Chern number and Z_2 invariant

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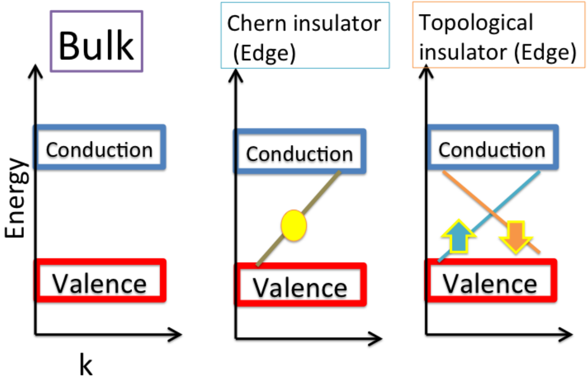
Introduction

Chern insulator, Topological insulator

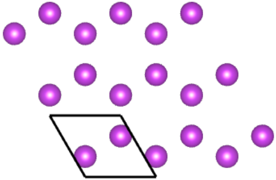
Topological material: Chern insulator[1] or Topological insulator[2] has special edge state(s).

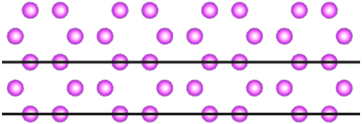


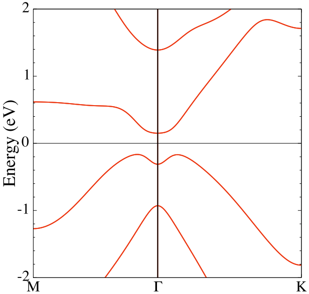
[1] Thouless-Kohmoto et al.,Phys. Rev. Lett. **49**, 405 (1982)
[2] L. Fu and C. Kane, Phys. Rev. B **74**, 195312 (2006)

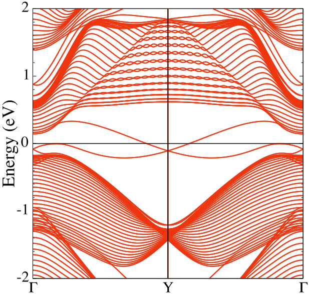
Example of edge states

Bi(111) film's(Topological insulator)[3] band dispersion









[3] S. Murakami, Phys. Rev. Lett. **97**, 236805 (2006).

Topological invariant(1)

Chern insulator is characterized by Chern number C defined as

Chern number

$$C = \sum_{n}^{occ.} \frac{1}{2\pi} \int_{\mathrm{BZ}} dk_x dk_y F_n = 0, \pm 1, \pm 2, \pm 3, \cdots$$

$$F_n = (\nabla \times \mathbf{A}_n)_z, \mathbf{A}_n = i \langle u_{n\mathbf{k}} | \frac{\partial}{\partial \mathbf{k}} | u_{n\mathbf{k}} \rangle$$

$C = 0$ corresponds to a trivial state and
$C = \pm 1, \pm 2, \pm 3, \cdots$ corresponds to a Chern insulator state.

Topological insulator is characterized by Z_2 invariant defined as

Z_2 invariant

$$Z_2 = \sum_{n}^{occ.} \frac{1}{2\pi} \left(\oint_{\mathrm{Half\ BZ}} \mathbf{A}_n \cdot d\mathbf{k} - \int_{\mathrm{Half\ BZ}} dk_x dk_y F_n \right) = 0 \text{ or } 1 \pmod 2$$

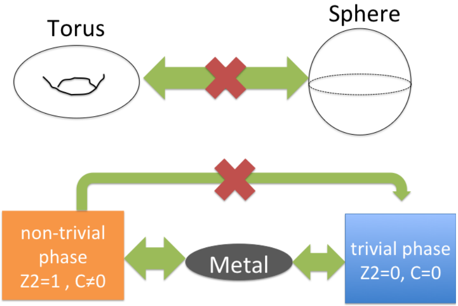
$Z_2 = 0$ corresponds to a trivial state and
$Z_2 = 1$ corresponds to a topological insulator state.

Topological invariant(2)

Why is Topological invariant, Chern number or Z_2 invariant important ?

We can predict if special edge state(s) exist
by calculating Chern number or Z_2 invariant in a bulk system
$\rightarrow$ **NO need to calculate edge states**.

Topological invariant, Chern number or Z_2 invariant doesn't change without gap closing. This fact is analogous to mathematical "Topology"



Fukui-Hatsugai method computing Chern number and Z_2 invariant

Chern number

Computing Chern number(1)-Overlap matrix-

The definition of Chern number:

$$C_n = \frac{1}{2\pi} \int_{\mathrm{BZ}} dk_x dk_y F_n = 0, \pm 1, \pm 2, \cdots$$

we define overlap matrix U (we can calculate U by "polB.c")[4]

$$U_{\boldsymbol{\mu}} = \det \langle u_m(\mathbf{k}) | u_n(\mathbf{k} + \Delta\boldsymbol{\mu}) \rangle$$

and, we can obtain A and F as

$$A_{\boldsymbol{\mu}}(\mathbf{k}) = \mathrm{Im} \log U_{\boldsymbol{\mu}}(\mathbf{k})$$
$$F_{k_x k_y}(\mathbf{k}) = \mathrm{Im} \log U_{k_x}(\mathbf{k}) U_{k_y}(\mathbf{k} + \Delta k_x) U_{k_x}^{-1}(\mathbf{k} + \Delta k_y) U_{k_y}^{-1}(\mathbf{k})$$

For obtaining Chern number, we need to calculate F on every "tile" in discretized Brillouin Zone and summate them [5].

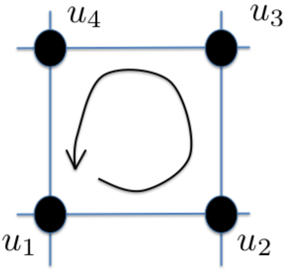
[4] Electric Polarization by Berry Phase:Ver. 1.1, Technical Notes on OpenMX

[5] T. Fukui, Y. Hatsugai and H. Suzuki, J. Phys. Soc. Jpn. **74**, 1674 (2005).

Computing Chern number(2)-Calculate F-

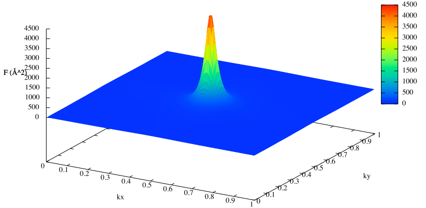
Discretized Brillouin Zone in the direction of k_x and k_y, and calculate on every "tile",

$$U_{12} = \det \langle u_1 | u_2 \rangle$$
$$U_{23} = \det \langle u_2 | u_3 \rangle$$
$$U_{34} = \det \langle u_3 | u_4 \rangle$$
$$U_{41} = \det \langle u_4 | u_1 \rangle$$
$$F_{\mathbf{k}} = \mathrm{Im} \log U_{12} U_{23} U_{34} U_{41}$$



and, we can obtain Chern number as

$$C = \sum_{n}^{\text{occ.}} C_n = \frac{1}{2\pi} \sum_{\mathbf{k}}^{\text{BZ}} F_{\mathbf{k}}$$



Z_2 invariant

The method of computing Z_2 invariant

There are three methods for computing Z_2 invariant

Method	Advantage	Disadvantage
Parity[6]	Easy	Only inversion symmetric system
WFC[7,8]	intuitive	indirect
Fukui-Hatsugai[9]	Direct	not intuitive

We implemented these three methods.

In this presentation, we introduce a Fukui-Hatsugai method.

Fukui-Hatsugai is direct method and suitable for **automatic** searching for topological insulators. (application to material informatics)

[6] L. Fu and C. Kane, Phys. Rev. B **76**, 045302 (2007).

[7] A. A. Soluyanov and D. Vanderbilt, Phys. Rev. B **83**, 235401 (2011).

[8] R. Yu, X. Qi, A. Bernevig, Z. Fang, and X. Dai, Phys. Rev. B **84**, 075119 (2011).

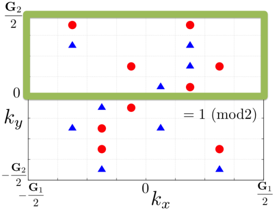
[9] T.Fukui and Y.Hatsugai, J. Phys. Soc. Jpn. **76**, 053702 (2007).

Computing Z_2 invariant -Fukui-Hatsugai method-

Computing Z_2 invariant by Fukui-Hatsugai method is almost same as computing Chern number.

$$Z_2 = \frac{1}{2\pi}\sum_n^{\text{occ.}}\left(\oint_{\text{Half BZ}} \mathbf{A}_n \cdot d\mathbf{k} - \int_{\text{Half BZ}} F_n dk_x dk_y\right) \pmod 2$$

$$U_{12} = \det \langle u_1 | u_2 \rangle$$
$$U_{23} = \det \langle u_2 | u_3 \rangle$$
$$U_{34} = \det \langle u_3 | u_4 \rangle$$
$$U_{41} = \det \langle u_4 | u_1 \rangle$$
$$F_{\mathbf{k}} = \mathrm{Im} \log U_{12} U_{23} U_{34} U_{41}$$
$$A_{ab} = \mathrm{Im} \log U_{ab}$$



$$n(\mathbf{k}) = \frac{1}{2\pi}[(A_{12} + A_{23} + A_{34} + A_{41}) - F_{\mathbf{k}}]$$

$$Z_2 = \frac{1}{2\pi}\sum_{\mathbf{k}}^{\text{Half BZ}} n(\mathbf{k}) \pmod 2$$

Test calculation and Application -Z_2 invariant -

How to use

we made two codes, "calB.c"(Chern number) and "Z2FH.c"(Z_2 invariant) by modifying "polB.c" (calculate polarization by Berry phase)
So, you have to prepare (system name).scfout file
by keyword specified in input file

```
HS.fileout                    on
```

and you can obtain Chern number or Z_2 invariant by

```
(PATH)/calB        (system name).scfout
(PATH)/Z2FH        (system name).scfout
```

Test calculation-Z_2 invariant (1)

Z_2 invariant calculated by Fukui-Hatsugai method which is implemented in OpenMX, completely agrees for all these materials.

Material	Method	Z_2	Fukui-Hatsugai	Previous study
Bi_2Te_3	Parity	1;(000)	1;(000)	[1]
Bi_2Se_3	Parity	1;(000)	1;(000)	[1]
Sb_2Te_3	Parity	1;(000)	1;(000)	[1]
Sb_2Se_3	Parity	0;(000)	0;(000)	[1]
Bi(111) film	Parity	1	1	[2]
$TlBiTe_2$	Parity	1;(000)	1;(000)	[3]
$TlBiSe_2$	Parity	1;(000)	1;(000)	[3]
$TlBiS_2$	Parity	0;(000)	0;(000)	[3]
$TlSbTe_2$	Parity	1;(000)	1;(000)	[3]
$TlSbSe_2$	Parity	1;(000)	1;(000)	[3]
$TlSbS_2$	Parity	0;(000)	0;(000)	[3]

Test calculation-Z_2 invariant (2)

Z_2 invariant calculated by Fukui-Hatsugai method which is implemented in OpenMX, completely agrees for all these materials.

Material	Method	Z_2	Fukui-Hatsugai	Previous study
$YBiO_3$	Parity	1;(111)	1;(111)	[4]
$YSbO_3$	Parity	1;(111)	1;(111)	[4]
AlBi,zincblende	WFC	1;(000)	1;(000)	[5]
BBi,zincblende	WFC	1;(000)	1;(000)	[5]
GaBi,zincblende	WFC	1;(000)	1;(000)	[5]
InBi,zincblende	WFC	1;(000)	1;(000)	[5]
$TlSbX_2$ film	WFC	1	1	[6]
$CsPbI_3$	WFC	1;(111)	1;(111)	[7]
$CsPbI_3$, FE	WFC	1;(111)	1;(111)	[7]

[1] H. Zhang, C. Liu, X. Qi, X. Dai, Z. Fang, and S. Zhang,Nat. Phys. **5**, 438 (2009).

[2] S. Murakami, Phys. Rev. Lett. **97**, 236805 (2006).

[3] B. Singh et al., Phys. Rev. B. **86**, 115208 (2012).

[4] H. Jin, S. Rhim, J. Im, and A. Freeman, Sci. Reports **3**, 1651 (2013).

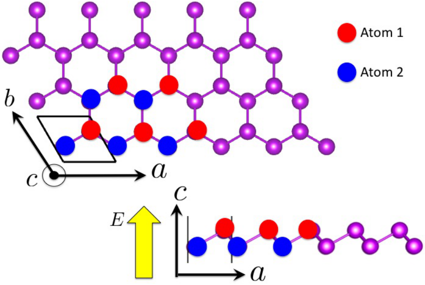
[5] H. Huang et al., Phys. Rev. B **90**, 195105 (2014).

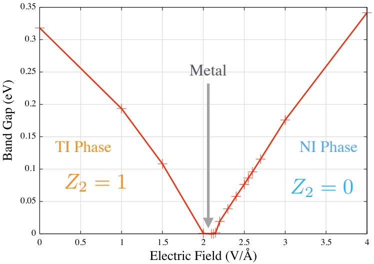
[6] R. W. Zhang et al. Sci. Reports **6**, 21351 (2016).

[7] S. Liu, Y. Kim, L. Tan, and A. Rappe, Nano. Lett. **16**, 1663 (2016).

Application(1)-Z_2 invariant-

We predict topological phase transition on Bi(111) film by electric field, topological insulator to normal insulator.



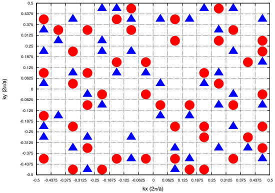


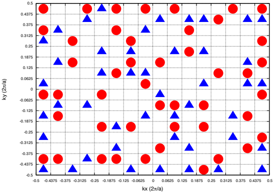
Application(2)-Z_2 invariant-

We confirmed Z_2 invariant by WFC and Fukui-Hatsugai.

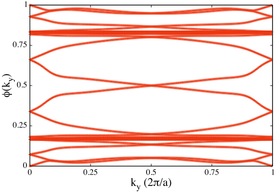
$E = 0\ \mathrm{V/Å}$ | $E = 2.5\ \mathrm{V/Å}$

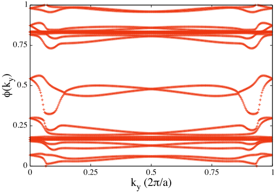
Fukui-Hatsugai





WFC





$Z_2 = 1$ | $Z_2 = 0$

Summary

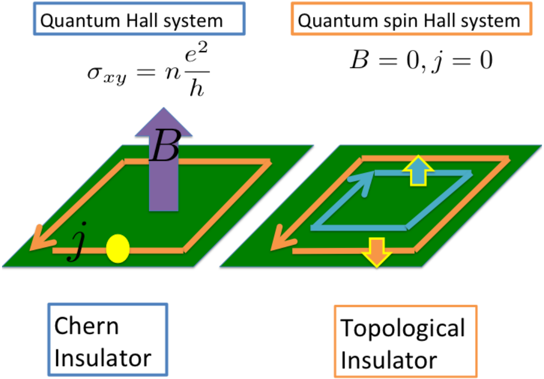
- Chern insulator or topological insulator has special edge states.
- Chern insulator is characterized "Chern number" and topological insulator is characterized "Z_2 invariant".
- These values are obtained by "Fukui-Hatsugai method"(calculation of Berry curvature F and Berry connection **A** by overlap matrix).
- This method is direct, so this is suitable for automatic searching for material, topological insulators or Chern insulators,

Appendix

Quantum Hall effect, Quantum spin Hall effect

Hall conductivity σ_{xy} described by Chern number as

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



Material	Chern insulator	Topological insulator
Symmetry	-	Time reversal symmetry
Edge state	Charge current	Spin current
Topological invariant	Chern number	Z_2 invariant

Calculate Z_2 invariant(1)-Calculate F and A-

The definition of Z_2 invariant:

$$Z_2 \quad = \frac{1}{2\pi} \sum_{n}^{\text{occ.}} \left(\oint_{\text{Half BZ}} \mathbf{A}_n \cdot d\mathbf{k} - \int_{\text{Half BZ}} F_n dk_x dk_y \right) \pmod 2$$

Computing Z_2 invariant is same as Chern number.
Calculate A and F by overlap matrix every "tile" and calculate $n(\mathbf{k})$ which is defined,

$$\begin{aligned} n(\mathbf{k}) \quad &= -\frac{1}{2\pi} [A_{k_y}(\mathbf{k} + \Delta k_x) - A_{k_y}(\mathbf{k}) \\ &-(A_{k_x}(\mathbf{k} + \Delta k_y) - A_{k_x}(\mathbf{k})) - F_{k_x k_y}(\mathbf{k})] \end{aligned}$$

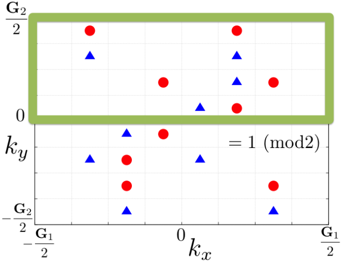
$n(\mathbf{k})$ is called "Lattice Chern number", we can obtain Z_2 invariant as,

$$Z_2 = \frac{1}{2\pi} \sum_{\mathbf{k}}^{\text{Half BZ}} n(\mathbf{k}) \pmod 2$$

Calculate Z_2 invariant(2)-Lattice Chern number-

Discretized Brillouin Zone in the direction of k_x and k_y, and calculate on every "tile",

$$U_{12} = \det \langle u_1 | u_2 \rangle$$
$$U_{23} = \det \langle u_2 | u_3 \rangle$$
$$U_{34} = \det \langle u_3 | u_4 \rangle$$
$$U_{41} = \det \langle u_4 | u_1 \rangle$$
$$F_{\mathbf{k}} = \mathrm{Im} \log U_{12} U_{23} U_{34} U_{41}$$
$$A_{ab} = \mathrm{Im} \log U_{ab}$$



Red circle is $+1$, blue triangle is -1, blank is 0

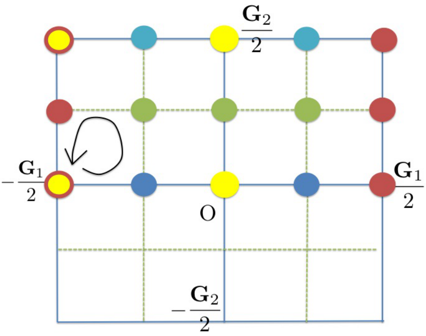
and, we can obtain Lattice Chern number as

$$n(\mathbf{k}) = \frac{1}{2\pi}[(A_{12} + A_{23} + A_{34} + A_{41}) - F_{\mathbf{k}}]$$

Calculate Z_2 invariant(3)-Gauge fix-

When we calculate Z_2 invariant, we summate only Half BZ, so summation is **gauge dependent**!! →we have to fix gauge

- Red point ⋯
  Translation symmetric points
- Blue point⋯
  Time reversal symmetric points
- Yellow point⋯
  Kramars degenerate points



I'll explain the details of fixing gauge if extra time is available