ecalj tutorial

Here are minimum GetStated to obtain QSGW band plot.

Qiita Japanese

Qiita English

Overview of QSGW calculation

- LDA calculations are performed with the program `lmf`. The initial setting file is `ctrl.foobar` (`foobar` is user-defined). Before running `lmf`, it is necessary to run `lmfa`, which is a spherically symmetric atom calculation to determine the initial conditions for the electron density (a calculation that finishes instantaneously).
- A file `sigm.foobar` is the key for QSGW calculations. The file `sigm.foobar` contains $V_{\rm xc}^{\rm QSGW}-V_{\rm xc}^{\rm LDA}$. By adding this potential term to the usual LDA calculation performed by `lmf`, we can perform QSGW calculations.
- Thus the problem is how to generate $V_{\rm xc}^{\rm QSGW}({\bf r},{\bf r}')$. This is calculated from the self-energy $\Sigma({\bf r},{\bf r}',\omega)$, which is calculated in the GW approximation. Roughly speaking, we obtain $V_{\rm xc}^{\rm QSGW}({\bf r},{\bf r}')$ with fixing the omega-dependence in $\Sigma({\bf r},{\bf r}',\omega)$.
- Therefore, the calculation of $V_{\rm xc}^{\rm QSGW}$ is the major part of the QSGW cycle , and is calculated in a double-structure loop. That is, there is an inner loop of `lmf`, and an outer loop to calculates $V_{\rm xc}^{\rm QSGW}$ using the eigenfunctions given by `lmf`. This outer loop can be executed with a python script called gwsc (which runs fortran programs). The computational time for QSGW is much longer than that of LDA calculation. As a guideline, it takes about 10 hours for 20 atoms (depending on the number of electrons).
- GPU can accelerate it, https://arxiv.org/abs/2506.03477. Thus we can handle large systems.
- Since automation is being promoted, there is almost no need to tweak parameters that are difficult to understand (if something strange, let me know). I think it is probably the GW kinds of computation codes which is the easiest to use. See band database in QSGW at https://github.com/tkotani/DOSnpSupplement/blob/main/bandpng.md (this is supplement of https://arxiv.org/abs/2507.19189)

PROF

Minimum flowchart to perform QSGW in ecalj.

1. Get ctrls from POSCAR

ctrls.foobar is the structure file in ecalj.
We obtain ctrls from POSCAR by a converter.

We already have POSCAR in ecalj/ecalj_auto/INPUT/testSGA/POSCARALL as

```
cd ecalj
mkdir TEST
cd TEST
mkdir test1
mkdir test2
cat ecalj_auto/INPUT/testSGA/joblist.bk
cp ../ecalj_auto/INPUT/testSGA/POSCARALL/POSCAR.mp-2534 test1
cp ../ecalj_auto/INPUT/testSGA/POSCARALL/POSCAR.mp-8062 test2
```

Then we convert POSCAR by vasp2ctrl. If you have cif, you need to convert the cif to POSCAR at firlst.

```
vasp2ctrl POSCAR.mp-2534
mv ctrls.POSCAR.mp-2534.vasp2ctrl ctrls.POSCAR.mp-2534
cat ctrls.mp-2534
```

ctrls.mp-2534 contains crystal structure equivalent to POSCAR:

```
cat ctrls.mp-2534
STRUC
     ALAT=1.8897268777743552
     PLAT=       3.52125300000       0.00000000000       2.03299700000
                 1.17375100000       3.31986900000       2.03299700000
                 0.00000000000       0.00000000000       4.06599300000
  NBAS=2
SITE
     ATOM=Ga POS=     0.00000000000       0.00000000000
0.00000000000
     ATOM=As POS=     1.17375100000       0.82996725000
2.03299675000
```

PROF

- MEMO:
  - ctrl2vasp ctrl.mp-2534 can convert back to VASP file. Check this by VESTA. We can use viewvesta (convert and invoke VESTA).
  - many unused files are generated (forget them).

2. Get ctrl from ctrls

ctrl is a basis input file for ecalj. We generate template of ctrl by ctrlgenM1.py.
Minimum explanations are embedded in the generated ctrl file.
Number of k points (nk1 nk2 nk3), APW cutoff (pwemax), nspin, so(spin orbit switch) are only what we need to tweak usually.

When we run lmf, we can add command line option such as -vnspin=2. Then const foobar=1 defined in the ctrl file is overridden (referred with {foobar}). save.* file show which -vfoobar you used.

It is possible to enforce symmetry, antiferro symmetry.

We only need ctrl file in the following calculations (while some tmp* kinds of files are generated).

```
ctrlgenM1.py mp-2534
cp ctrlgenM1.ctrl.mp-2534 ctrl.mp-2534
```

- importand settings in ctrl
  - nk1,nk2,nk3
  - xcfun
  - ssig
  - pwemax
  - gmax
  - so
  - socaxis

Here is a list of ctrl file.

3. LDA計算

Run lmfa at first. It is for spherical atomic electron density. It ends instantaneously.
If you run `lmfa foobar|grep conf`, we can see electronic configulation. No side effects if you repeat lmfa.

```
lmfa ctrl.mp-2534
```

gives spherical atom calculation for initialization. No side effects to repeat.

> lmfa ctrl.mp-2534 |grep conf
> show atomic configuration (not necessary).

PROF

Files:

> save.* : computational history. DFT total energy is shown at each iteration (See lmf next).
> atmpnu* : ratial derivative file. Used at lmf
> atm.* : atom potential Used at lmf (only init)
> ves* : obsolate
> log* : just for debug log

Main part calculation:

```
mpirun -np 8 lmf mp-2534 |tee llmf
```

- mp-2534 gives 5.75 \AA for GaAs, while the experimental value is 5.65\AA

- llmf contains iteration log. band eigenvalue, and so on. Check band gap.
- rst.mp-2534 is generated. Self-consistent charge included.
- You can change lattice constant as ALAT=1.8897268777743552*5.65/5.75 in ctrl file. simple math can be possible in ctrl
- Note: ctrlp is intermediate file generated by python from ctrl. Fortran calls a python code internally.
- check save.mp-2534. Show history of lmfa and lmf. one line per iteration. Show your console options. c,x,i,h
  LDA energy shown two values need to be the same (but slight difference).
  Repeat lmf stops with two iteration.

- SiteInfo.lmchk : Site infor
- PlatQlat.chk : Lattice info
- estaticpot.dat : electrostatic potential of smooth part.

4. job_pdos,job_tdos, job_fermisurface,job_band

For band plot, we use job_band. Before this, we need to generate symmetry lines writtenin syml.foobar。This can be generated by getsyml foobar.

```
getsyml mp-2534
```

This generates syml.mp-2534.
BZ.html contains BZ and symmetry lines.
For bandplot,

```
job_band mp-2534 -np 8 [options]
```

At the end of job_band, you can add options for lmf as -vso=1 -vnspin=2.
(these are for SOC as perturbation)
We use gnuplot for band plot bandplot.isp1.glt.

In the similar manner, we can run job_pdos, job_tdos, job_fermisurface.

5. QSGW calcualtion

We need one additional input file GWinput, whose template can be ganerated by mkGWinput→GWinput as

```
mkGWinput ctrl.mp-2534
```

The edit GWimput.tmp to GWinput.
n1n2n3 should be something smaller thatn nk1 nk2 nk3 in ctrl file.

If 6x6x6 for Si, it is reasobale. Except k points, not need to modify so much
(ask us).

QSGW計算の流れ

We can run QSGW calculation with gwsc. For semiconductors, several iterations are fine.QPU file contains diagonal components of GW calculations.
Note that our Mixed Produce basis is a key technology for the GW calculation.

```
gwsc -np NP [--phispinsym] [--gpu] [--mp] nloop extension
```

(--phispinsym is for magnetic materials to keep the same basis for up and down)

Then console outputs of gwsc is somthing like

```
### START gwsc: ITERADD= 1, MPI size=  4, 4 TARGET= si
===== Ititial band structure ======
---> No sigm. LDA caculation for eigenfunctions
0:00:00.226245   mpirun -np 1 /home/takao/ecalj/SRC/TestInstall/bin/lmfa
si     >llmfa
0:00:00.807062   mpirun -np 4 /home/takao/ecalj/SRC/TestInstall/bin/lmf
si     >llmf_lda
===== QSGW iteration start iter 1 ===
0:00:03.071054   mpirun -np 1 /home/takao/ecalj/SRC/TestInstall/bin/lmf
si     --jobgw=0 >llmfgw00
0:00:03.904403   mpirun -np 1
/home/takao/ecalj/SRC/TestInstall/bin/qg4gw    --job=1 > lqg4gw
0:00:04.431022   mpirun -np 4 /home/takao/ecalj/SRC/TestInstall/bin/lmf
si     --jobgw=1 >llmfgw01
0:00:05.918216   mpirun -np 1
/home/takao/ecalj/SRC/TestInstall/bin/heftet --job=1    > leftet
0:00:06.444439   mpirun -np 1
/home/takao/ecalj/SRC/TestInstall/bin/hbasfp0 --job=3    >lbasC
0:00:07.064558   mpirun -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hvccfp0 --job=3    > lvccC
0:00:07.812283   mpirun -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hsfp0_sc --job=3    >lsxC
0:00:08.545956   mpirun -np 1
/home/takao/ecalj/SRC/TestInstall/bin/hbasfp0 --job=0    > lbas
0:00:09.156775   mpirun -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hvccfp0 --job=0    > lvcc
0:00:09.884064   mpirun -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hsfp0_sc --job=1    >lsx
0:00:10.644292   mpirun -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hrcxq   > lrcxq
0:00:11.482931   mpirun -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hsfp0_sc --job=2    > lsc
0:00:12.460776   mpirun -np 1
/home/takao/ecalj/SRC/TestInstall/bin/hqpe_sc    > lqpe
```

```
0:00:13.019735   mpirun -np 4 /home/takao/ecalj/SRC/TestInstall/bin/lmf
si     >llmf
===== QSGW iteration end   iter 1 ===
OK! ==== All calclation finished for  gwsc ====
 Comparison OK! max(abs(QPU-QPU))= 0.005000000000002558  <etol= 0.011
for QPU
 Comparison OK!  MaxDiff= 0.00019999999999997797 < tol= 0.003  for
log.si
=== EndOf si_gwsc  at  /home/takao/ecalj/SRC/TestInstall/work/si_gwsc
```

...

The log files of console outputs are staring from l. C at the ends means Core-releated parts. lsxC is the exchange self-energy due to cores.
lsx is for exchange. lsc is correlation. lvcc is for Coulomb matrix。
In this calculation we run `gwsc -np 8 1 si`, where 1 is the number of QSGW iteration.

If you repeat gwsc, you can add additional QSGW iterations added to your previous calculations.

How to start over calcualtions

Remove mix* rst* (mix* is mixing files)
If MT changes, start over from lmfa (remove atm* files)

- As long as converged, no problem.
- If you have 3d spagetti bands at Ef, need caution.

6. Dielectric function, ESM, spin fluctuation, life time of QP, Wannier method,...

Ask us.

7.lmchk

PROF

lmchk mp-2534
is to check the crystal symmetry. In addition determine MT radius. and Check the ovarlap of MTs.
Defaults setting is with -3% overlap.(no overlap).

- symmetry
- MT overlap
  If you have less symmetry rather than than the symmetry of lattice for magnetic systems, you have to set crystal symmetry by hand.
  This can be done by adding space group symmetry generator to SYMGRP (instead of find).
  We need to pay attention for this point in the case of SOC.

memo

band plot with spin orbit coupling.

method 1: only band plot

```
job_band mp-2534 -np 8 -vso=1 -vnspin=2: band plot only
```

Caution: when you set nspin=2, rst is twiced. No way to move it back to rst for nspin=1.

method 2. single iteration and SO=1

```
mpirun -np 8 lmf -vso=1 -vnspin=2 -vnit=1
```

job_band mp-2534 -np 8 : band plot only

method 3. full iteration SO=1

```
mpirun -np 8 lmf -vso=1 -vnspin=2 -vnit=1
```

job_band mp-2534 -np 8 : band plot only

Caution: when you set nspin=2, rst is twiced. No way to move it back to rst for nspin=1.

ecalj/Samples/MgO_PROCAR

This is a sample of fat band. Run job_procarを実行する。You will have eps file.