Topological properties with WannierTools

Tutorial I: Haldane model

Hands-on session

Hands-on based on WannierTools v2.5.1

Useful information about WannierTools:
Documentation: www.wanniertools.com
Forum: www.wanniertools.org
Open source: https://github.com/quanshengwu/wannier_tools

Tips: Open file.eps, file.pdf file in Linux, you can use command "evince". such as

```
$ evince file.eps
```

Open file.png file in Linux, you can use command "eog". such as

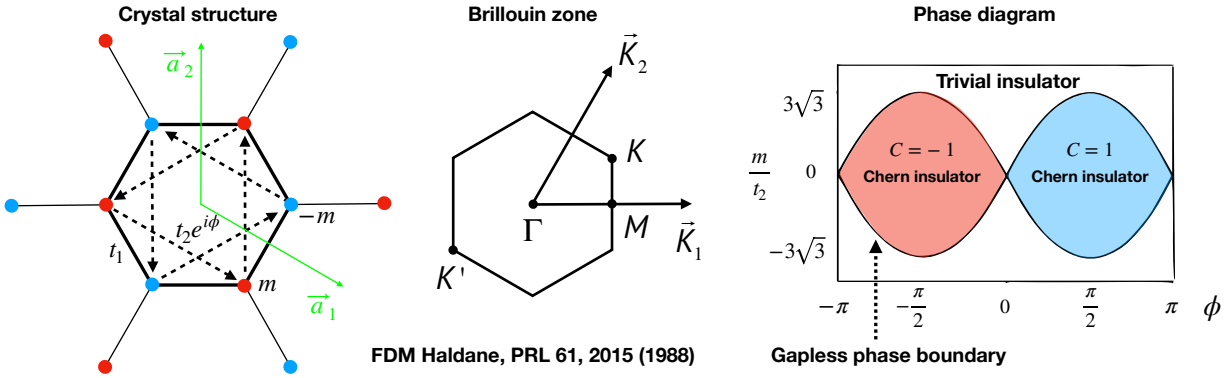
```
$ eog file.png
```

In this session we will study topological properties of a given tight binding model using WannierTools. First copy the tutorial input files of the exercise:

```
$ git clone https://github.com/wannier-developers/wannier-tutorials.git
$ cd 2020_03_Oxford/1_topological/Haldane_model/
```

Haldane model (Ref:PRL 61,2015 (1988))

In this exercise we will study three phases of the Haldane model, trivial insulator ($\phi = \pi/2,\ m = 0.2; t_1 = 1.0, m/t_2 < -3\sqrt{3}$ or $m/t_2 > 3\sqrt{3}$) , gapless semimetal ($\phi = \pi/2,\ m = 0.2; t_1 = 1.0, m/t_2 = \pm 3\sqrt{3}$) and Chern insulator ($\phi = \pi/2,\ m = 0.2; t_1 = 1.0)., -3\sqrt{3} < m/t_2 < 3\sqrt{3}$)



0.0.1 Trivial insulator

▶ **Generate tight-binding model:**
First, we need to generate the tight-binding model *Haldane_hr.dat* with script *haldane_hr_gen-trivial-insulator.py*.

```
$ python haldane_hr_gen-trivial-insulator.py
```

▶ **Generate the wt.in file:**

```
$ cp wt.in-trivial-insulator  wt.in
```

If you open and check the *wt.in* file, you will find that we are going to calculate the bulk band structure in both kpath and kplane mode, slab band structure, Wannier charge center at $k_z = 0$ plane and Berry curvature at $k_z = 0$ plane.
Necessary parameters for all calculations are

```
--                                                                                    wt.in
&TB_FILE
Hrfile = "Haldane_hr.dat"
/

&SYSTEM
SOC = 0                 ! soc
E_FERMI = 0        ! e-fermi
/

LATTICE
Angstrom
2.1377110  -1.2342080   0.0000000
0.0000000   2.4684160   0.0000000
0.0000000   0.0000000   10.000000

ATOM_POSITIONS
2                              ! number of atoms for projectors
Direct                         ! Direct or Cartisen coordinate
C 0.333333 0.666667 0.500000 C
C 0.666667 0.333333 0.500000 C

PROJECTORS
1 1          ! number of projectors
C pz
C pz
```

Band structure in kpath mode is controlled by the following parameters:

```
--                                                                                    wt.in
&CONTROL
BulkBand_calc         = T  ! calculate band structure in kpath mode
/

&PARAMETERS
Nk1 = 60            ! number k points along each kpath
/

KPATH_BULK            ! k point path in unit of reciprocal lattce vectors
3             ! number of k line only for bulk band
  M   0.50000  0.00000  0.00000   K' -.33333   -.33333  0.00000
  K'  -.33333  -.33333  0.00000   G  0.00000   0.00000  0.00000
  G   0.00000  0.00000  0.00000   K  0.33333   0.33333  0.00000
```

Band structure in k-plane mode is controlled by the following parameters:

```
--                                                                                    wt.in
&CONTROL
BulkBand_plane_calc         = T  ! calculate band structure in kpath mode
/

&SYSTEM
NumOccupied = 1  ! we will only write out two energy eigenvalue close to NumOccupied'th band
/
```

```
&PARAMETERS
Nk1 = 60            ! number k points
Nk2 = 60            ! number k points
/

KPLANE_BULK
 0.00  0.00  0.00   ! central point for 3D k slice
 1.00  0.00  0.00   ! The first vector to define 3d k space slice
 0.00  1.00  0.00   ! The second vector to define 3d k space slice
```

Berry curvature calculation of a given k-plane is controlled by the following parameters:

```
--                                                                                wt.in
&CONTROL
BerryCurvature_calc   = T
/

&SYSTEM
NumOccupied = 1    ! We assume the band below NumOccupied'th band are full occupied.
/

&PARAMETERS
Nk1 = 60            ! number k points
Nk2 = 60            ! number k points
/

KPLANE_BULK
 0.00  0.00  0.00   ! central point for 3D k slice
 1.00  0.00  0.00   ! The first vector to define 3d k space slice
 0.00  1.00  0.00   ! The second vector to define 3d k space slice
```

Wannier charge center (Wilson loop) calculation of a given k-plane is controlled by the following parameters:

```
--                                                                                wt.in
&CONTROL
Wanniercenter_calc   = T
/

&SYSTEM
NumOccupied = 1    ! We assume the band below NumOccupied'th band are full occupied.
/

&PARAMETERS
Nk1 = 60            ! number k points
Nk2 = 60            ! number k points
/

KPLANE_BULK
 0.00  0.00  0.00   ! Starting point of the k-slice
 1.00  0.00  0.00   ! The first vector is used for integration.
 0.00  1.00  0.00   ! the WCC is along this vector.
```

Note that the usage of the first vector of KPLANE_BULK card in Wanniercenter_calc= T is different from that in BerryCurvature_calc=T and BulkBand_plane_calc=T. You can read details of the usage of KPLANE_BULK card from the documentation.
Band calculation for a slab system along a given kpath is controlled by the following parameters:

```
--                                                                                wt.in
&CONTROL
SlabBand_calc   = T
```

```
/

&SYSTEM
NSLAB =60    ! We assume the band below NumOccupied'th band are full occupied.
/

&PARAMETERS
Nk1 = 60             ! number k points
/

SURFACE             ! See doc for details
 0  0  1
 1  0  0
 0  1  0

KPATH_SLAB
1         ! numker of k line for 2D case
K0 0.0 0.0      K1 0. 1.0  ! k path in unit of 2D reciprocal lattice vectors
```

▶ Run WannierTools:

```
$ mpirun -np 2 wt.x &
```

If everything works well, then you will find a "See you next time :)" message at the end of file $WT.out$ by running:

```
$ tail WT.out
```

The tail of *W*T.out should look like this

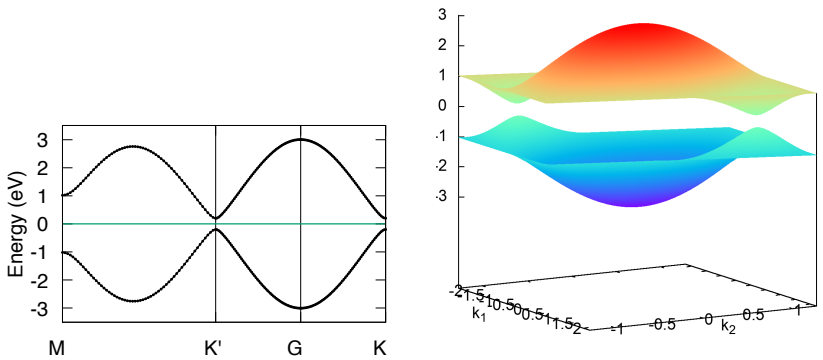
```
--                                                                                WT.out
  WannierTools : An open-source software package for novel topological materials
  QuanSheng Wu and ShengNan Zhang and Hai-Feng Song and Matthias Troyer and Alexey A. Soluyanov
  Computer Physics Communications 224, 405 (2018)
  https://doi.org/10.1016/j.cpc.2017.09.033

  For bugs, please report to wuquansheng@gmail.com
  or wanniertools@groups.google.com.
  More information could find on www.wanniertools.com
  See you next time :)
  ============================================================================
```

▶ Visualize the results using Gnuplot

1). Now we can plot the band structure with

```
$ gnuplot bulkek.gnu
$ gnuplot bulkek_plane.gnu
```

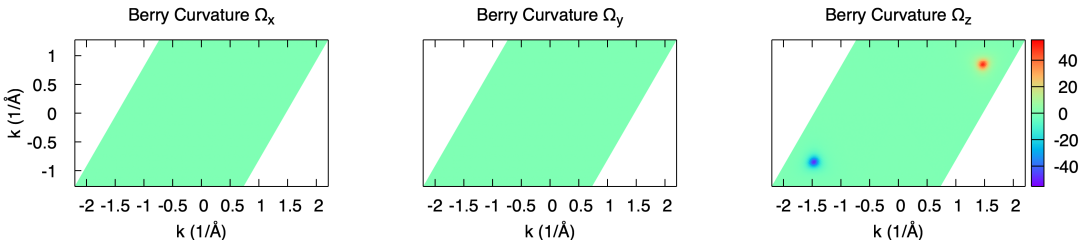
Two plots are named as bulkek.pdf and bulkek_plane.png. They should look like this:



The band structure of this phase shows that it is a insulator.
2). Then we can plot the Berry curvature with

```
$ gnuplot Berrycurvature.gnu
```

The plot are named as Berrycurvature.png. It should look like this:



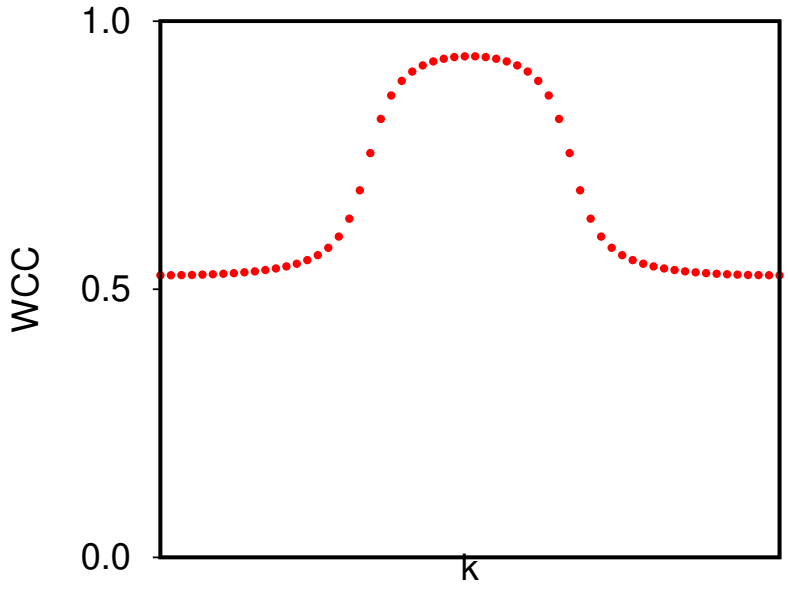
It's shown that Ω_x, Ω_y are zero since it's a two dimensional system. Ω_z has positive and negative value which cancel with each other. Eventually

$$C = \frac{1}{2\pi}\int_{BZ} d\mathbf{k}\Omega_z(\mathbf{k}) = 0 \tag{1}$$

3). We can also plot the Wannier charge center (Wilson loop) to get the Chern nubmer.

```
$ gnuplot wcc.gnu
```

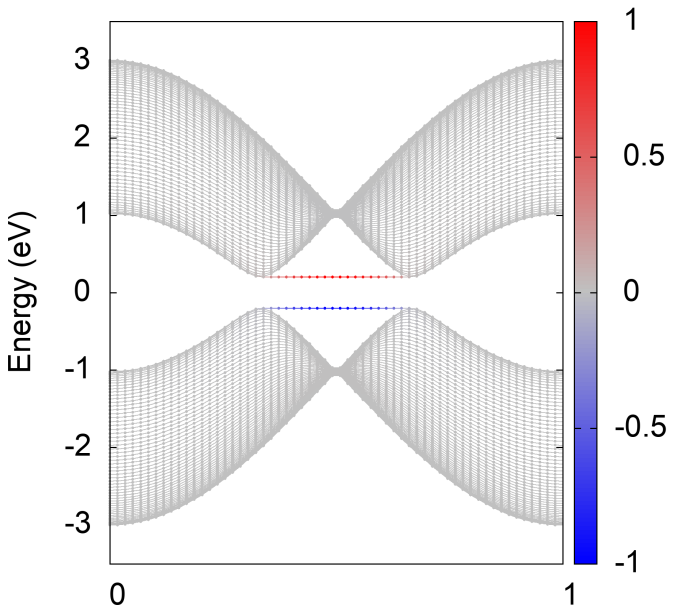
The plot are named as *w*cc.eps. It should look like this:



This WCC shows a trivial insulator $C = 0$ since there is no winding.
4). In the end, we can show the band structure of a slab system. Here, a slab means a ribbon since Haldane model is a 2D system. However, WannierTools always treat it as a 3D system by making it periodic along z direction with a thick vacuum.

```
$ gnuplot slabek.gnu
```

We will get slabek.png which looks like this:



Where the red and blue color shows the weight that projected onto top and bottom surface respectively. This shows that the edge states are trivial since they don't connect valence band and conduction band together.

0.0.2 Chern insulator

Now we are going to study the Chern insulator with parameters $\phi = \pi/2$, $m = 0.2; t_1 = 1.0, m/t_2 = 3\sqrt{3}/2$, which is in the region of $C = 1$.

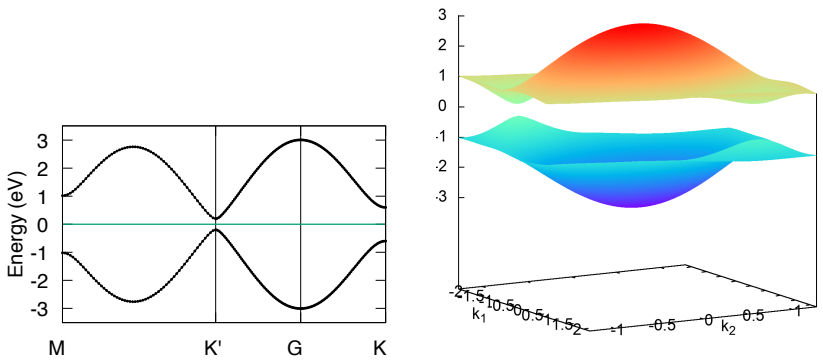
▶ **Generate a tight-binding Hamiltonian and the input file wt.in**

```
$ python haldane_hr_gen-chern-insulator.py
$ cp wt.in-chern-insulator wt.in
```

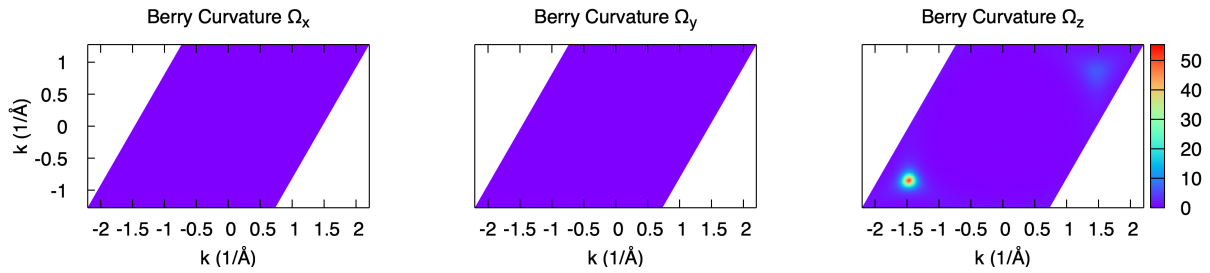
When it's done, we start to run *wt*.x

```
$ mpirun -np 2 wt.x &
```

▶ **Plot the results as the above procedure.** The bulk band structure, Berry curvature, Wannier charge center and slab band structure.



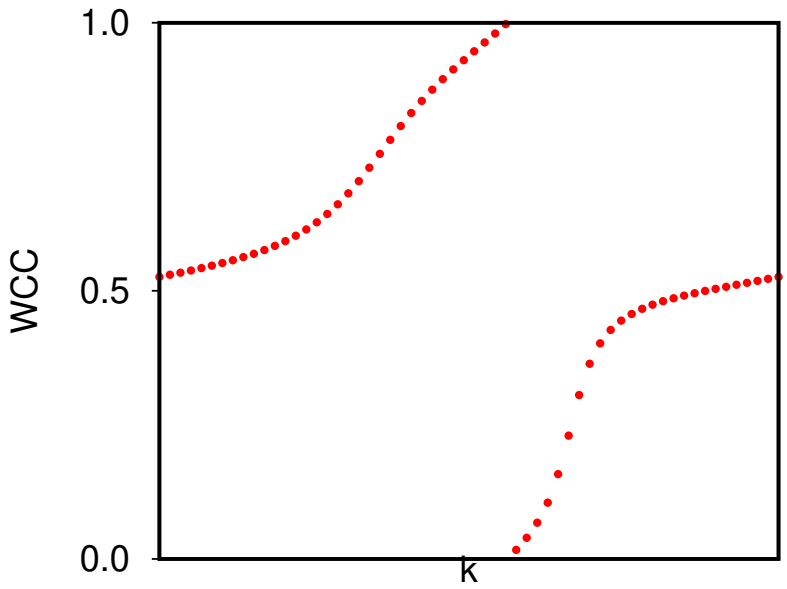
The bulk band structure looks almost exact the same as that of trivial insulator phase.



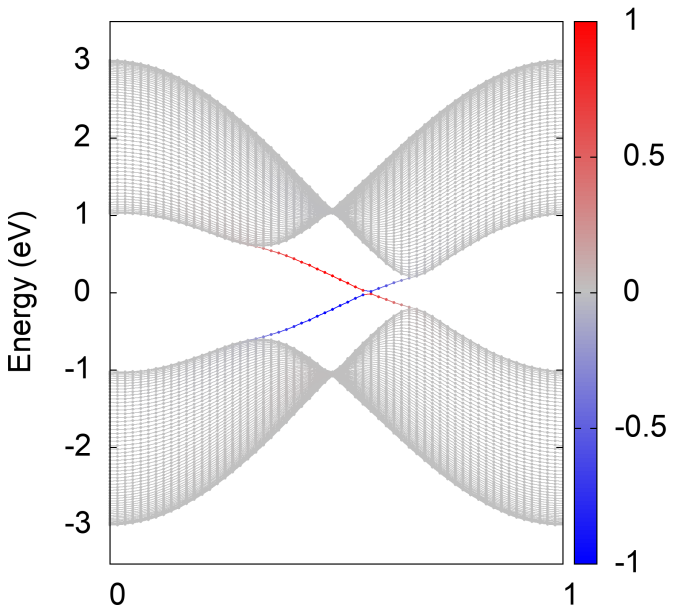
The Berry curvature is different from that of trivial phase. There is no negative value in Ω_z. The integration of $\Omega_z(\mathbf{k})$ over BZ should be 1.

$$C = \frac{1}{2\pi}\int_{BZ} d\mathbf{k}\Omega_z(\mathbf{k}) = 1 \tag{2}$$

This topological number can be validated through the Wannier charge center plot shown as:



The Chern number of this WCC plot is one according to the winding number.
Due to the equivalence between WCC and edge states, the edge states should looks the same feature.



The two edge states marked as red and blue color are located on the left and right side. On each side, the edge states in the gap are chiral states whose velocity keep the same sign.

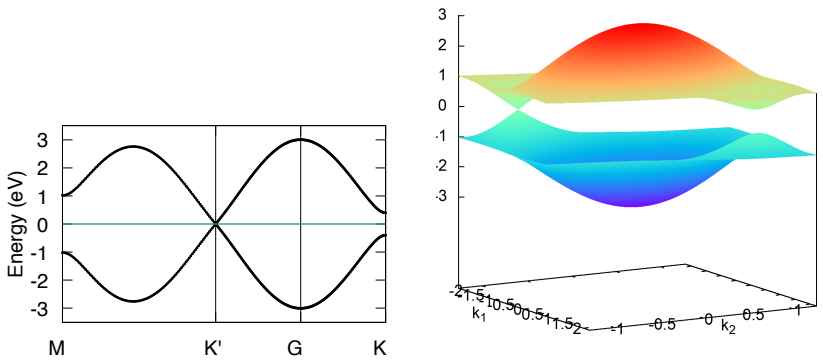
0.0.3 Gapless semimetal

Gapless semimetal is an intermediate phase linking the trivial insulator and Chern insulator phase. The parameters to generate this phase is $\phi = \pi/2$, $m = 0.2; t_1 = 1.0, m/t_2 = 3\sqrt{3}$

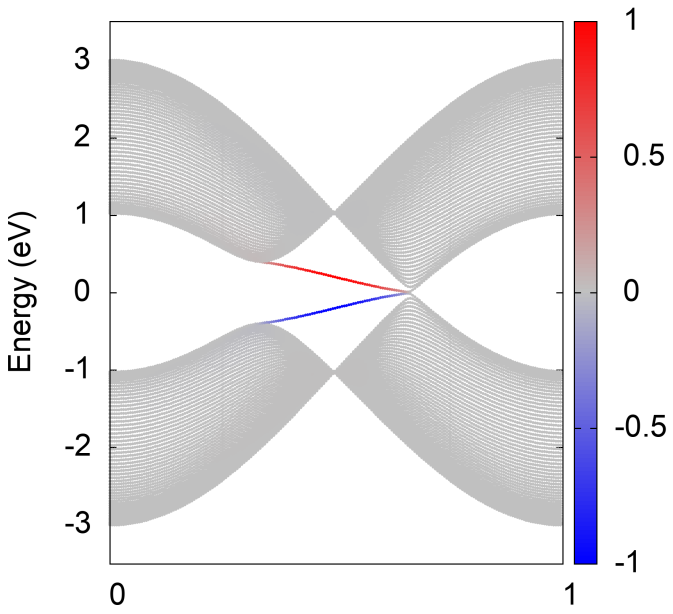
▶ **Do the same procedures to run WannierTools.**

```
$ python haldane_hr_gen-gapless.py
$ cp wt.in-gapless wt.in
$ mpirun -np 2 wt.x &
```

If you check the input file *wt.in*, you will find that we set *Wanniercenter_calc* = *F*, *BerryCurvature_calc* = *F* in order not to calculate Wannier charge center and Berry curvature. The reason is that these two quantities are not well defined if there is gapless state in the k-plane that we are interested in. The band structure of the bulk and slab system look like this:



The energy gap at K' point is closed while the energy gap at K point is still open. By comparing the Berry cuvature of the trivial insulator phase and that of Chern insulator phase, it's clear that the gap closing is the source of Berry curvature.



▶ Exercises

1. Compare the energy bands of Graphene and the gapless phase in Haldane model.

   Tips: the tight binding model of Graphene can be obtained by setting parameters $\phi = 0$, $m = 0; t_1 = 1.0, t_2 = 0$

2. Study the Berry curvatures and Wannier charge center of two phases close to the gapless phases by modifying parameter t_2 a little bit larger or smaller than $m/3/\sqrt{3}$.