User guide of Wannier_tools

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1. Installaion

(a) Check out the repository by " git clone https://github.com/quanshengwu/wannier_tools.git" or download the zip file.
(b) cd wannier_tools/soc directory, Edit Makefile, Change the blas library " libs= " to your mkl library, you can use your own blas and lapack library. Then type make. The executive binary is copied to directory wannier_tools/bin
(c) add the wannier_tools/bin path to your PATH by "export PATH=yourdirecory/wannier_tools/bin:$PATH"

2. The introduction of input file

Before execute wann_tools, you should edit the input file in the directory wannier_tools/example by your own necessary. Here we take Bi2Se3 as an example.

At present, The input file is not very flexible. It is a normal fortran free format file.

```
 1|  wannier90_hr.dat ! input file
 2|  output          ! output file's filename
 3|  T               ! BulkBand_calc
 4|  F               ! SlabBand_calc
 5|  F               ! WireBand_calc
 6|  F               ! SlabSS_calc
 7|  F               ! SlabArc_calc
 8|  F               ! SlabSpintexture_calc
 9|  F               ! wanniercenter_calc
10|  F               ! berry
```

```
  11|  40               ! Nk
  12|  100              ! omega number
  13|  -2.00 2.00       ! omegamin omegamax
  14|  0                ! E_arc
  15|  10               ! nslab
  16|  1                ! np
  17|  18               ! NumOccupied
  18|  18               ! ntotch
  19|  2                ! soc
  20|  0.001            ! eta
  21|  4.4195           ! e-fermi
  22|  0.0              ! surf_onsite
  23|  0 0 0            ! Bx By Bz
  24|  -2.069  -3.583614  0.000000     ! crystal lattice information
  25|   2.069  -3.583614  0.000000
  26|   0.000   2.389075  9.546667
  27|  5                            ! number of atoms in unit cell
  28|  Direct                       ! Direct or Cartesian coordinate
  29|   Bi 0.3990    0.3990    1.1970
  30|   Bi 0.6010    0.6010    1.8030
  31|   Se 0     0     0
  32|   Se 0.2060    0.2060    0.6180
  33|   Se 0.7940    0.7940    2.3820
  34|   3 3 3 3 3          ! number of projectors
  35|  Bi px py pz         ! projectors
  36|  Bi px py pz
  37|  Se px py pz
  38|  Se px py pz
  39|  Se px py pz
  40|       5              ! number of k line only for bulk band
  41|  G 0.00000 0.00000 0.0000 X 0.50000 0.00000 0.5000  ! k
point path
  42|  X 0.50000 0.00000 0.5000 W 0.75000 0.25000 0.5000
  43|  W 0.75000 0.25000 0.5000 L 0.50000 0.50000 0.5000
  44|  L 0.50000 0.50000 0.5000 G 0.00000 0.00000 0.0000
  45|  G 0.00000 0.00000 0.0000 K 0.75000 0.37500 0.3750
  46|  1 0 0    ! Umatrix for new lattice 001
```

```
  47|  0 1 0
  48|  0 0 1
  49|  2        ! numker of k line for 2D case
  50| X 0.5 0.0 G 0.0 0.0  ! k path for 2D case
  51| G 0.0 0.0 Y 0.5 0.0
  52| 0.0 0.0 0.0 0.5  ! define 2d k space plane for arc plots
  53| 0.0 0.0 0.5 0.5
  54| 0.0 0.0 0.0  0.5  0.0 0.0  ! define 3d k space plane for gap
plots
  55| 0.0 0.0 0.0  0.0  0.5 0.0
```

line 1 : wannier90_hr.dat ! input file
The file name of wannier90_hr.dat, which is generate from wannier90 package (http://www.wannier.org).
Currently, we support two formats, one is from wannier90. One is from Openmx, which rewrite
wannier90_hr.dat.

line 2 : output ! output file

Filename for some outputs. You can check this file for running status.

From line 3-10 : give some control parameters for this program. The value should be F or T relate t
False and True respectively.

Flag option	Function	Output	Test
BulkBand_calc	Band structure for bulk	bulkek.dat, bulkek.gnu	yes
SlabBand_calc	Band structure for slab system	slabek.dat,slabek.gnu	yes
	Band structure for	ribbonek.dat,ribbonek.g	

WireBand_calc	ribbon system	nu	yes
SlabSS_calc	Surface spectrum A(k,E) along a k line and energy interval	dos.dat_l, dos.dat_r surfdos_l.gnu,surfdos_r.gnu	yes
SlabArc_calc	Surface spectrum A(k1,k2,E0) for a fixed energy E0	arc.dat_l, arc.dat_r arc_l.gnu,arc_r.gnu	yes
SlabSpintexture_calc	calculate spin texture for slab system	spindos.dat	No
wanniercenter_calc	calculate wannier centers for slabs	wanniercenterky0.dat	No
berry_calc	calculate berry phase along one k line		No

For Bulkband calculation, you should specify number of k lines and the special klines in line
41-45 (these line number is relatively). The output for this subroutine are bulkek.dat and bulkek.gnu. You
can run "gnuplot bulkek.gnu", or "xmgrace bulkek.dat" to get bandstucture plot.

For Slab band calculation, you only need to change Nk in line 11 to get more points for k line.
The output for this subroutine are slabek.dat and slabek.gnu. You can run "gnuplot slabek.gnu", or "xmgrace
slabek.dat" to get bandstucture plot. If you use gnuplot, you should check the png files.

The procedure for ribbon band calculation is similar to slab band

calculation. the data is different by the
names.

For surface state calculation, the output files are dos.dat_l, dos.dat_r, surfdos_l.gnu, surfdos_r.gnu. dos.dat_l and dos.dat_r are the spectrum weight for each k point and each energy,
related to the top and bottom surface state respectively.
You can run "gnuplot surfdos_l.gnu" to get surfdos_l.png.

For Fermi arc calculation, basically, the principle for this calculation is similar to surface state
calculation. The difference is to get spectrum A(k, ω) for a fixed energy ω but (kx, ky) in
2D in this calculation, while get get spectrum A(k, ω) for some special k lines and an energy
interval for the surface state calculation.

SlabSpintexture_calc and wanniercenter_calc are not tested yet.

line 11 : 40 ! Nk
Number of k points for any necessary subroutines, like bulk, slab, ribbon band structure calculation

line 12 : 500 ! omega number

Number of energies when calculate surface state, this value determines
the resolution of the surface state pictures. If it's large, the calculation will be slow linearly scaling.
You can set it to be 200 at first, if the resolution of the picture is not enough, then increase it.

line 13 : -2.00 2.00 ! omegamin omegamax

Energy interval for surface state calculation.

line 14 : 0 ! E_arc

Energy at which the fermi arc is calculated.

line 15 : 10 ! nslab

Number of slabs for slab band. If you calculate the band structure for nanoribbon, it represent the thickness of one direction. The thickness for the other direction is Np.
see Np.

line 16 : 1 ! Np

Number of principle layers for calculating surface state and fermi arc. If your wannier function is not
enough localized. For instance, there are big hoppings beyond the home unit cell. Then we should set
this value to 2 or 3 or 4. In principle, you should check the convergency of the surface state by increasing
this value. The computation will be cubically grows as a functional of Np. at the beginning, you can set
Np=1.

If you calculate band structure for nanoribbon, then this value is the thickness of another direction of nanoribbon. See slab.

line 17 : 18 ! NumOccupied

This value is not valid at present, leave it alone. However, don't delete this line.

line 18 : 18 ! Ntotch
number of electrons, if you want to determine the fermi level, this value will work.

line 19 : 1 ! soc

The flag for soc, if there is no spin-orbital included in your

wannier90_hr.dat, then set it to be zero. else, set it to be 1.

line 20 : 0.001 ! eta

Broadening of green's function when calculate the surface states. If you don't know what it is, leave it unchanged.

line 21 : 4.4195 ! e-fermi in eV

Fermi level of your wannier90_hr.dat.

line 22-24 :

```
-2.069  -3.583614  0.000000     ! crystal lattice information
 2.069  -3.583614  0.000000
 0.000   2.389075  9.546667
```

Three lattice vectors coordinates.

line 25- 33 :

```
5                          ! number of atoms for projectors
Direct                       ! Direct or Cartesian coordinate
Bi 0.3990    0.3990    0.1970
Bi 0.6010    0.6010    0.8030
Se 0     0     0
Se 0.2060    0.2060    0.6180
Se 0.7940    0.7940    2.3820
```

Set the number of atoms in your wannier90_hr.dat when you constructed it. Notice, this is the atoms that has projectors contribution to Wannier functions, not the whole atoms in the unit cell.
Set the coordinate system type, Direct or Cartesian. Direct means the coordinates based on primitive unit cell.
Set the name and coordinate of each atoms. this coordinate is based on the three lattice vectors. It's easy to find it for through the wannier90.win.

line 34- 39 :

```
 3 3 3 3 3          ! number of projectors
Bi px py pz
Bi px py pz
Se px py pz
Se px py pz
Se px py pz
```

Number of projectors for each atom when you construct your wannier functions. And the name of projectors.

line 40- 45 :

```
     5        ! number of k line\\
G 0.00000 0.00000 0.0000 X 0.50000 0.00000 0.5000  ! k point path\\
X 0.50000 0.00000 0.5000 W 0.75000 0.25000 0.5000\\
W 0.75000 0.25000 0.5000 L 0.50000 0.50000 0.5000\\
L 0.50000 0.50000 0.5000 G 0.00000 0.00000 0.0000\\
G 0.00000 0.00000 0.0000 K 0.75000 0.37500 0.3750
```

Number of high-symmetric k point lines. Look the format carefully. This k lines are in unit of the reciprocal lattice built by the lattice vector given in line 24-26

line 46-48 :

```
1 0 0   ! Umatrix for new lattice   a11, a12, a13\\
0 1 0   ! a21 a22 a23\\
0 0 1   ! a31 a32 a33
```

These three lines are very important for slabs and ribbon calculation. It defines the surface we needed. Basically, you should know of which surface you want to get the surface, and of which direction you want to simulate the ribbon. So we need to define the new lattice vector system like this, choose two vectors on the surface we want to study, and choose another vector which is not in this plane. The volume of the cell constructed by these three vectors should be the same of the previous one. And the orientation should

be the same by checking $R_1'\cdot(R_2'\times R_3')= R_1\cdot(R_2\times R_3)$. The relations between old and new basis are

\begin{eqnarray}
R_1'= a_{11} R_1 + a_{12} R_2 + a_{13} R_3 \\
R_2'= a_{21} R_1 + a_{22} R_2 + a_{23} R_3 \\
R_3'= a_{31} R_1 + a_{32} R_2 + a_{33} R_3
\end{eqnarray}

The slab calculations are base on the surface constructed by vector R_1', R_2'. The ribbon is along R_3' direction, two surfaces are constructed by vector R_1', R_3' and R_2', R_3' respectively.

\end{enumerate}

line 49-51 :

```
2       ! numker of k line for 2D case
X 0.5 0.0 G 0.0 0.0  ! k path for 2D case
G 0.0 0.0 Y 0.5 0.0
```

Number of high-symmetric k point lines for 2D system, such as the surface state spectrum or the band structure for slab system . Look the format carefully. This k lines are in unit of the reciprocal lattice built by the lattice vector for 2D system given in line 46-48. Number of k points along each line is Nk, which is set in line 11.

line 52-53 :

```
0.0 0.0 0.0 0.5  ! define 2d k space plane for arc plots
0.0 0.0 0.5 0.5
```

Define a 2D k space plane for arc plots. The first two numbers in line 52 is the start point of the first arrow, the second two numbers in line 52 is the end points of the first arrow. The same means for line 53.

line 54-55 :

```
0.0 0.0 0.0  0.5  0.0 0.0  ! define 3d k space plane for gap plots
0.0 0.0 0.0  0.0  0.5 0.0
```

The same set as line 52-53, but for 3D case. We can use these two vectors to calculate the band gap of a plane in 3D BZ, then we can check whether there are Weyl points in that plane. Notice that these

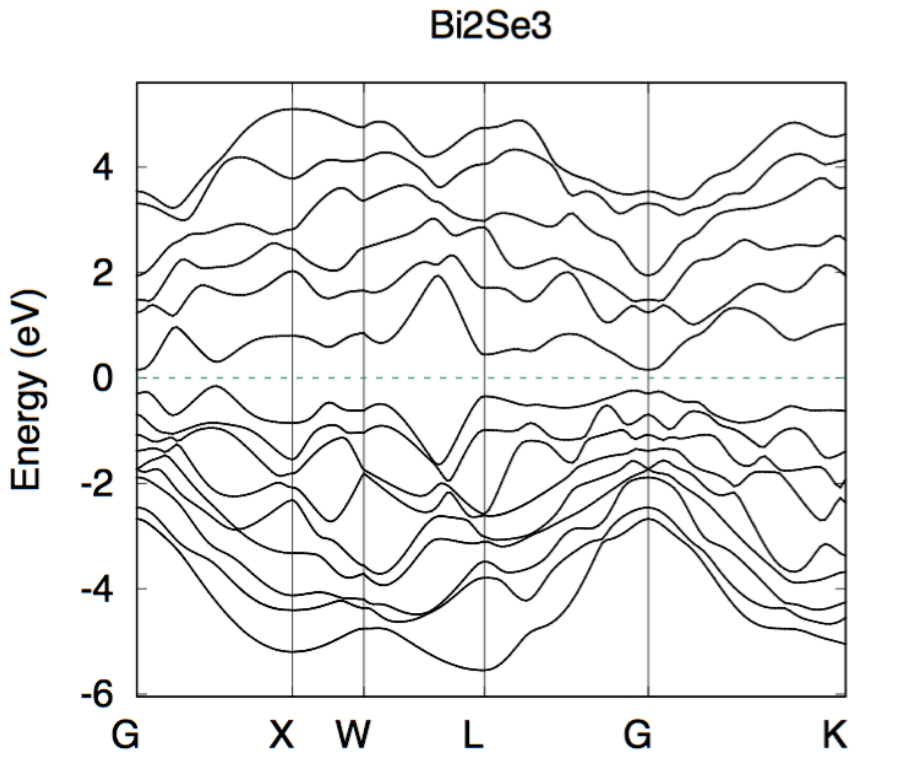
vectors is in unit of reciprocal vectors.

If you want to calculate Wannier charge center, which is sometimes called Wilson loop, you should notice that the first vector is the integration direction, the difference between two vectors should be in one primitive reciprocal lattice vector. Such as 0.0 0.0 0.0 1.0 0.0 0.0. After the calculation, you can get the Wannier charge center along the second k line.

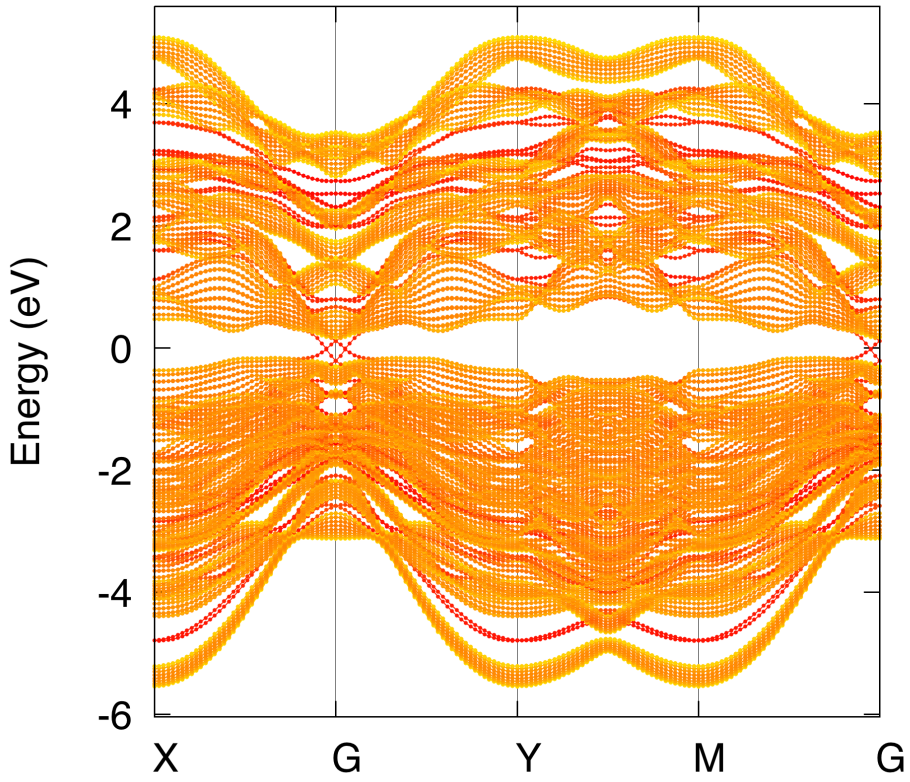
Examples (Bi2Se3)

The wannier90_hr.dat is compressed as Bi2Se3_hr.tar.gz in examples/ folder. You can decompressed by a command “tar xzvf Bi2Se3_hr.tar.gz”. The input.dat file can also be found in that folder.

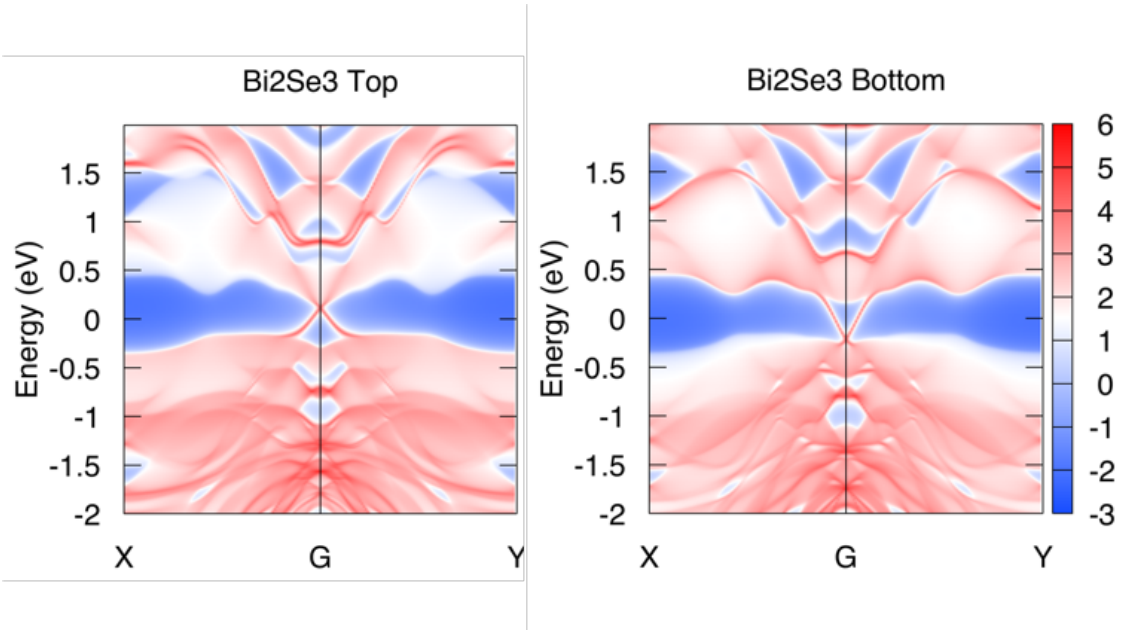
(1). Bulk band structure



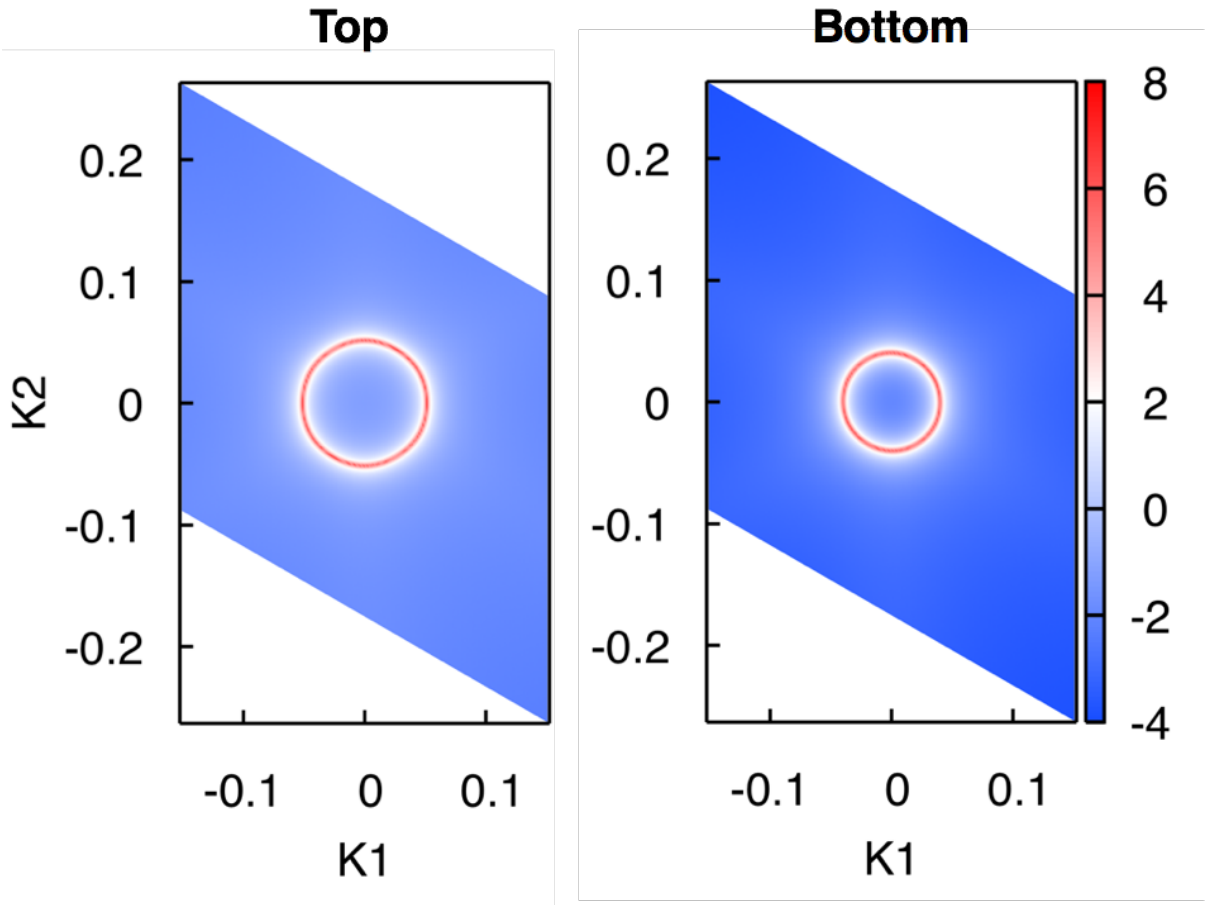
(2). (001) oriented slabs.



(3). (001) surface state



(4). (001) surface spectrum for a fixed energy E=0eV



Comment: The Wannier TB constructed here has not perfect symmetry, which will cause different chemical potential on both surfaces. So The top and bottom surface states are not exactly the same. However the topological properties will not be changed by change the surface chemical potential.

4. License and agreement.

If you use our code, please cite this website "Q.S.Wu, https://github.com/quanshengwu/wannier_tools" . If you have good ideas to improve this code, do not hesitate to contact me. Your contribution will be recorded.

5. Enjoy and good luck.