

UsageDetailed

console output

Console output is now mainly for debug purpose.

But we still need to read some of output data from the console output (we are trying to modify this).

From console output, we can check convergence behavior, band energies, Fermi energies, whether `sigm`, `rst` are correctly read in or not.

save.foobar

- `save.foobar` records starting history invoking `lmf`, `lmchk`, and `lmfa`. In addition, it give total energies, a line per iteration of `lmf`. At each line, 'i: intermediate, c: converged, x: iteration max without converged'.
- In addition, `-vfoobar=xxx` is recorded (overriding variables in `ctrl`).
- Two total energies Kohn-Sham and Harris-Folker is given---both should be virtually the same. But some differences for bigger systems. Take one of them.
- log file
`log.foobar` generated by `lmf`, `lmchk`, `lmfa` are currently used for debuggging purpose.

Spin polarized case without SOC

To treat magnetic systems, we have to set `MMOM` (ititial condition of spin magnatic moments) in addition to set `nspin=2` in `ctrl.foobar`. The spin magnetic moments are specified as the difference of number of electrons between spin channels, `isp=1` and `isp=2`.

For example, run

```
./job_materials.py NiO
```

at `ecalj/MATERIALS/`. For safe, it might be better to remover `ecalj/MATERIALS/NiO/` in advance. Then we see console output ending with

```
...
Finished!: tail NiO/save.nio:c mmom= 0.0000 ehf(eV)=-86704.349038
ehk(eV)=-86704.348942 sev(eV)=-142.498970
===== end =====
```

. Try `cat save.nio` at `ecalj/MATERIALS/NiO/`. It shows iteration history of `lmf`. Last line in `save.nio` should show `c mmom= 0.0000 ehf(eV)=-86704.349038 ehk(eV)=-86704.348942 sev(eV)=-142.498970` (energies may be slightly different). `c` means converged.

ehf and ehk are [total energies by two formulas](#).
Note that total energy is not meaningful in QSGW

Look into ctrl.nio, which is generated from ctrl.nio supplied by the mini database handled by [job_materials.py](#)
ctrl.nio contains

```
SITE      ATOM=Niup POS=  .0    .0    .0 # ← Niup site
          ATOM=Nidn POS= 1.0    1.0    1.0 # ← Nidn site
          ATOM=O   POS=  .5    .5    .5
          ATOM=O   POS= 1.5    1.5    1.5

SPEC
  ATOM=Niup Z=28 R=2.12
    MMOM=0 0 1.2 0          # ← initial spin
    EH=-1 -1 -1 -1 RSMH=1.06 1.06 1.06 1.06
    EH2=-2 -2 -2 -2 RSMH2=1.06 1.06 1.06
    KMXA={kmtx} LMX=3 LMXA=4 NMCORE=1
  ATOM=Nidn Z=28 R=2.12
    MMOM=0 0 -1.2 0         # ← initial spin
    EH=-1 -1 -1 -1 RSMH=1.06 1.06 1.06 1.06
    EH2=-2 -2 -2 -2 RSMH2=1.06 1.06 1.06
    KMXA={kmtx} LMX=3 LMXA=4 NMCORE=1
```

Here we have two sites named Niup and Nidn. **MMOM=0 0 1.2 0** means initial spin moment within MTs: that is **MMOM= {s} {p} {d} {f}**, where **{s} {p} {d} {f}** are number of spin moments for each \$l\$ at atomic sites.

Separators after MMOM can be space or comma. In addition, we set **nspin=2** defined at the **% const** line in ctrl file.

Calculated spin moments within MT are at 'true mm' column in the console output, and shown in the [mmom.nio.chk](#) as

```
# Qtrue      MagMom(up-dn) Rmt    MT
1 8.527587   1.200085  2.120000 Niup
2 8.527604  -1.200081  2.120000 Nidn
3 5.380352  -0.000002  1.700000 0
4 5.380352  -0.000002  1.700000 0
```

Note it is overwritten at every iteration. These are shown in concole output as `true mm' as well. Atomic site index are given in 'Siteinfo.chk'. Total Magnetic Moments are shown as

Magnetic moment= 2.241805 !this is a case of bulk Fe

With the setting in GWinput generated by [job_materials.py NiO](#), we can run gWSC as

```
gwsc -np 32 5 nio
```

I needed 275 sec with 32 MPI per QSGW cycle. I used this qsub script.

```
#!/bin/sh
#$ -N NioTest
#$ -pe smp 32
#$ -cwd
#$ -M takaokotani@gmail.com
#$ -m be
#$ -V
#$ -S /usr/bin/bash
export OMP_NUM_THREADS=1
EXEPATH=/home/takao/bin/
$EXEPATH/gwsc -np 32 5 nio >& lgwsc
```

After calculations, remove temporary files with `rm __*` or `cleargw .`, which were already in your bindir.

You can run `job_band` and so on in the same manner of DFT with `nspin=1`.

- cat save.nio shows total energies (but not meaningful)
- We can effectively use [antiferro symmetry for calculation \(only for so=0,2\)](#)

orbital moments

When `so=1`, orbital moments within MTs are shown at `IORBTM:` in the console output as

```
IORBTM: orbital moments :
ibas Spec      spin  Moment decomposed by l ...
  1   Pr        1    0.000000  -0.011483  -0.010535  -4.881144
0.000234
  1   Pr        2    0.000000   0.012332   0.003604   0.000373
-0.000090
total orbital moment  1:  -4.886708
  2   N         1    0.000000  -0.004174   0.001584   0.000291
0.000129
  2   N         2    0.000000   0.004622   0.000236   0.000045
0.000006
total orbital moment  2:   0.002738
```

Antiferro symmetry without SOC

We can perform LDA/QSGW calculation with the AF symmetry (not for SOC=1).

Only up spin are calculated. Then charge density and eigenvalues are symmetrized for the antiferro symmetry.

See ~/ecalj/Samples/AFsymmetry.

To set AF symmetry, We have to set a line in ctrl file as

```
SYMGRPAP i:(1,1,1) #Antiferro symmetry operation
```

Here SYMGRPAP is the generator of the antiferro magnetic symmetry that

$\vec{g} = i:(1,1,1) * \sigma_y$ should be the generator of magnetic space group, whereas

```
SITE      ATOM=Niup POS=  .0  .0  .0  AF=1      #Antiferro pair
          ATOM=Nidn POS= 1.0 1.0 1.0 AF=-1
```

should contains the AF= to specify antiferro pairs.

Note that the space group operation $i:(1,1,1)$ (this is inversion with translation) is explained at SYMGRP.

In addition, we have an example of ctrl.nise for NiSe.

```
SYMGRPAP i:(0,0,1/2)
ATOM=Niup POS= 0.00 0.000 0.000 AF=1
ATOM=Nidn POS= 0.00 0.000 0.500 AF=-1
```

, where inversion with (0,0,1/2) translation gives AF symmetry.

(README_mmtarget.afest.txt shows the fixed-moment method for antiferro symmetry ---> need to be fixed).

Spin-orbit coupling

We have a switch HAM_SO in the ctrl file

- For LDA/GGA, set nspin=2 and so=1. Then we can perform calculations including SOC. so=1 is for soc included (so=2 is for LzSz mode neglecting LxSz+LySy).
- In the case of semiconductors such as GaAs, we need to include so=1 to see the band structure at the top of valence.
- Currently, QSGW can not be performed with so=1. So we first have to run gwsc with so=0 or 2. After we get sigm file, we run lmf with --vso=1 (nit=1 can be fine) as a perturbation.
- We can treat only colinear spins. Spin axis is along (0,0,1) as default. We can choose other direction with SOCAXIS. See ecalj/Samples/SOCAXIS. Not checked completely, but it seems work well.

Band plot with spin orbit coupling.

- method 1: only apply SOC for band plot

```
job_band mp-2534 -np 8 -vso=1 -vnspin=2
```

Caution: when you set nspin=2, the size of rst is twiced. No way to move it back to rst for nspin=1. So you may need to keep rst.

- method 2. single iteration and SO=1

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

Then we have revised rst.foobar. Then run `job_band mp-2534 -np 8 -vso=1 -vnspin=2`.

- method 3. full iteration SO=1

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

Then run `job_band mp-2534 -np 8 -vso=1 -vnspin=2`

Forces and Atomic position relaxiation

See [ecalj/Samples/LaGaO3_relax](#).

We have to set **DYN** category. In addition, we can set directions for relaxation. No cell optimizations.

Fermi surface

See a sample at [ecalj/Samples/FermiSurface](#)

PROCAR mode

See a sample at [ecalj/Samples/MgO_PROCAR](#)

We can generate PROCAR file containing the size of eigenfuncitons**2.

The sample (run job file) generates eps file showing fat band of O2 components.

Run jobprocar. This gives *.eps file which shows Fat band picture.

PROCAR (vasp format) is generated and analysed by a script BandWeight.py.

LDA+U

We have samples

- <https://github.com/tkotani/ecalj/tree/master/Samples/GdNldau>
- `~/ecalj/Samples/ReNcub`
- IDU=, UH=, JH= specify parameters for LDA+U. IDU=#,#,#,... specifies which l-channels are to have U and the type of LDA+U implementation.
0 in a particular l-channel means no U is to be applied, 1 or 2 are for particular forms of LDA+U. For

example,
IDU= 0 0 0 1 UH= 0 0 0 -0.28 JH=0 0 0 0

BoltTrap

--boltztrap option is to generate files required for boltztrap.

See [~/ecalj/Samples/Boltztrap](#)

Dielectric function

[~/ecalj/Samples/EPS](#)

Dielectric functions for Cu and GaAs. For Cu, we have intraband and interband contributions separately.

See [dielectric fuctnion](#).

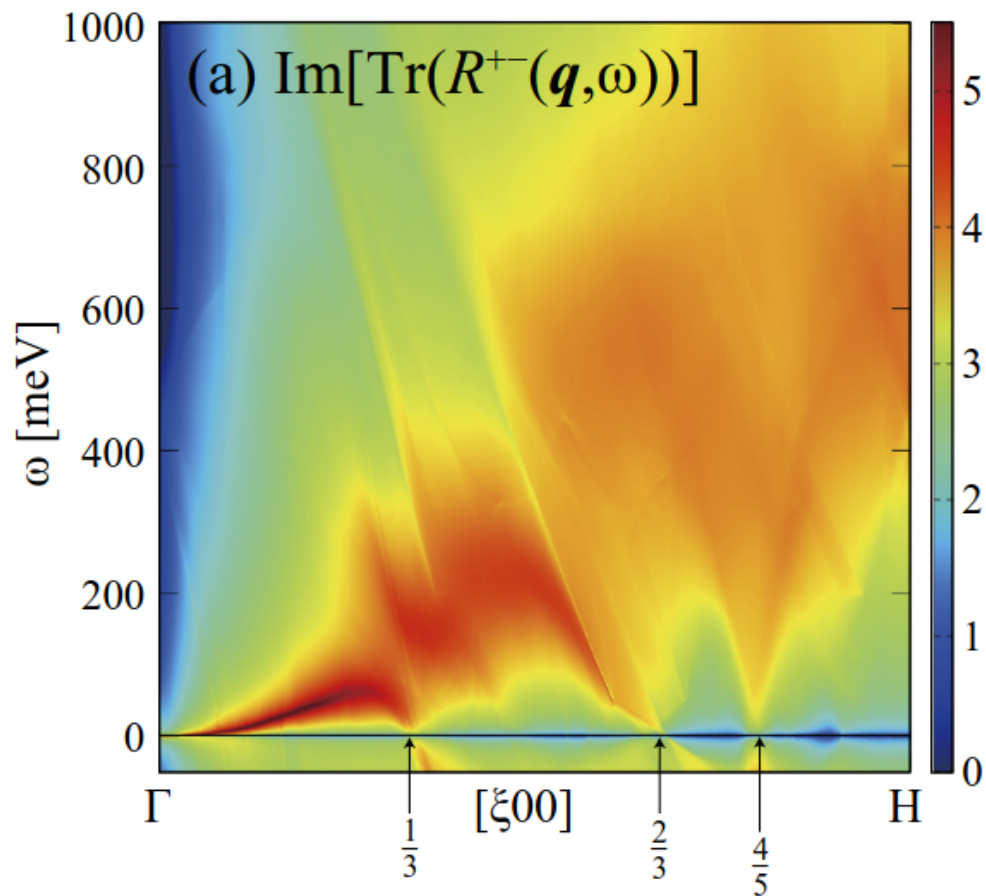
Impact ionization rate

[~/ecalj/Samples/IIR](#)

Spin fluctuation

[~/ecalj/Samples/Magnon](#)

It is via the MaxlocWannier. We are going to move to MLO instead. Here is a figure (this is on top of LDA)



Effective Screening Medium (ESM)

We can apply electric field to slab model. ESM combined with QSGW is quite unique.

Used in the paper <https://journals.aps.org/prb/abstract/10.1103/PhysRevB.101.205120>

Ask us.

lmf and ctrl

See [lmf and ctrl](#)

gwsc and GWinput

See [gwsc](#).

For GPU, see [ecaljgpu](#) and [gwsc for GPU for ISSP](#) together.

See [explanation of GWinput](#).

getsym1: automatic symmetry line and BZ for band plot

See [sym1](#)

These citations are required.

1.Y. Hinuma, G. Pizzi, Y. Kumagai, F. Oba, I. Tanaka, Band structure diagram paths based on crystallography, Comp. Mat. Sci. 128, 140 (2017)

2.Cite spglib that is essential for getsym.

ecalj/Samples/

- MLO: new localized basis
Maximally localized Wannier function and cRPA interaction
- MLWF_samples
Wannier function generator and cRPA
wannier90 method implemented in ecalj and cRPA.
(a cRPA method by Juelich group).
See Samples_MLWF/README.
~/ecalj/README_wannier.md This is going to be replaced with README_MLO.md
- mass_fit_test
Effective mass calculation. See README. probably not maintained\dots

ecalj_auto

This is a suit of python scripts to run thousands of gwsc calculations automatically.

[ecalj_auto](#)

Background charge and fractional Z

[background charge](#)

How to perform paper-quality QSGW calculations with minimum costs.

The accuracy of band gaps can be ~ 0.1 eV or larger for larger band gap materials..

In cases, it is easy, but in cases not so easy. So, it is better to use your own "simple criterion".

"Not stick to convergence so much. Just stick to Reproducibility."

PROF

4f and 5f atoms

We need special care to treat atoms where 4f and 5f are fractionally filled.

We have not yet include following setting in ctrlgenM1.py as for 4f/5f atoms (2025-08-07).

Here is the setting for RareEarth rocksalt nitrides ReN such as ErN.

1. Set nsp=2, so=2 (since QSGW can not treat so=1 now). (If necessary set so=1 after QSGW).
2. SYMGRP r4z. This is needed since we have lower symmetry rather than the lattice. It fixes the direction of spins and orbital moments.
3. Our setting is

```
--- ctrl.ern
  ATOM=Er Z=68 R=2.58
    PZ=0, 5, 0, 5
```



```

IDU=0 0 0 12 UH=0 0 0 0.773 JH=0 0 0 0.0945 MMOM=0 0 0 3
EH=-1 -1 -1 -1 RSMH=1.29 1.29 1.29 1.29
EH2=-2 -2 -2 -2 RSMH2=1.29 1.29 1.29 1.29
KMXA={kmtx} LMX=3 LMXA=6 NMCORE=1
(pwemax=2, nk=8 8 8 was used)
--- GWinput
(n1n2n3 6 6 6 was used)
(tol 1d-2 was used)
lcutmx(atom)
6 2

```

Here PZ is the principle quantum number of local orbitals. This sets 5p and 5f as local orbitals. Run **lmfa crn|grep conf** to check atomic configuration.

- IDU,UH,JH are the LDA+U parameters, only for initial condition. Since IDU is 10+2, we skip U effect when sigm exists.
- MMOM is the initial magnetic moments.
- LMXA=6 to expand augmented waves is needed.
- Make sure READP=T.

With these settings, we have series of calculations finished for 4f ReN.
So input files are available. Ask us.

QPU and QPD files

This contains the contents of self-energy

Papers

It is instructive to reproduce samples in [Deguchi paper](#).

We can set up templates for your calculations. Ask us.

We have a latest paper at <https://arxiv.org/abs/2506.03477> for GPU version.

It shows some details of computational steps in ecalj.

In Japanese, pages by Dr.Gomi at <http://gomisai.blog75.fc2.com/blog-entry-675.html> and <https://qiita.com/takaokotani/items/9bdf5f1551000771dc48>.

How to perform paper-quarilty QSGW calculations with minimum costs.

We expect that the accuracy of band gaps can be ~0.1eV (or larger for larger band gap materials).

In cases, it is easy but in cases not so easy (magnetic metals requires many number of iterations).

So, it is better to use your own "simple criterion".

"Not stick to convergence so much. Just stick to Reproducibility."

LDA calculation

We need to confirm LDA-level of calculations first.

The ctrl file is generated just from ctrl.* (crystal structure file)

For calculation of QSGW, use large enough NKABC, so as to avoid convergence check on them.

QSGW: how to check convergence

QSGW iteration cycle by gwsc contains (1) and (2)

- (1) One-body self-consistent calculation
(where we add $\text{sigm} = \text{Sigma} - V_{xc}^{\text{LDA}}$ to one-body potential).
to determine one-body Hamiltonian H_0 .
- (2) For given H_0 , we calculate sigm file.

Big iteration cycle of QSGW is made from (1)+(2).

(gwsc script. not run_arg is a subroutine of bash script)

With (1), we have small iteration cycle of one-body calculation with keeping given sigm.

In `save.*`, we see total energy (but not the total energy in the QSGW mode with sigm file), a line per each iteration of (1). A line "c ..." is the final iteration cycle of (1). "x ..." is unconverged (but no problem as long as we finally see "c ...").

The command `grep '[cx]' save.*` gives an indicator for going to be converged or not.

Or you can take `grep gap llmf.*run` (see it bottom.)

Another way:

`dqpu QPU.3run QPU.6run`

is to compare two QPU files which contains QP energies.

(note: QP energies shown are calculated just at the beginning of iteration).

For insulator, (I think), comparing band gap for each iteration is good enough to check convergence. But for metal, it is better to plot energy bands for some of final iterations, and overlapped (`cd QSGW.*run` and run `job_band`).

PROF Another way is `grep rms lqpe*`. This gives rmsdel. Difference of self-energy (at least we see it is getting smaller for initial first cycles).

How to make 80%QSGW +20% LDA, and SO setting

Note that sigm file contains $V_{xc}^{\text{QSGW}} - V_{xc}^{\text{LDA}}$.

If sigm exists, lmf read it, and run self-consistent calculations with adding sigm to the one-body potential.

See Table I in

<https://iopscience.iop.org/article/10.7567/JJAP.55.051201/pdf>

1. QSGW80(NoSC)

For practical prediction of band structure, such as band gap and so on, it may be better to use 80% QSGW +20% LDA procedure when you

make band plot. After, you have rst and sigm files determined self-consistently

Run

```
job_band gaas -np 4 -vssig=0.80
```

(Confirm ssig is defined and cited as **ScaledSigma={ssig}** in the ctrl file). This gives a result of QSGW80nosc in the TableII.

2. QSGW80(Nosc)+SO

80%QSGW+20%LDA with SO=1 (L.S method).

If you like to include L.S method

```
mpirun lmf gaas -np 4 -vssig=0.80 -vso=1 -vnspin=2
```

This procedure makes self-consistency with keeping the sigm file. This may/(or may not) required. If you expect large orbital moment this procedure may be needed.

```
job_band gaas -np 4 -vssig=0.80 -vso=1 -vnspin=2
```

NOTE: nspin=2 is required for so=1. rst and sigm are expanded for npsin=2 (you can not run with nspin=1, after rst and sigm are expanded).

3. QSGW80

With ssig=0.80, you can run QSGW calculaiton in gwsc.

Then you have self-consistent results of QSGW80.

You can simultaneously use the setting so=2 (Lz.Sz scheme).

Be careful for z-direction and setting of SYMOPS (so as to keep the z-axis), for so=2.

If you like to get results of QSGW80+SO, you need to set so=1 after self-consistent of sigm attained.

4. Example of GaAs

Good example to check band gap, and SO splitting at top of valence of Gamma point for ZB structure as GaAs.

Before run it, make sure your ctrl file include variables ssig, so, nspin by

```
>grep ssig ctrl.gaas  
>grep so ctrl.gaas  
>grep nspin ctrl.gaas
```

to know the variable `ssigm` is defined and used as

`ScaledSigma={ssig}`, `NSPIN={nspin}`. For `-vso=1` work, you also need to so is defined and `S0={so}` is set in ctrl.

How to do version up? git minimum

Be careful to do version up ecalj. It may cause another problem.

If you are not good at git, make another clone.

Do not mix up with previous version (e.g. where you install)

```
cd ecalj
git log
This shows what version you use now.
```

```
git diff > gitdiff_backup
This is to save your changes added to the original (to a file git_diff_backup ) for safe.
I recommend you do take git diff >foobar as backup.
git stash also move your changes to stash.
```

```
git checkout -f
CAUTION!!!!: this delete your changes in ecalj/.
This recover files controlled by git to the original which was just downloaded.
```

```
git pull
This takes all new changes. It is safer to use git fetch and gitk --all (git checkout FETCH_HEAD -b youbranch) to checkout your local branch.
```

I think it is recommended to use

```
gitk --all
```

and read this document. Difference can be easily taken,
e.g. by

```
git diff d2281:README 81d27:README
(here d2281 and 81d27 are several digits of the begining of its version id).
```

```
git show 81d27:README
```

is also useful.

History (not latest description)

Relation with Questaal at <http://www.questaal.org/>:

Questaal is one-another package to perform QSGW distributed by Mark van Schilfgaarde mainly in FP-LMTO, not in the PMT. In the package, there is the driver to use a modified version of the GW code in `ecalj` (GW part in Questaal is originated in `ecalj`). The FP-LMTO in questaal and ecalj have some similarities (for input files and outputs).

History

T.Kotani learned the LMTO-ASA-GW code by F.Aryasetiawan, which is on top of the Stuttgart's LMTO-ASA, mainly by van Schilfgaarde under O. Jepsen and O. K. Andersen

<http://www2.fkf.mpg.de/andersen/LMTODOC/LMTODOC.html> A FP-LMTO package is originally given by M.Methfessel, Mark van Schilfgaarde and their collaborators. T.Kotani developed an all-electron full-potential GW method on top of the FP-LMTO during his sabbatical at 1999-2000 at the lab of M.Schilfgaarde. Then the QSGW method has developed with the help of S.Faleev and M.Schilfgaarde, first published in 2004. Then T.Kotani was adding new functionality such as spin fluctuation, impact ionization. In year 2008, T.Kotani started the PMT=LMTO+LAPW method to remove problem of the FP-LMTO. After T.Kotani moved to Tottori-u at 2009, he spends time for the improvement of PMT method. T.Kotani and H.Kino showed that PMT can describe even the diatomic molecules efficiently and accurately. It turns out very limited number of APWs can remove such problems. Then T.Kotani have developed PMT-QSGW method. It is now stable, easy, and reliable rather than the previous version of QSGW on top of FP-LMTO. We can perform calculations just from given crystal structures usually, but still some problem in cases with complicated electronic structures.