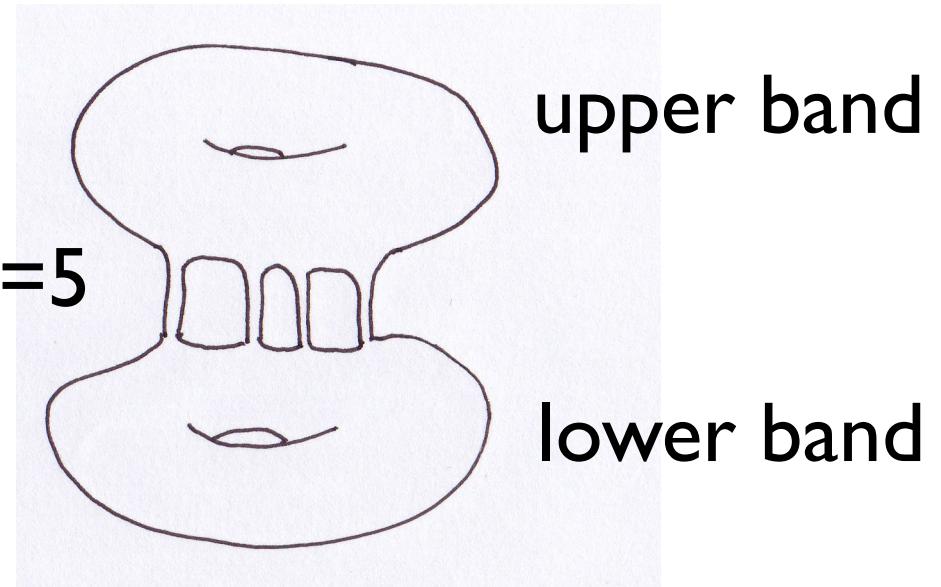
$$\frac{dx^a}{dt} = \frac{1}{\hbar} \nabla_k^a \epsilon_n(\mathbf{k}) + F_n^{ab}(\mathbf{k}) \frac{d\mathbf{k}_b}{dt}$$

Topology of 2D bands with time-reversal symmetry



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

genus=1

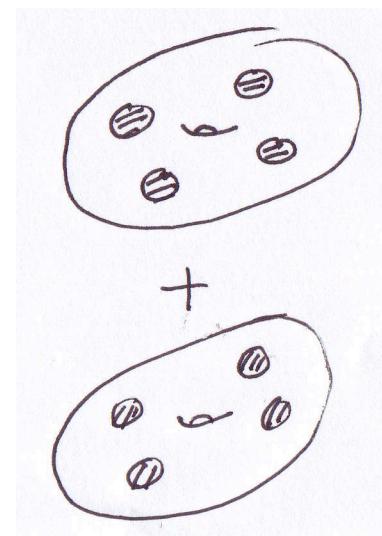


upper band
lower band

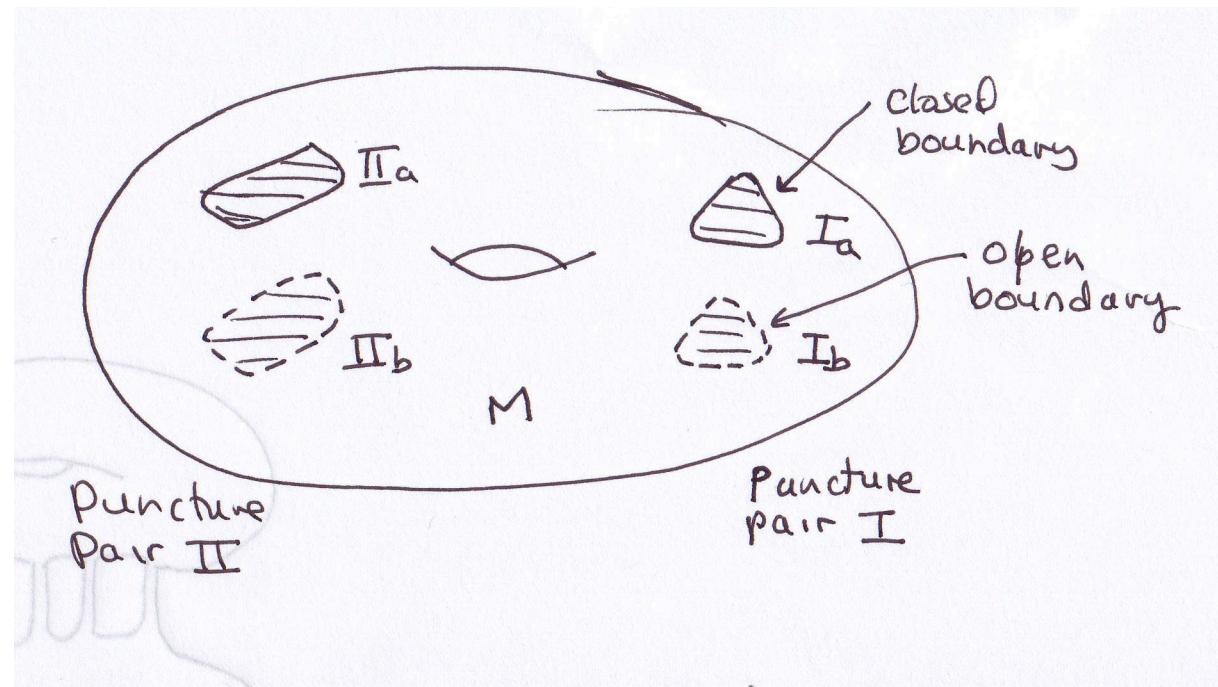
A 2D band with SOC (and no inversion symmetry) is topologically two 2-tori, punctured and joined at the four T-reversal-invariant k-points to make a genus-5 two manifold, (on which every point has a Kramers-conjugate antipode)

basic idea

- If the genus-5 2-manifold is sliced into the upper band and 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 ∂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

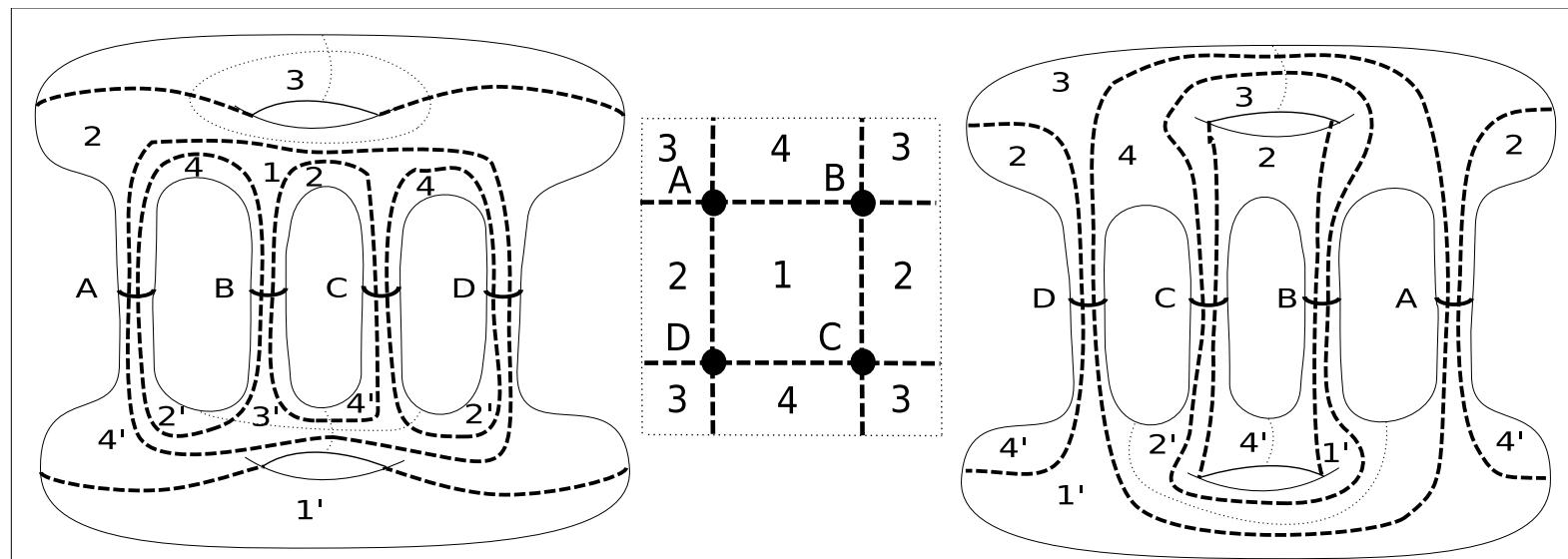
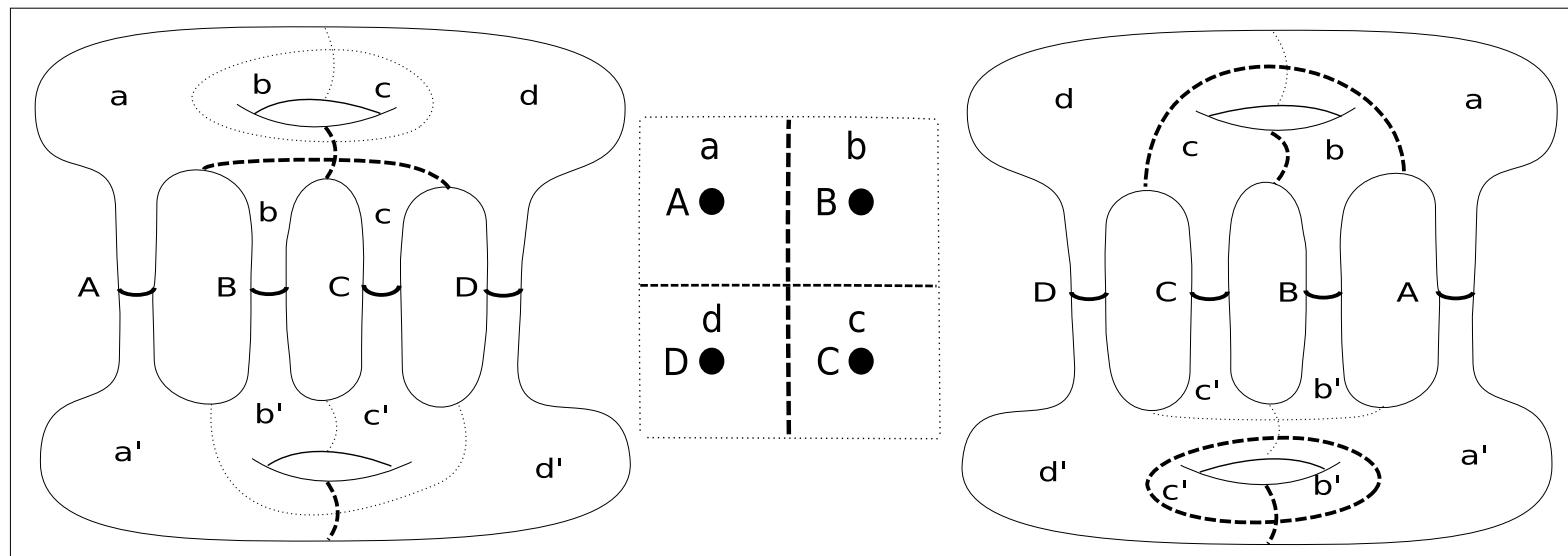
- In general, no topological Chern invariant survives on a punctured manifold.
- Here, each member of a pair of Kramers-conjugate puncture boundaries has the **same** Berry phase factor!

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

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, ± 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”?.