1.21.8 wannier_tools introduction

1. Installaion

check out the repository by " git clone https://github.com/quanshengwu/wannier_tools.git" or download the zip file.

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

2. add the wannier_tools/bin path to your PATH by

export PATH=yourdirecory/wannier_tools/bin:$PATH

3. Edit the input file in the directory wannier_tools/example by your own necessary. Then execute wann_tools.

```
wusocBi2Se3.HWR ! input file
output        ! output file
F             ! BulkBand_calc
T             ! SlabBand_calc
F             ! WireBand_calc
F             ! SlabSS_calc
F             ! SlabArc_calc
F             ! SlabSpintexture_calc
F             ! wanniercenter_calc
40            ! Nk
500           ! omega number
-2.00 2.00    ! omegamin omegamax
0             ! E_arc
20            ! nslab
2             ! np
18            ! NumOccupied
1             ! soc
0.05          ! eta
-0.183283       ! e-fermi
  -3.90984   -2.25735   18.04058  ! lattice vector
   3.90984   -2.25735   18.04058
   0.00000    4.51470   18.04058
   5
Se -0.794  0.206  0.206      ! atom position
Bi -0.601  0.399  0.399
Se  0.0    0.0    0.0
Bi  0.601 -0.399 -0.399
Se  0.794 -0.206 -0.206
 3 3 3 3 3          ! number of projectors
Se px py pz
Bi px py pz
Se px py pz
Bi px py pz
Se px py pz
     5         ! number of k line
```

```
36 G 0.00000 0.00000 0.0000 X 0.50000 0.00000 0.5000  ! k point path
37 X 0.50000 0.00000 0.5000 W 0.75000 0.25000 0.5000
38 W 0.75000 0.25000 0.5000 L 0.50000 0.50000 0.5000
39 L 0.50000 0.50000 0.5000 G 0.00000 0.00000 0.0000
40 G 0.00000 0.00000 0.0000 K 0.75000 0.37500 0.3750
41 1 0 0   ! Umatrix for new lattice
42 0 1 0
43 0 0 1
```

1. the first line : wusocBi2Se3.HWR ! 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.

2. the second line : output ! output file

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

3. From line 3-9, give some control parameters for this program. The value should be F or T relate to False and True respectively.

表 1.2: Control parameters

BulkBand_calc	Band structure for bulk	supported
SlabBand_calc	Band structure for slab system	supported
WireBand_calc	Band structure for ribbon system	supported
SlabSS_calc	Surface state	supported
SlabArc_calc	Calculate Fermi-Arc for slabs.	supported
SlabSpintexture_calc	calculate spin texture for slabs	Not supported yet
wanniercenter_calc	calculate wannier centers for slabs	Not supported yet

For Bulkband calculation, you should specify number of k lines and the special klines in line 35-40 (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 should only change Nk in line 10 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 supported yet.

4. line 10 : 40 ! Nk

   Number of k points for any necessary subroutines.

5. line 11 : 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.

6. line 12 : -2.00 2.00 ! omegamin omegamax

   Energy interval for surface state calculation.

7. line 13 : 0 ! E_arc

   Energy at which the fermi arc is calculated.

8. line 14 : 20 ! nslab

   Number of slabs for slab band and surface state calculation. 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.

9. line 15 : 2 ! 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.

10. line 16 : 18 ! NumOccupied

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

11. line 17 : 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.

12. line 18 : 0.05 ! eta

    Broadening of green´s function when calculate the surface states. If you don´t know what it is, leave it unchanged.

13. line 19 : -0.183283 ! e-fermi in eV

    Fermi level of you wannier90_hr.dat.

14. line 20-21
    -3.90984 -2.25735 18.04058 ! lattice vector
    3.90984 -2.25735 18.04058
    0.00000 4.51470 18.04058

    Three lattice vector coordinates.

15. line 22- 27 :
    5

Se -0.794 0.206 0.206 ! atom position

Bi -0.601 0.399 0.399

Se 0.0 0.0 0.0

Bi 0.601 -0.399 -0.399

Se 0.794 -0.206 -0.206

Set the number of atoms in your wannier90_hr.dat when you constructed it. 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.

16. line 28- 34

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

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

17. line 35- 40

    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.

18. line 41-43

    1 0 0 ! Umatrix for new lattice a11, a12, a13

    0 1 0 ! a21 a22 a23

    0 0 1 ! a31 a32 a33

    This 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

$$R'_1 = a_{11}R_1 + a_{12}R_2 + a_{13}R_3 \tag{1.94}$$

$$R'_2 = a_{21}R_1 + a_{22}R_2 + a_{23}R_3 \tag{1.95}$$

$$R'_3 = a_{31}R_1 + a_{32}R_2 + a_{33}R_3 \tag{1.96}$$

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.

3. Enjoy and good luck.