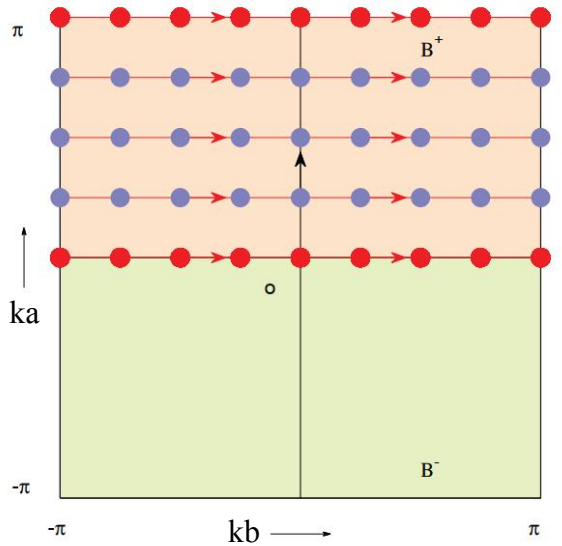
Use VASP2mat (vmat=14) to do Wilson loop calculations

Wilson loop calculation
For Bi2Se3, considering spin-orbit coupling(SOC),
in the kc=0 plane, loop along kb direction to get Wannier charge center (WCC),
WCC evolves along the ka direction.

1）make self-consistent calculation
Use INCAR :
ISTART = 0
ICHARG = 2
LWAVE= .TRUE.
LCHARG=.TRUE.
LSORBIT =.TRUE.
MAGMOM = 15*0.0

Use POSCAR:
Bi2 Se3
1.0
4.045513 0.000000 -0.869980
1.929214 3.555884 -0.869980
0.000000 0.000000 9.841060
Bi Se
2 3
Cartesian
2.383916 1.418798 1.244445
3.590811 2.137087 6.856656
0.000000 0.000000 0.000000
1.230794 0.732512 5.723343
4.743933 2.823372 2.377757

2）make non-self-consistent calculation to get WAVECAR
for a series of k points along kb direction.
Use INCAR :
ISTART = 1
ICHARG = 11
LWAVE= .TRUE.
LSORBIT =.TRUE.
MAGMOM = 15*0.0



3) Run vasp2mat to get WCC
Use INCAR :
ISTART = 1
LSORBIT =.TRUE.
MAGMOM = 15*0.0

Use INCAR.mat :
&vmat_para
print_only_diagnal = .true.
vmat = 14
vmat_name = 'Berry_K'
bstart=11, bend=28 #band range
/

use the following script for steps 2 and 3

loop_run.sh

```
#!/bin/bash
for((i=0;i<=11;i+=1))
do
kl=$(printf "%.10f" $(echo "scale=10;(0.0+0.5*1/11*$i)/1"|bc))

j=`echo 11*0+$i|bc -l`

if [ ! -d "k$j" ]; then
echo k$j
cp -r loop_seed k$j
cd  k$j

cat > KPOINTS << eof
k-points along high symmetry lines
56
Line-mode
rec
 $kl  0.0  0.0
 $kl  1.0  0.0
eof

qsub ../loop_vasp.pbs >jobid
cd ../
fi
done
```

mkdir loop_seed
prepare CHGCAR, WAVECAR form scf—calculation and etc.

- CHGCAR
- INCAR
- INCAR.mat
- POSCAR
- POTCAR
- WAVECAR

loop_vasp.pbs :
$mpirun —machinefile $PBS_NODEFILE —np $ncpu $vasp >> out
/home/soft/vasp2mat >>log

Run:
bash loop_run.sh

Run:
python split_n_1D.py

output

MAT_Berry_K.m

```
%                                vmat
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%     k      =   0.00000000   0.00000000   0.00000000   in b_i
%     B1     =   0.82187814  -0.44590285   0.00000000   in bohr^-1
%     B2     =   0.00000000   0.93504701   0.00000000   in bohr^-1
%     B3     =   0.07265656   0.04324185   0.33786185   in bohr^-1
% Number of k-points along the wilson loop:        56
% On bands :    11    12    13    14    15    16    17    18
% On bands :    19    20    21    22    23    24    25    26
% On bands :    27    28
% Berry's phase in 2pi
   Berry_K( 1:   18, 1:2)=[
       11    (  -0.50000  +0.87475i)
       12    (  +0.50000  +0.87475i)
       13    (  -0.28043  +0.96755i)
       14    (  -0.28043  +0.96755i)
       15    (  +0.28043  +0.96755i)
       16    (  +0.28043  +0.96755i)
       17    (  +0.20329  +0.90890i)
       18    (  +0.20329  +0.90890i)
       19    (  -0.20329  +0.90890i)
       20    (  -0.20329  +0.90890i)
       21    (  +0.08383  +0.93568i)
       22    (  +0.08383  +0.93568i)
       23    (  -0.08383  +0.93568i)
       24    (  -0.08383  +0.93568i)
       25    (  -0.00000  +0.93157i)
       26    (  -0.00000  +0.93157i)
       27    (  +0.00000  +0.97251i)
       28    (  +0.00000  +0.97251i)
];
% trace = (    +0.00000    +0.00000i)
```

—WCCs for 11—28 bands