Berry phases and topological materials

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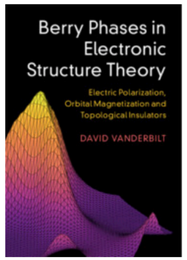
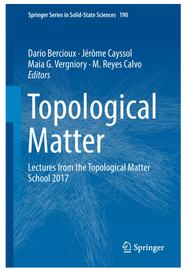
References:

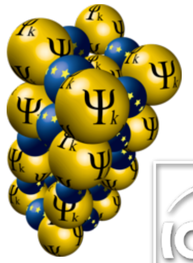


Vanderbilt, D. (2018). *Berry phases in electronic structure theory: Electric polarization, orbital magnetization and topological insulators*. Cambridge University Press.



Bercioux, D., Cayssol, J., Vergniory, M. G., & Reyes Calvo, M. (Eds.). (2019). *Topological matter: Lectures from the topological matter school 2017*. Springer Nature.

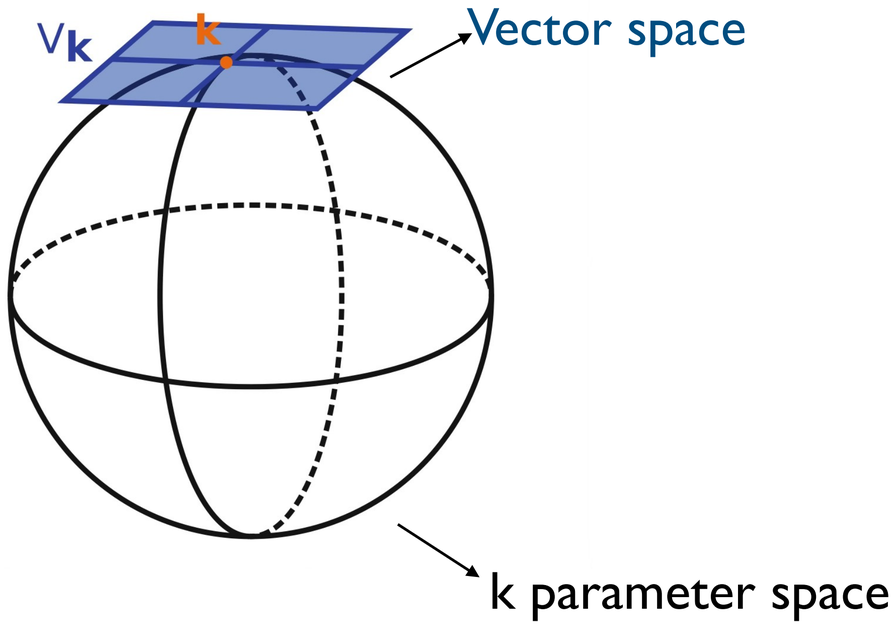
Financial support:

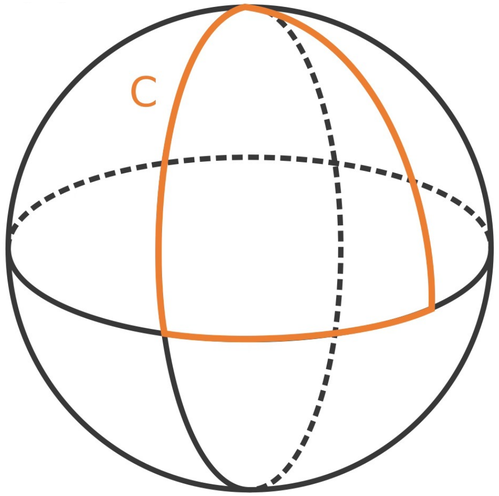


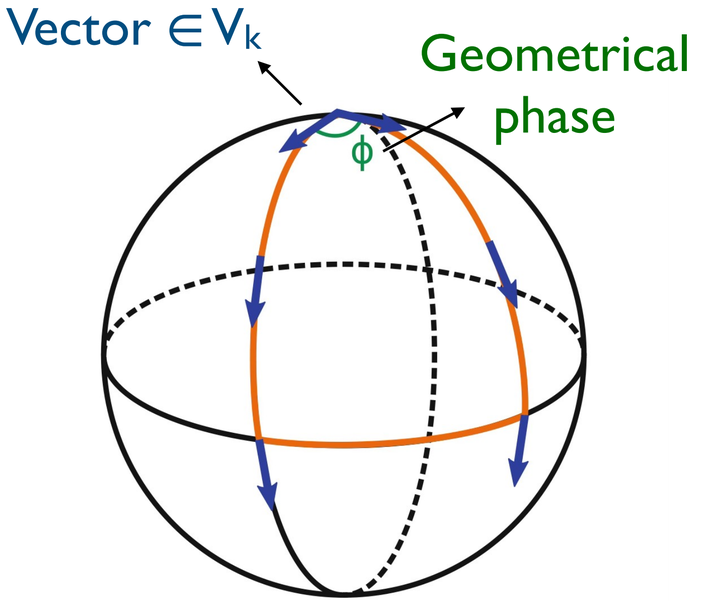
Outline

- Berry phase
  - Geometrical phase
  - Berry/Zak's phase
- Modern theory of polarization
  - Polarization of crystalline materials
  - Spontaneous polarization and Born effective charges
- Topology in band theory
  - Topology
  - Topological invariants
  - Geometry of the reciprocal space
  - Berry phase, curvature and connection.
- Topological materials: types and characterization (WIEN2k & BerryPI)
  - Bulk boundary correspondence principle
  - Chern Insulators: CherN.py(FeBr3 monolayer)
  - Berry curvature maps: CherN.py(MoS_2 monolayer)
  - $\mathbb{Z}_2$ topological insulators: wcc.py(Bi_2Se_3)
  - Characterization of Weyl semimetals: WloopPHI(TaAs)

Geometrical (Patcharatnam) phase

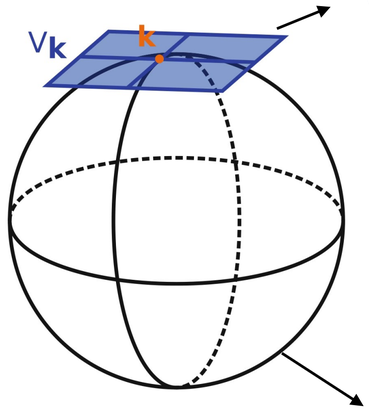






Source: "*Topological matter, Chapter 3*" by D. Gresch and A. Soluyanov

Geometrical (Patcharatnam) phase in QM: discrete formulation

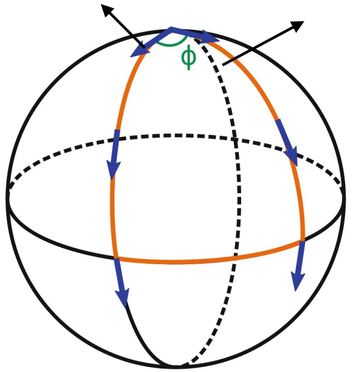


Vector space

k parameter space

Vector $\in V_k$

Geometrical phase



Source: "*Topological matter, Chapter 3*" by D. Gresch and A. Soluyanov

Hilbert space (k)

$$H(k)\,|\psi(k)\rangle = E(k)\,|\psi(k)\rangle$$

$|\psi_o(k)\rangle \in$ Hilbert Space(k) ⟶ Considering only ground eigenstates at different k (Adiabatic evolution)

$$e^{-i\Delta\varphi_{12}} = \frac{\langle\psi(k_1)\,|\,\psi(k_2)\rangle}{|\,\langle\psi(k_1)\,|\,\psi(k_2)\rangle\,|} \longrightarrow \Delta\varphi_{12} = -\,\mathrm{Im}\ln\langle\psi(k_1)\,|\,\psi(k_2)\rangle$$

Relative phase difference

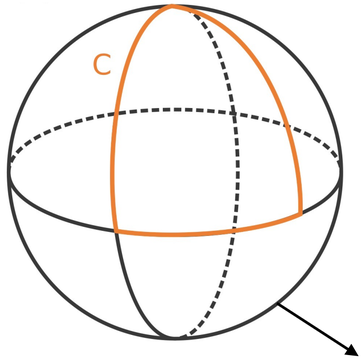
No physical meaning as a gauge transformation of the form:

$$|\psi(k_2)\rangle \to e^{-i\delta\varphi_2}\,|\psi(k_2)\rangle \qquad |\psi(k_1)\rangle \to e^{-i\delta\varphi_1}\,|\psi(k_1)\rangle$$

Leads to a change

$$\Delta\varphi_{12} \to \Delta\varphi_{12} + (\delta\varphi_1 - \delta\varphi_2)$$

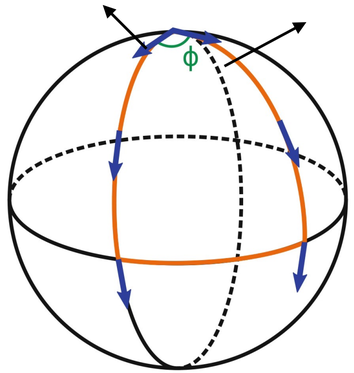
Geometrical (Patcharatnam) phase in QM: discrete formulation



k parameter space

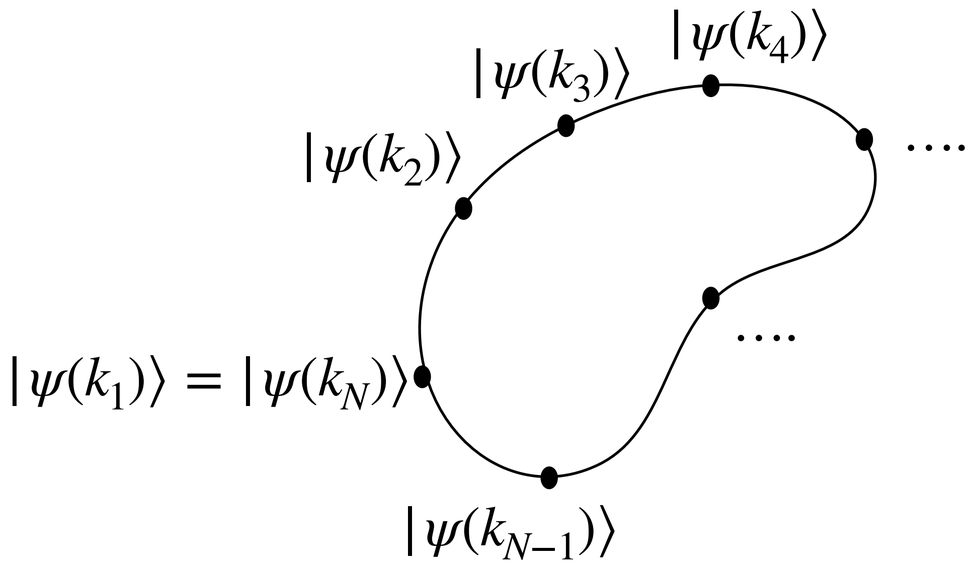
Vector $\in V_k$

Geometrical phase



Source: "*Topological matter, Chapter 3*" by D. Gresch and A. Soluyanov

But, what if we take a closed sequence of inner products or loop ?



The total phase difference is given by

$$\gamma = \Delta\varphi_{12} + \Delta\varphi_{23} + \Delta\varphi_{34} + \ldots + \Delta\varphi_{(N-1)N}$$

$$\gamma = = -\operatorname{Im}\ln\langle\psi(k_1)|\psi(k_2)\rangle\langle\psi(k_2)|\psi(k_3)\rangle\langle\psi(k_3)|\psi(k_4)\rangle\ldots\langle\psi(k_{N-1})|\psi(k_{N=1})\rangle$$

$$\gamma = = -\operatorname{Im}\ln\prod_{i=1}^{N-1}\langle\psi(k_i)|\psi(k_{i+1})\rangle$$

Which is a gauge invariant quantity as the gauge-arbitrary phases cancel in pairs.

Berry/Zak's phase: continuum formulation

In the continuum formulation given k a real variable

$$\ln\langle\psi(k)\,|\,\psi(k+dk)\rangle \approx \langle\psi(k)\,|\,\partial_k\psi(k)\rangle dk$$

We can define

Berry potential:

$$\mathbf{A}(k) = -i\langle\psi(k)\,|\,\partial_k\,\psi(k)\rangle$$

Berry curvature:

$$\mathbf{\Omega}(k) = \nabla_{\mathbf{k}} \times \mathbf{A}(k)$$

Berry phase is given as closed line integral of the Berry potential in k parameter space and equivalently as a flux of the Berry curvature through a surface S (Stokes' theorem)

$$\gamma_{\partial S} = \oint_{\partial S} \mathbf{A}(k)\cdot dk = \iint_S \mathbf{\Omega}(k)\cdot d\mathbf{S}$$

Berry curvature is also gauge invariant!

Berry, Proc. R. Soc. London A **392**, 45 (1984)
Zak, Phys. Rev. Lett. **62**, 2747 (1989)

For electrons in a crystal, the Bloch theorem states

$$\psi^{(n)}_{\mathbf{k}}(\mathbf{r}) = u^{(n)}_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{kr}} \qquad u^{(n)}_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u^{(n)}_{\mathbf{k}}(\mathbf{r})$$

Cell periodic: well behaved

$$\left[\frac{1}{2m}p^2 + V(\boldsymbol{r})\right]\psi^{(n)}_{\mathbf{k}}(\boldsymbol{r}) = \varepsilon^{(n)}(\boldsymbol{k})\psi^{(n)}_{\mathbf{k}}(\boldsymbol{r})$$

$$\left[\frac{1}{2m}(\boldsymbol{p}+\hbar\mathbf{k})^2 + V(\boldsymbol{r})\right]u^{(n)}_{\mathbf{k}}(\boldsymbol{r}) = \varepsilon^{(n)}(\mathbf{k})u^{(n)}_{\mathbf{k}}(\boldsymbol{r})$$

Mapping from k independent Hamiltonian to H(**k**) with **k**-independent boundary conditions ($u^{(n)}_{\mathbf{k}}$ belong to the same Hilbert space).

$$\gamma^{(n)}_{\partial S} = \oint_{\partial S} i\langle u_{nk}\,|\,\nabla_{\boldsymbol{k}}\,|\,u_{nk}\rangle\cdot d\mathbf{k} = \iint_S \mathbf{\Omega}^{(n)}(\mathbf{k})\cdot d\mathbf{S}$$

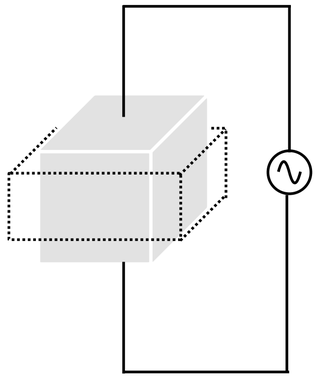
Is there any application?

Modern theory of polarization: pioneered by *King-Smith*, *David Vanderbilt* and *Raffaele Resta*

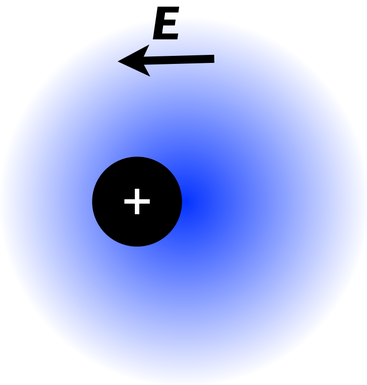
Polarization: Fundamental quantity essential to the electronic response of the system.

Some related properties:

Piezo- and Ferroelectricity



Dielectric screening



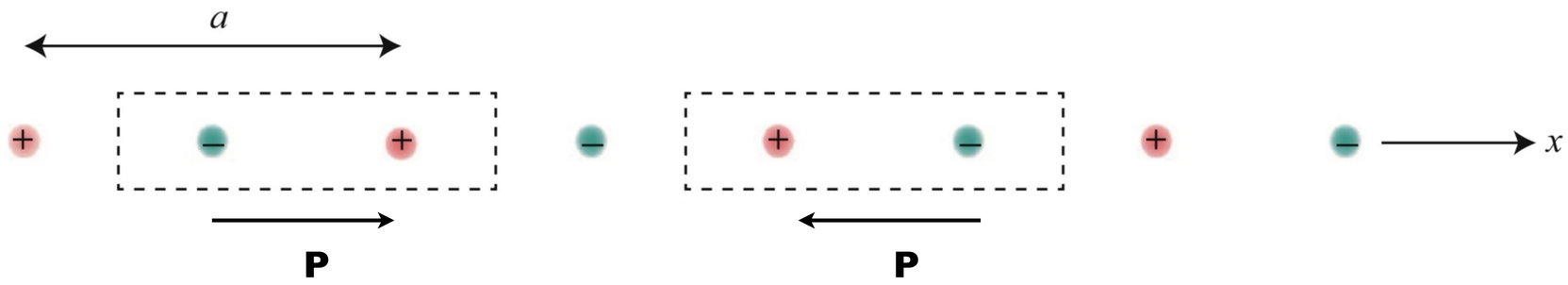
For the case of a collection of charges in the ionic limit or charge densities $n(\mathbf{r})$ the dipole moment:

$$\mathbf{d} = \sum_i q_i \mathbf{r}_i \qquad \mathbf{d} = \int en(\mathbf{r})\mathbf{r}\, d\mathbf{r}$$

Well defined provided there is no net charge.

Modern theory of polarization

Now, for a solid we want to convert this idea to a bulk property: dipole moment per unit volume.



Spaldin, N.A. Solid State Chemistry, 195,2-10, (2012).

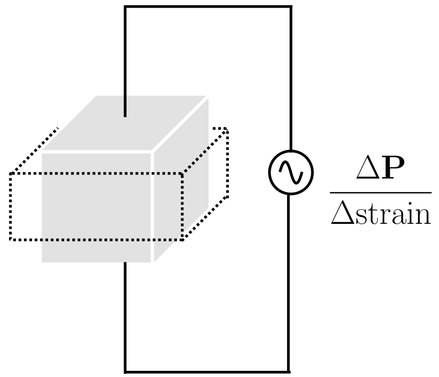
Problem: No existence of a proper microscopic theoretical description of polarization in crystals, the charge distribution is periodic in space and this leads to the dipole operator to not be well defined.

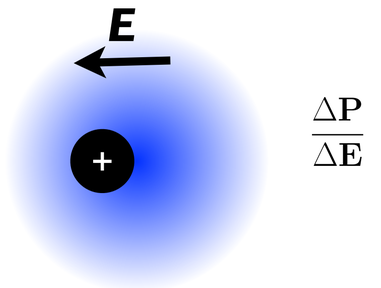
Reason: The polarization of a periodic system is a lattice rather than a vector, it is a multivalued quantity property which is a natural consequence of the periodicity in a bulk solid.

Consequence: Obtaining different values depending on the choice of the unit cell

Modern theory of polarization

Solution: Only the change in polarization has physical meaning! $\Delta\mathbf{P} = \mathbf{P}^{(1)} - \mathbf{P}^{(0)}$





Supported by the experimental fact that measurements of absolute polarization of a crystal have never been measured as a bulk property.

Well known properties are derivative of the polarization with respect to suitable perturbations.

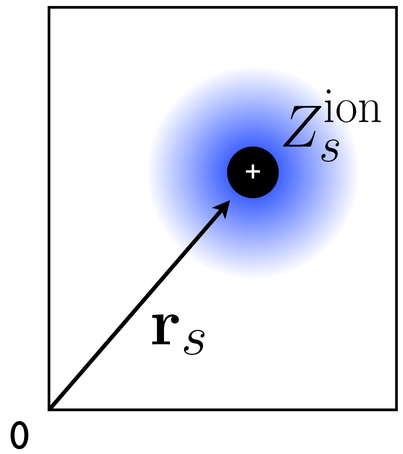
Modern theory of polarization

The change in polarization is singled valued provided we stick with the same choice of unit cell and basis throughout the analysis and can be quantified by employing the Berry phase of the electronic wavefunction

$$\Delta\mathbf{P} = \mathbf{P}^{(1)} - \mathbf{P}^{(0)}$$

Components of total microscopic polarization

$$\mathbf{P} = \mathbf{P}_{ionic} + \mathbf{P}_{electronic}$$



$$\mathbf{P}_{ionic} = \frac{e}{\Omega}\sum_{s}^{\text{atoms}} Z_s^{\text{ion}}\mathbf{r}_s \qquad \mathbf{P}_{electronic} = \Omega^{-1}\int d\mathbf{r}\,\mathbf{r}\rho(\mathbf{r}) = \Omega^{-1}\sum_{n}^{\text{bands}}\langle\psi_n|\mathbf{r}|\psi_n\rangle$$

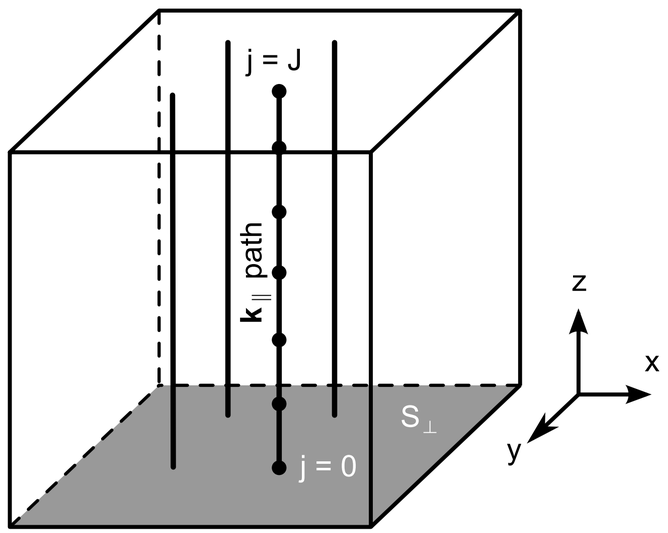
$\hat{\mathbf{r}} = i\nabla_{\mathbf{k}}$ (position operator in k-space)

$$\mathbf{P}_{electronic} = -\frac{2e}{(2\pi)^3}\sum_{n}^{\text{bands}}\int_{\text{BZ}} \mathrm{d}\mathbf{k} i\langle u_{n\mathbf{k}}|\nabla_{\mathbf{k}}|u_{n\mathbf{k}}\rangle$$

Berry phase

King-Smith and David Vanderbilt, Phys. Rev. B **47**, 1651 (1993)

Polarization: BerryPI



The Berry phase is computed for individual **k**-paths parallel to an axis in the Brillouin zone and the average for all paths is taken.

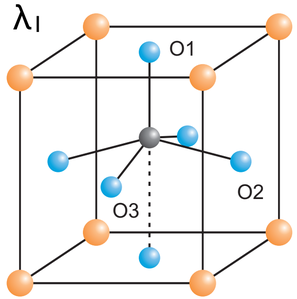
These strings are equivalent to a closed loop due to the Born–von Karman boundary conditions.

An electric field causes linear variation in **k**. A closed path is achieved when **k** sweeps the whole Brillouin Zone. (Other way to induce loops in parameter space is through magnetic-induced cyclotron Orbits)

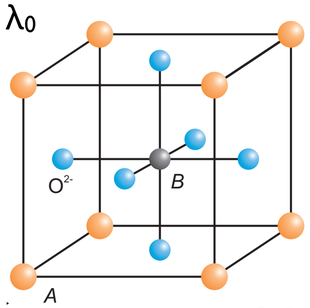
Spontaneous polarization: $P_s = P_{nc} - Pc$

Requires 2 structures

Non-centrosymmetric



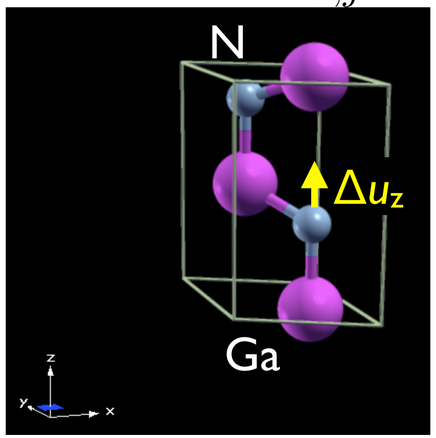
Centrosymmetric



Characteristic of ferroelectric materials

Born effective charge

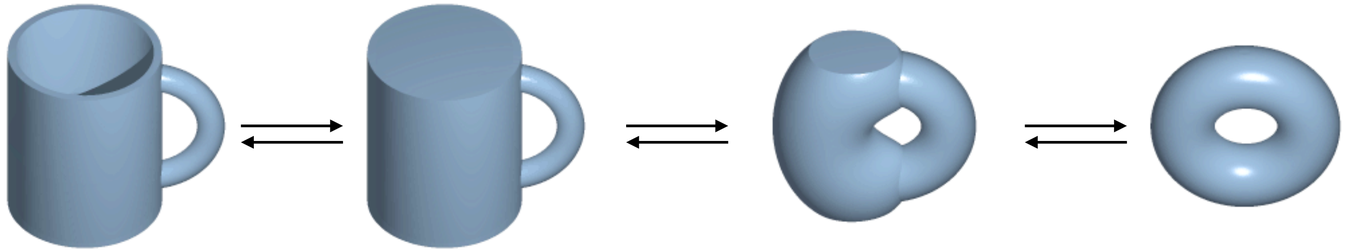
$$Z^*_{s,ij} = \frac{\Omega}{e}\frac{\Delta P_i}{\Delta r_{s,j}}$$



Amount of charge that contributes to the polarization during the displacement of the ions

Topology

Topology is the study of the properties of geometrical objects that remain invariant as the object is continuously deformed.



Genus = 1

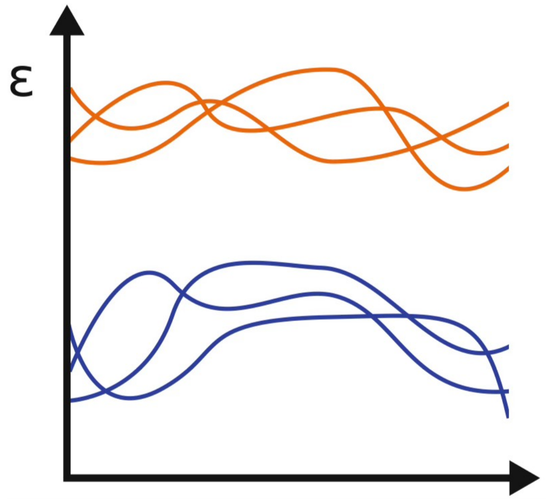
Torus to mug morphing animation, by Lucas Vieira, License: Public Domain

Topological Invariant:

- Allows the classification of objects in discrete classes
- Integer quantity that cannot be changed without changing the whole topological class.
- Encodes information about the global structure of the object/space
- Can not vary in a continuous fashion, which points to potential great stability of a property.

Topological materials: what is topological about them?

The relevant topology is *not related to* the shape in real space nor reciprocal space!

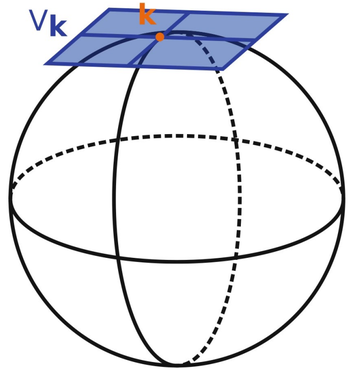


$$\{|u_{n\mathbf{k}}\rangle\}_{\in\ occupied}$$

↓ Span

$$V_{\mathbf{k}}(\mathbf{C})\ \forall\ \mathbf{k}$$

Hilbert space (k)



Vector (Groundstate)

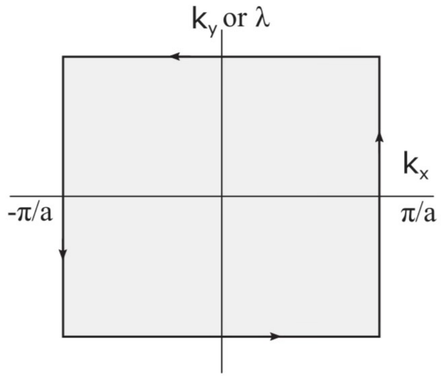
∈

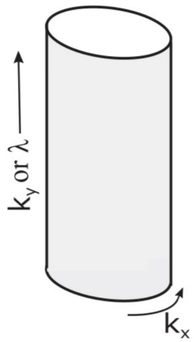
Hilbert space

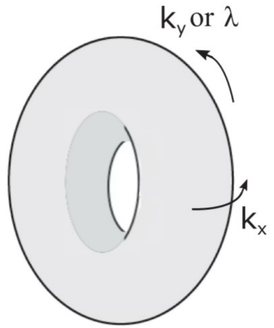
k-parameter space = Brillouin Zone

The topology is defined by the way the eigenvectors change as a function of k in the Brillouin zone.

From the boundary conditions: the BZ is a closed space.





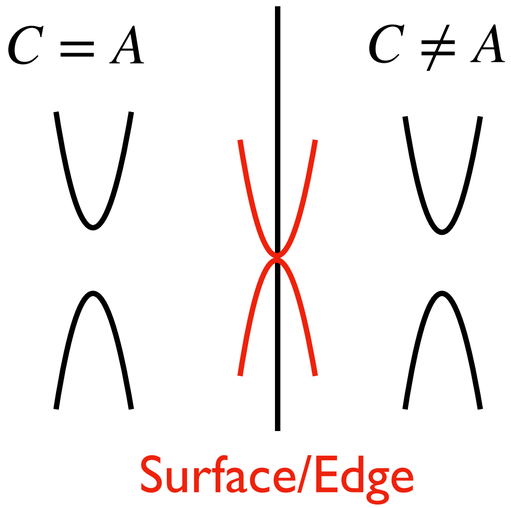


Source: "Electronic structure: Basic theory and practical methods., *Chapter 25.4*" by Martin, R. M.

2D BZ is a T^2

Topological materials: Classification

Topological Insulator



- Vacuum is topologically trivial ($C = 0$)
- Bulk boundary correspondence principle: gapped bulk and conductive surface/edge states.
- Topologically protected: as long as the gap remains open, surface states exist.
- Topology is global property of the bulk electronic structure with measurable effects on the interface.
- Potential application in quantum computing

Berry curvature, when cannot be neglected? $\boldsymbol{\Omega}(k) = \nabla_{\mathbf{k}} \times \mathbf{A}(k)$

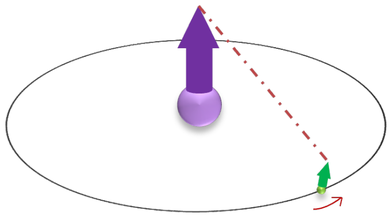
TRS invariant: $\boldsymbol{\Omega}(-\mathbf{k}) = -\boldsymbol{\Omega}(\mathbf{k})$

(Magnetic fields breaks TRS)

P-symmetric: $\boldsymbol{\Omega}(-\mathbf{k}) = \boldsymbol{\Omega}(\mathbf{k})$

(Spatial inversion symmetry)

Both present $\rightarrow \boldsymbol{\Omega} = \mathbf{0}$



An important contributor to topological phenomena is the spin-orbit interaction.

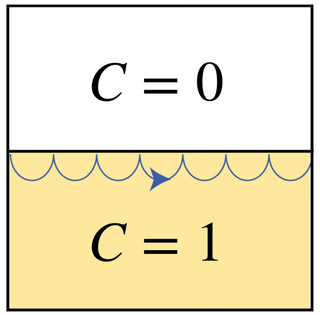
Chern Insulator/ Quantum anomalous Hall phase

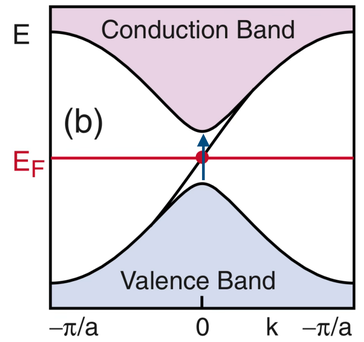
It is regarded as the basic tological insulator from which other topological states are derived.

Characteristics:

- 2D system
- Magnetic: Time Reversal Symmetry spontaneously broken
- Insulating
- High SOC (band inversion)

Physical consequence





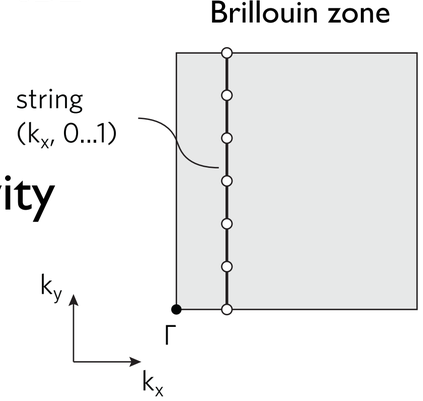
Spin filtered conductive edge states(number of crossing states = ΔC)

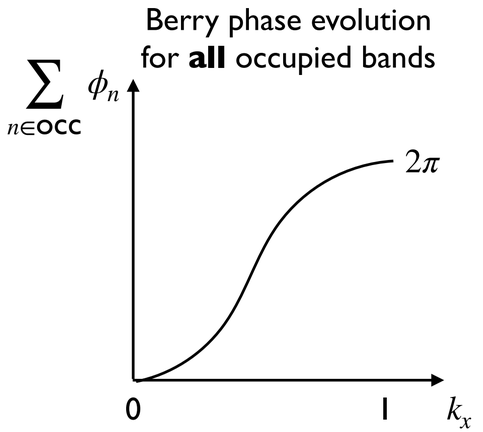
Modified from: Hasan, M. Z., & Kane, C. L. (2010). *Rev Mod Phys*, *82*(4)

Topological Invariant: Chern Number

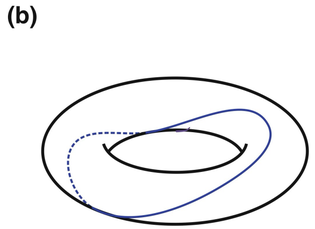
$$C = \frac{1}{2\pi}\sum_{n}^{\text{occ.}}\int_{\text{BZ}} \Omega^{(n)}(\mathbf{k})\cdot d\mathbf{S} = \frac{1}{2\pi}\sum_{n}^{\text{occ.}}\gamma_{\partial BZ}$$

Characterization



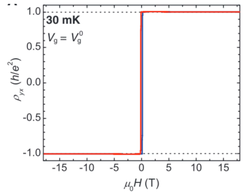


Winding of the Berry phase around the BZ



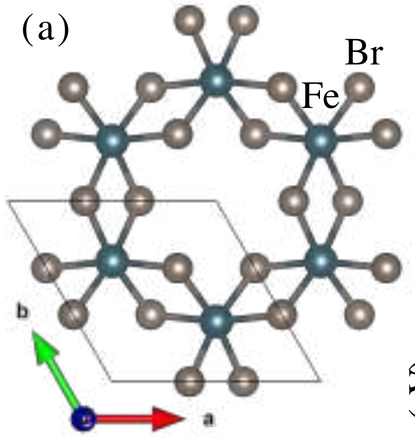
Linked to the Quantum anomalous Hall conductivity

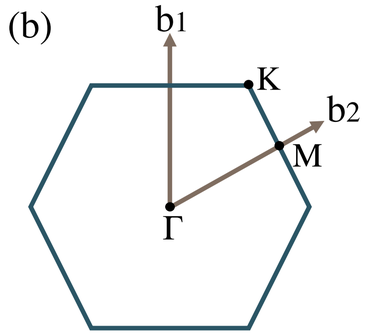
$$\sigma_{\text{AHC}} = C\frac{e^2}{h}$$

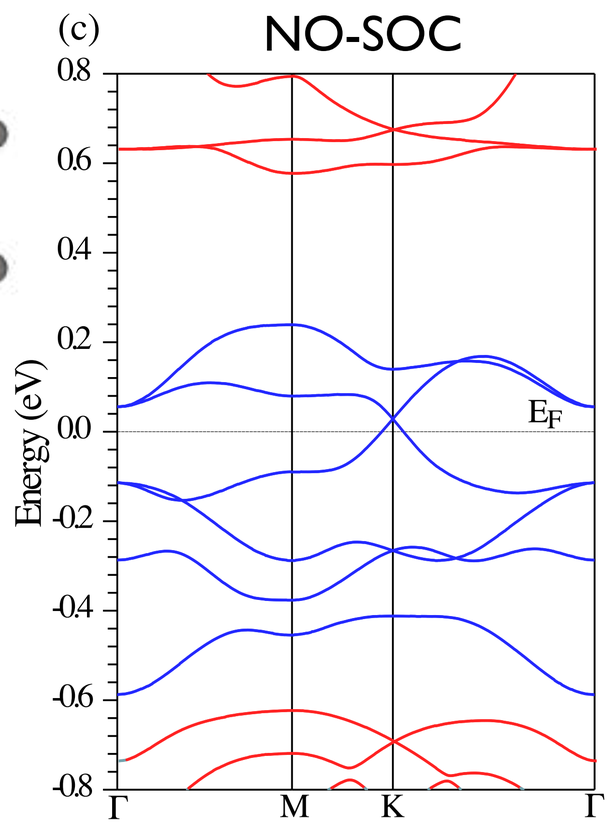


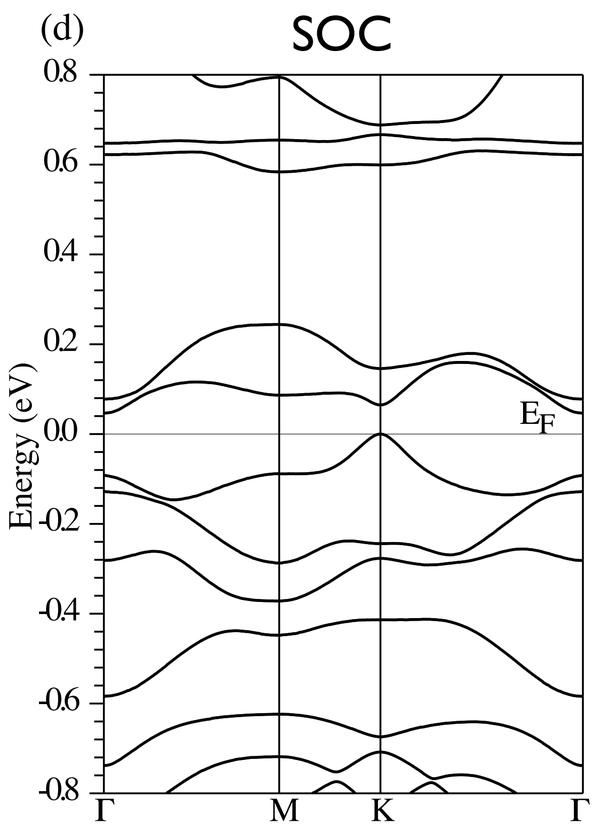
Xue, Q.K. , et. Al. (2013). *Science*, *340*(6129), 167–170.

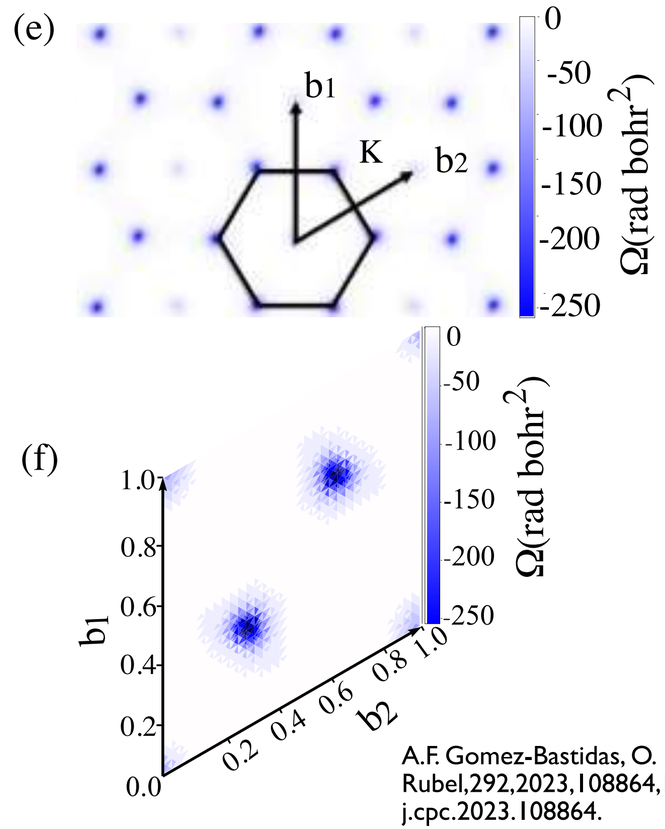
Chern Insulator: 2D-FeBr3 (CherN.py)







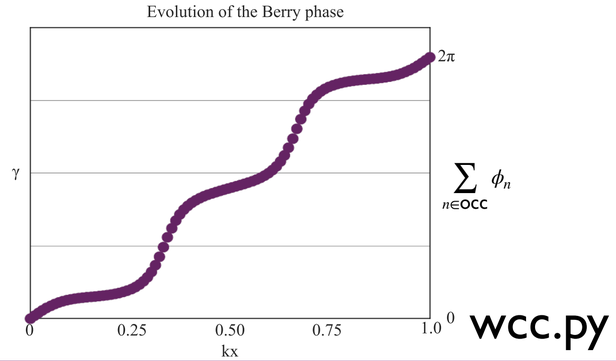




A.F. Gomez-Bastidas, O. Rubel,292,2023,108864,10.1016/j.cpc.2023.108864.

Chern number:

$$C = (2\pi)^{-1} \iint_{BZ} \mathbf{\Omega}(\mathbf{k}) \cdot d\mathbf{S} = -1$$

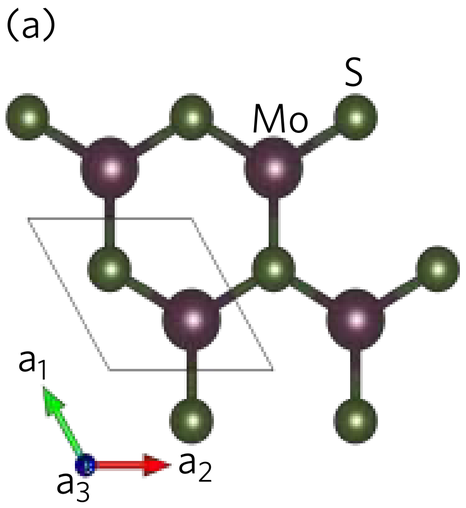


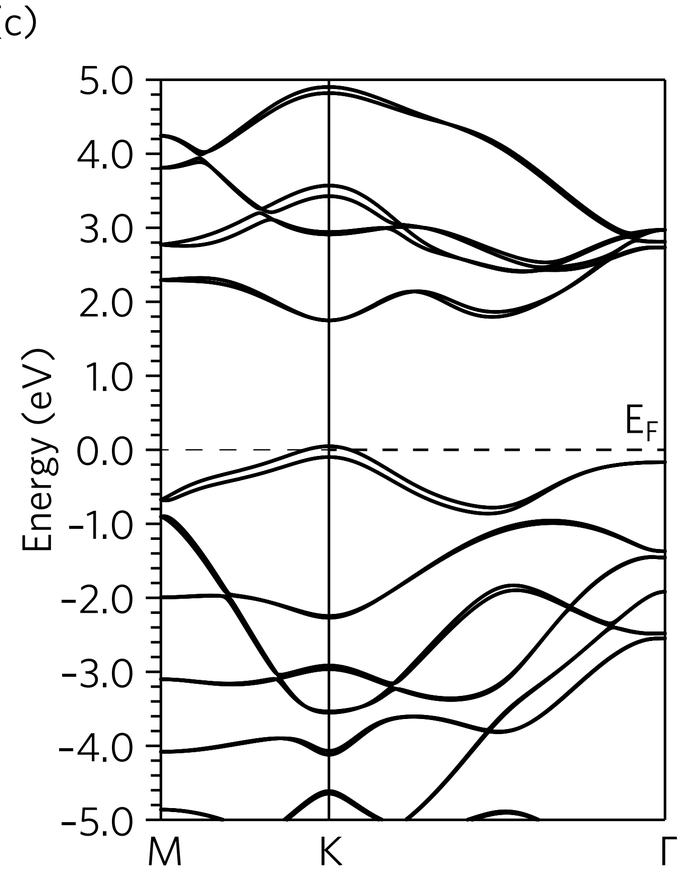
wcc.py

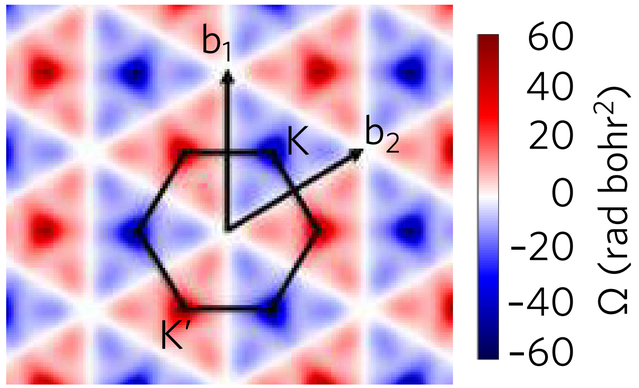
Berry Curvature

$$\Omega_{\alpha\beta}(\mathbf{k}) = -2\,\mathrm{Im}\left[\sum_{n\neq occ} \frac{\langle u_{\mathbf{k}}^{(0)} | \partial \hat{H}_{\mathbf{k}}/\partial k_\alpha | u_{\mathbf{k}}^{(n)} \rangle \langle u_{\mathbf{k}}^{(n)} | \partial \hat{H}_{\mathbf{k}}/\partial k_\beta | u_{\mathbf{k}}^{(0)} \rangle}{\left(\epsilon_{\mathbf{k}}^{(0)} - \epsilon_{\mathbf{k}}^{(n)}\right)^2}\right]$$

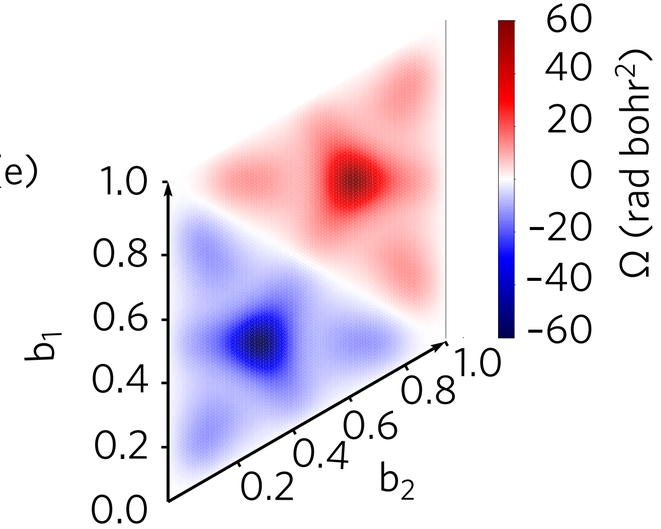
Berry curvature map: 2D-MoS_2 (CherN.py)







Curvature is local



A.F. Gomez-Bastidas, O. Rubel,292,2023,108864,10.1016/j.cpc.2023.108864.

Honeycomb lattice with different sites breaks the spatial inversion symmetry

It is not magnetic, hence invariant under TRS

Chern number:

$$C = (2\pi)^{-1} \iint_{BZ} \mathbf{\Omega}(\mathbf{k}) \cdot d\mathbf{S} = 0$$

Used to obtain a global property

Berry curvature map workflow (CherN.py)

1) Construct a structure file

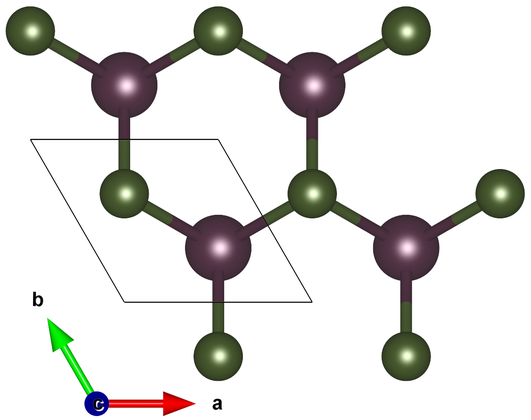
2) Perform SCF-SOC calculation

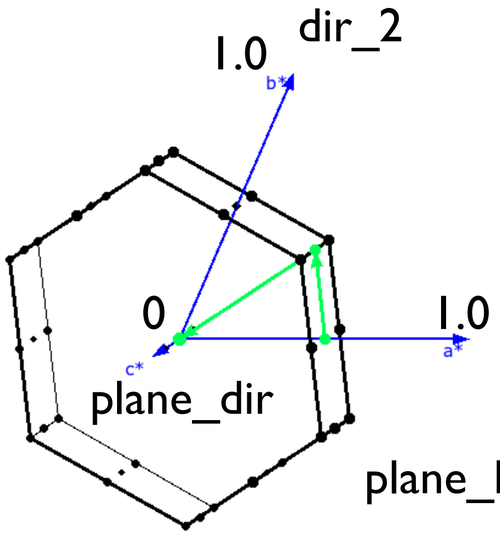
To calculate the Berry curvature map on the z=0 plane of the BZ.

3) Edit and run CherN.py script

bands = [1,26] → grep ':NOE' case.scf

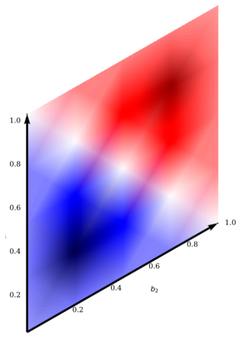
```
n_1 = 6    #discretization in dir_1
n_2 = 6    #discretization in dir_2
plane_dir = 3  # direction normal to the plane
plane_height = 0.0            # value of the constant plane
boundary = [0 , 1.0 , 0 , 1.0] #boundary selection
spinpolar = False             # spin polarized
orbital = False               # additional orbital potential
parallel = False              # parallel calculation
```





plane_height = 0

5 x 5



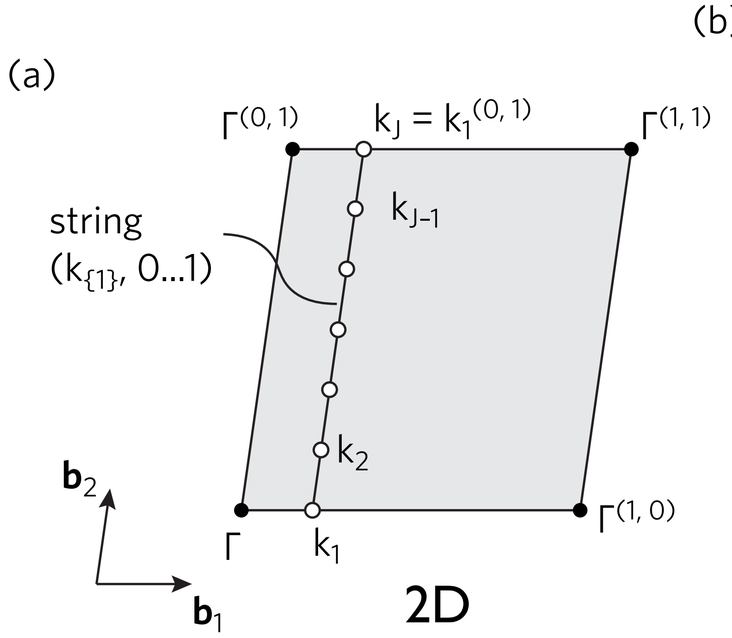
```
The total Chern number is:  0.0
```

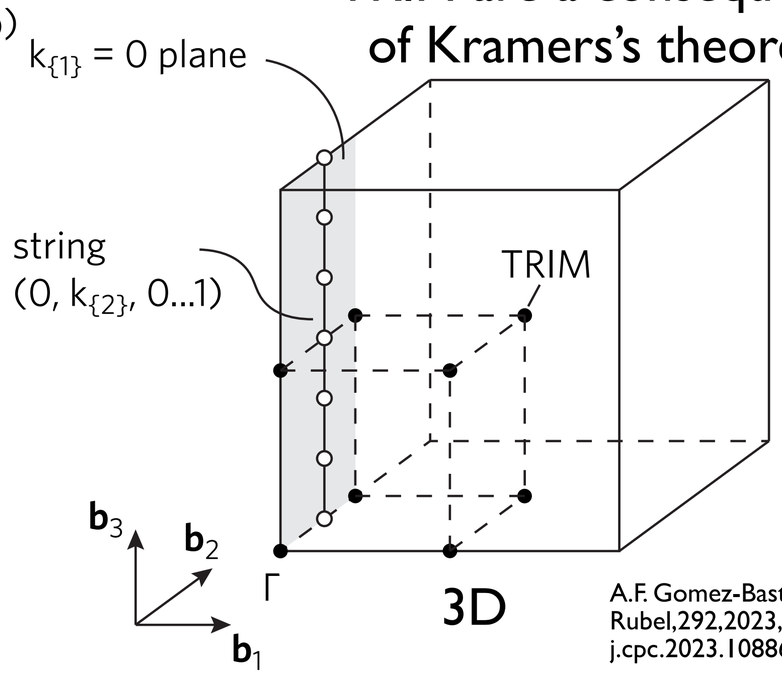
.pdf , .csv, .png

Tutorial

Kane-Mele-Fu Z2 insulator

- Time Reversal Symmetry is conserved

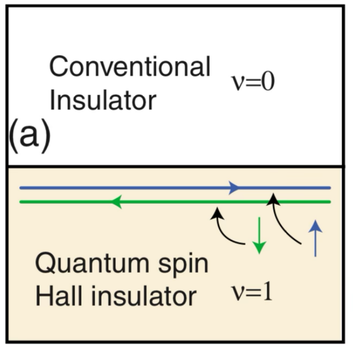


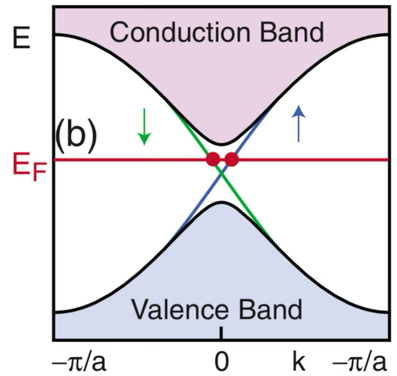


TRIM are a consequence of Kramers's theorem

A.F. Gomez-Bastidas, O. Rubel,292,2023,108864,10.1016/j.cpc.2023.108864.

Physical consequence



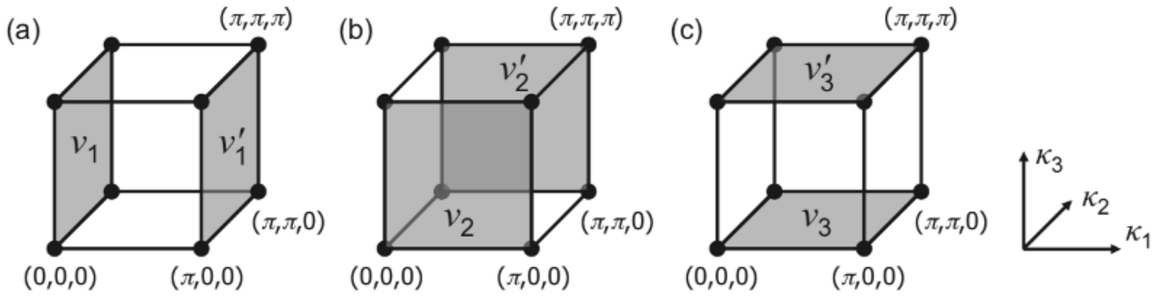


Hasan, M. Z., & Kane, C. L. (2010). *Rev Mod Phys*, *82*(4)

Conductive edge states but no net Hall conductivity

- Characterization through the evolution of the hybrid Wannier charge centers.

$$\bar{x}_n = \frac{a}{2\pi}\gamma_n$$



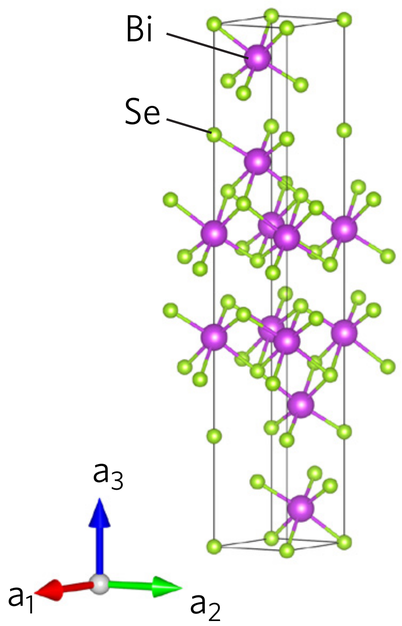
Topological Invariant

$\mathbb{Z}_2$ index = $(\nu_0;\ \nu'_1\nu'_2\nu'_3)$ tells us on which face to expect edge states.

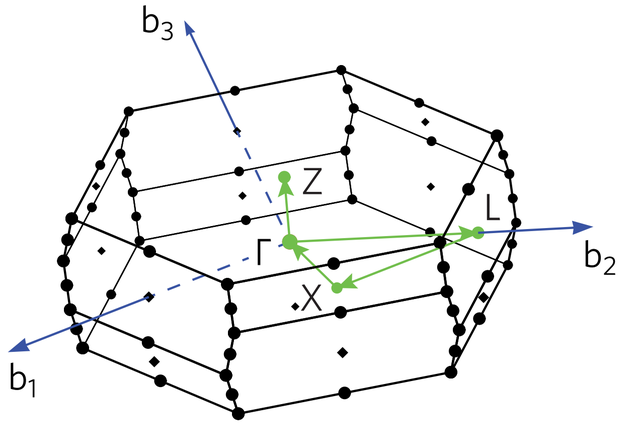
Soluyanov, A. A.; Vanderbilt, D. ***Phys. Rev. B* 2011, *83*** (23)

Kane-Mele-Fu Z2 insulator: Bi_2Se_3

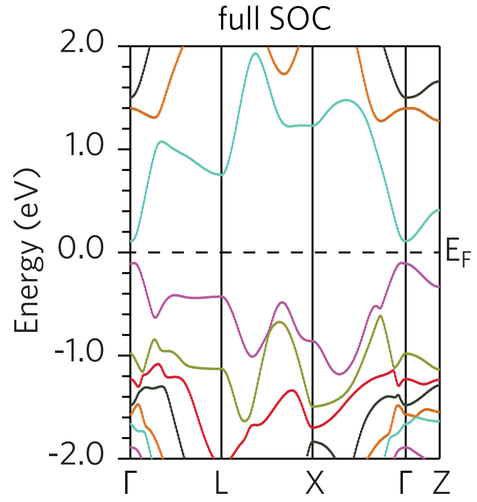
(a)



(b)

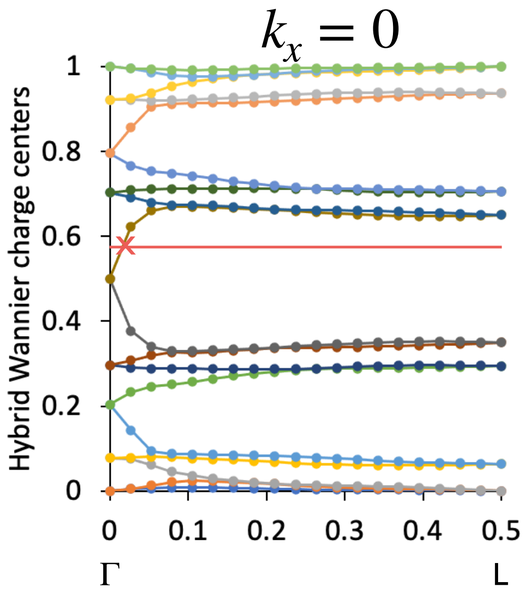


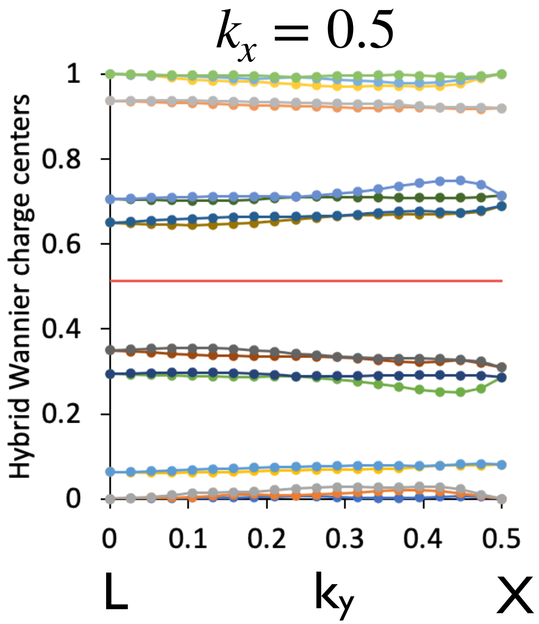
(c)



Information beyond the electronic band-structure?

Evolution of hybrid Wannier charge centers





one crossing, thus $\nu_1 = 1$

no crossings, thus $\nu'_1 = 0$

$$\nu_0 = \nu_1 + \nu'_1 = \nu_2 + \nu'_2 = \nu_3 + \nu'_3 \mod 2$$

$\mathbb{Z}_2$ index = $(1; 000)$

Strong topological insulator: all faces present conductive states

Hybrid Wannier charge centers workflow (wcc.py)

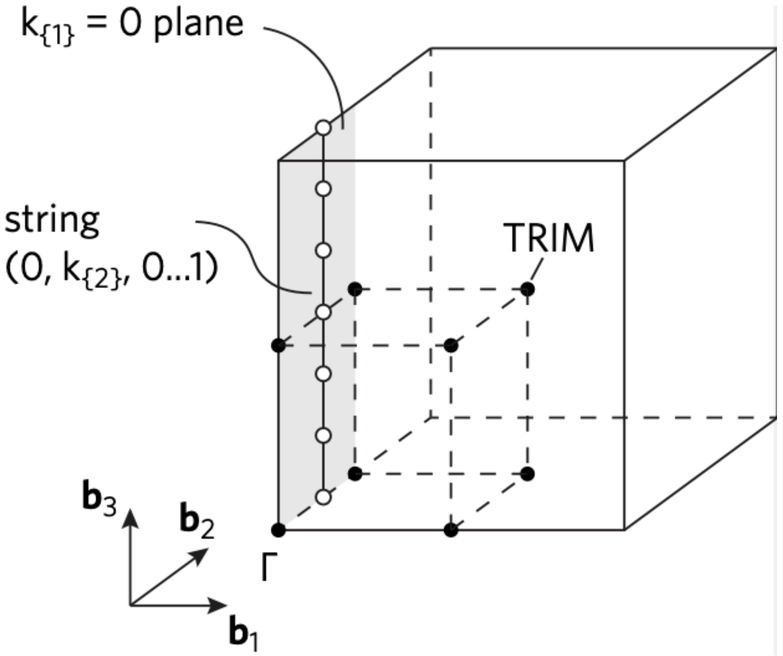
1) Construct a structure file

2) Perform SCF-SOC calculation

To calculate the HWCC:

3) Edit and run wcc.py script

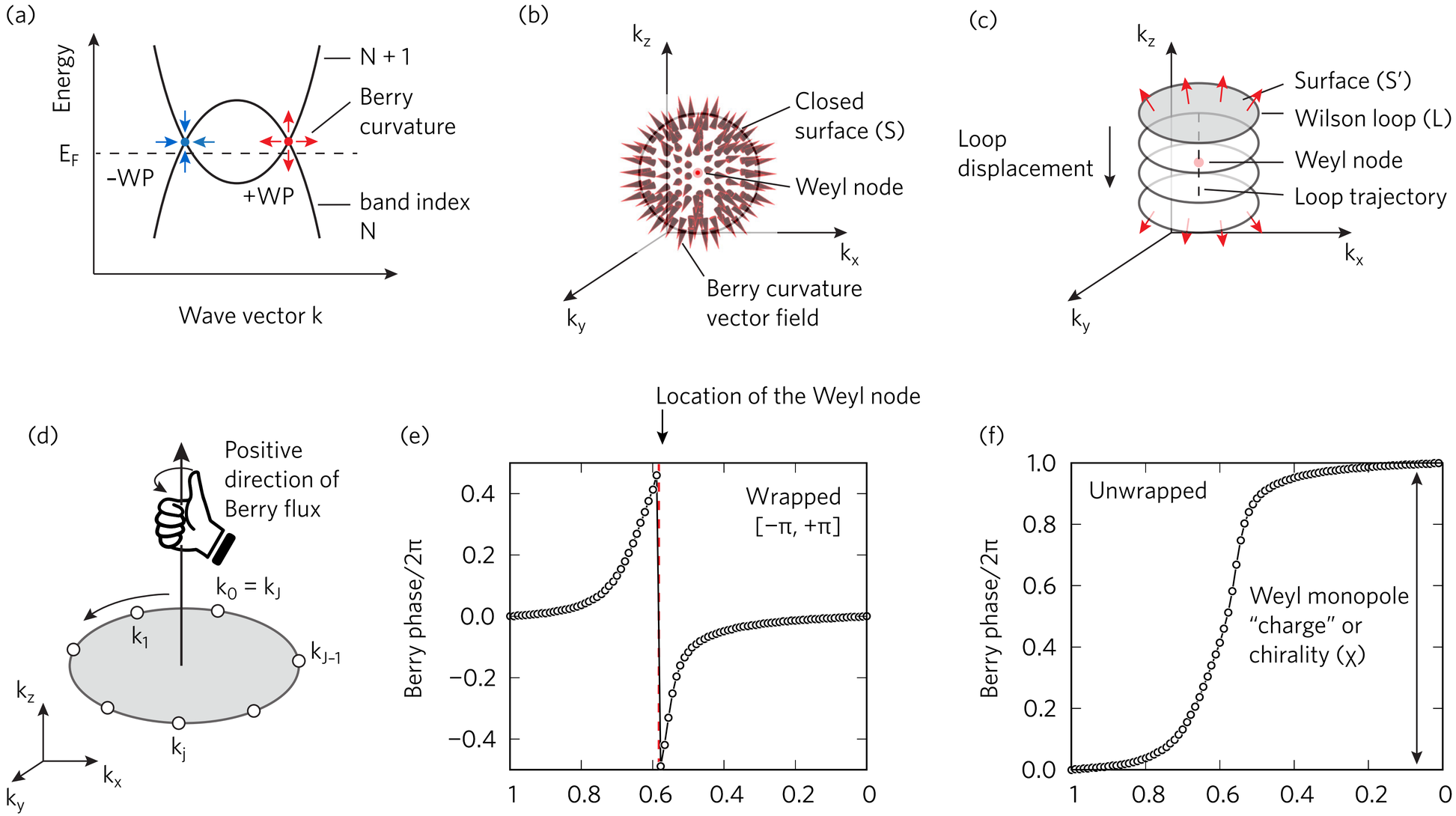
```
kevoldir = 2       # b2 (Wilson loops are constructed perpendicularly)
kevol = [0, 0.5]   # start and end fraction of b2 in this case from Gamma to L
nkevol = 20        # discretization intervals (Number of lines constructed)
kwlsndir = 3       # b3 (Hybrid Wannier centers calculation direction)
nkwlsn = 10        # discretization intervals (Points along the line)
kfix = 0.0         # in fraction of reciprocal lattice vectors (b1)
bands = [61, 78]   # select an isolated group
parallel = True    #
spinpolar = False  #
orbital = False    #
```



4) wcc.csv file

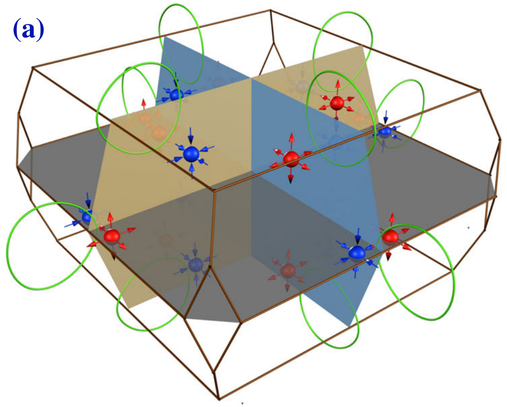
Input

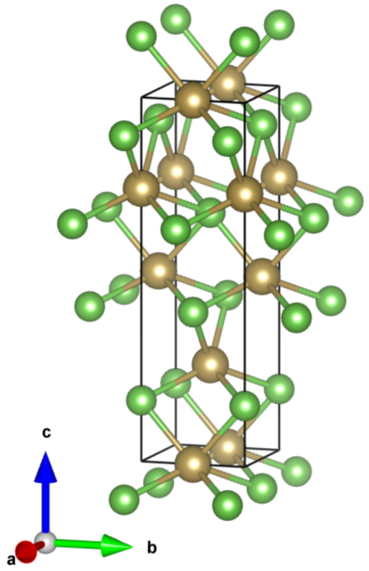
Topological materials: Weyl semimetals, Weyl fermion chirality (WlooPHI)

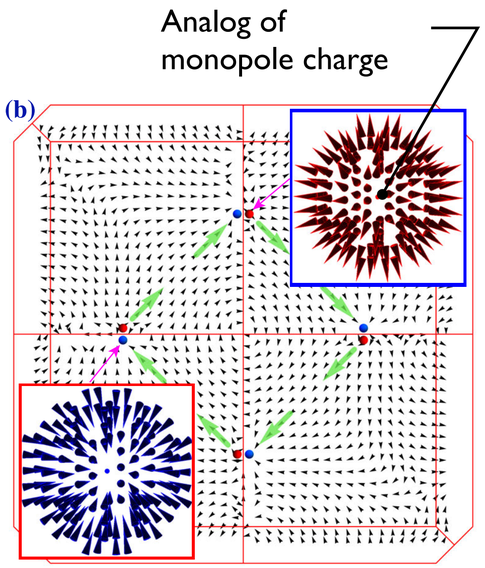


Topological materials: Weyl semimetals

TaAs

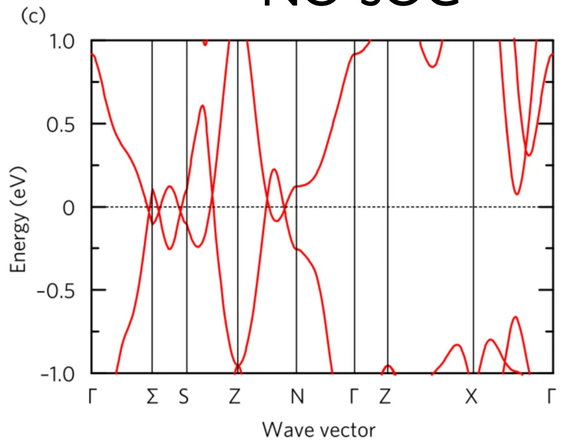


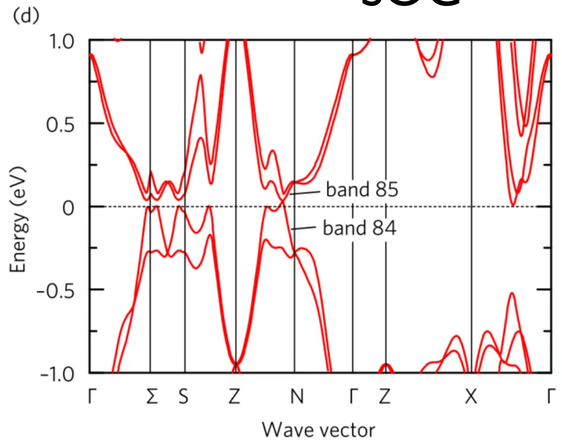


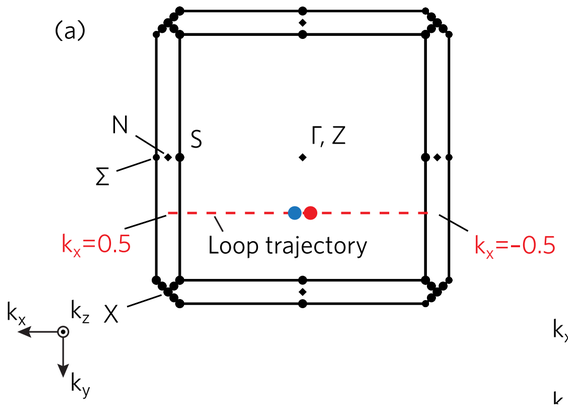


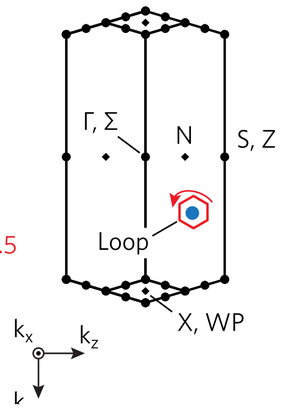
Weng et al.,
Physical Review X 5, 011029 (2015)

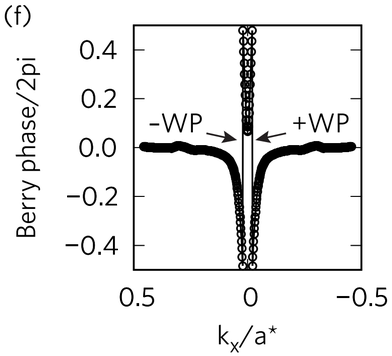
Results











Summary

- The accumulation of Berry phase is a phenomena with physical consequences. It is needed to explain the polarization in solids and as an addition to the band-theory of solids.

- Insulators can be classified based on the topology of their electronic bandstructure, which leads to the prediction of conductive states at the interface of topological phases.

- It is possible to employ WIEN2k+BerryPI for:

  - Polarization
  - Chern Insulators: CherN.py
  - Berry curvature maps
  - $\mathbb{Z}_2$ topological insulators
  - Characterization of Weyl semimetals

Thank you!