EPFL Ecole polytechnique fédérale de Lausanne

Berry phase and topological properties

Wannier tutorial March 25, 2020
Virtual conference edition

QuanSheng Wu

École polytechnique fédérale de Lausanne, Switzerland

EPFL

MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

OUTLINE

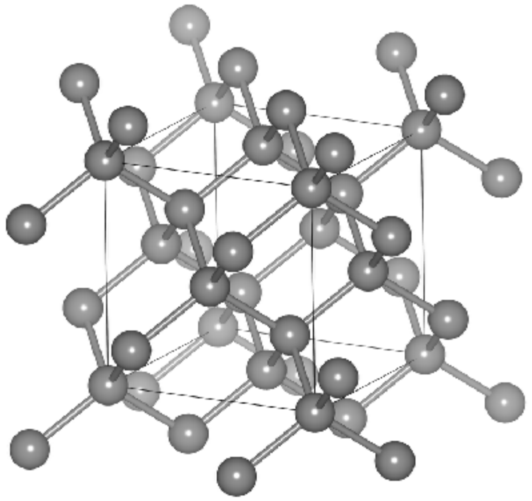
- Theory
  - Berry phase, Berry curvature
  - Wannier charge center
  - Bulk-edge correspondence
- Applications
  - Haldane model
  - Weyl semimetal
  - QSHE and topological insulator

TYPE OF ORDERS

Until 1980, all ordered phases could be understood as "symmetry breaking"

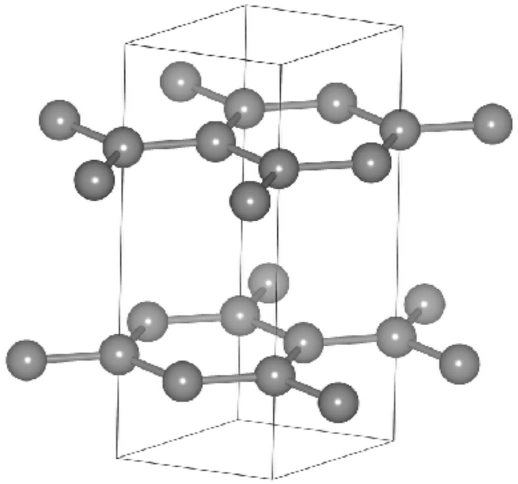
Carbon gas

Symmetries:
1. O(3) Rational
2. Continuous translation



Diamond

Cubic: Fd-3m #227



Graphite

Hexagonal: P6_3/mmc #194

Examples:
Magnets breaks time-reversal symmetry and the rotational symmetry of spins
Superfluid breaks an internal U(1) gauge field symmetry.

Modified from Topological effects in metals - Moore 2015

TYPE OF ORDERS

QHE is the first ordered phase beyond symmetry breaking discovered in 1980.

Current I along x and measure V along y

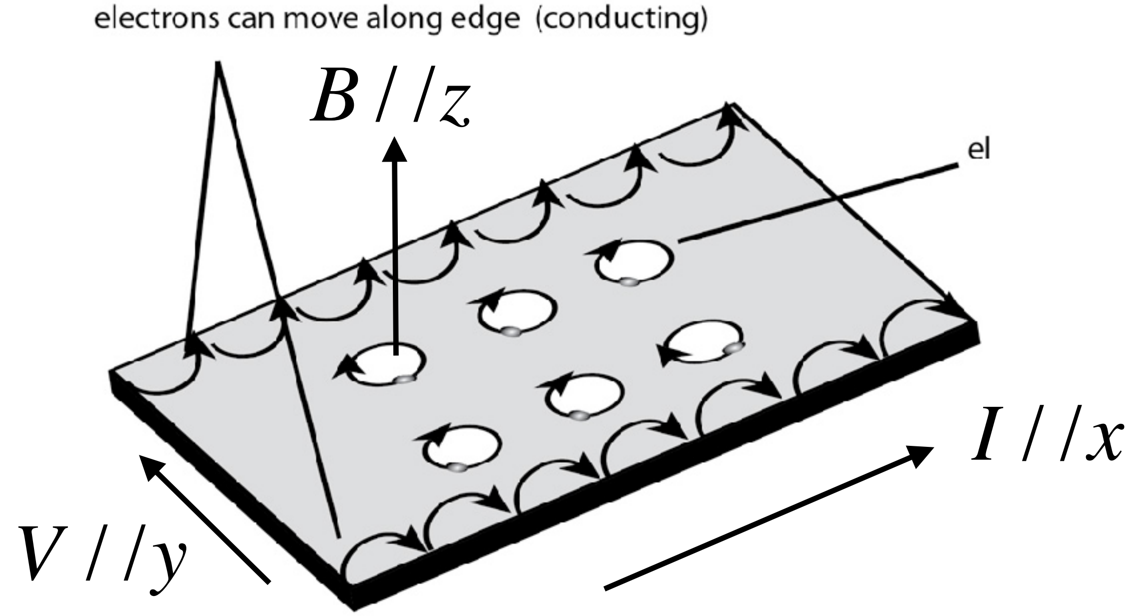
$$\sigma_{xy} = n\frac{e^2}{h}$$

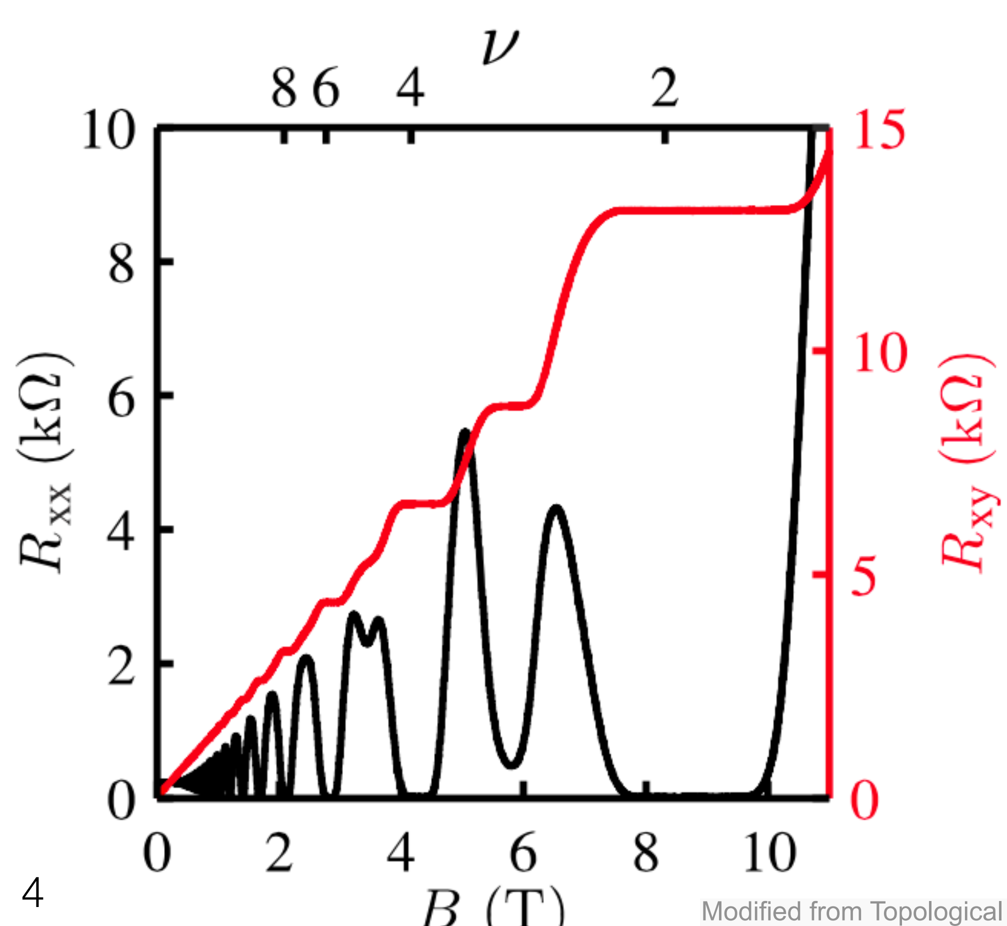
n is an integer

The precision of conductance is super high up to 10^{-9}.

Note that the material is not perfect and at room temperature.

Why so precise?

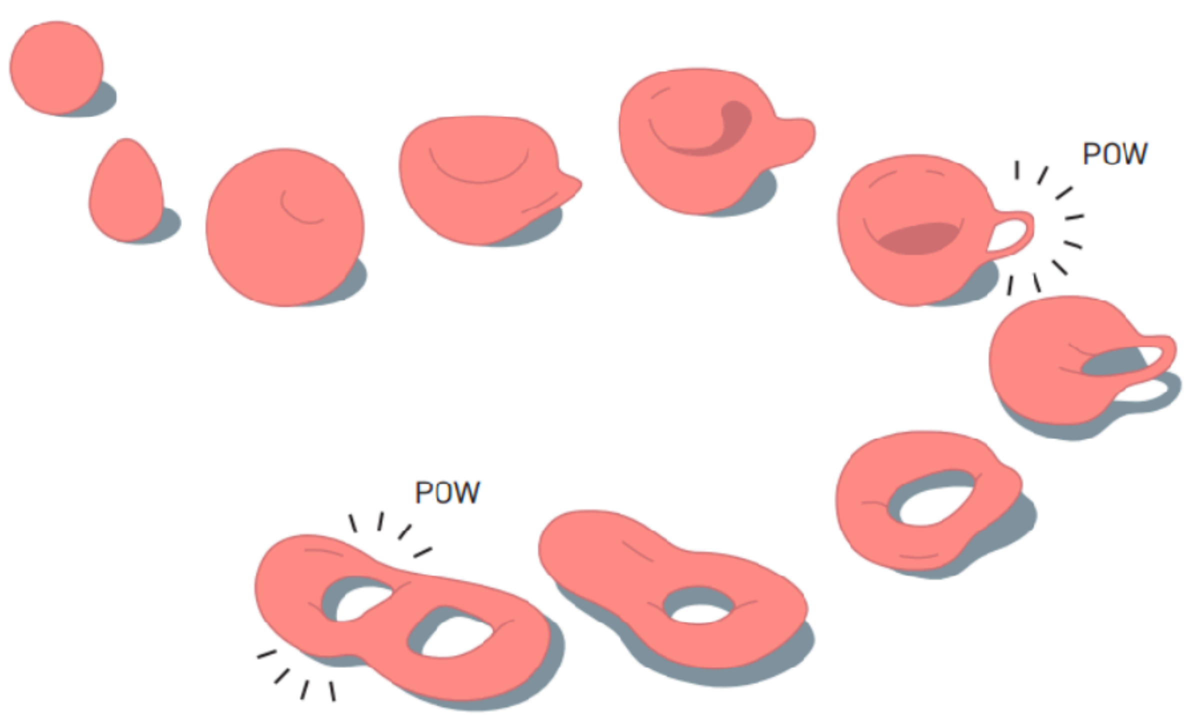




Modified from Topological effects in metals - Moore 2015

TOPOLOGICAL INVARIANTS

Two objects are topologically the same if they can be deformed continuously into each other without cutting and pasting.



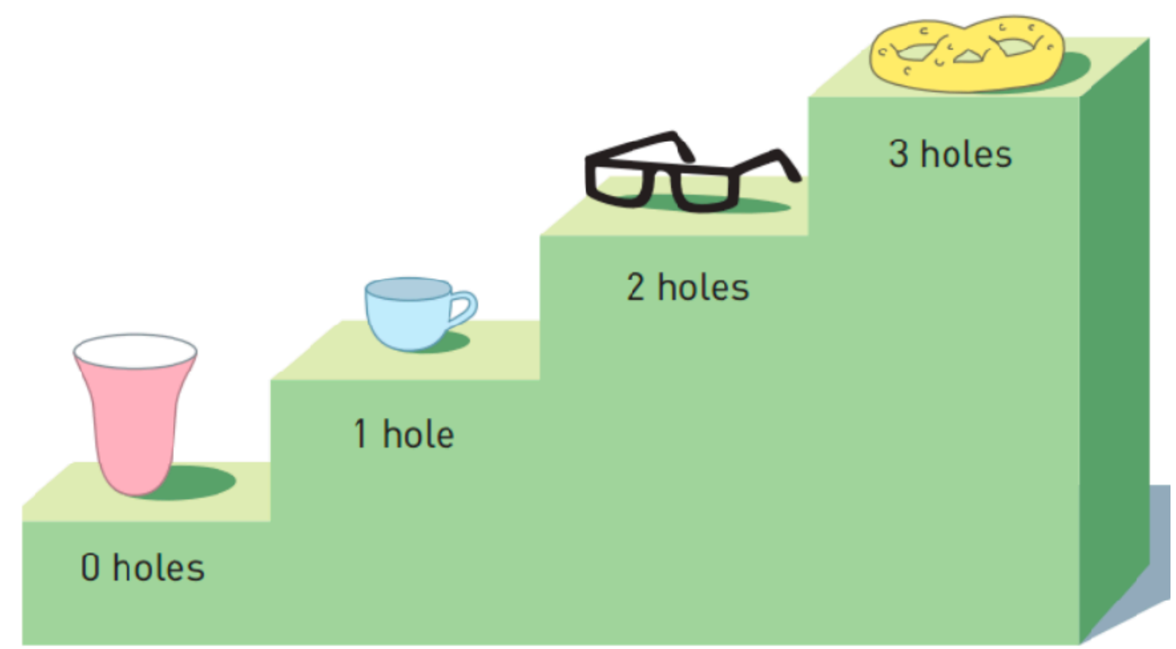


Illustration: ©Johan Jarnestad/The Royal Swedish Academy of Sciences

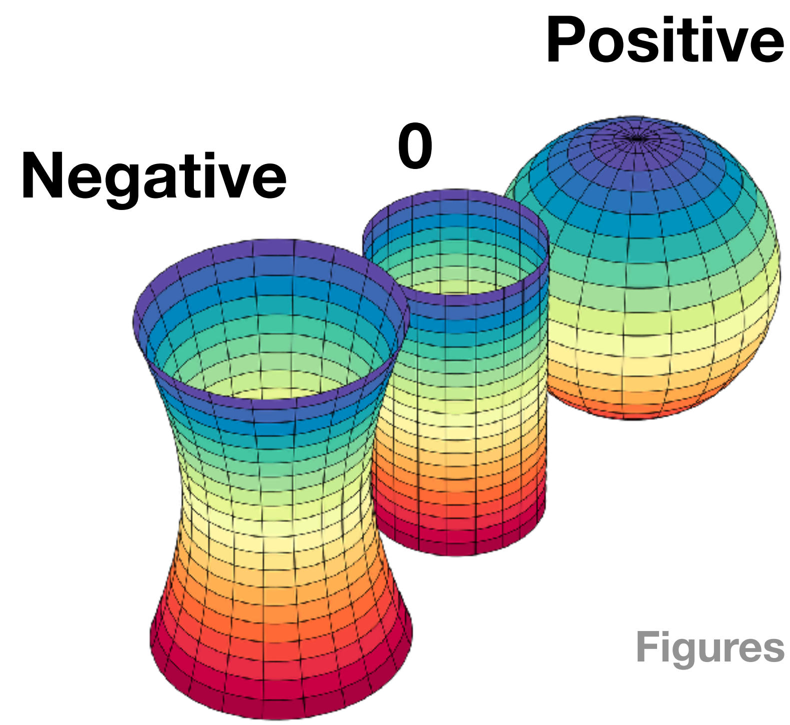
Topological invariant = number of ‘holes’

TOPOLOGICAL INVARIANTS

Consider a two-dimensional surface

The Gaussian curvature is defined as the inverse of two radii of curvature

$$K = (r_1 r_2)^{-1}$$

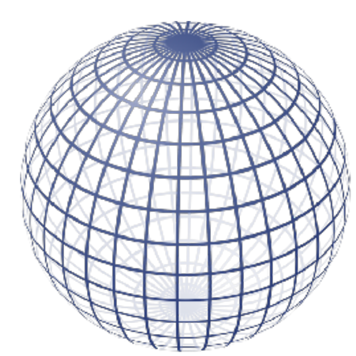


Figures from wikipedia

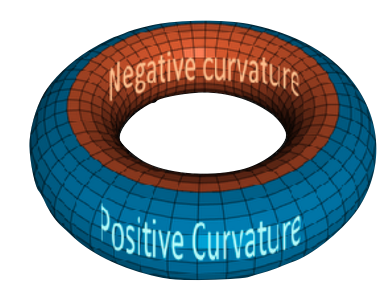
Gauss-Bonnet theorem: The area integral of curvature over a closed surface M is "quantized" and is a topological invariant.

$$\iint_M K\, dA = 2\pi\chi = 2\pi(2-2g)$$

$$K = \frac{1}{r^2}$$



$$\chi = 2$$
$$g = 0$$



$$\chi = 0$$
$$g = 1$$

Most topological invariants in physics arise as integrals of some geometric quantity.

Modified from Topological effects in metals - Moore 2015

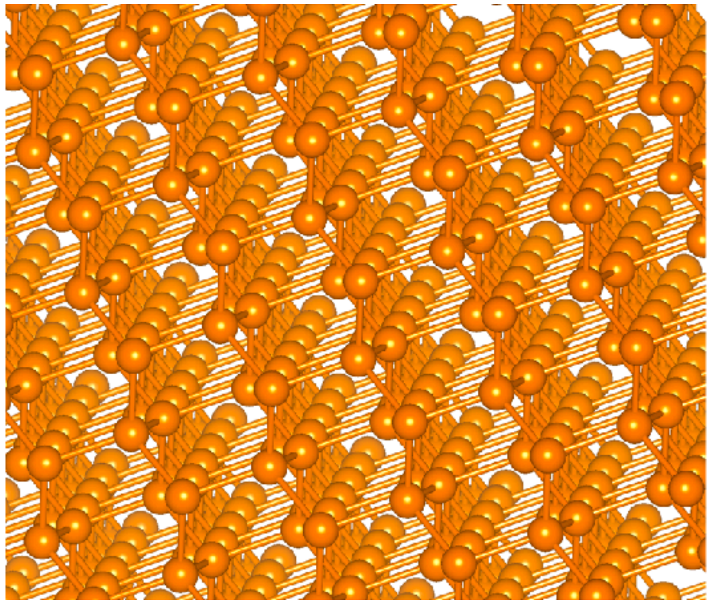
TOPOLOGICAL INVARIANTS

Bloch theorem:

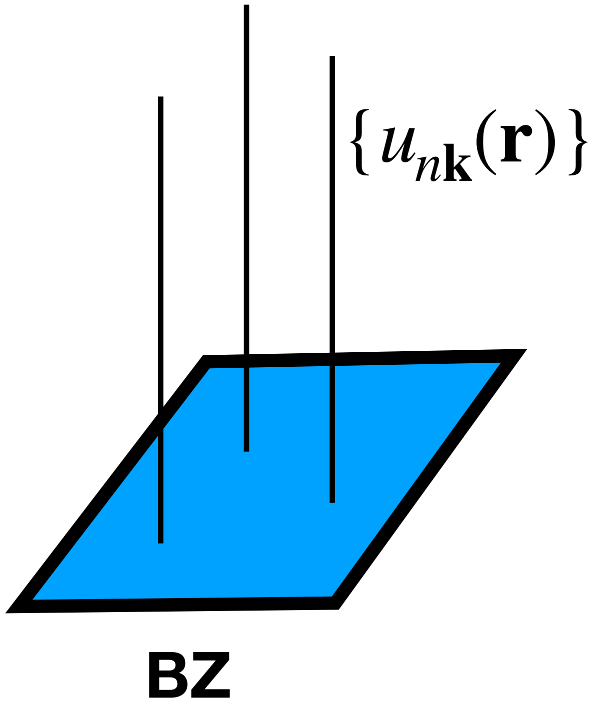
One-electron wave function in a crystal can be written

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

where k is "crystal momentum" and u is periodic.



Analog to the previous case:



1. A closed surface M can be made by a closed first BZ in 2D materials or a closed surface in 3D BZ.

2. Gauss curvature -> Berry curvature

How can we define Berry curvature?

BERRY PHASE

Berry phase is the starting point to get Berry curvature

In the adiabatic limit, the Hamiltonian is changed slowly. The system remains in its time dependent ground states. The wave function evolves as

$$\Psi(t) = \psi_n(\lambda(t)) e^{-i\int_0^t dt'\varepsilon_n/\hbar} e^{-i\gamma_n}$$

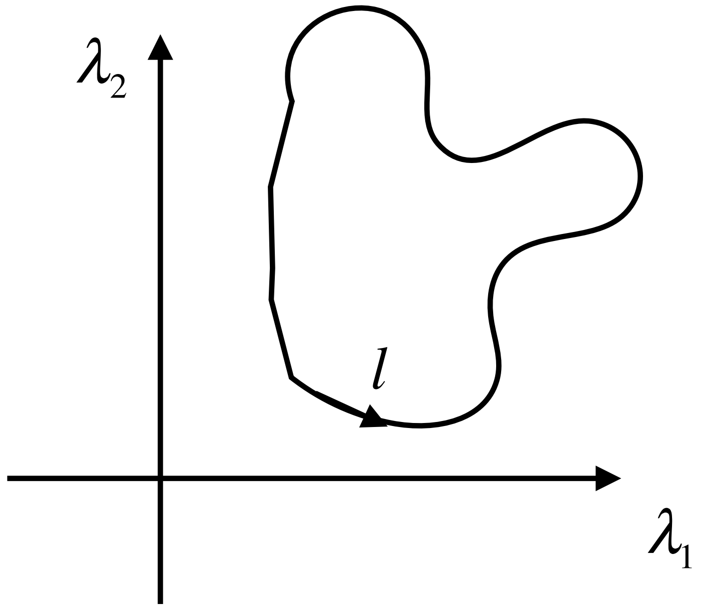
γ_n **is called the Berry phase which is a geometric phase. It doesn't depend on time, only depend on the geometry of the path.**

$$\gamma_n = \oint_l d\lambda \langle \psi_n | i \frac{\partial}{\partial \lambda} | \psi_n \rangle$$

In crystal system, k is the parameter λ

Berry phase: $\gamma_n = \oint_l dk A(k)$

Berry connection: $A(k) = \langle u_{nk} | i\nabla_k | u_{nk} \rangle$



Modified from Topological effects in metals - Moore 2015

BERRY PHASE

The property of Berry phase

Berry phase: $$\gamma_n = \oint_l dk A(k)$$

Berry connection: $$A(k) = \langle u_{nk} | i\nabla_k | u_{nk} \rangle$$

There is a freedom choice of phase factor of wave function which is called U(1) gauge freedom.

$$u_{nk} \rightarrow e^{i\chi(k)} u_{nk}$$

Under this change, the Berry connection A(k) changes by a gradient.

$$A(k) \rightarrow A(k) + \nabla_k \chi$$

This is analogy to the vector potential in electrodynamics.

Just like how we obtained the magnetic field strength B from vector potential, We can get the Berry curvature by taking the curl of A(k)

$$\Omega(k) = \nabla \times A(k)$$

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BERRY PHASE—ANALOGIES

Berry connection

$$A(k) = \langle u_{nk} | i\nabla_k | u_{nk} \rangle$$

Vector potential

$$A(r)$$

Berry curvature

$$\Omega(k)$$

Magnetic field

$$B(r)$$

Berry phase

$$\oint_l A(k)\,dk = \iint dS \cdot \Omega(k)$$

Aharonov-Bohm phase

$$\oint_l A(r)\,dr = \iint dS \cdot B(r)$$

Chern number

$$\frac{1}{2\pi} \oiint dS \cdot \Omega(k) = \text{integer}$$

Dirac monopole

$$\oiint dS \cdot B(r) = \text{integer}\ \frac{h}{e}$$

BERRY PHASE—ANALOGIES

Berry connection

$$A(k) = \langle u_{nk} | i\nabla_k | u_{nk} \rangle$$

Berry curvature

$$\Omega(k) = \nabla \times A(k)$$

Berry curvature is gauge invariant. So it may be connected with some physical quantity.

In 1982, TKNN pointed out that the integer quantum hall effect in a 2D crystal follows from the integral of Ω(k).

$i\Omega(k)$

$$\sigma_H = \frac{ie^2}{2\pi h} \sum \int d^2k \int d^2r \left(\frac{\partial u^*}{\partial k_1} \frac{\partial u}{\partial k_2} - \frac{\partial u^*}{\partial k_2} \frac{\partial u}{\partial k_1} \right)$$

$$= \frac{ie^2}{4\pi h} \sum \oint dk_j \int d^2r \left(u^* \frac{\partial u}{\partial k_j} - \frac{\partial u^*}{\partial k_j} u \right), \qquad (5)$$

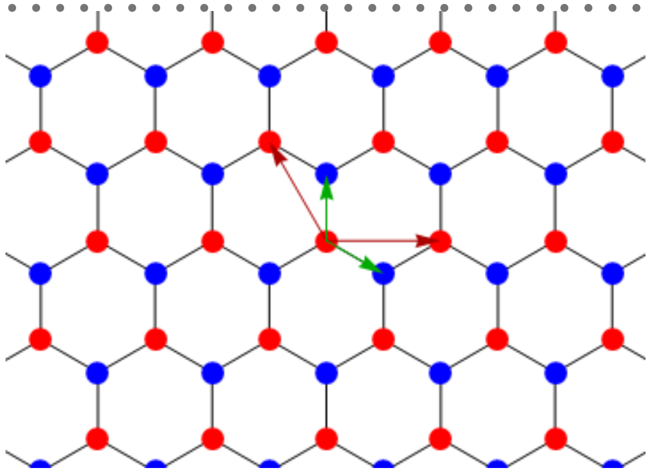
TKNN, PRL 49, 405 (1982)

$$\sigma_H = n\frac{e^2}{h}$$

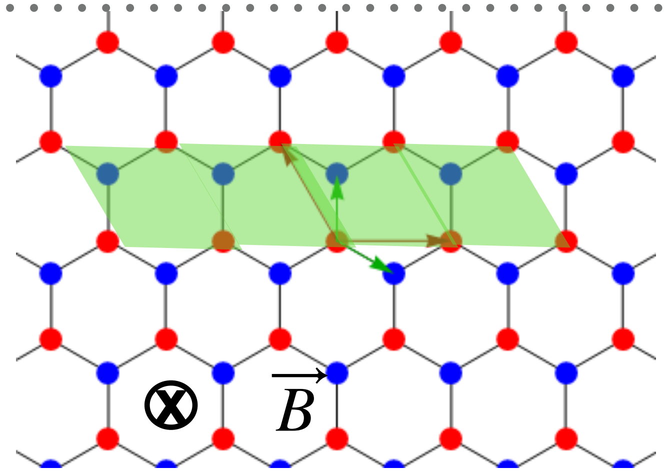
"n" is the TKNN number which is also called the first Chern number.

Modified from Topological effects in metals - Moore 2015

INTRODUCTION: QUANTUM HALL EFFECT II



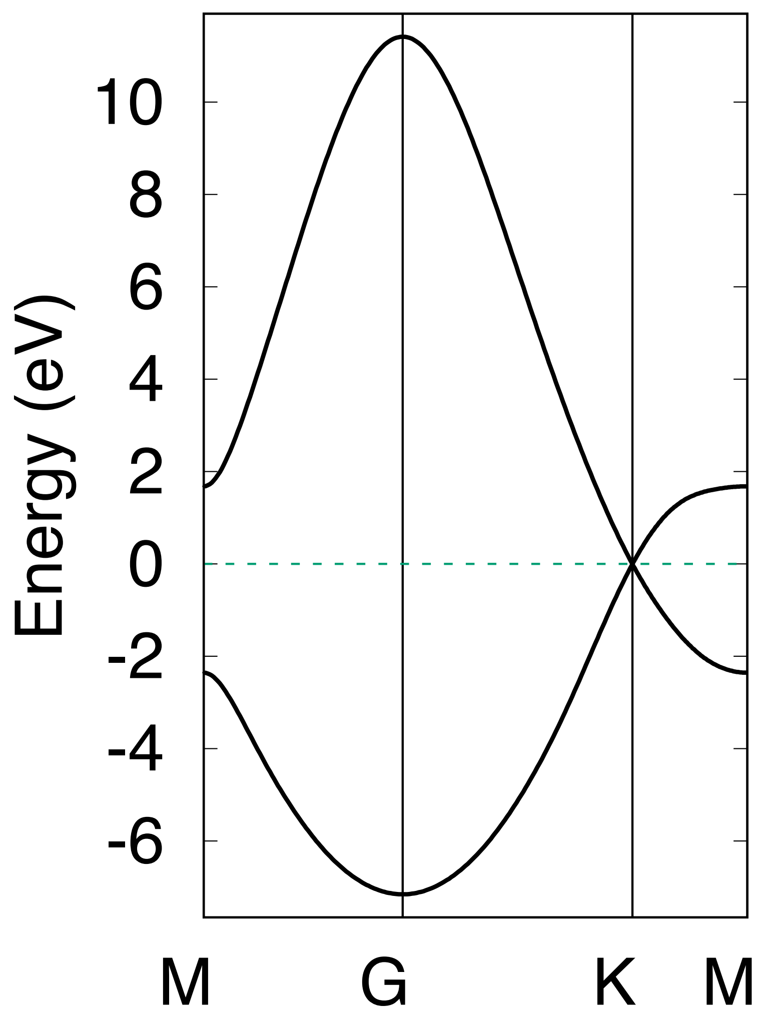
$\phi = 0$

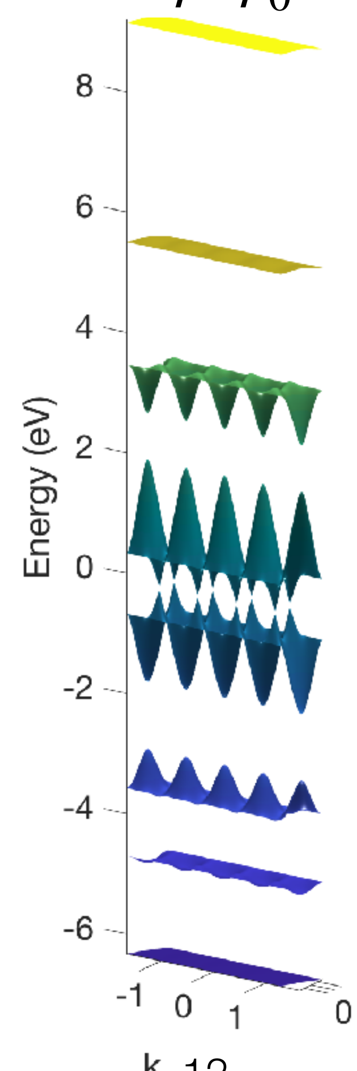


$\phi/\phi_0 = 1/4$

$$\phi = BS_0$$

$$\mathbf{\Omega}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}_n(\mathbf{k})$$
$$= i\langle \nabla_{\mathbf{k}} u_{n\mathbf{k}} \times | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle$$





C=-1

C=-2

C=-1

C=0

C=1

C=2

C=1

$$C = \frac{1}{2\pi} \oint_{MBZ} d^2k \Omega_{xy}$$

MBZ: magnetic Brillouin zone

Hofstadter D. R. PRB 14, 2239

WANNIER FUNCTIONS

There is another way called Wannier charge center to calculate the Chern number.

Let's start with Wannier functions.

Fourier transform

$$|w_{n\mathbf{R}}\rangle = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} e^{-i\mathbf{k}\cdot\mathbf{R}} |\psi_{n\mathbf{k}}\rangle \, d^3k$$

$$\Updownarrow \text{FT}$$

$$|\psi_{n\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} |w_{n\mathbf{R}}\rangle \, .$$

Wannier center is defined as

$$\begin{aligned}
\bar{\mathbf{r}}_n &= \langle w_{n\mathbf{0}}|\mathbf{r}|w_{n\mathbf{0}}\rangle \\
&= \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} \langle u_{n\mathbf{k}}|i\nabla_{\mathbf{k}} u_{n\mathbf{k}}\rangle \, d^3k \\
&= \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} \mathbf{A}_n(\mathbf{k}) \, d^3k
\end{aligned}$$

In one-dimension

$$\begin{aligned}
\bar{x}_n &= (a/2\pi) \int_0^{2\pi/a} \langle u_{nk}|i\partial_k u_{nk}\rangle \, dk \\
&= a \, \frac{\phi_n}{2\pi}
\end{aligned}$$

Where ϕ_n is just the Berry phase.

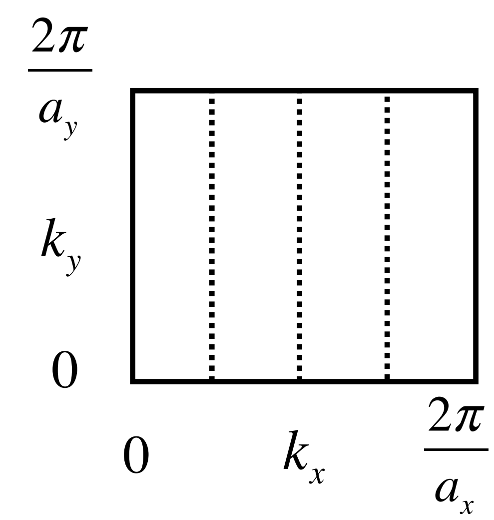
In other words, a Berry phase evolving from 0 to 2π would just correspond to a Wannier center evolving from x= 0 to x=a

Vanderbilt book (2019)

WANNIER CHARGE CENTER (WCC)

Let's define a hybrid Wannier function (HWF) in a 2D crystal

$$\left|n;l_y,k_x\right\rangle = \frac{a_y}{2\pi}\int_0^{2\pi/a_y} e^{ik_y l_y a_y}\left|\psi_{n,k_x,k_y}\right\rangle dk_y$$



The center of HWF is

$$\bar{y}_n(k_x) = \left\langle n;0,k_x\right|\hat{y}\left|n;0,k_x\right\rangle$$

$$= \frac{a_y}{2\pi}\int_0^{2\pi/a_y} A_n(k_x,k_y)\,dk_y$$

Where

$$A_n(k_x,k_y) = i\left\langle u_{nk}\right|\partial_{k_y}\left|u_{nk}\right\rangle$$

$\bar{y}_n(k_x)$ **is the Berry phase for a given kₓ.**

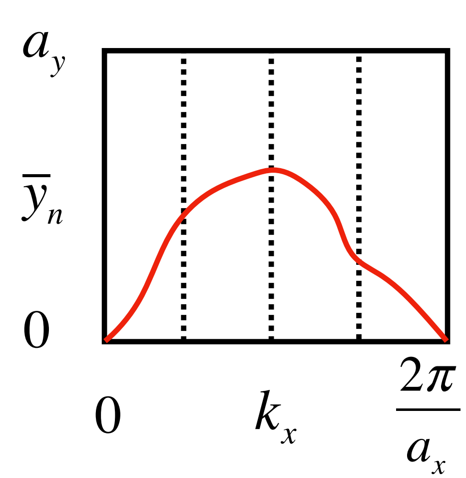
Using the Stokes' theorem, we can get

$$\bar{y}_n(k_x = 2\pi/a_x) - \bar{y}_n(k_x = 0)$$

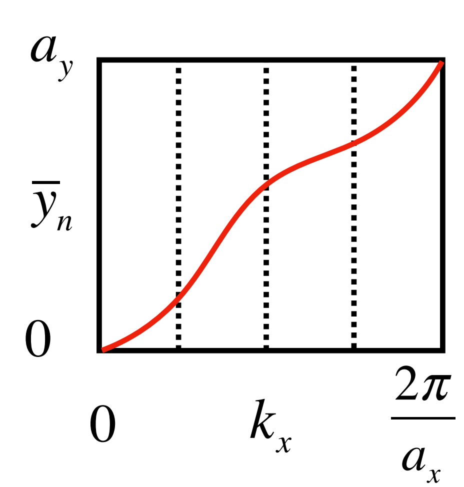
$$= \frac{a_y}{2\pi}\left[\oint A_n(k_x = 2\pi/a_x, k_y)\,dk_y - \oint A_n(k_x = 0, k_y)\,dk_y\right]$$

$$= \frac{a_y}{2\pi}\iint_{BZ} \nabla_k \times A_n(k)\,dk_x dk_y = \frac{a_y}{2\pi}\iint_{BZ} \Omega_n(k)\,dk_x dk_y = a_y C$$

$C=0$



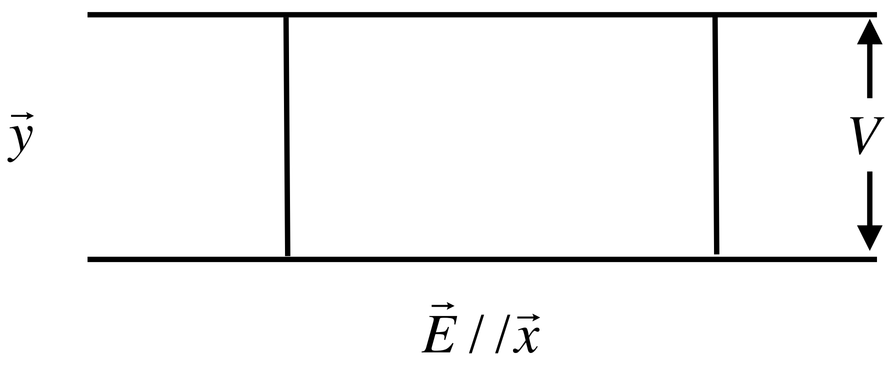
$C=1$



Soluyanov 2011, Yu 2011, Alexandradinata 2014

WANNIER CHARGE CENTER (WCC)

Let current along x direction, measure voltage along y direction



Momentum k evolves under electric field

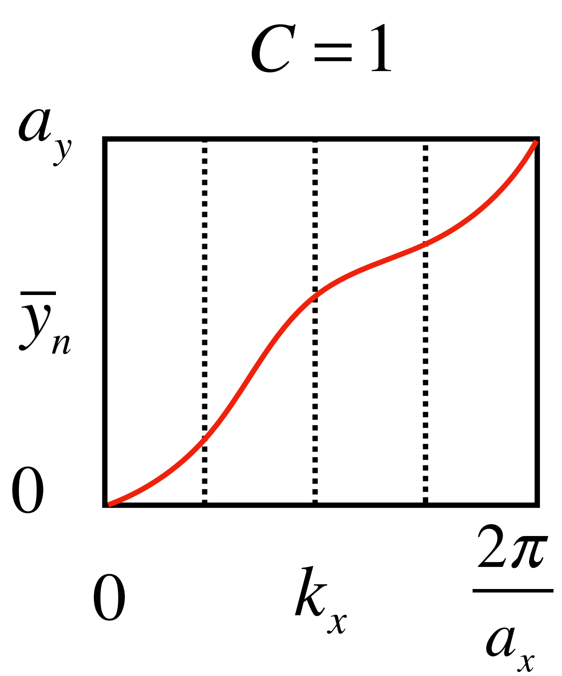
$$\frac{d\vec{k}}{dt} = -\frac{e}{\hbar}\vec{E}$$

So

$$k_x(t) - k_x(0) = -\frac{e}{\hbar}Et$$

By change k_x with 2pi/a, we can get the time

$$\frac{2\pi}{a_x} = -\frac{e}{\hbar}Et_0 \Rightarrow t_0 = -\frac{2\pi\hbar}{ea_xE}$$



During this time t0, There are C number of electrons moving along y direction, So the current

$$I_y = \frac{eC}{t_0} = -\frac{e^2 a_x EC}{h}$$

$$j_y = \frac{I_y}{a_x} = -C\frac{e^2}{h}E = -\sigma_{yx}E \Rightarrow \sigma_{yx} = C\frac{e^2}{h}$$

Vanderbilt book (2019)

MULTI-BAND SYSTEM

The Chern number of multi-band system is

$$C = \sum_{n \in occupied} [\bar{y}_n(k_x = 2\pi / a_x) - \bar{y}_n(k_x = 0)] / a_y$$

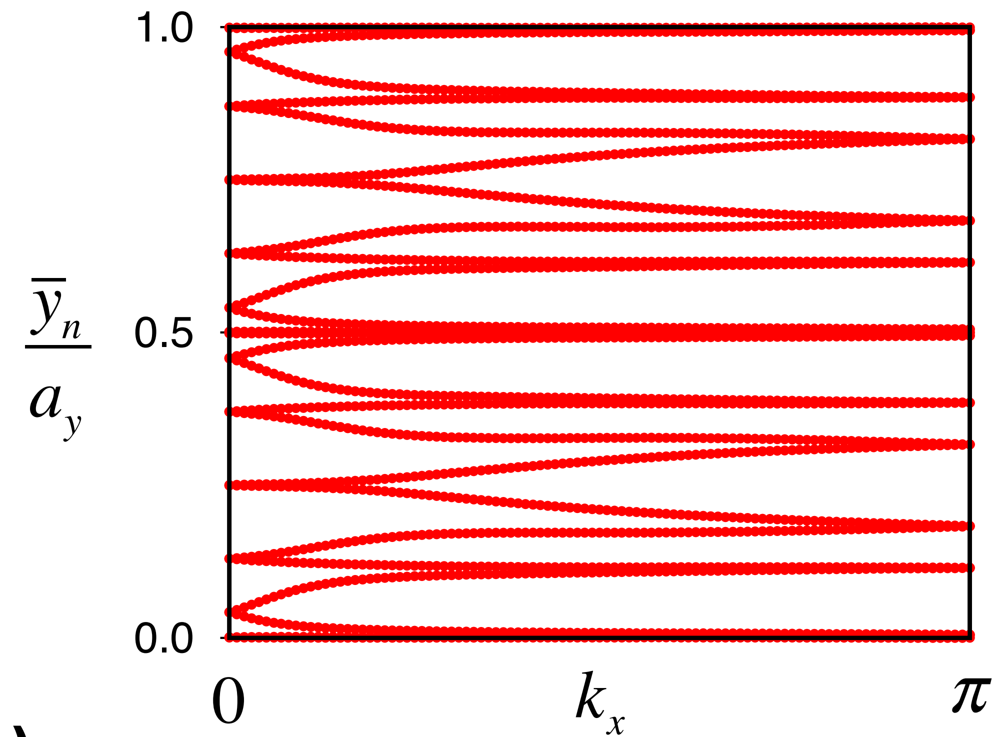
Let's define a projector for all occupied states

$$P(k) = \sum_{n \in occupied} \int_0^{2\pi} \frac{dk_y}{2\pi} \left| \psi_{n,k_x,k_y} \right\rangle \left\langle \psi_{n,k_x,k_y} \right|$$

It's clearly that $\bar{y}_n(k_x)$ **is the eigenvalue of**

$$P\hat{y}P$$

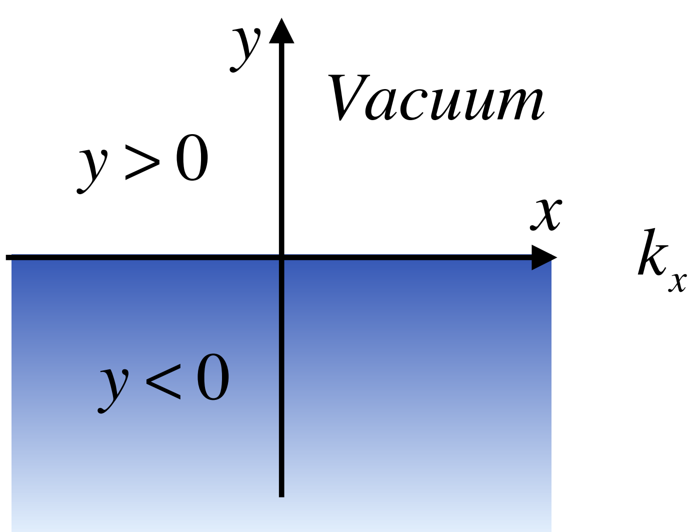
$\bar{y}_n(k_x)$ **are called Wannier charge centers (WCCs)**

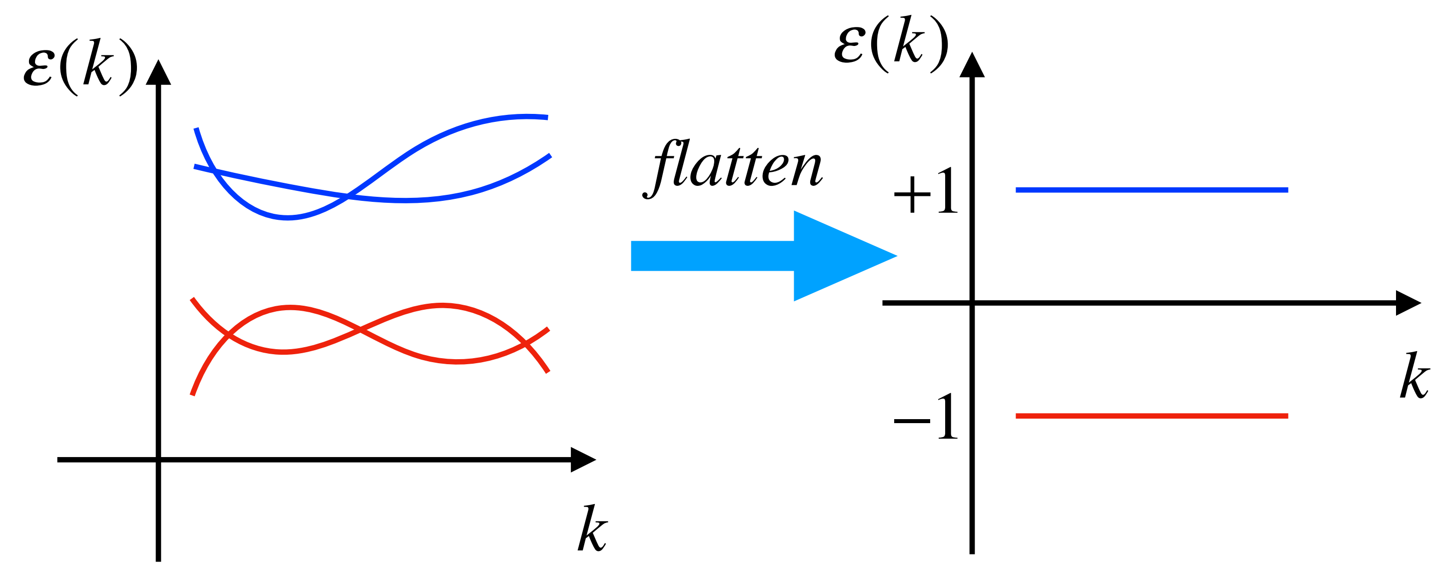


WCCs not only can be used to get the topological number, but also it's related to the surface/edge state spectrum.

BULK EDGE CORRESPONDENCE

Let's study a semi-infinite system





$$H = \sum_n |\psi_{nk}\rangle \varepsilon_n(k) \langle \psi_{nk}| \quad \longrightarrow \quad \tilde{H} = 1 - 2 \sum_{n \in occupied} |\psi_{nk}\rangle\langle \psi_{nk}|$$

$$P = \sum_{n \in occupied} \int_0^{2\pi} \frac{dk_y}{2\pi} \left|\psi_{n,k_x,k_y}\right\rangle\left\langle\psi_{n,k_x,k_y}\right|$$

The flattened Hamiltonian should be

$$\tilde{H}_{\text{semi-infinite}}(y < 0) = 1 - 2P$$

$$\tilde{H}_{\text{semi-infinite}}(y \geq 0) = 1$$

In compact

$$\tilde{H}_{\text{semi-infinite}} = PV_0(y)P + (1 - P)$$

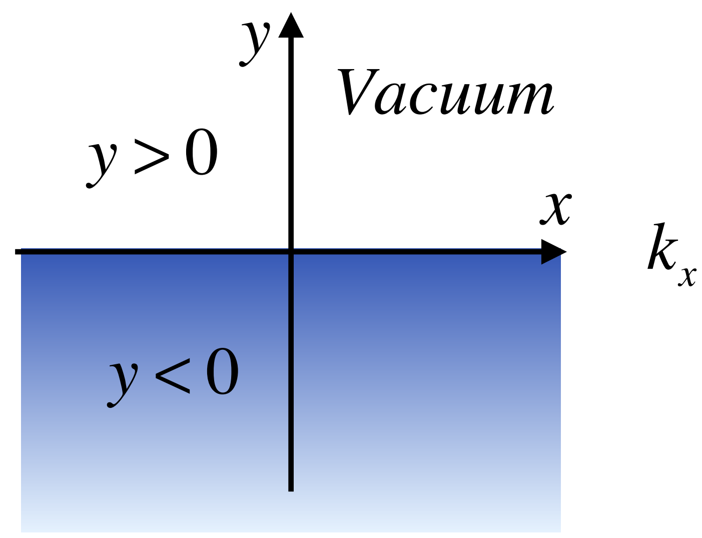
$$V_0(y) = \begin{cases} 1 & \text{for } y \geq 0 \\ -1 & \text{for } y < 0 \end{cases}$$

Fidkowski, Jackson, Klich PRL 107, 036601 (2011)

BULK EDGE CORRESPONDENCE

Let's study a semi-infinite system

$$\tilde{H}_{\text{semi-infinite}} = PV_0(y)P + (1-P)$$



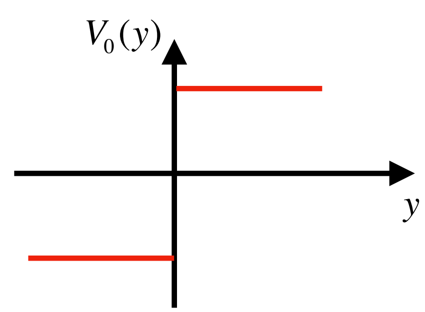
$\tilde{H}_{\text{semi-infinite}}$ **includes the spectrum +1 and -1**

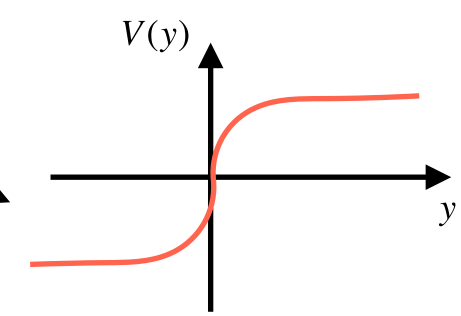
The boundary states are included in this term

$$PV_0(y)P$$

Where

$$V_0(y) = \begin{cases} 1 & \text{for } y \geq 0 \\ -1 & \text{for } y < 0 \end{cases}$$



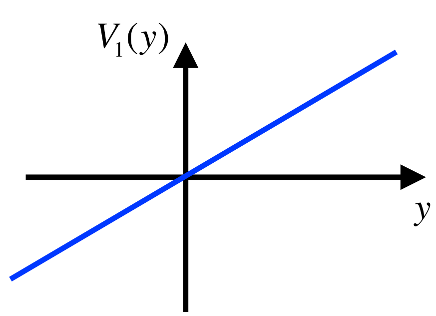


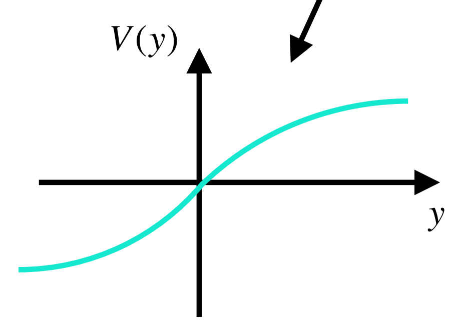
Wannier charge centers (WCCs) $\bar{y}_n(k_x)$

are the eigenvalues of $PV_1(y)P$

Where

$$V_1(y) = \hat{y}$$



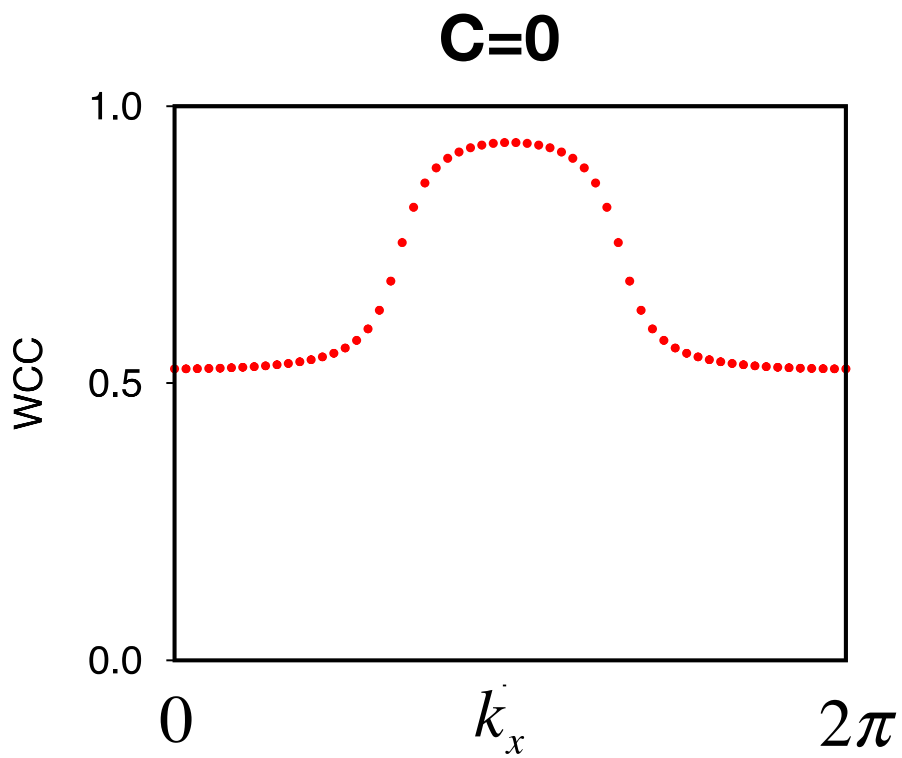


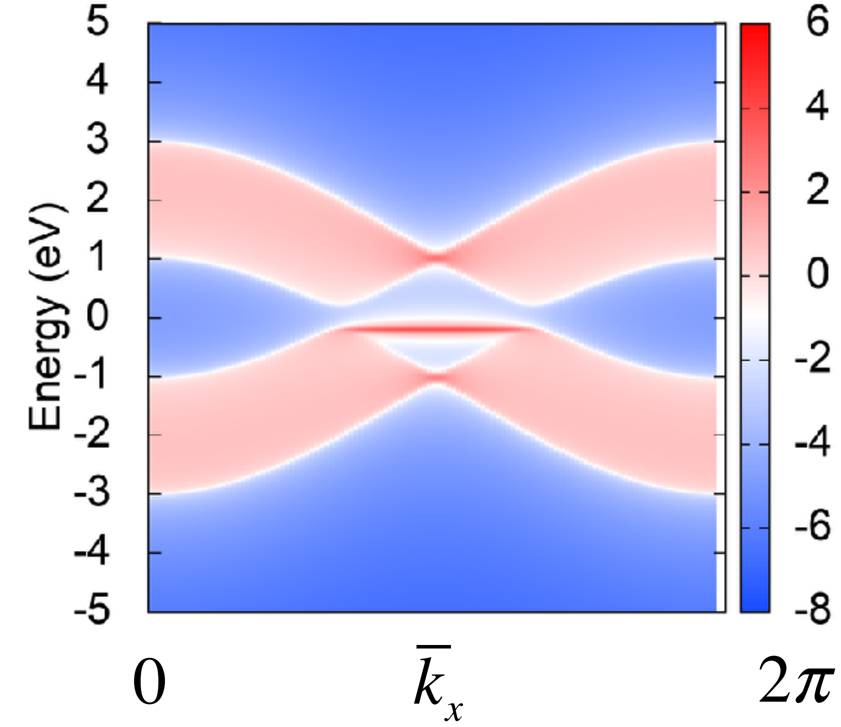
Conclusion:

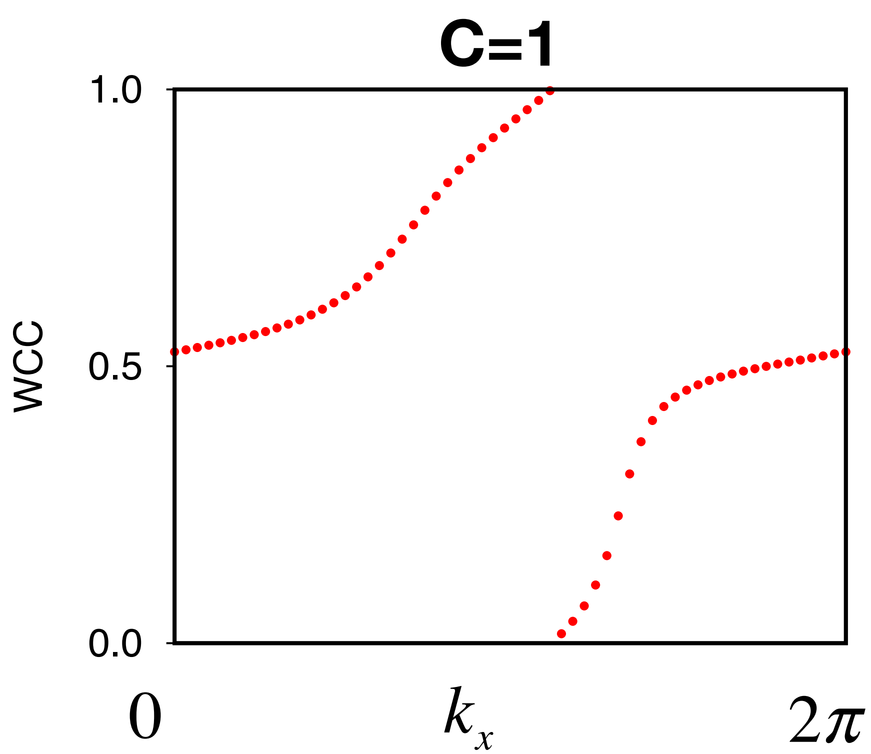
The topology of the WCCs spectrum and the physical boundary spectrum is thus identical!

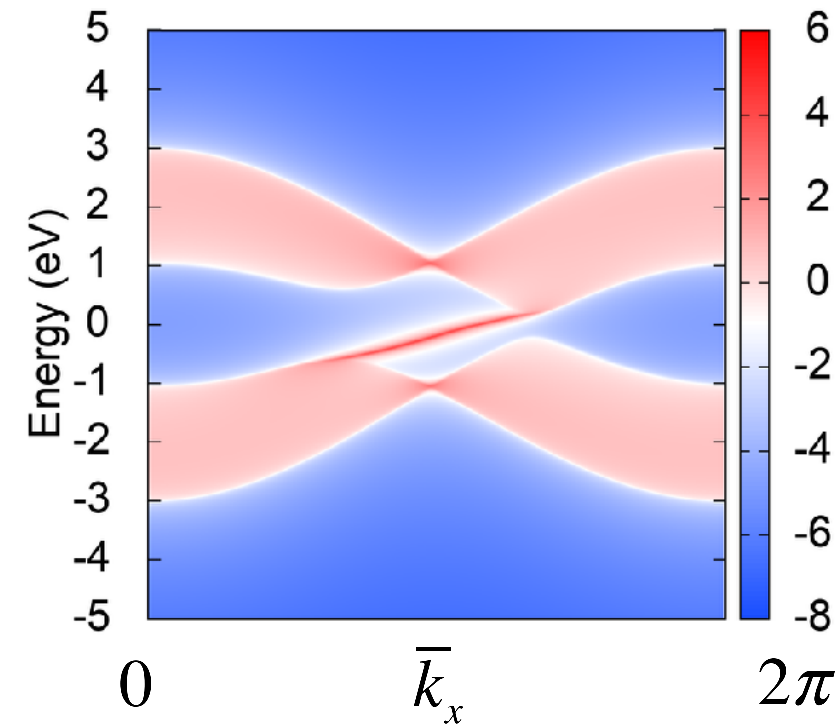
Fidkowski, Jackson, Klich PRL 107, 036601 (2011), Neupert, Schindler arXiv:1810.03484

BULK EDGE CORRESPONDENCE







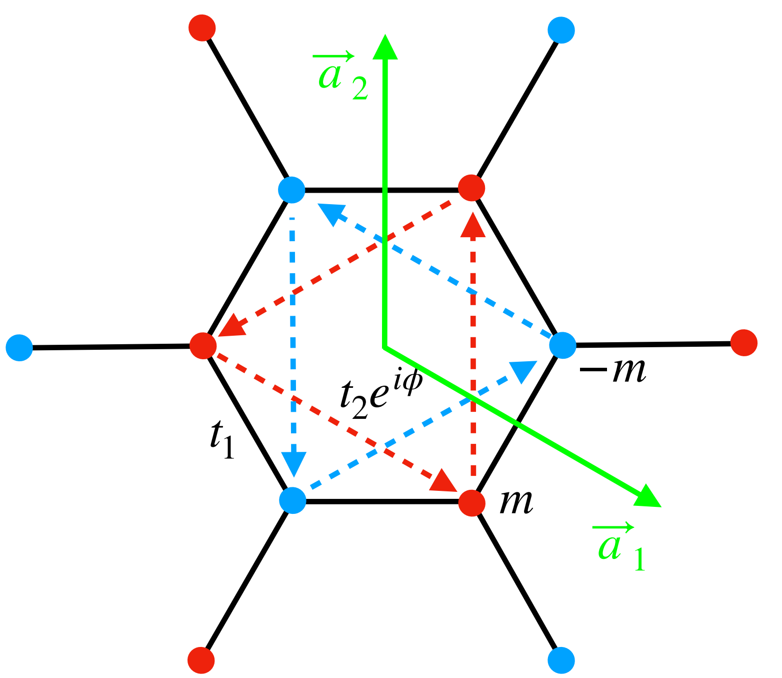


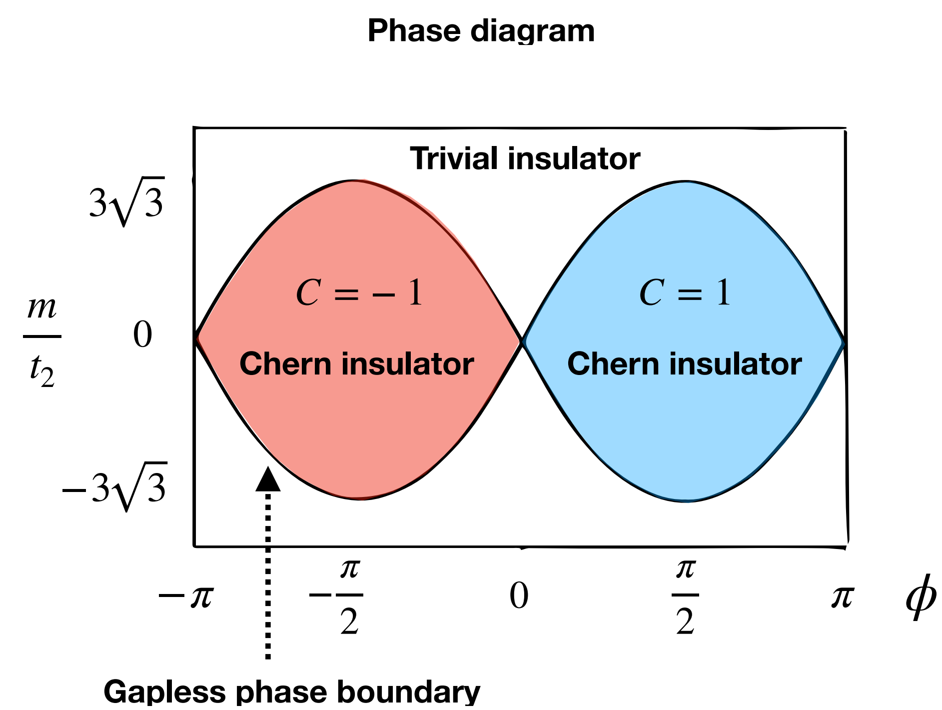
OUTLINE

- Theory
  - Berry phase, Berry curvature
  - Wannier charge center
  - Bulk-edge correspondence
- Applications
  - Haldane model
  - Weyl semimetal
  - QSHE and topological insulator

HALDANE MODEL

A toy model to realize quantum anomalous Hall effect.





The next nearest hopping t_2 breaks the time reversal symmetry.

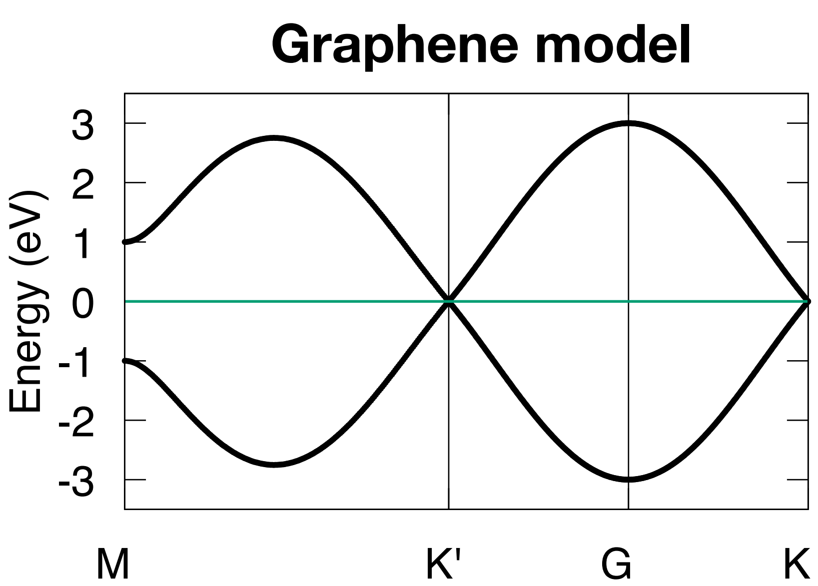
Onsite energy m breaks the sublattice symmetry.

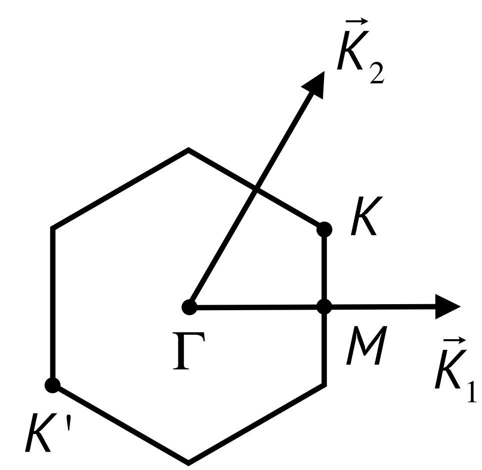
When t_2=0 and m=0, it becomes a model of Graphene

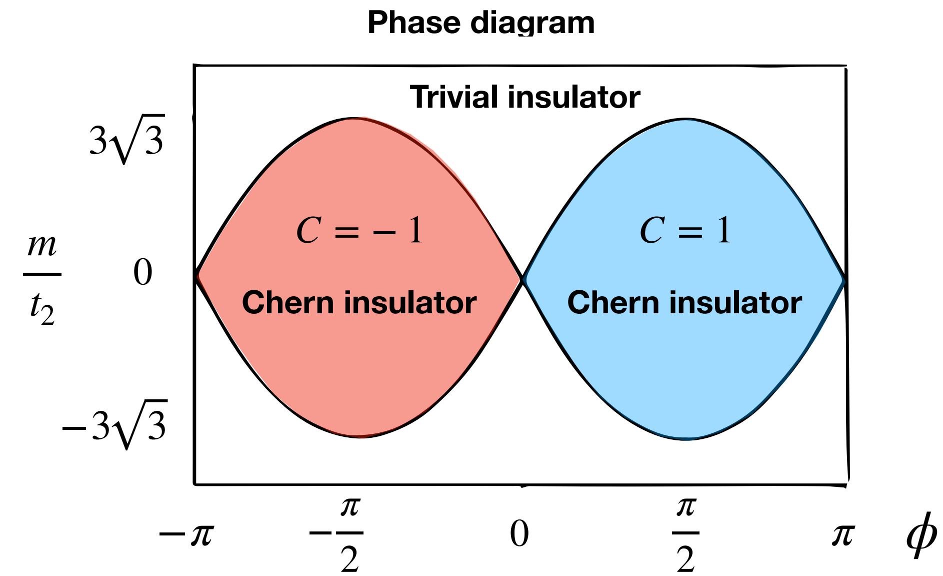
FDM Haldane, PRL 61, 2015 (1988)

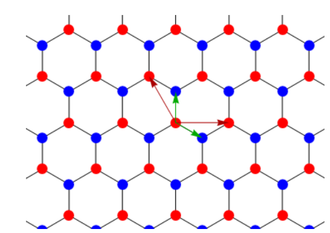
HALDANE MODEL-TRIVIAL INSULATOR PHASE

$t_1 = 1; t_2 = 0; m = 0$

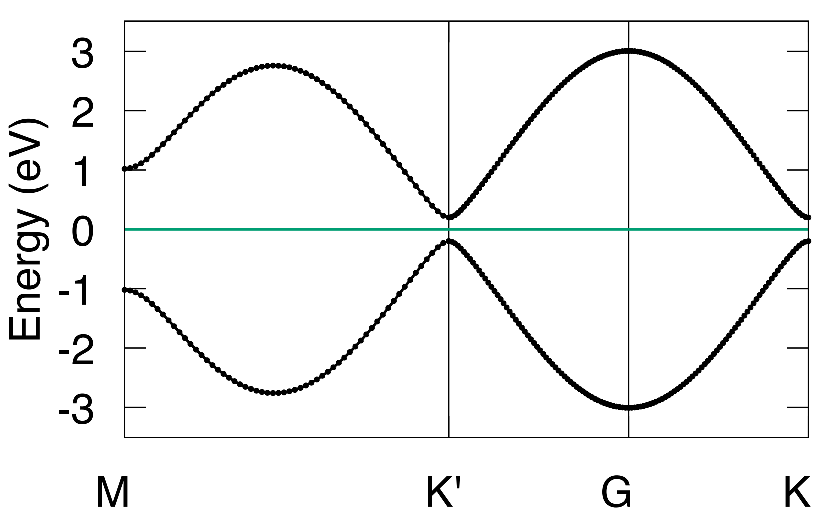


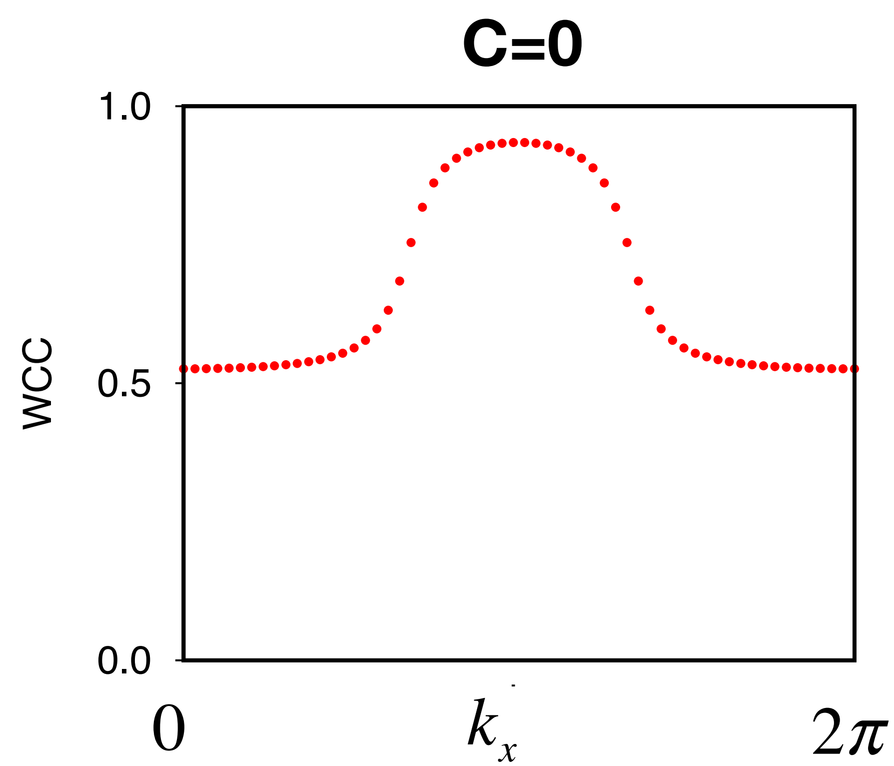


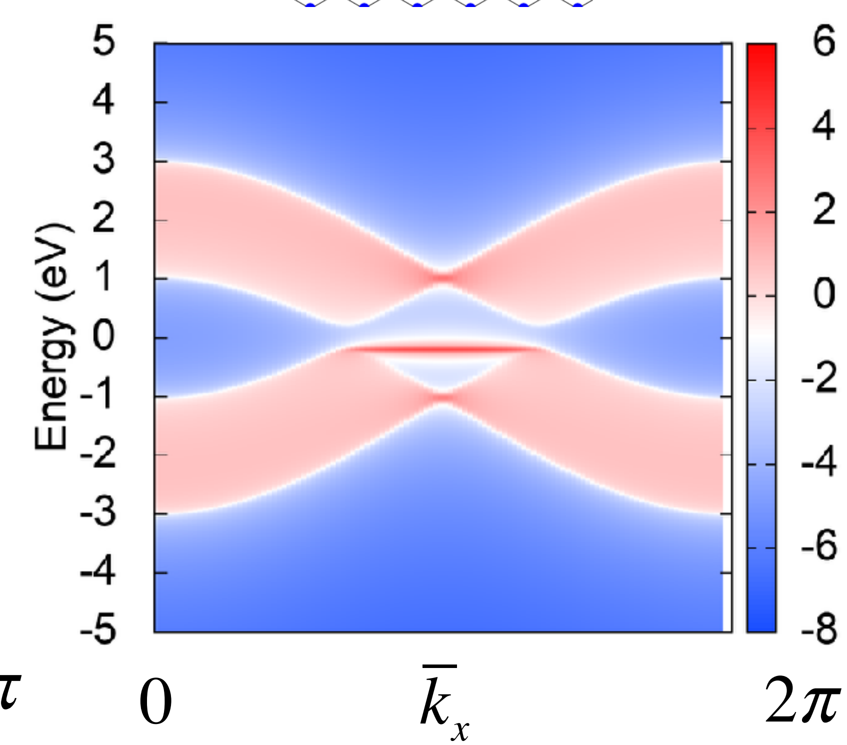




$t_1 = 1; t_2 = 0; m = 0.2; m / t_2 = \infty$

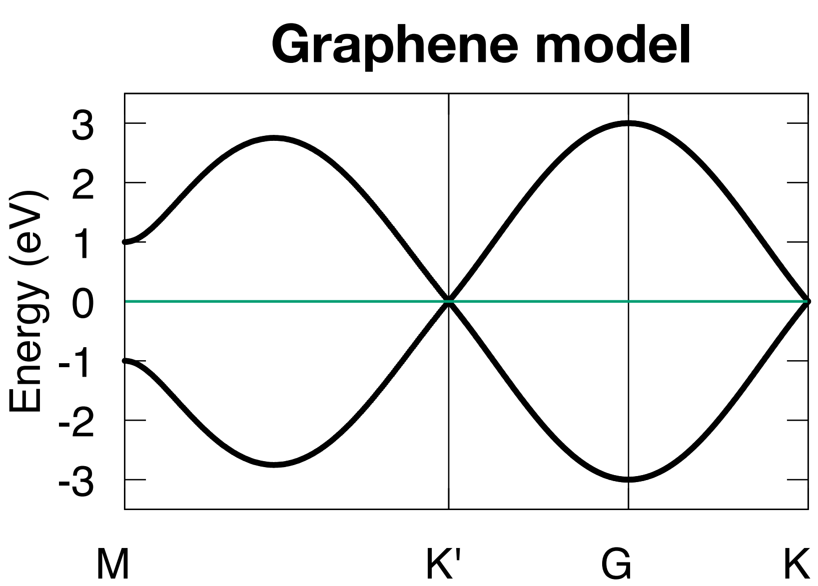


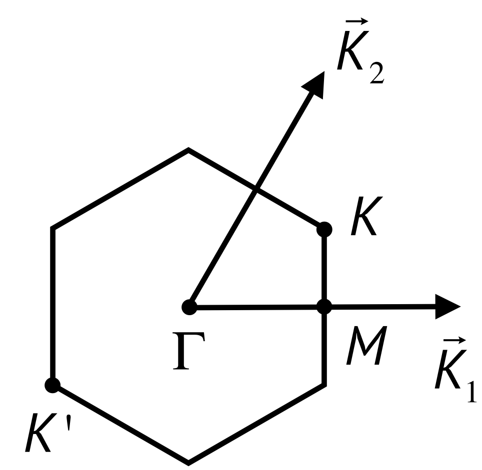


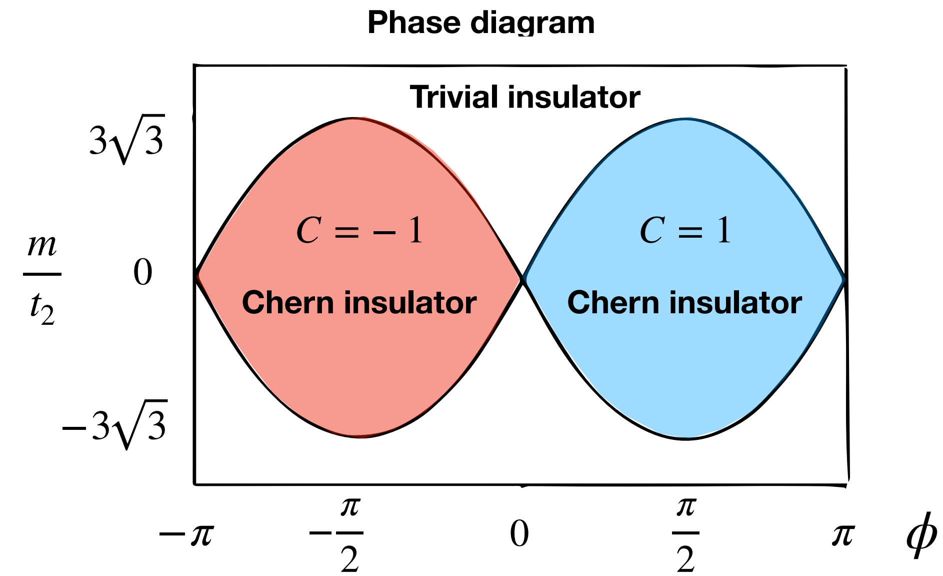


HALDANE MODEL-CHERN INSULATOR PHASE

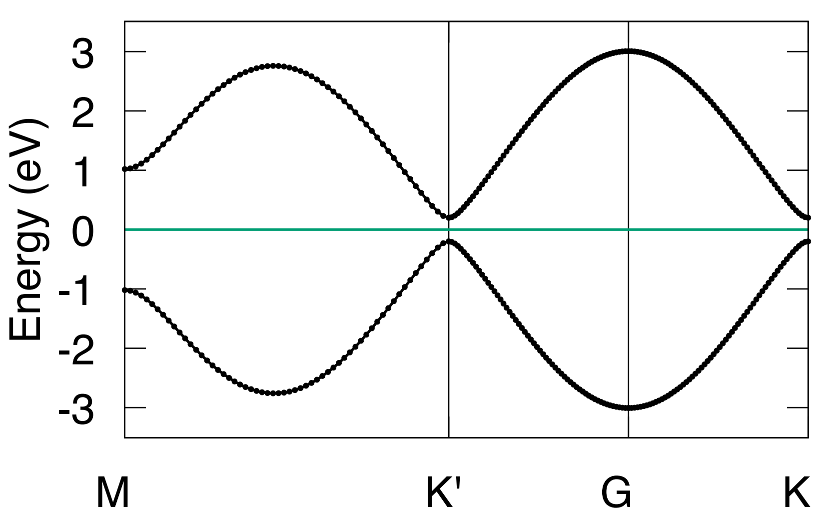
$t_1 = 1; t_2 = 0; m = 0$

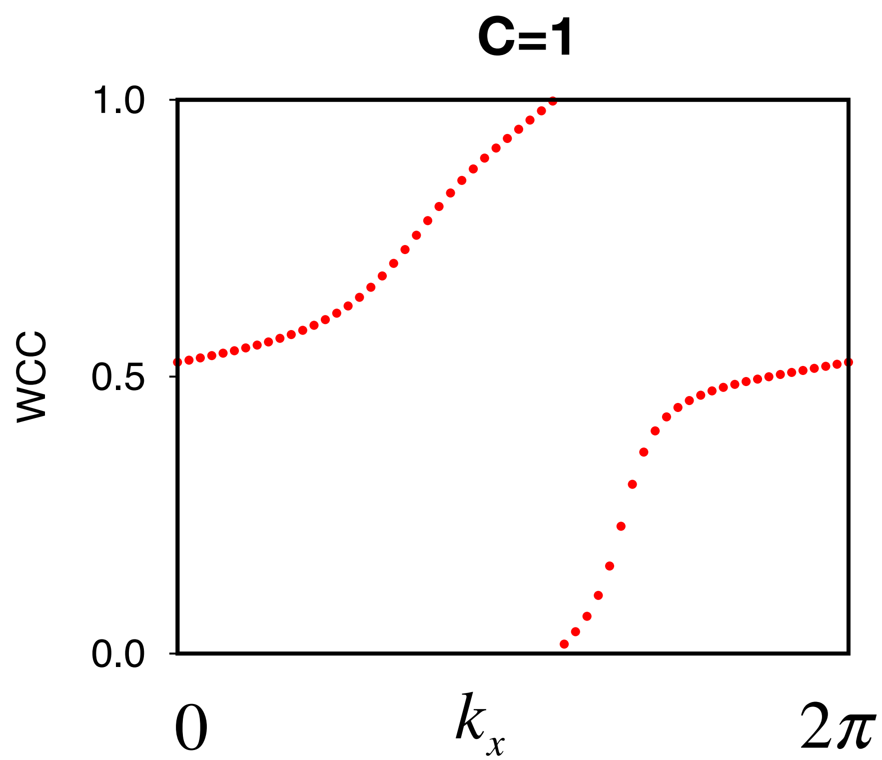


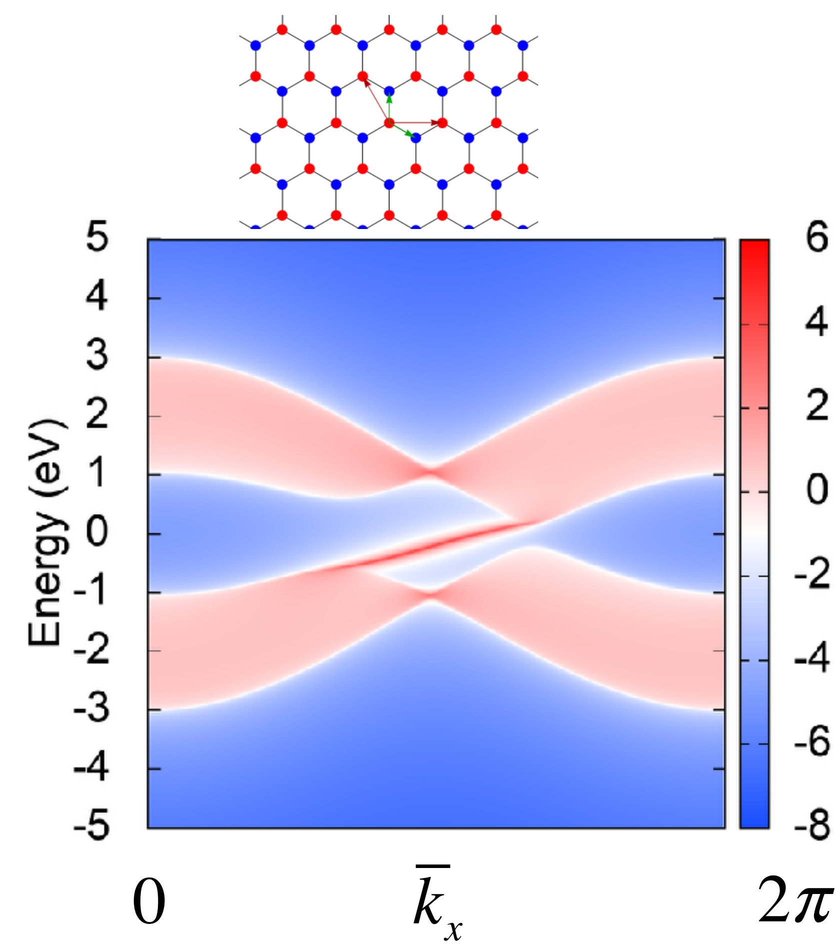




$t_1 = 1; m = 0.2; m / t_2 = 3\sqrt{3}/2; \phi = \frac{\pi}{2}$







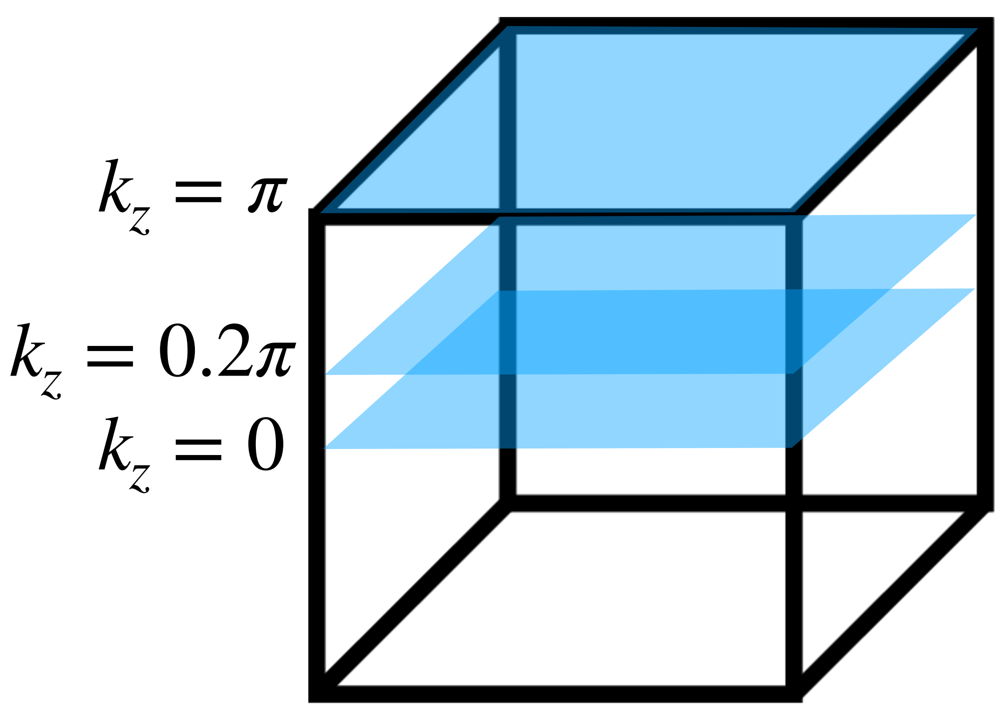
In the tutorial session, we will dig more about Haldane model!

WEYL SEMIMETAL

Chern number is defined as integral of Berry curvature in a closed surface in momentum space. For a 2D system, BZ is a closed surface.

$$C = \frac{1}{2\pi} \oint_{BZ} d^2k \Omega_{xy}$$

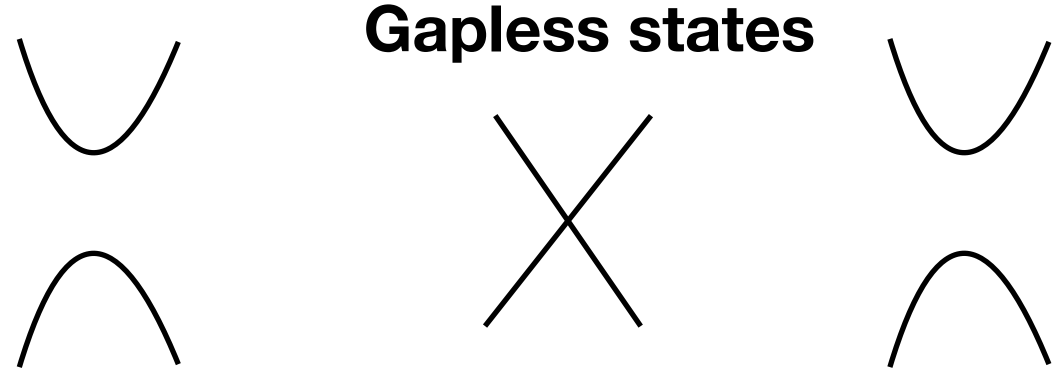
In 3D case, we can choose a slice of BZ as a close surface.



What if the Chern numbers of slices are different? For example

$C(k_z = 0) = 1$ $\qquad$ $C(k_z = \pi) = 0$

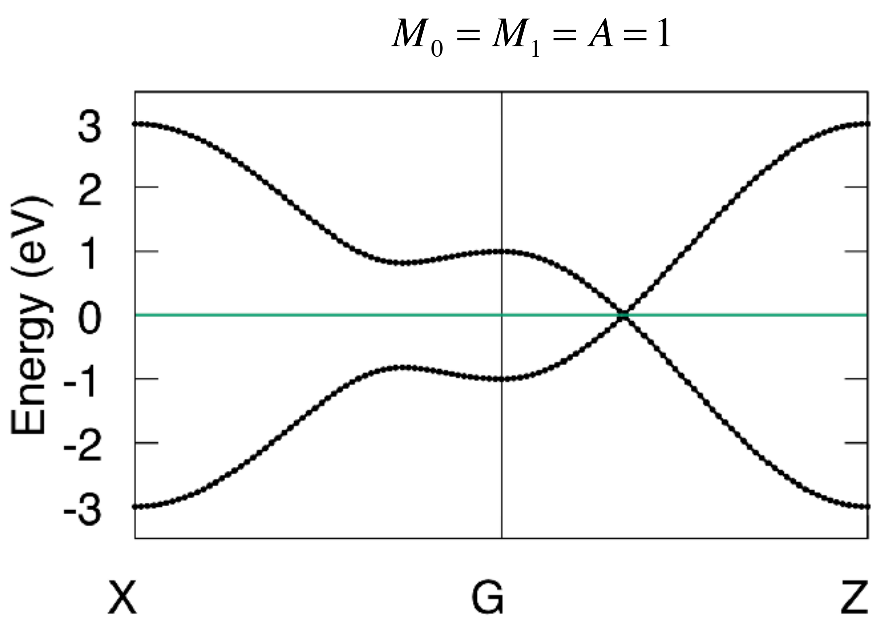
Gapless states

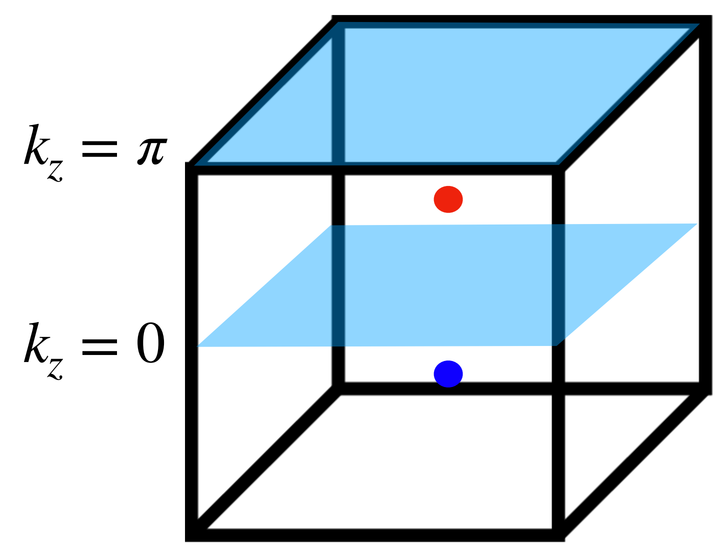


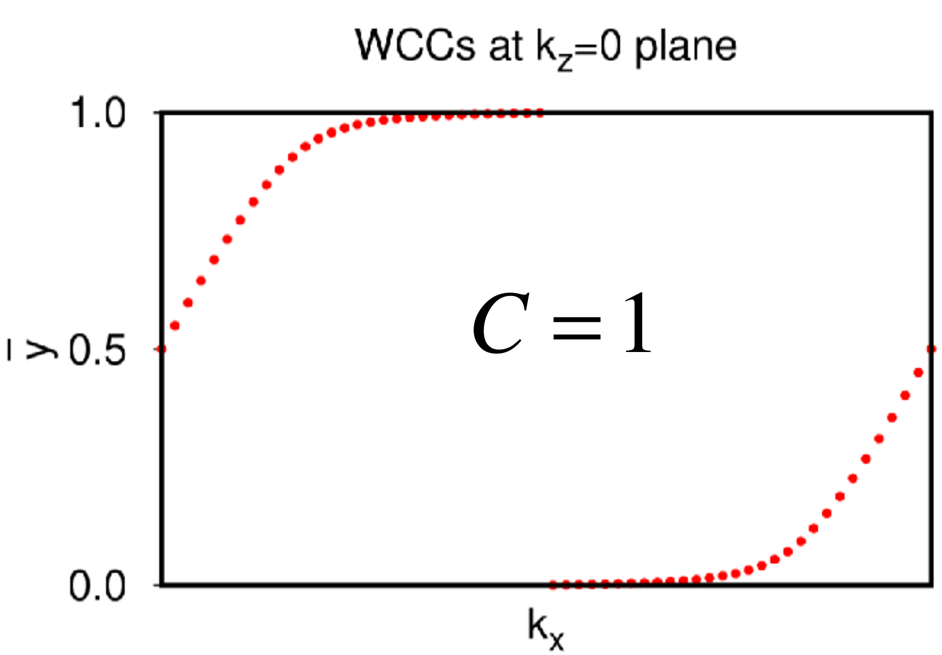
WEYL SEMIMETAL

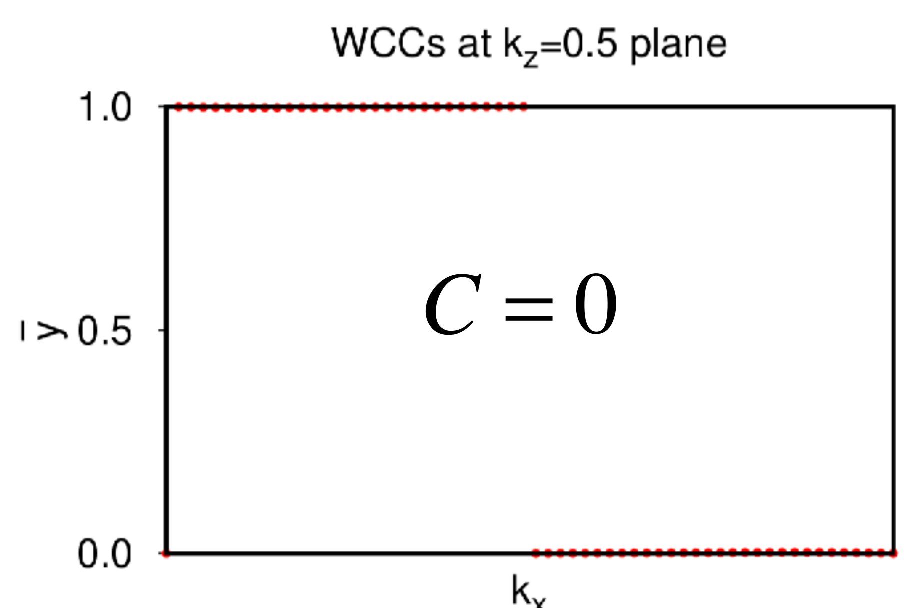
A 2-band toy model

$$H = A(k_x\sigma_x + k_y\sigma_y) + [M_0 - M_1(k_x^2 + k_y^2 + k_z^2)]\sigma_z$$



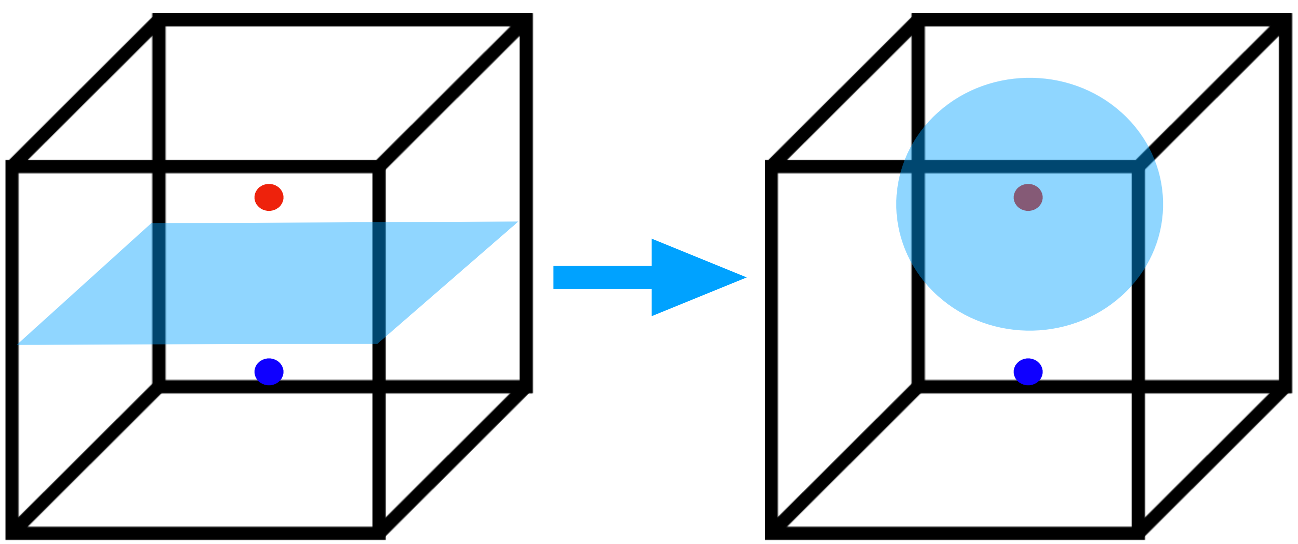


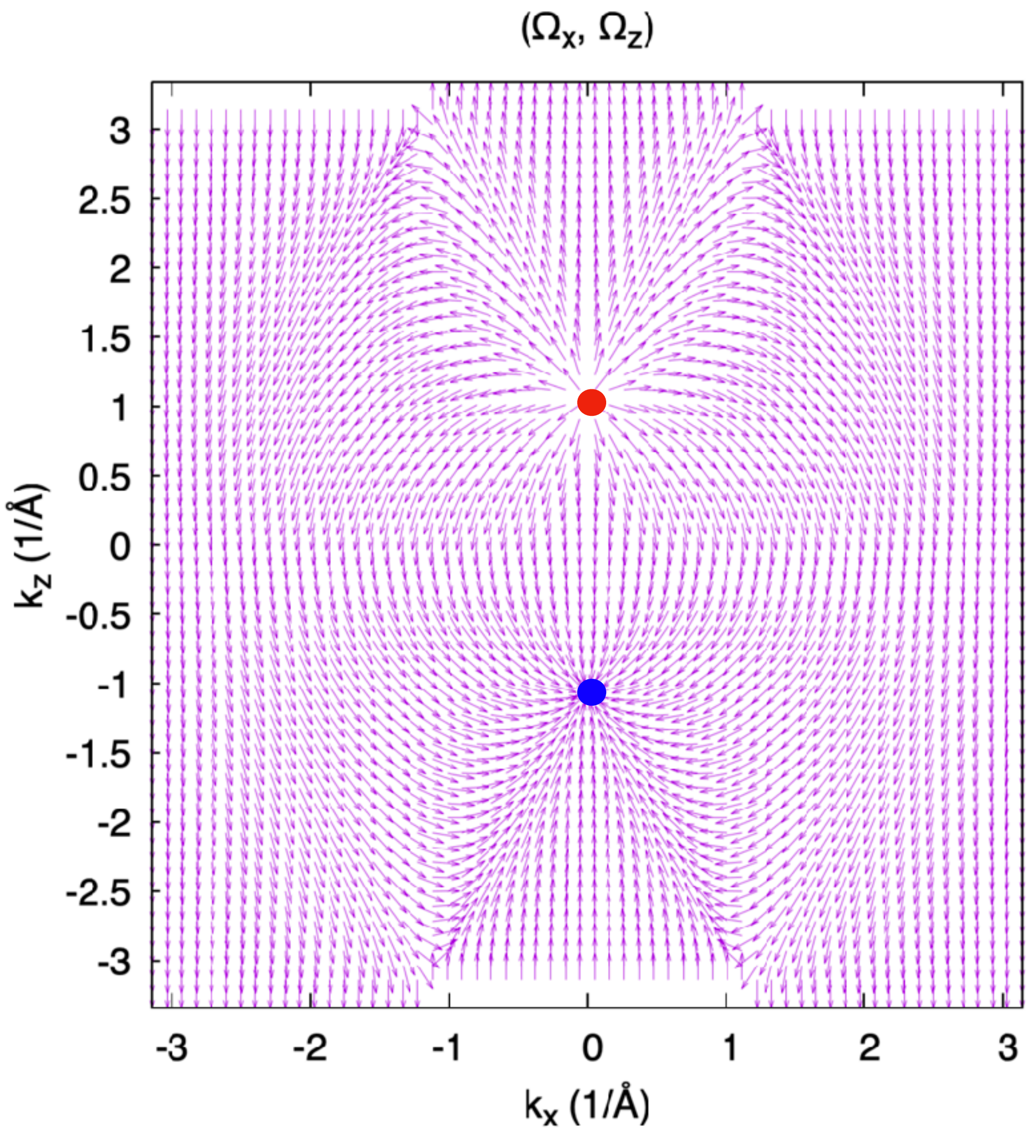




WEYL SEMIMETAL

We can continuous modify the closed slice at kz=0 such that it becomes a sphere enclosing the Weyl points.





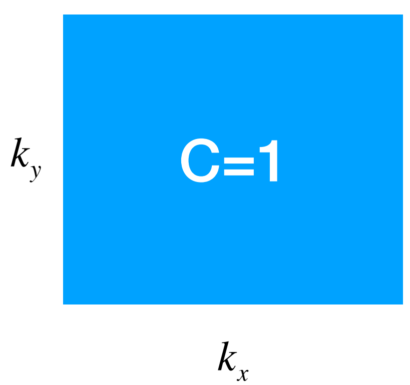
$$C = \frac{1}{2\pi}\oint_S \Omega \cdot dS$$

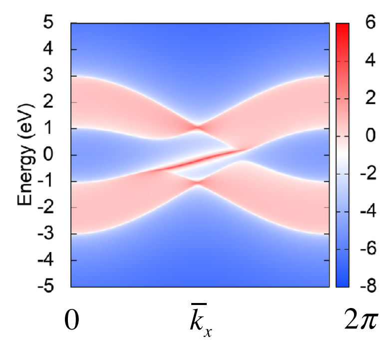
Non-trivial Chern number means that the Berry curvature is not trivial. Positive Chern number indicates that the Weyl point is the source of Berry curvature.

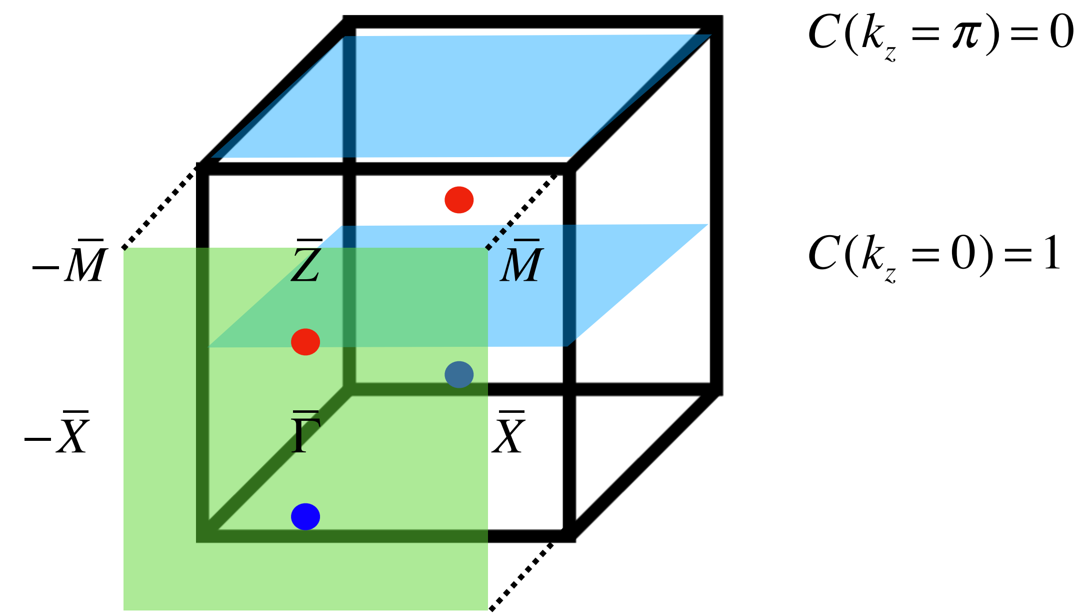
WEYL SEMIMETAL

What kind of surface states would Weyl semimetal has?

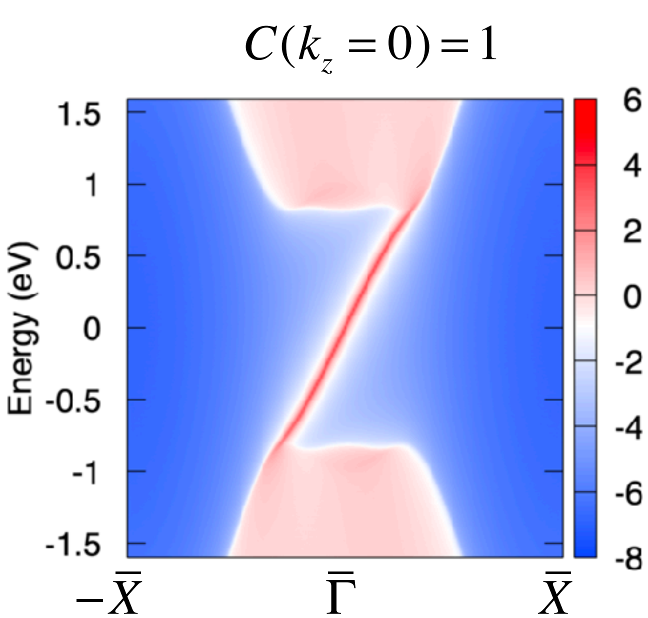
Review:

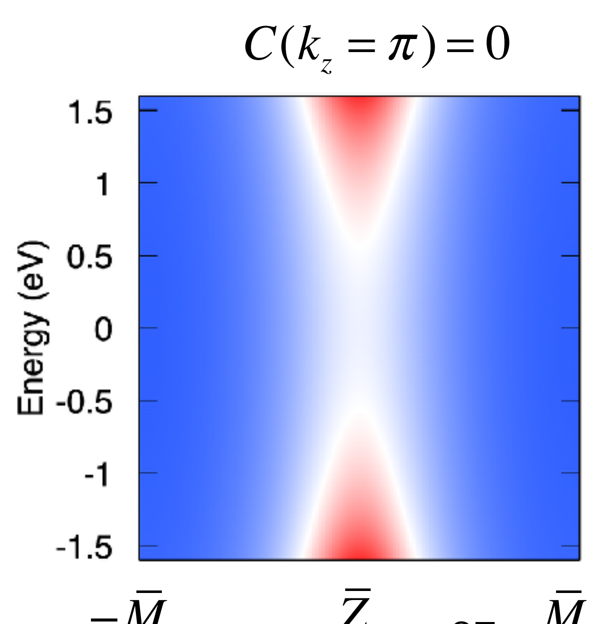


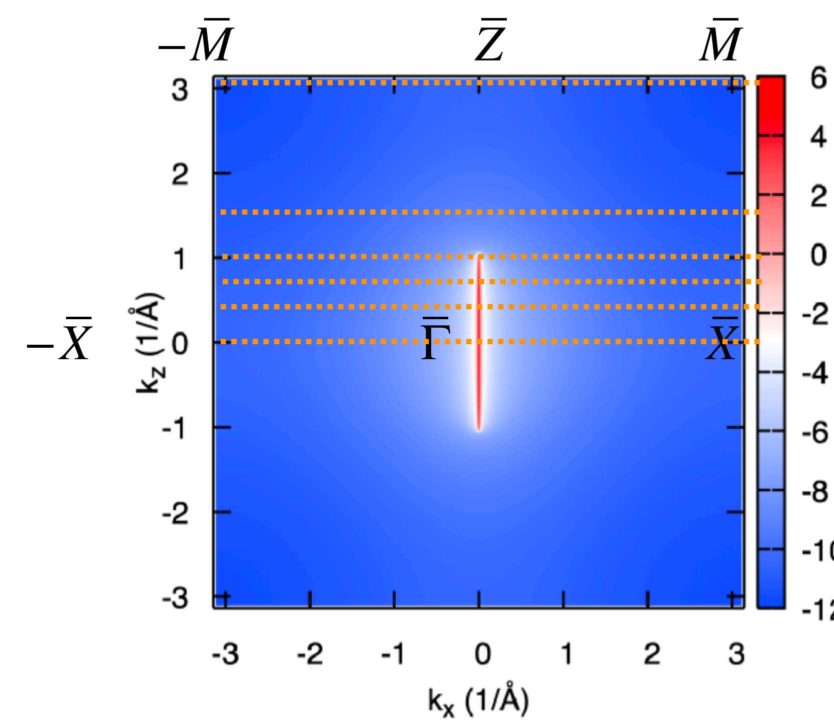




Let's study the (010) surface where there is no periodicity along y direction.







QUANTUM SPIN HALL EFFECT

If a system has time reversal symmetry

$$\Omega(k) = -\Omega(-k)$$

Then Chern number vanishes!

$$C = \frac{1}{2\pi}\oint_{BZ} d^2k\Omega(k) = 0$$

Are all time reversal symmetry preserved systems trivial?

The answer is no!

Consider this case:

You have two spaces which are related by time reversal symmetry. And two spaces has opposite non-trivial Chern number C_+ and C_-.

Then we may define a new topological number Z= C_+ -C_-. This number is not zero even with time reversal symmetry.

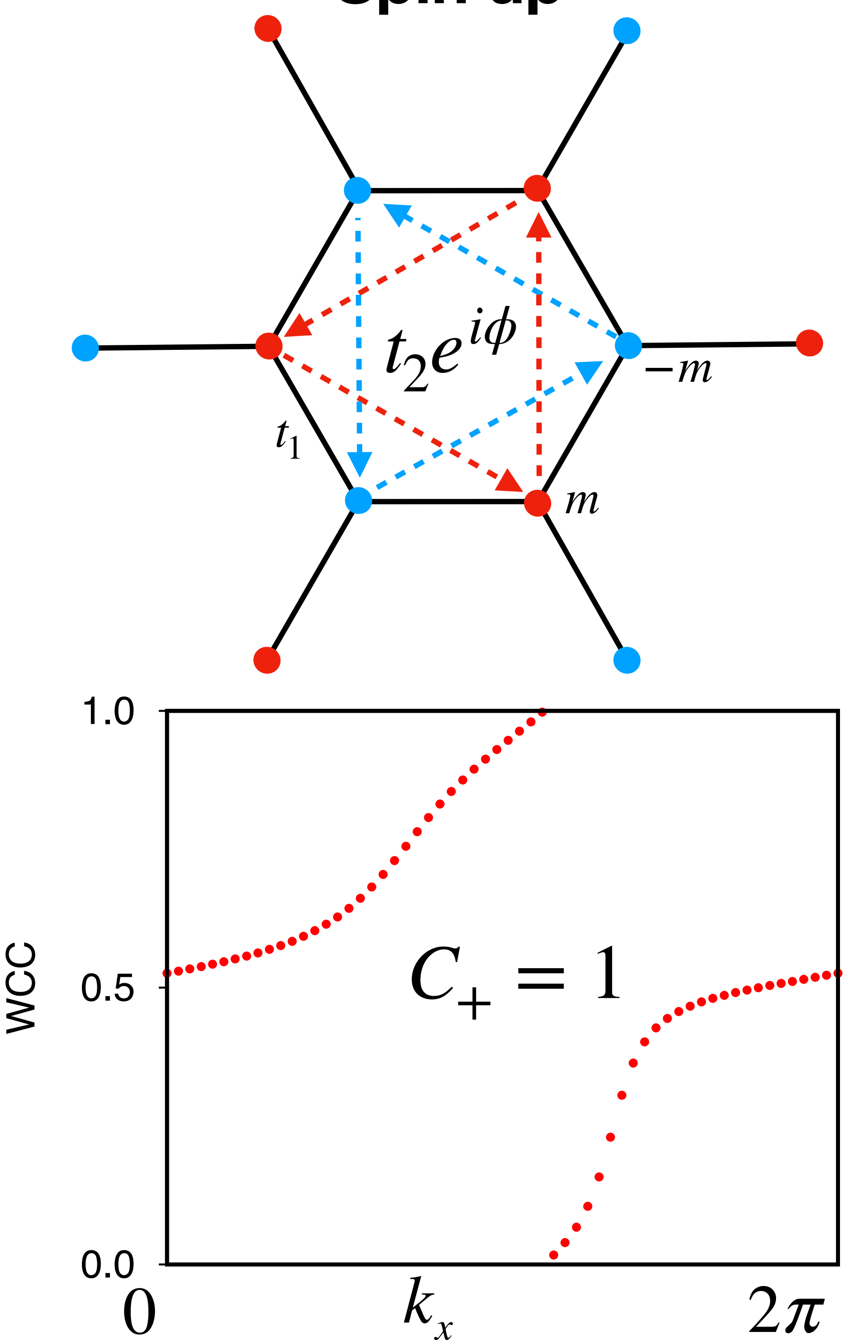
QUANTUM SPIN HALL EFFECT

One example of such a system with time reversal symmetry is the Kane-Mele model.

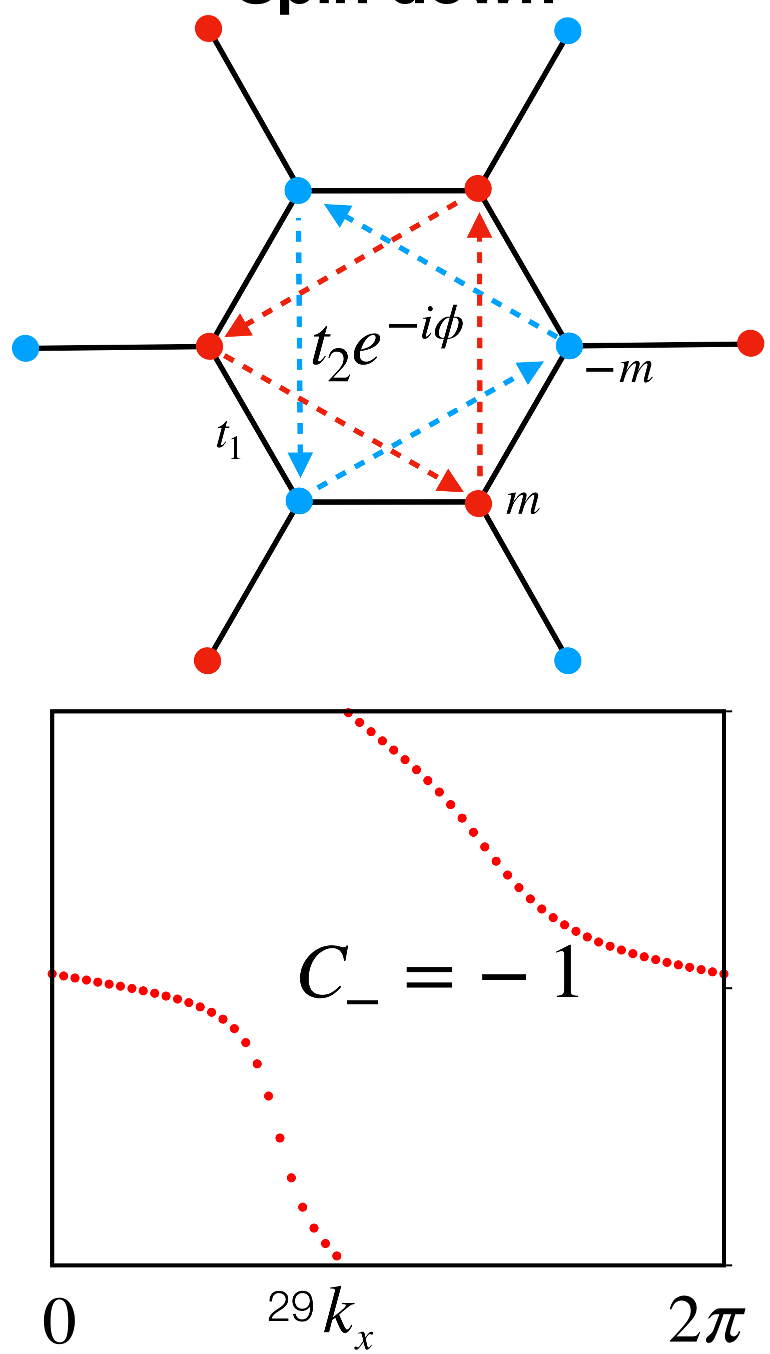
Kane-Mele model is a doubled copy of Haldane model.

Kane & Mele PhysRevLett.95.226801 (2005)

Spin up



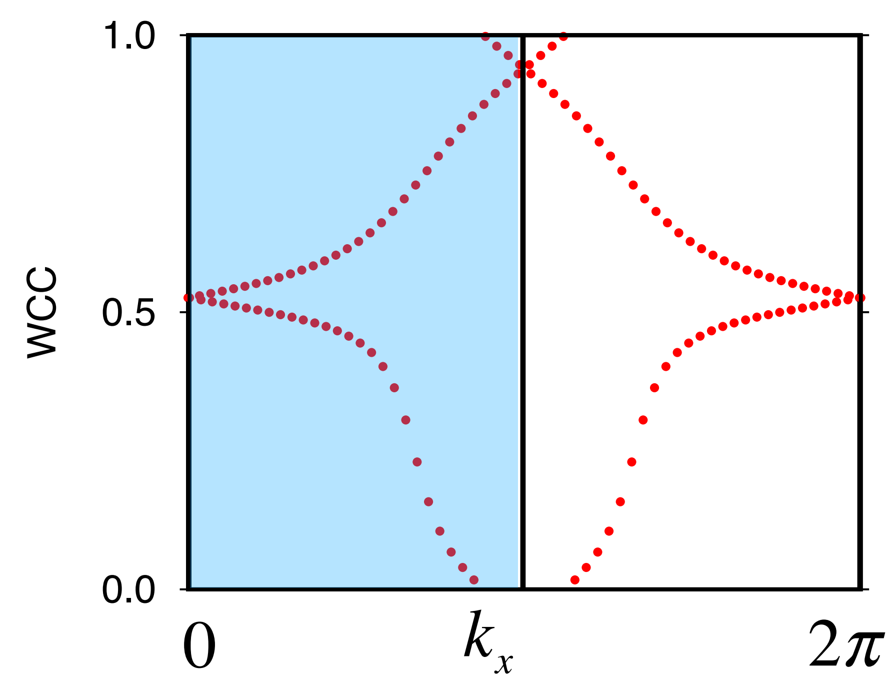
Spin down



Topological number

$$Z_2 = mod(C_+ - C_-, 2) = 1$$

In total



QUANTUM SPIN HALL EFFECT

How to realize such QSHE states?

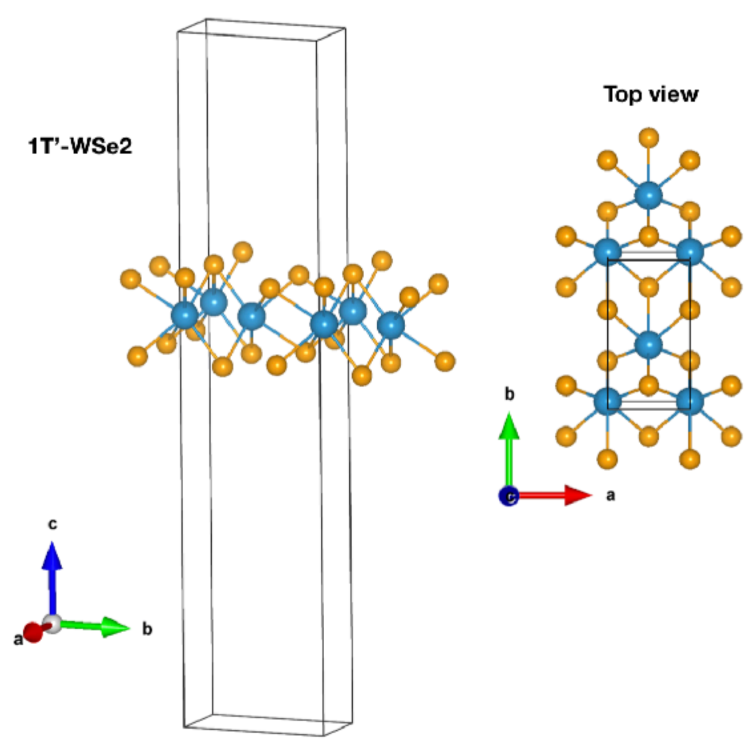
Kane-Mele point out that the imaginary next-nearest hopping can be realized if we take into account the spin-orbital coupling (SOC) effect. A sad thing is that the SOC effect in Graphene is negligible.

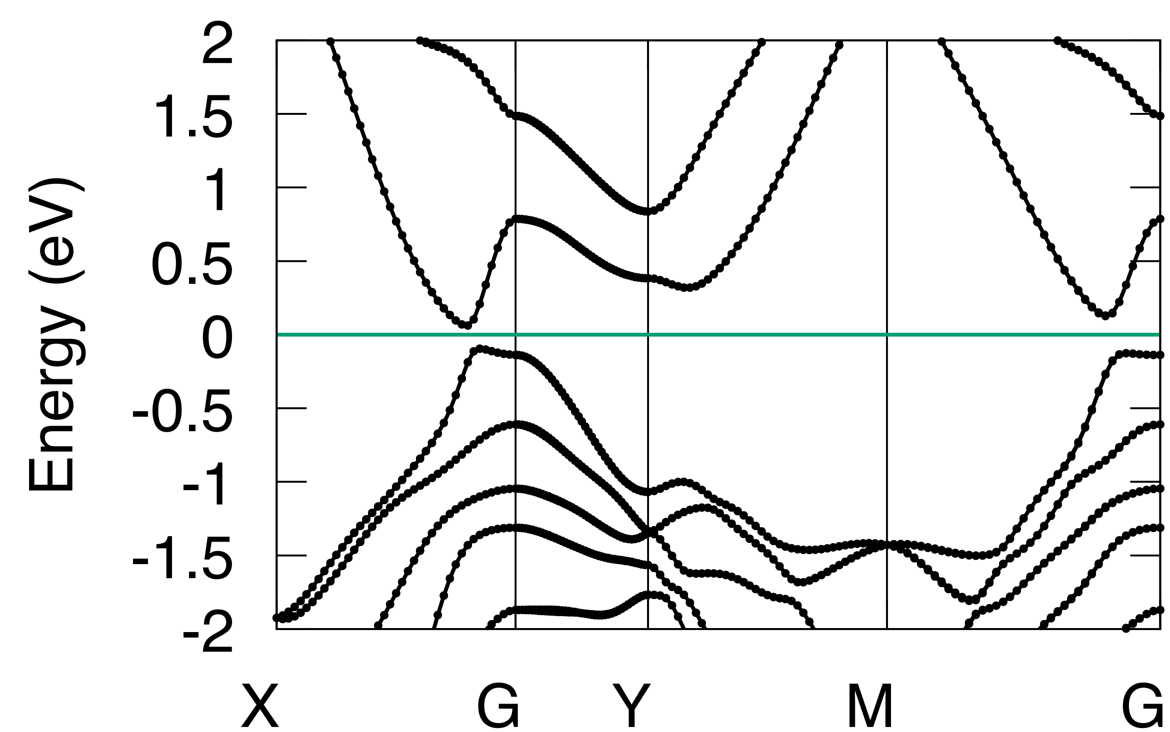
Kane & Mele PhysRevLett.95.226801 (2005)

In 2006, Bernevig, Hughes, Zhang noticed that QSHE can be realized when the energy bands get inverted by SOC. It can be realized in HgTe QWs.

Bernevig, Hughes, Zhang, Science 314, 1757 (2006)

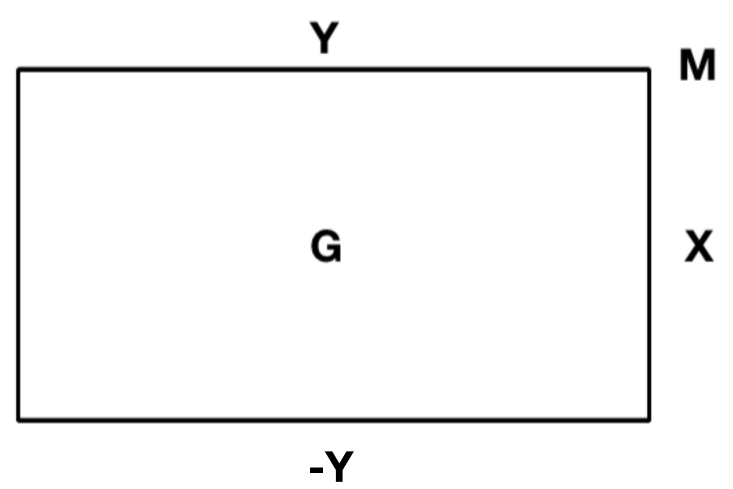
One example: 1T'-WSe2

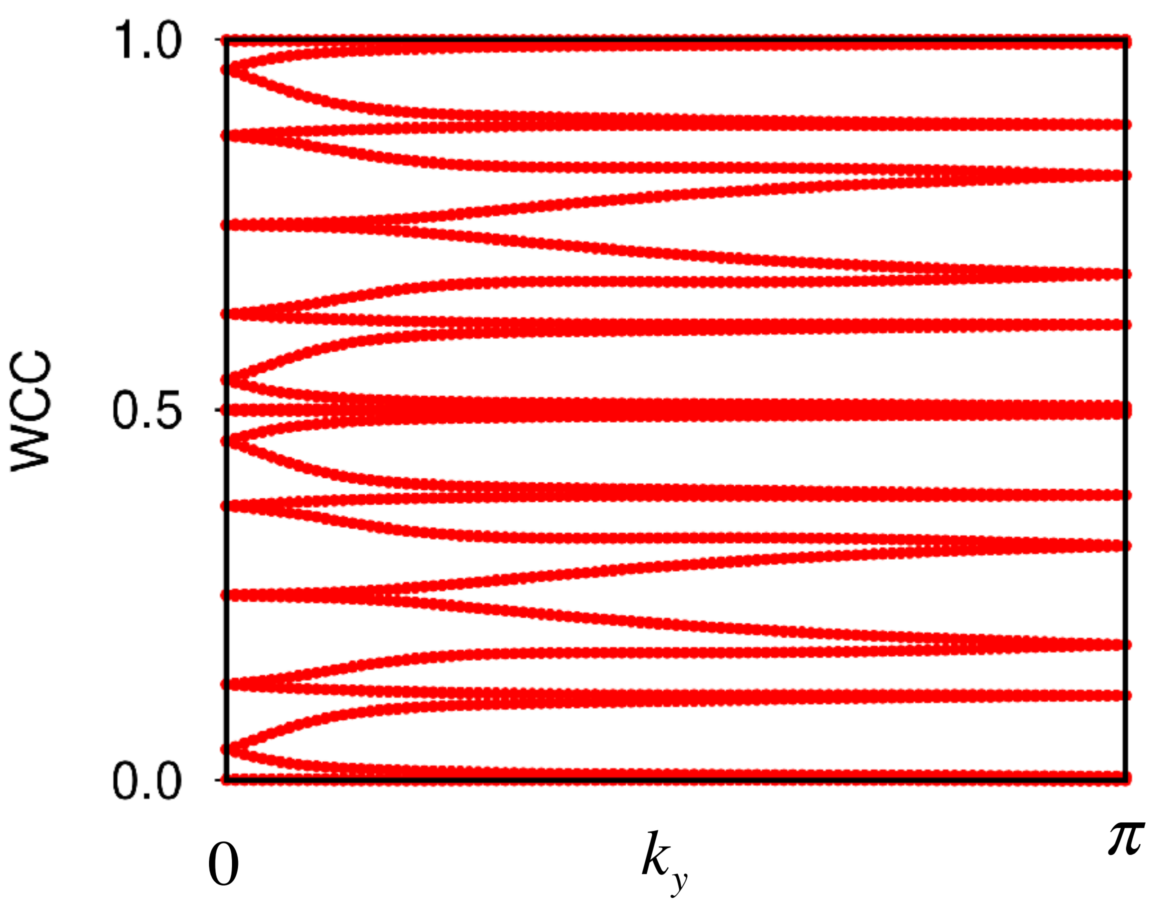




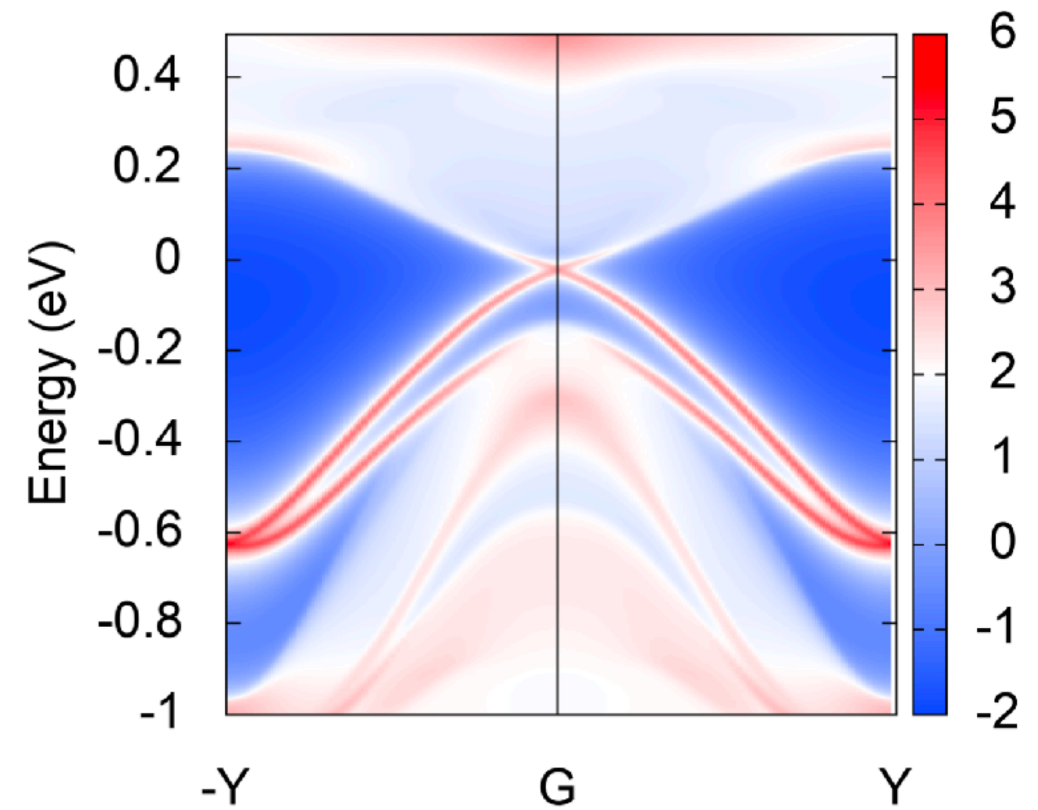
QUANTUM SPIN HALL EFFECT

One example: 1T’-WSe2



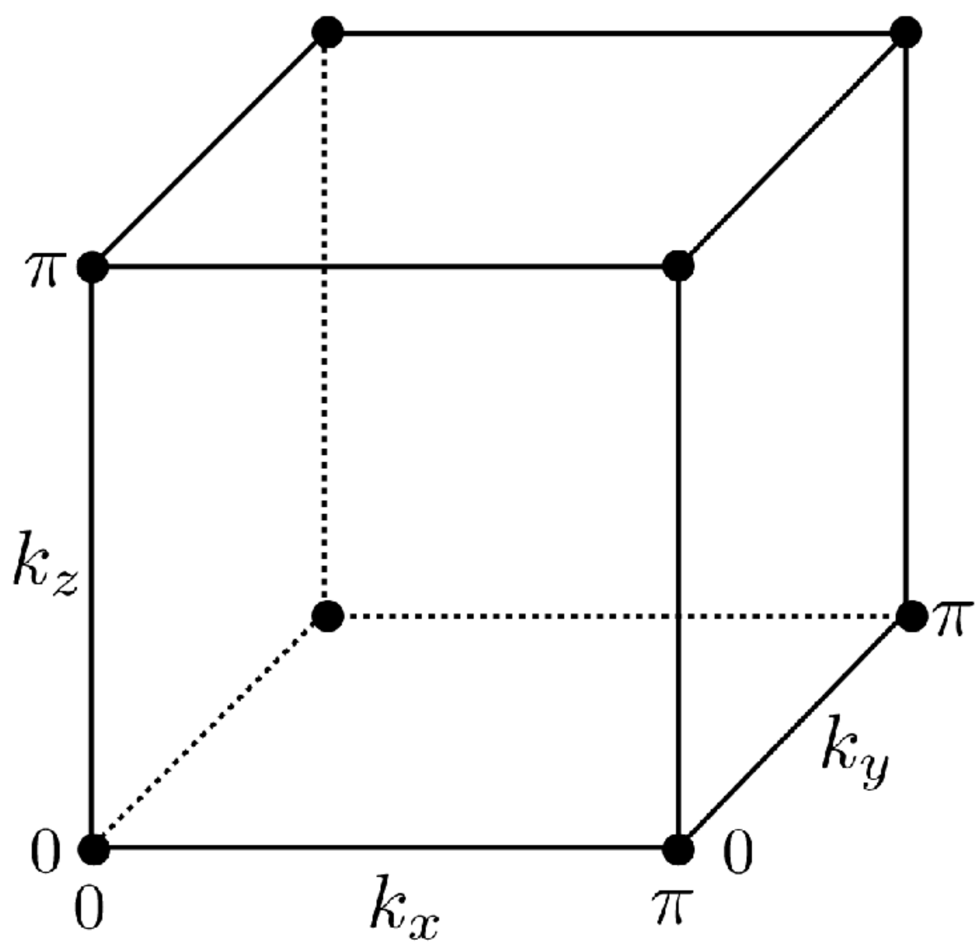


Z2=1



3D TOPOLOGICAL INSULATOR

Extent QSHE to 3D topological insulator (TI) is not a trivial thing, since there are four topological numbers named ($v_0;v_1v_2v_3$) in 3D TI.



Z2 number is calculated in the time-reversal invariant plane. There are six such planes. Each of them can give you one Z2 number, which give us 6 numbers. However not all of them are independent. Specifically, there is a constraint.

$$Q(k_x = 0)\, Q(k_x = \pi) \equiv Q(k_y = 0)\, Q(k_y = \pi) \equiv Q(k_z = 0)\, Q(k_z = \pi)$$

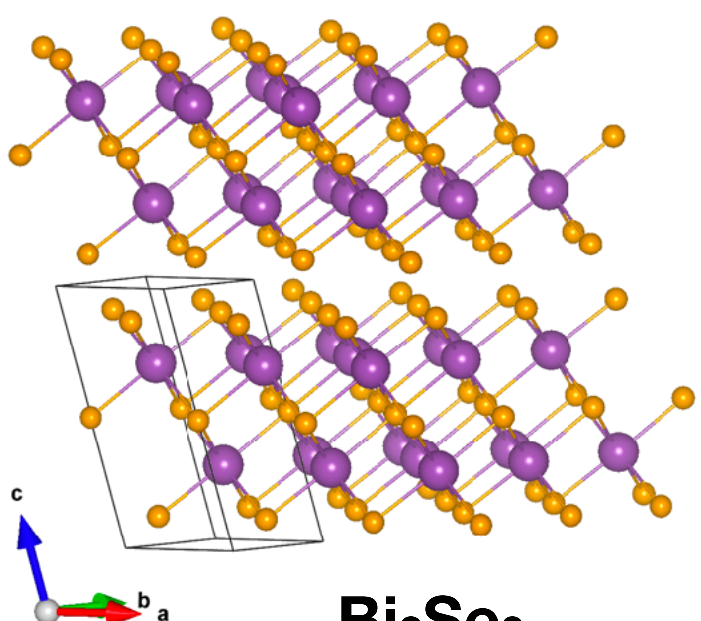
This product is called the strong topological invariant v_0.

$$Q(k_x = \pi),\ Q(k_y = \pi),\ Q(k_z = \pi)$$

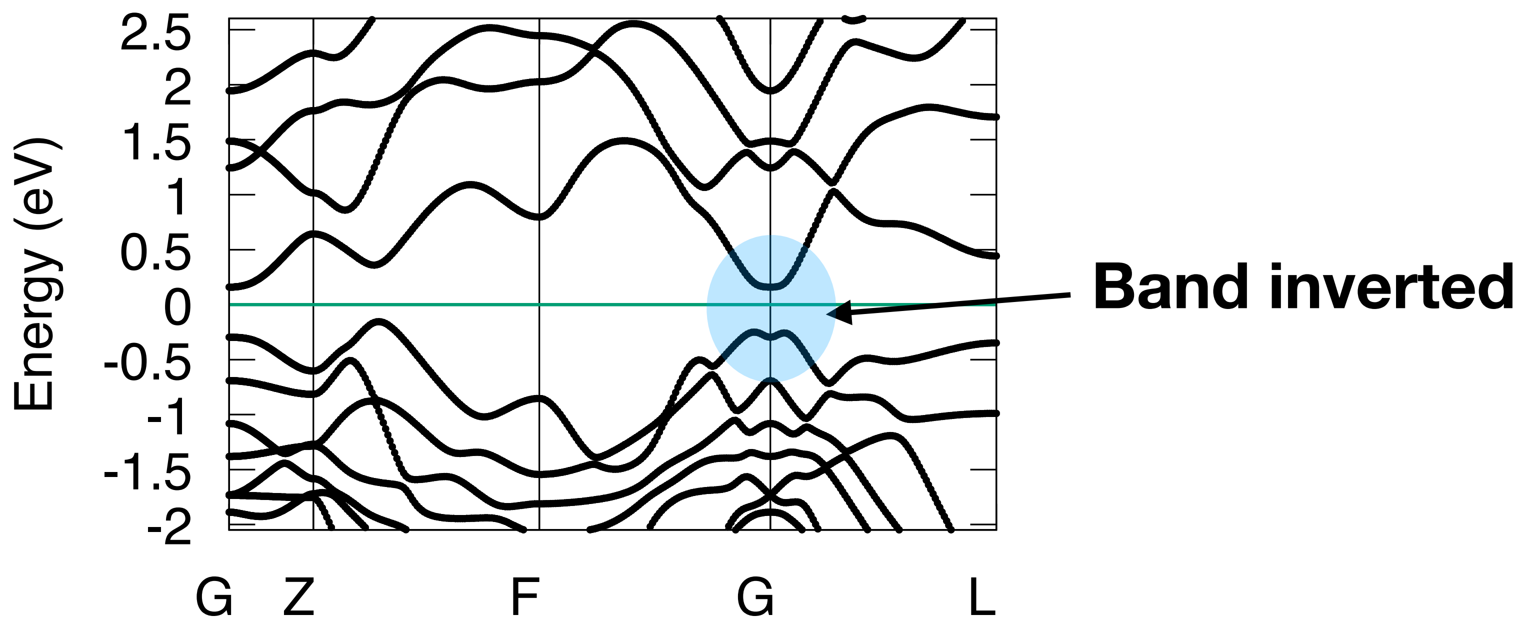
are chosen as v_1,v_2,v_3.

3D TOPOLOGICAL INSULATOR

Bi_2Se_3 is theoretical predicted and experimental validated as a strong 3D TI.

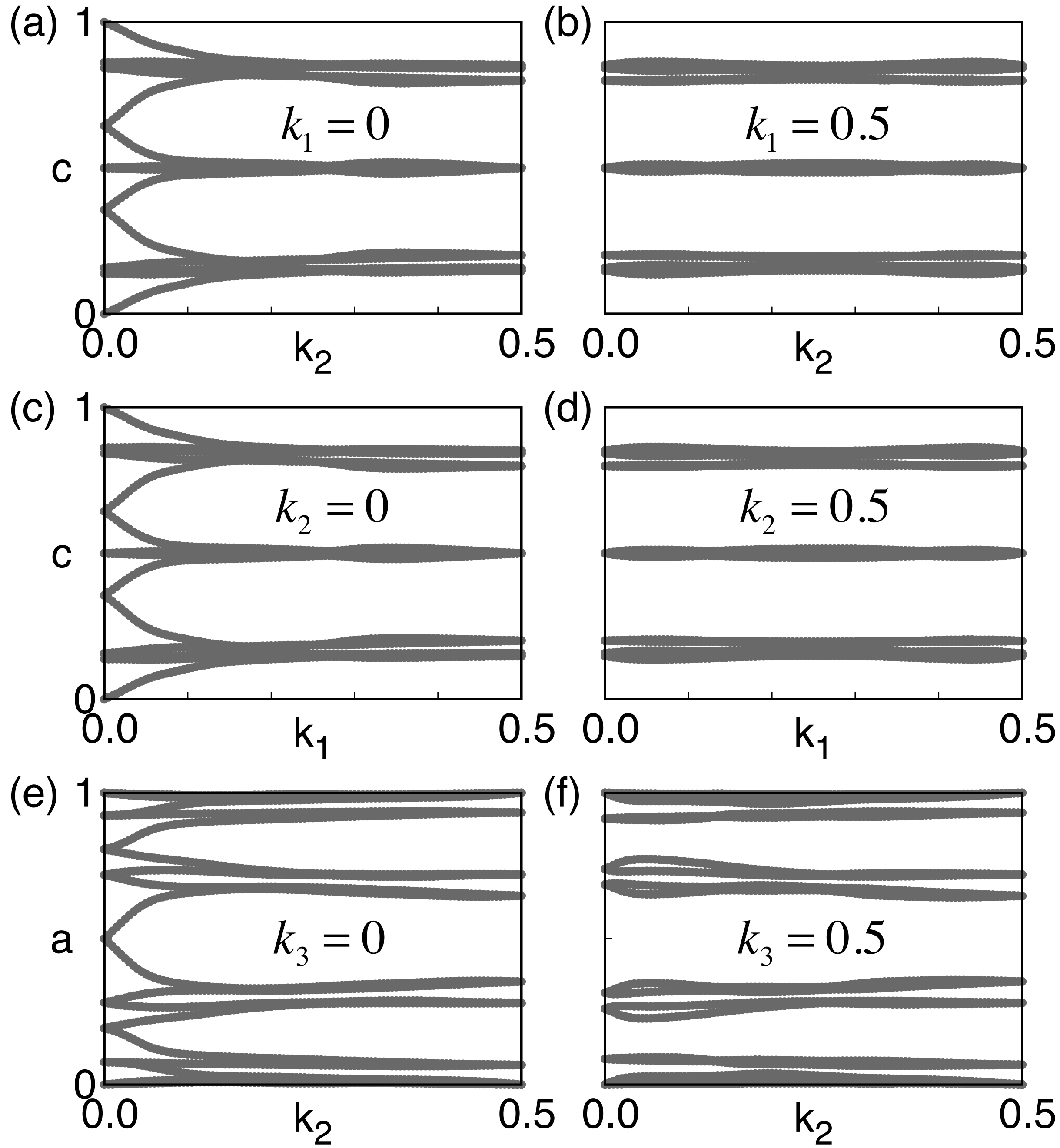


Bi_2Se_3



3D TOPOLOGICAL INSULATOR

Bi_2Se_3 is theoretical predicted and experimental validated as a strong 3D TI.

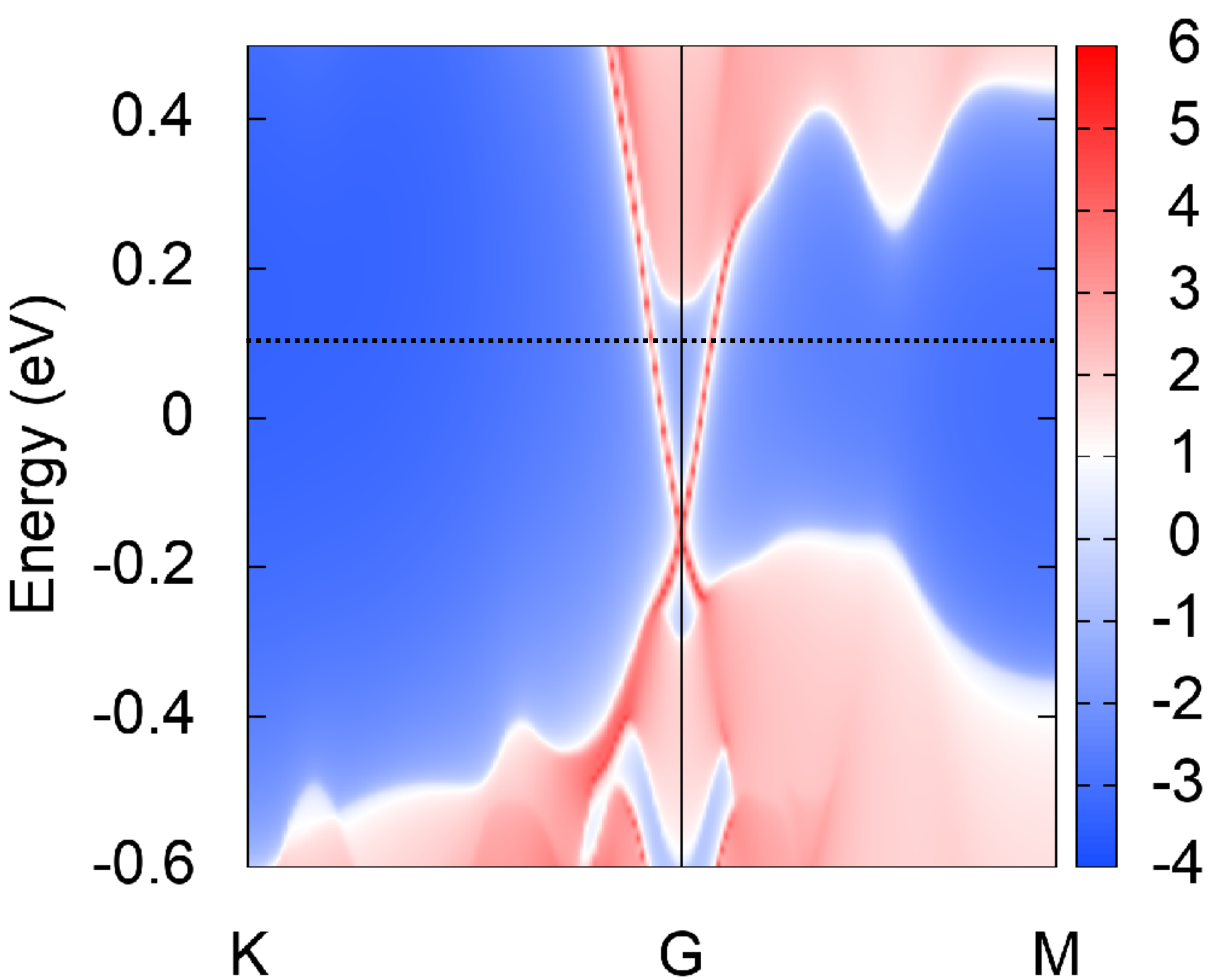


Topological number is
$(v_0;v_1v_2v_3)=(1;000)$

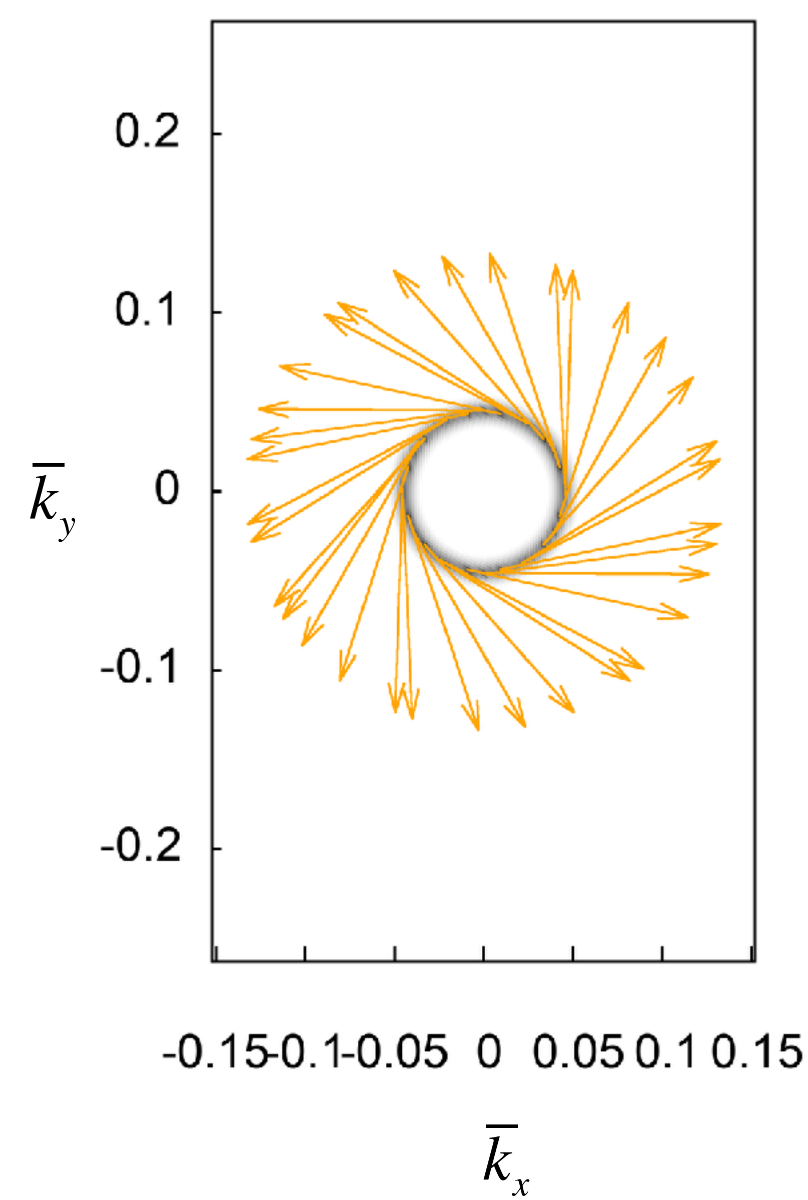
3D TOPOLOGICAL INSULATOR

Bi_2Se_3 is theoretical predicted and experimental validated as a strong 3D TI.

Surface states



Spin texture



CONCLUSION

1. Introduced some preliminaries of Berry phase and topological properties.

2. Introduced Haldane model, Weyl semimetal, QSHE and 3D TI.

CONCLUSION

There are a lot of physical properties that related to the bulk topology that are not introduced in this talk due to the time limit, includes

- **anomalous Hall conductivity**
- **orbital magnetization**
- **spin Hall conductivity**
- **the Berry curvature dipole**
- **the kinetic magnetoelectric effect (kME)**
- **Shift current**
- **…**

Those properties can be calculated using the latest Wannier90 v3.1.0.

Thank you for your attention!