Hopf Insulators: Localized Representation and Surface Properties

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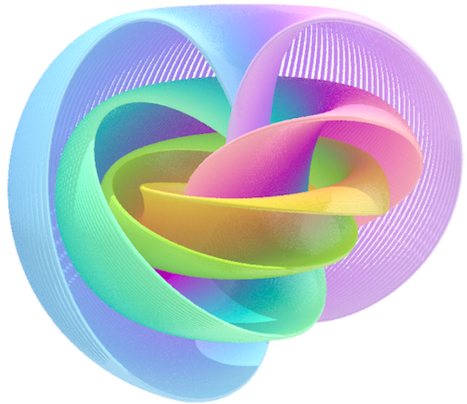
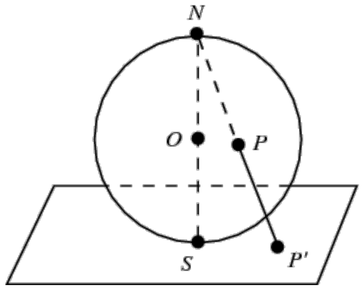
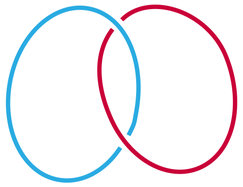
Hopf insulators

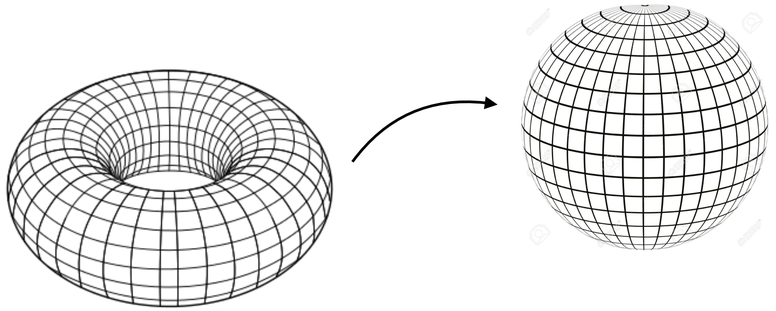




stereographic projection



Hopf map from S^3 to S^2



$$\hat{H}(k_x, k_y, k_z) = \sum_{i=x,y,z} H_i(k_x, k_y, k_z)\sigma_i$$

$$\vec{H} \in S^2, \ \vec{k} \in T^3$$

Hopf insulator

$$\chi = -\frac{1}{4\pi^2}\int_{BZ} d^3k\, \vec{\mathcal{F}} \cdot \vec{A}$$

$$\vec{A}(k) = -i\langle u_k^{occ} | \vec{\nabla}_k | u_k^{occ} \rangle$$

$$\vec{\mathcal{F}}(k) = \vec{\nabla}_k \times \vec{A}(k)$$

Hopf invariant

J. Moore, Y. Ran and X.-G. Wen, Phys. Rev. Lett. ***101****, (2008)*

Plan of the talk

- Localized Wannier representation

    1. Possibility to localize Wannier functions

    2. Centers of localization

- Surface behavior

    3. Robustness of surface states

    4. Bulk-edge correspondence

    5. Explanation by magnetoelectric polarizability

- Phase transition point

Exponential localization of Wannier functions

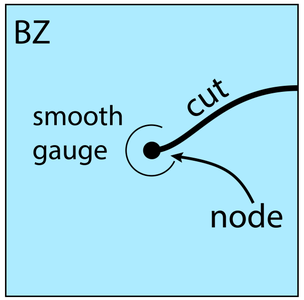
Bloch → Wannier

$$\Psi_k(r) = e^{ikr}u_k(r)$$

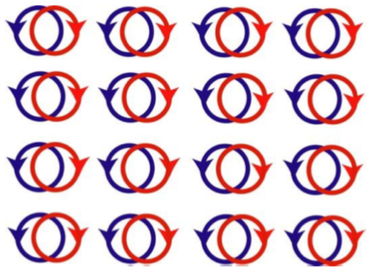
$$w_R(r) = \frac{1}{\sqrt{N}}\sum_k e^{-ikR}\Psi_k(r)$$

No symmetric localized Wannier function

Chern insulator



Z_2 insulator



Hopf insulator

- Zero Chern number
- No symmetry related band subsets

Example: Moore-Ran-Wen model

Tight-binding Hamiltonian:

$$H = \sum_i c^\dagger \sigma_i c \sigma_i$$

$$c_1 = \sin k_x + i \sin k_y$$

$$c_2 = \sin k_z + i(\cos k_x + \cos k_y + \cos k_z + h)$$

σ_i - Pauli matrices, $k_x, k_y, k_z \in BZ$

Solutions:

$u_+ = (c_1, c_2)^\dagger, u_- = (c_2^*, -c_1^*)^\dagger$ - analytic functions

$$E_\pm = \pm\sqrt{|c_1|^2 + |c_2|^2}$$

Fourier expansion of analytic function gives exponentially decaying coefficients

J. Moore, Y. Ran and X.-G. Wen, *Phys. Rev. Lett.* **101**, (2008)

Centers of localization

Atomic limit

- One-site localization of Wannier functions
- No hoppings between sites

Any trivial insulator is equivalent to the atomic limit

General argument

Assume one-site-localized Wannier functions $\Psi_{\pm,\mathbf{R}} \propto \delta_{\mathbf{R},\mathbf{0}}$

Fourier transform $u_{\pm} \propto const$

Nontrivial map from T^3 to S^2 is homotopically inequivalent to the constant map.

Example: Moore-Ran-Wen model

Atomic limit

$$\bar{z} = \overline{\langle w \,|\, z \,|\, w \rangle} \in \mathbb{Z}$$

Hopf topological phase

$$\bar{z} \notin \mathbb{Z}$$

$$w(\mathbf{k}_\perp, z) = \int dk_z e^{-ik_z z} u(\mathbf{k}) -$$

Hybrid Wannier function

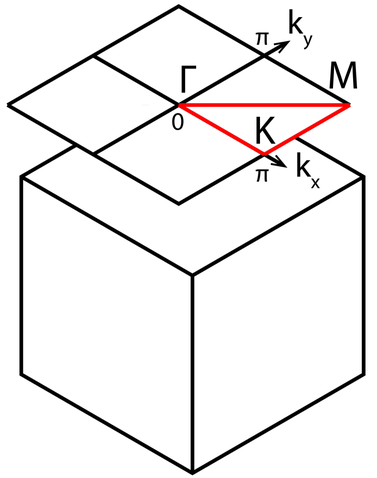
$$\bar{z}(\mathbf{k}_\perp) = \frac{1}{2\pi} \int dk_z \mathbf{A}_z(\mathbf{k}_\perp) -$$

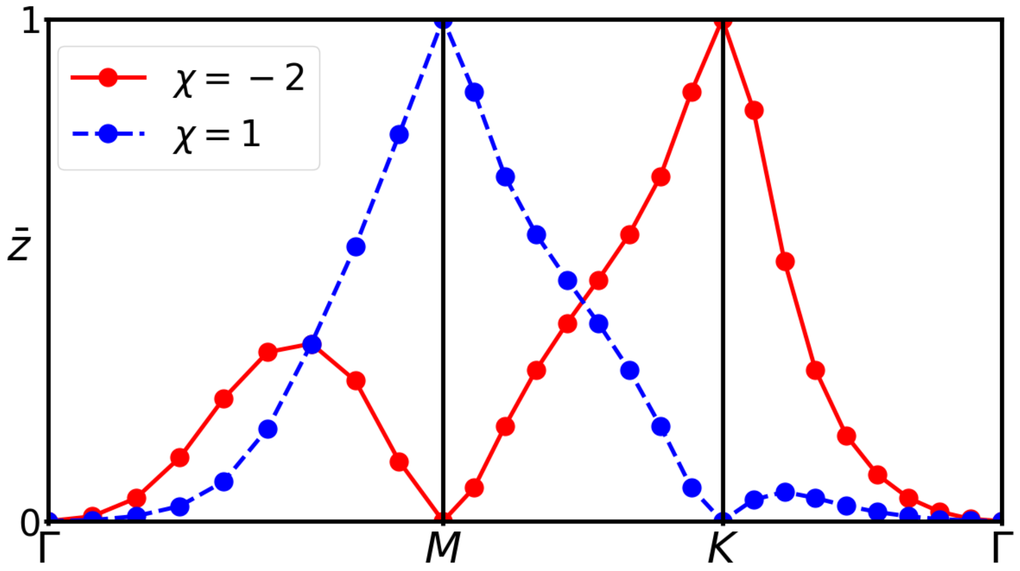
centers of Hybrid Wannier functions

Particle-hole symmetry

$$\Xi H(k_{inv}, k_z) \Xi^\dagger = -H(-k_{inv}, -k_z)$$

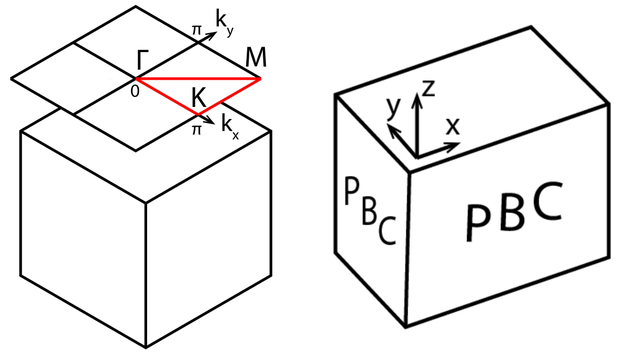
$$\bar{z}(k_{inv}) = 0 \mod 1, k_{inv} \in \{\Gamma, K, M\}$$





N. Marzari and D. Vanderbilt, *Phys. Rev. B* **56** (1997)

Robustness of surface states



General statement

If the Hamiltonian

- has the symmetry of a d-spatial-dimensional space group G,
- Hilbert space is a direct sum of two unit-rank band representations of G,
- analytic and has a finite spectral gap in the BZ,

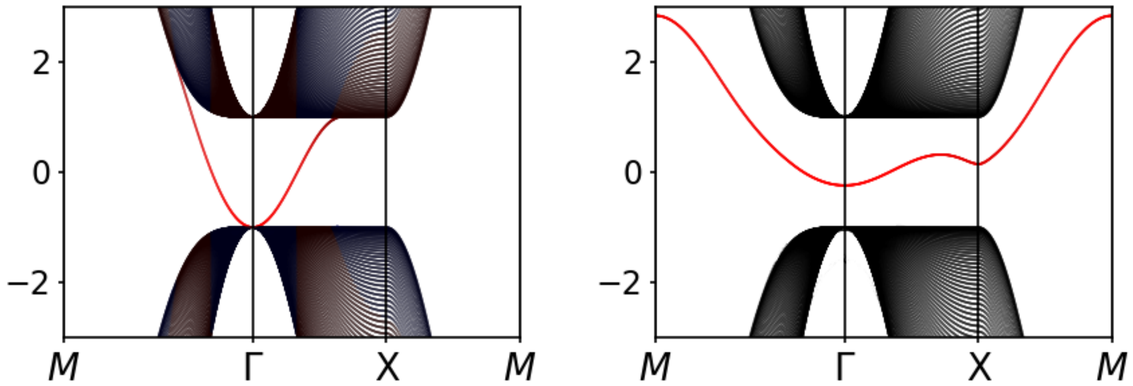
and the first Chern number for the lower state is zero

⇩

Surface states are not robust

Example

Finite slab with 100 layers in z direction



By applying surface potential we detach surface state from the bulk

$$H_{surface} \rightarrow 0.25 H_{surface}$$

Bulk-edge correspondence

Hopf invariant

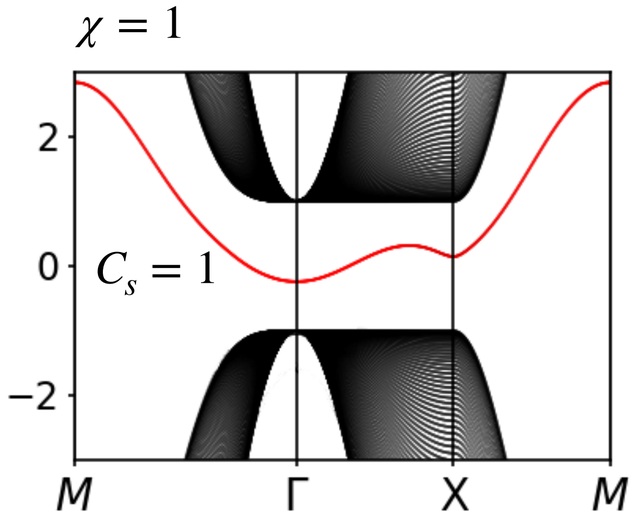
$$\chi = -\frac{1}{4\pi^2}\int_{BZ} d^3k\,\overrightarrow{\mathscr{F}}\cdot\overrightarrow{A}$$

Surface Chern number

$$C_s := \frac{1}{2\pi}\int_{rBZ} Tr[\mathscr{F}(\mathbf{k})\cdot\hat{\mathbf{n}}]d^2k$$

Surface states are detachable

$$\chi = C_s$$



Invariance of surface Chern number

C_s is invariant under continuous deformation of H:

- Assume C_s and C_s' correspond to the same χ
- Corresponding Hamiltonians are smoothly connected in parameter space $H(\mathbf{k}, \lambda)$, $\lambda \in [0,1]$
- In 4D space the transferred quanta of Berry curvature $C_s - C_s'$ corresponds to the second Chern number C_2
- $C_2 = \frac{1}{32\pi^2} \int_{BZ} d^4k \epsilon_{lmno} Tr[F_{lm} F_{no}]$ - nonlinear response to E, B in 4D systems
- Second Chern number is zero $C_2 = 0$ for systems with occupied subspace spanned by single analytic Bloch function

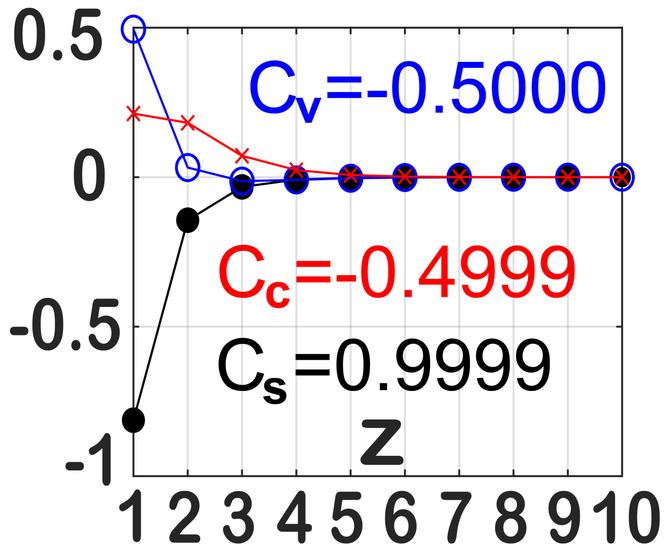
Berry-curvature polarization

From geometric theory of polarization:

$$\vec{P} = \int_{BZ} \vec{A}\, dk$$

In a finite slab it reveals as a charge accumulated on the surface.

Similarly define $\chi = \int_{BZ} \vec{A}\,\vec{\mathcal{F}}\, dk -$ polarization of Berry curvature, with $\vec{\mathcal{F}} = \vec{\nabla} \times \vec{A}$.



From the theory of magneto-electric polarizability:

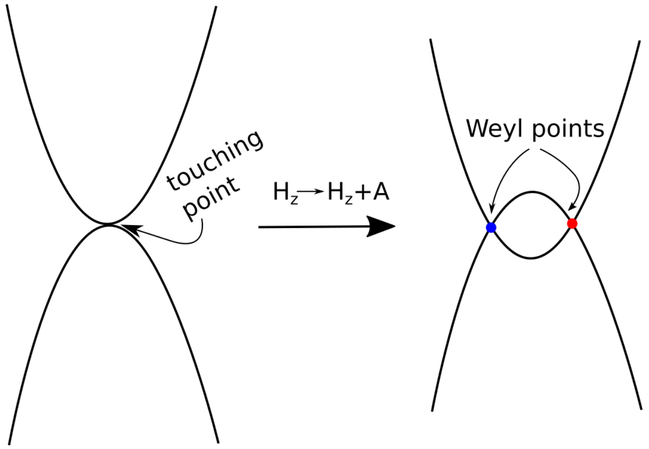
- Both valence and conductance bands with Berry polarization χ give $-\chi/2$ contribution to surface Chern number.
- This must be compensated by Chern number of the surface state $C_s = \chi$

A. M. Essin et. al., Phys. Rev. Lett. ***102****, 146805 (2009)*

Phase transition points

Quadratic band touching point ($E_+ = E_-$) is the Weyl dipole

Adding a splitting term → Weyl dipole splits into two Weyl points of opposite chirality



Continuum limit — illustration of Weyl dipole:

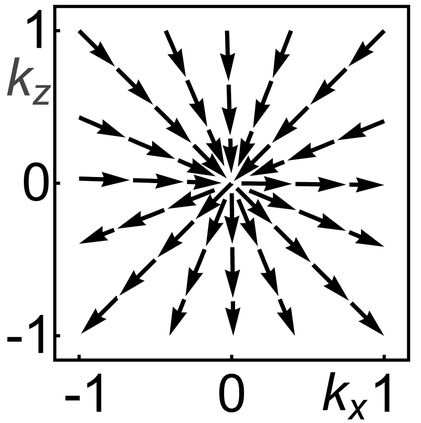
$$H = \sum_i c^\dagger \sigma_i c \sigma_i$$

$$c_1 = k_x + i k_y, \;\; c_2 = k_z + i\phi$$

Berry curvature polarization in continuous limit:

$$\frac{1}{4\pi^2} \int_{\mathbb{R}^3} \mathscr{F} \cdot A \, d^3k = \frac{1}{2} \text{sign}[\phi]$$

Berry curvature of the Weyl dipole



Conclusions

- Localized Wannier representation is possible for Hopf insulators
- There’s always a finite width of Wannier localization for nontrivial Hopf phases
- Surface states are not robust in Hopf insulators
- Berry curvature polarization of the bulk leads to nonzero Chern number of the surface
- At phase transition points Weyl dipoles change Hopf invariant by one for every band touching point