ecalj main documents

This is a main document of ecaljdoc. All files in ecaljdoc are linked from this file.

- Qiita Japanese may be a help, but most of all are here.
- Here we give GetStarted and UsageDetailed, followed by install and Overview section.

Licence

- AGPLv3
- For publications, we hope to make a citation cleary to this homepage such as;

  [foobar] ecalj available from https://github.com/tkotani/ecalj/.

Install

To install ecalj, look into install, as well as install for ISSP

Overview of QSGW calculation

- band calculations calculations (LDA level) 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 (`lmfa` finishes instantaneously).
- A file `sigm.foobar` is the key for QSGW calculations. The file `sigm.foobar` contains the non-local potential $V_{\rm xc}^{\rm QSGW}-V_{\rm xc}^{\rm LDA}$. 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 removing 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). See https://arxiv.org/abs/2506.03477
- We have GPU acceleration for QSGW, https://arxiv.org/abs/2506.03477. Thus we can handle large systems. With 4 GPU, we can compute systems with 40 atoms per cell with surfaces.
- We intend to perform calculations **without parameter settings by hands**.
  Thus I think ecalj is one of the easiest code to perform GW for users. See band database in QSGW

PROF

at
https://github.com/tkotani/DOSnpSupplement/blob/main/bandpng.md
(this is supplement of https://arxiv.org/abs/2507.19189). This is away from complete one, but showing the abity of ecalj.

GetStarted

We explain DFT/QSGW calculations with ecalj. Then we explain how to make band plots.
For simplicity, we treat paramagetic cases (nsp=1), no 4f, no SOC.
We explain things step by step.

Further details are explained at AdvancedUsage.

0. POSCAR

We first need POSCAR (crystal structure in VASP format).
You can find samples of 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
```

For example, POSCAR of mp-2534 GaAs is given as:

```
Ga1 As1
1.0
   3.5212530000000002    0.0000000000000000    2.0329969999999999
   1.1737510000000000    3.3198690000000002    2.0329969999999999
   0.0000000000000000    0.0000000000000000    4.0659929999999997
Ga As
1 1
direct
   0.0000000000000000    0.0000000000000000    0.0000000000000000 Ga
   0.2500000000000000    0.2500000000000000    0.2500000000000000 As
```

This is another POSCAR for ba2pdo2cl2:

```
POSCAR_ba2pdo2cl2
1.0
```

```
-2.06443 2.06443 8.40383
2.06443 -2.06443 8.40383
2.06443 2.06443 -8.40383
Ba Pd O Cl
2 1 2 2
Cartesian
0.0 0.0 6.5153213224
0.0 0.0 10.2923386776
0.0 0.0 0.0
0.0 2.06443 0.0
2.06443 0.0 0.0
0.0 0.0 3.1625293056
0.0 0.0 13.6451306944
```

If you have cif and like to convert it to `POSCAR`, do
`cif2cell foobar.cif -p vasp --vasp-cartesian --vasp-format=5`.

Step 1. convert POSCAR to ctrls file

Then we convert POSCAR to ctrls by vasp2ctrl.
ctrls is the structure file used in ecalj.

```
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
```

- 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).

Step 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
```

Edit `ctrl.foobar` if necessary. Explanations are embedded in ctrl.foobar (please let me know wrong descriptions). Possible points to rewrite in ctrl.foobar:

1. Number of k points (nk1,nk2,nk3).
2. nsp=2 if magnetic
3. SpinOrbitCoupling: so=0 (none), so=1 (LdotS), 2 (LzSz). nsp=2 is required for so=1,2. so=1 does not yet support QSGW. SOC axis can also be freely selected, but currently (0,0,1) default and (1,1,0) are supported (m_augmbl.f90). If you want to set SO=1 in QSGW, currently, run QSGW calculation with so=0 or so=2 to obtain ssig file, then set so=1
4. xcfun (choice of LDA exchange correlation term). Only =1:BH, =2:VWN, =103:PBE-GGA.
5. LDA+U settings (not explained yet).
6. ssig=1.0 (If you choose QSGW80, use ssig=0.8. Effective for QSGW calculations.
   $V^{\rm xc QSGW}-V^{\rm xc LDA}$ is stored in a file `sigm.foobar`. We add ssig $\times (V^{\rm xc QSGW}-V^{\rm xc LDA})$ to the potential in the lmf calculation as long as `sigm.foobar` file is available.

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- `lmchk --pr60 foobar` allows you to check the recognized symmetries by `lmf`. Turning off --pr60 or reducing 60 will reduce the verbosity of output.

At this point, you can visually check the following check files.

- SiteInfo.chk
  MT radius Atomic positions
- PlatQlat.chk
  Primitive lattice vector (plat) Primitive reciprocal lattice vector (qlat)

Here we explain details of ctrl file.

Hereafter, we only use `ctrl.foobar` (`ctrls.foobar` is used hereafter.). We can delete temporary files.

Install VEST

It is convenient to see crystal structures with VESTA.
(I installed VESTA-gtk3.tar.bz2 (ver. 3.5.8, built on Aug 11 2022, 23.8MB) on ubuntu 24)
At ecalj/StructureTool/, we have 'viewvesta' command. Try

```
viewvesta ctrl.si
```

to see the structure in VESTA. At /StructureTool, we have converters,
`vasp2ctrl` and `ctrl2vasp`.
(We have ~/ecalj/GetSyml/README.org. Not need to see this)

Step 3. LDA calculation

1. Run lmfa at first. It is for spherical atomic electron densities, contained in the crystals. lmfa ends instantaneously.

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

   gives spherical atom calculation for initialization.`lmfa` calculates spherically symmetric atoms and generates the files required for lmf below.
   Check `conf` section in the console output as

   ```
   lmfa ctrl.mp-2534 |grep conf
   ```

   . This shows atomic configuration (there are no side effects even if `lmfa` is repeated). The initial condition of electron density for lmf is given as the superposition of spherically symmetric atomic densities given by lmfa. In addition, lmfa calculations are performed with the logarithmic derivative of the radial wave function at the MT sphere edge fixed (READP True in default ctrlgenM1.py setting). The derivatives are contained in `atmpnu.*` files. So, `atmpnu.*` are needed for `lmf`.

2. After `lmfa`, we run LDA calculation as:

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

   - mp-2534 (GaAs) gives 5.75 $\AA$ for GaAs, while the experimental value is 5.65$\AA$.
   - llmf contains information of iterations, check eigenvalue and fermi energies, 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 operators such as `* + - / **` can be possible in ctrl.

- Note: ctrlp is intermediate file generated by python from ctrl. Fortran calls a python code internally.(ctrl2ctrlp.py is responsible for the math)
- 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.

NOTE:
We have deguchi paper https://sci-hub.tw/https://doi.org/10.7567/JJAP.55.051201
All calculation is by the default setting in QSGW on the PMT method.

> No empty spheres. EH=-1,EH=-2, MT radius is -3% untouching.
> RSMH=RSMH2=R/2

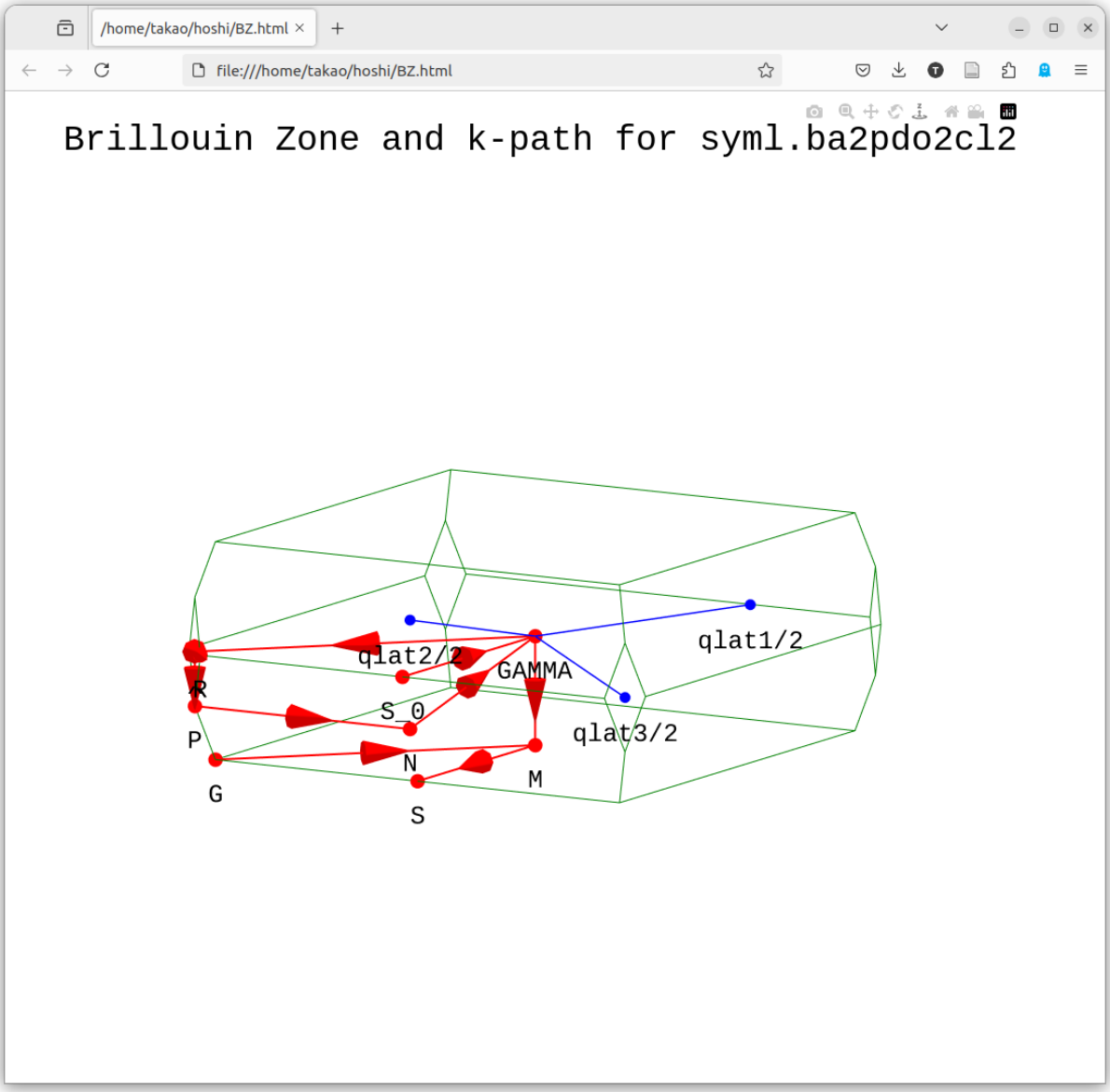
Step 4. Create k-path and BZ for band plot

After the calculation converges, it might be necessary to make a band plot with `job_band` command explain later on. The normality of the calculation of bands can be confirmed by the band plot (for magnetic systems, check the total magnetic moment and the magnetic moment for each site).

Before `job_band`, run `getsyml gaas`. Install any missing packages with pip. It is on spglib by Togo and seekpath. After finished, view BZ.html. It shows the k-path in the BZ ashow show below for ba2pdo2cl2. It is an interactive figure written with plotly, so you can read the coordinate values.

```
getsyml mp-2534
```

- Samples of BZ.html by getsyml are seen at https://ecalj.sakura.ne.jp/BZ/.



Step 5. band plot

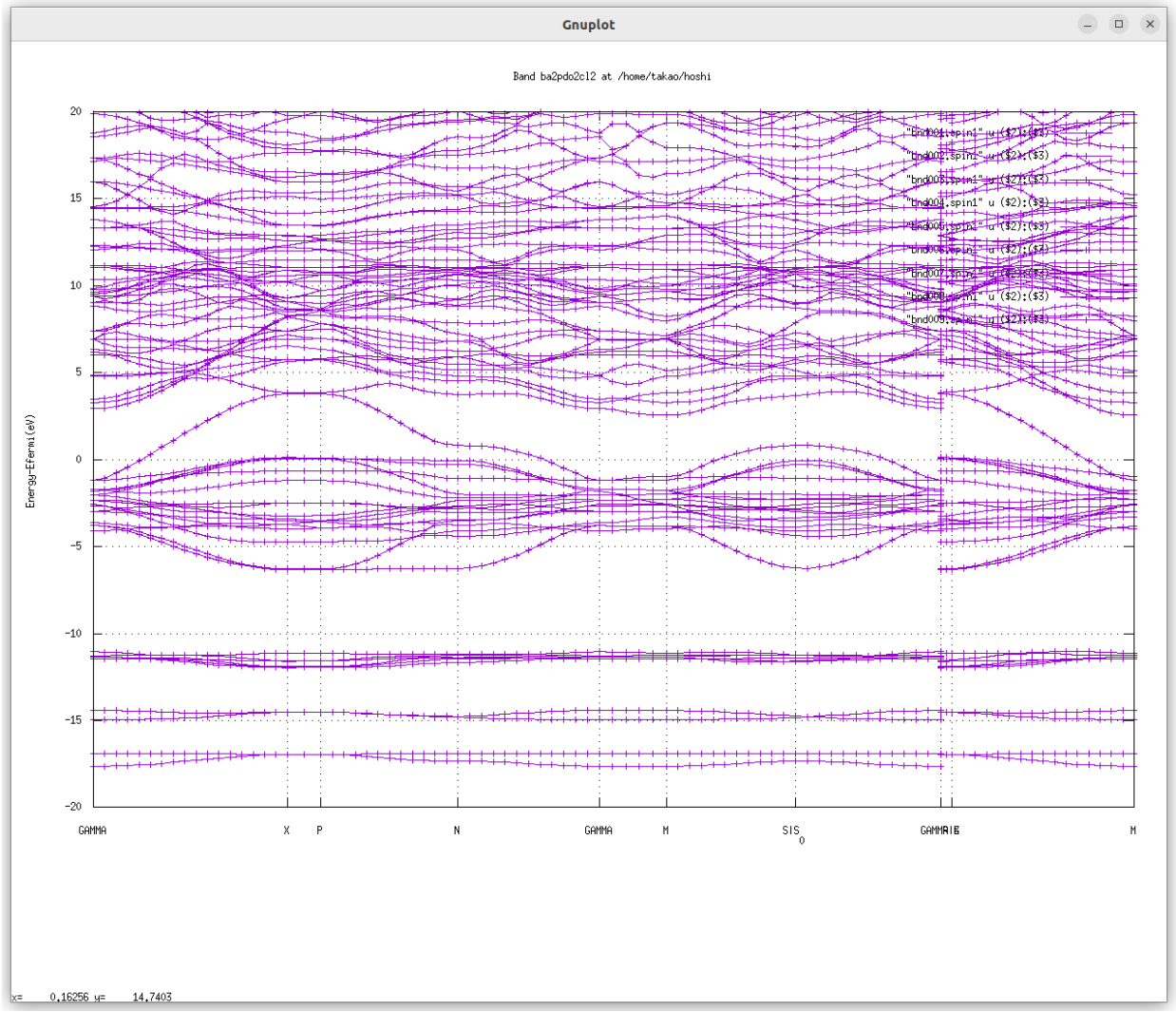
PROF

(this is a case for ba2pdo2cl2)

```
>job_band ctrl.ba2pdo2cl2 -np 8
```

A gnuplot script can be created. Edit it if necessary. If you edit syml.ba2pdo2cl2 before `job_band`, you can adjust the symmetry line and mesh size.

- The following picture is the LDA bands for the default calculation of ba2pdo2cl2 (the names of the symmetric points can be confirmed with BZ.html. In addition, look into `syml.foobar`). 0 eV is the Fermi energy. Since this is metallic, we see no band gap.



.

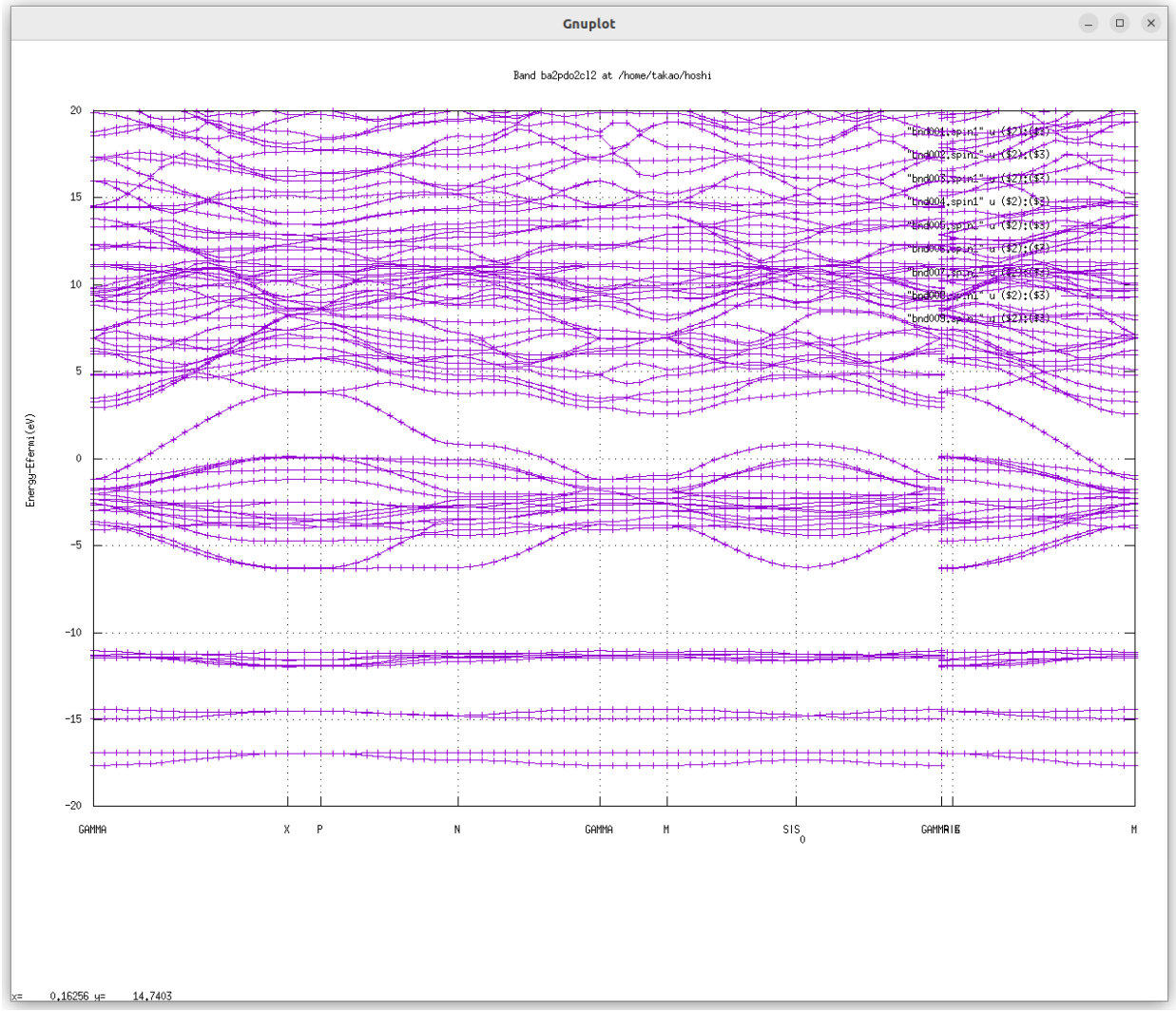
- The defaults are fine except for the k-mesh setting. For example, it is better to increase the k mesh for Fe. In general, for semiconductors, 4 4 4 for Si is a reasonable level, 6 6 6 is a level that can be used for a paper, and 8 8 8 is a level for checking accuracy. For metals such as Fe, 8 8 8 is a reasonable level.

PROF Here we are talking about band energies.

- In ecalj, the k mesh for `lmf` (ctrl) and the k mesh for GW (n1n2n3 specified in GWinput) can be different. The former has affected little on computational time, but the latter has a large effect (thus we want to reduce `n1n2n3` in `GWinput`).

- In ecalj's band plot mode, theoretically degenerated bands because of symmetry at the BZ edge are not degenerated. This is because there are limited numbers of APW basis functions, so run the

band plot with pwemax=4, etc. (Temporary solution: We want to automate it).



job_tdos, job_fermisurface, job_pdos

`job_pdos` calculates PDOS, `job_tdos` calculates total DOS, and `job_fermisurface` draws the Fermi surface with Xcrysden.
`job_fermisurface` can be used to draw the shape of the CBM bottom as ellipsoid of Si.
xxx

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Step 6. QSGW calculation

We now run QSGW calculations. qSGW is compuationally very expensive. So we recommend you to run smaller systems at first.

For QSGW calculations, we need one additional input file `GWinput`, whose template is generated by mkGWinput GWinput as

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

Then copy and edit GWimput.tmp to GWinput.

In `GWinput`, n1n2n3 should be smaller than nk1 nk2 nk3 in ctrl file
in order to reduce computational time (1/2 or 2/3 of ctrl, for example)
If 6x6x6 for Si, it is reasoble. Except k points, not need to modify so much (ask us).
`GWinput` is explained here. Input system is different from ctrl.

flow of QSGW calculation with the script gwsc

We run the QSGW calculations with gwsc. For semiconductors, several QSGW iterations are fine, close enough to final results.
QSGW is to obtain band structures (or one-body Hamiltonian), the total energy is not yet.

`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/bin/lmfa si     >llmfa
0:00:00.807062   mpirun -np 4 /home/takao/bin/lmf  si     >llmf_lda
===== QSGW iteration start iter 1 ===
0:00:03.071054   mpirun -np 1 /home/takao/bin/lmf si     --jobgw=0
>llmfgw00
0:00:03.904403   mpirun -np 1 /home/takao/bin/qg4gw    --job=1 > lqg4gw
0:00:04.431022   mpirun -np 4 /home/takao/bin/lmf si     --jobgw=1
>llmfgw01
0:00:05.918216   mpirun -np 1 /home/takao/bin/heftet --job=1    > leftet
0:00:06.444439   mpirun -np 1 /home/takao/bin/hbasfp0 --job=3    >lbasC
0:00:07.064558   mpirun -np 4 /home/takao/bin/hvccfp0 --job=3    > lvccC
0:00:07.812283   mpirun -np 4 /home/takao/bin/hsfp0_sc --job=3    >lsxC
0:00:08.545956   mpirun -np 1 /home/takao/bin/hbasfp0 --job=0    > lbas
0:00:09.156775   mpirun -np 4 /home/takao/bin/hvccfp0 --job=0    > lvcc
0:00:09.884064   mpirun -np 4 /home/takao/bin/hsfp0_sc --job=1    >lsx
0:00:10.644292   mpirun -np 4 /home/takao/bin/hrcxq   > lrcxq
0:00:11.482931   mpirun -np 4 /home/takao/bin/hsfp0_sc --job=2    > lsc
0:00:12.460776   mpirun -np 1 /home/takao/bin/hqpe_sc    > lqpe
0:00:13.019735   mpirun -np 4 /home/takao/bin/lmf si     >llmf
===== QSGW iteration end   iter 1 ===
OK! ==== All calclation finished for  gwsc ====
```

...

The log files of console outputs are `l*`. C at the end of the lof file means Core-related 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, we have additional QSGW iterations on top the previous calculations.

Here is a case of ba2pdo2cl2.

Run

```
mkGWinput ba2pdo2cl2
```

to generate GWinput.tmp, which is a setting file for QSGW.
After copying this to GWinput, you may need to edit GWinput.
Minimum thing to edit is the number of k points for the self energy (n1n2n3).
Compared with k points in ctrl (nk1,nk2,nk3), we use small numbers.
(We often use 1/2 or 2/3 of k points given in ctrl as nk1,nk2,nk3).

There are another setting in GWinput. However, we usually do not need to touch things except n1n2n3 if you treat non-magnetic semiconductors.

Then you can run QSGW calculation with

```
gwsc -np 32 1 ba2pdo2cl2
```

. Here 1 means the number of QSGW iterations. QSGW iteration is quite time-consuming. `gwsc` gives minimum help (we need to explain options elsewhere).

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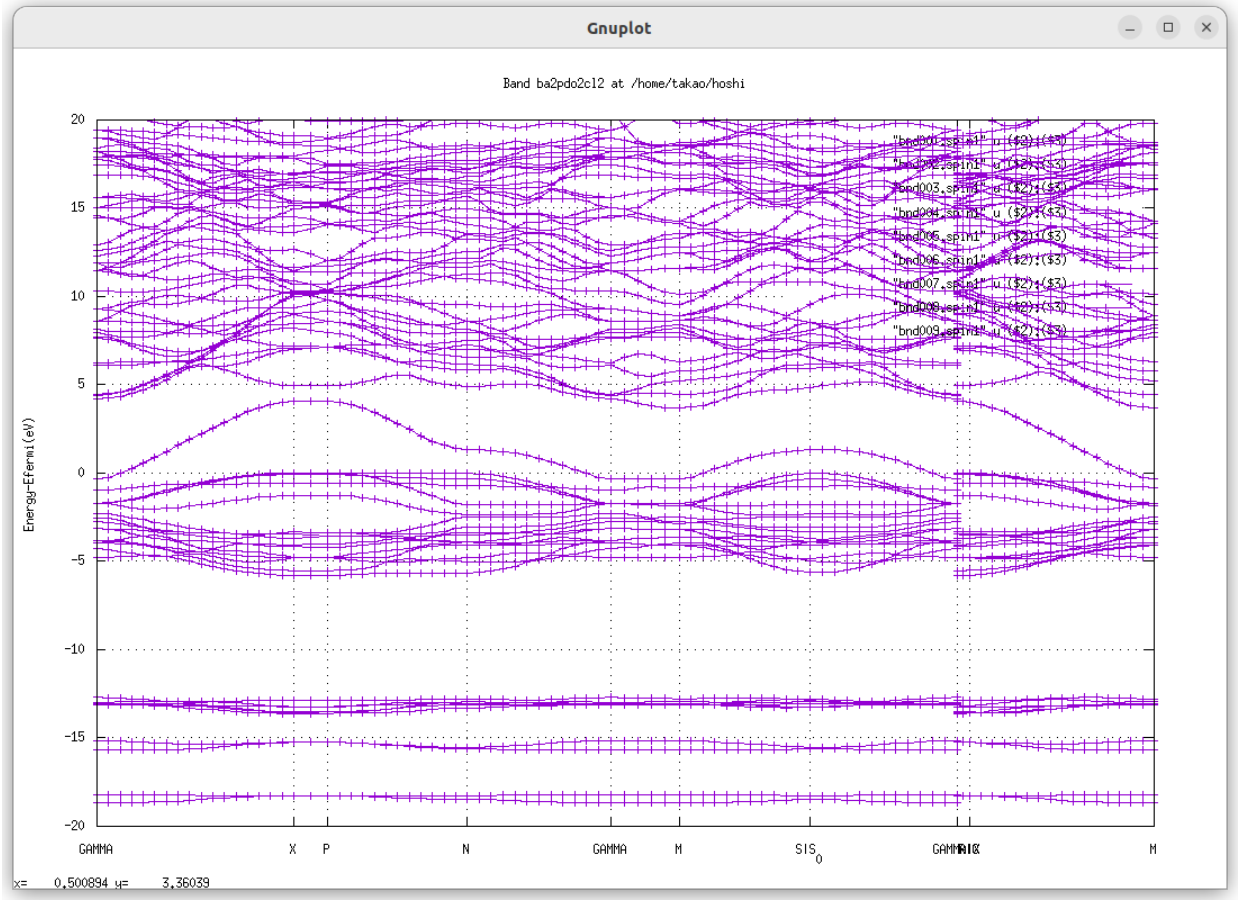
The iteration is kept in `rst.foobar`:electron density, `sigm.*`:vxcqsgw.
(Remove these files in addition to *run files/directories if you like to start from the beginning).

- It requires 53 minutes to run one iteration of QSGW.
- job_band ba2pdo2cl2 -np 32 gives the following picture. QSGW one-shot changes band structure around Ef from that in LDA.But still metallic, no band gaps.



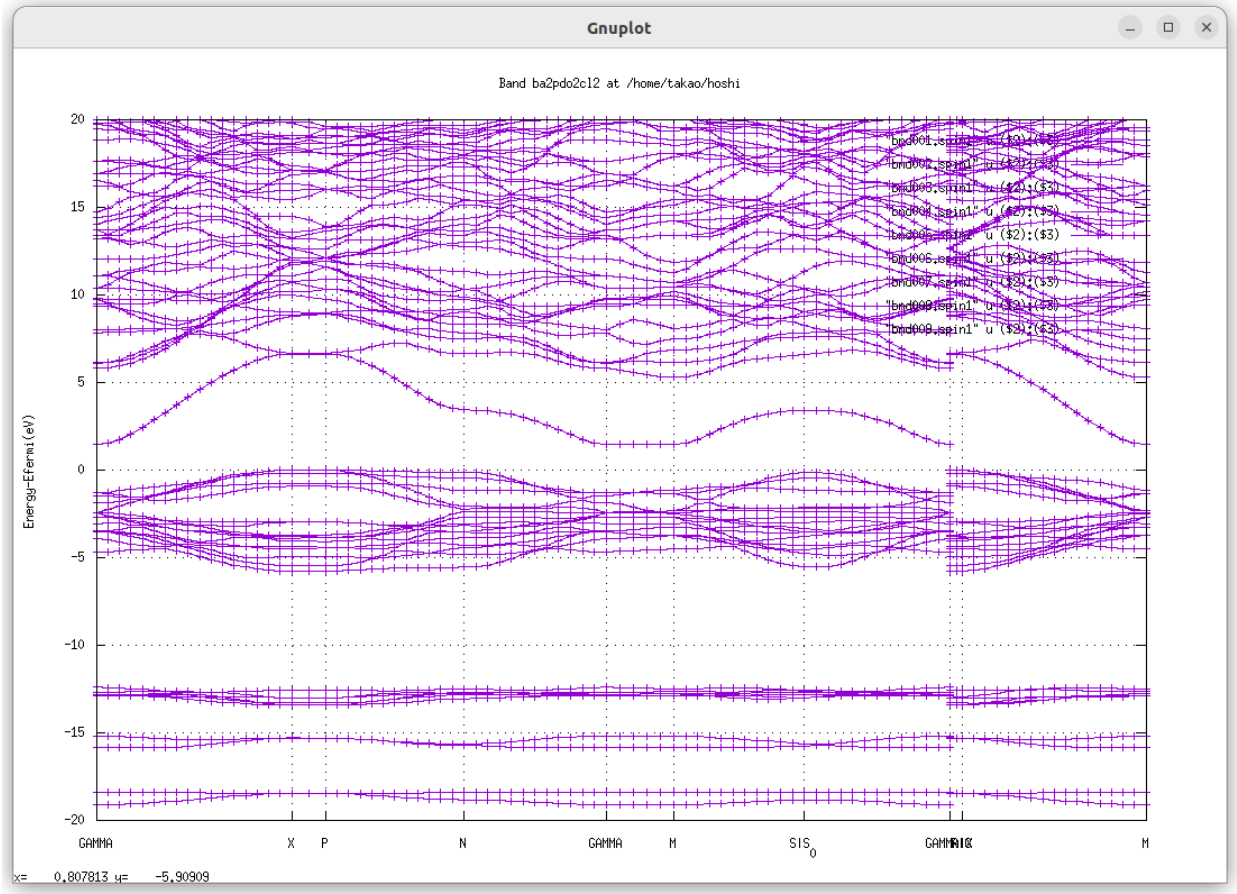
- To continue QSGW iteration, run

```
gwsc -np 32 nx ba2pdo2cl2
```

Since you did 1 already. You will have the results of 1+nx QSGQ iteration.

- when we run 8 iterations as for ba2pdo2cl2, we had band gap 2.1 eV. We saw band gap after 4th iteration.

PROF



- For comparison with experiments, we recommend to use ssig=0.8
  (set in ctrl.foobar file), which is called as QSGW80.
- Spin-orbit coupling. After you obtain `sigm.foobar`, you set SO=1 (LdotS scheme) and run lmf.
  Then you can include effect of SOC. Sinc SO=1
  is not implemented in the whole gwsc cycle, we have to include SOC just at the end step (We include SOC after we fix VxcQSGW).
- If you run

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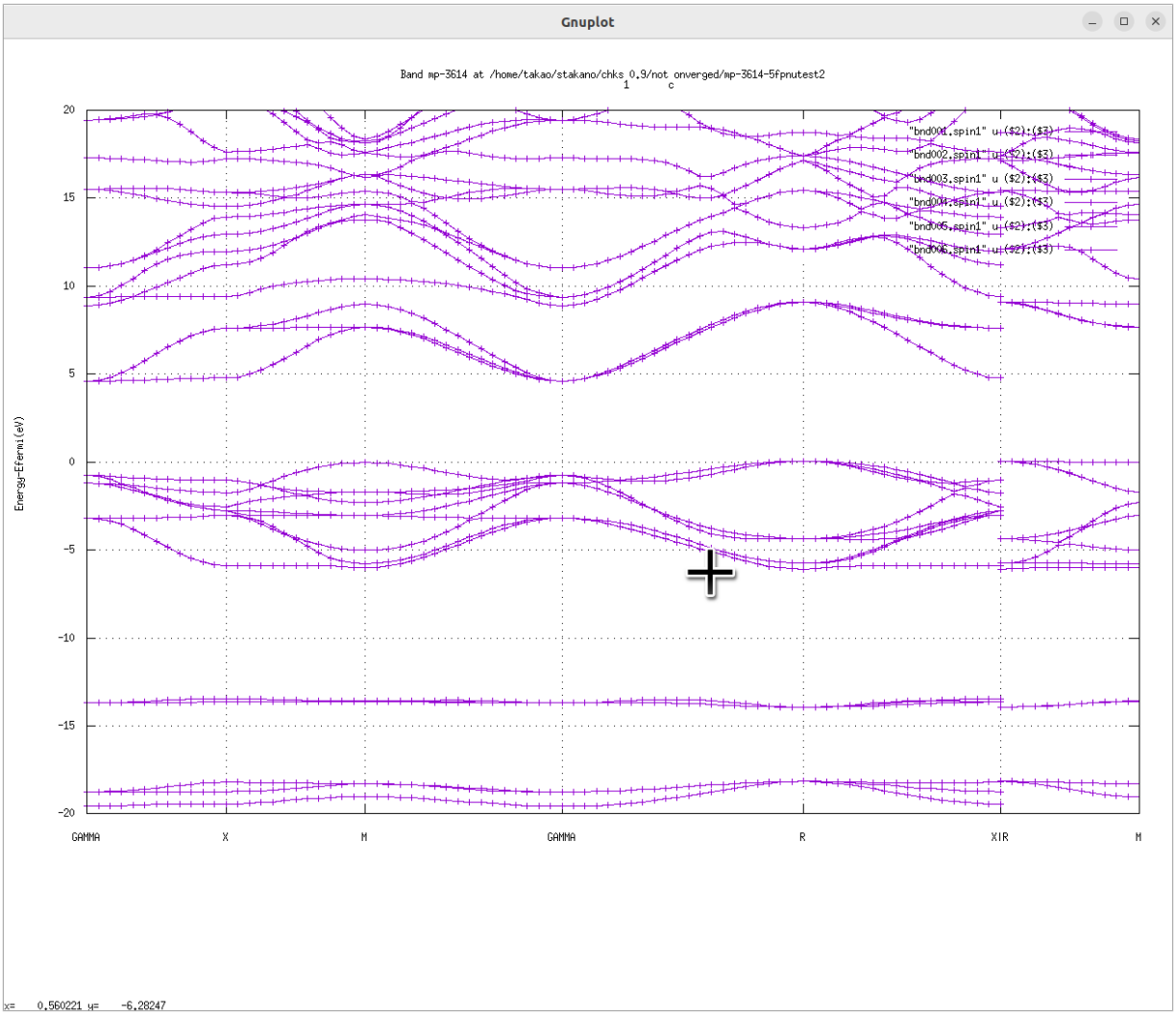
```
gwsc -np 32 5 ba2pdo2cl2 -vssig=0.8
```

, this overide ssig, which is defined in ctrl.ba2pdo2cl2, in lmf calculations. (Check it in save.ba2pdo2cl2)

- Example of QSGW for KTaO3 (perovskite,mp-3614)



How to start over calcualtions

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

PROF

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

A mini database for tests.

At ecalj/MATERIALS/, you can run ./jobmaterials.py. It shows a help with a list of materials.
It contains samples of simple materials.It performs LDA calculations and generates GWinput for materials.
Run as follows. Then we perform LDA calculations where crystal structures are already contained in a mini database.

```
./job_materials.py
```

gives a help, showing a list of materials. Then

```
./job_materials.py Si
```

performs LDA calculation of Si at ecalj/MATERIALS/Si/. '--all' works as well instead of 'Si'.

> job_materials.py works as follows for given names.
> Step 1. Generate ctrls.* file for Materials.ctrls.database. (names are in DATASECTION:)
> Step 2. Generate ctrl by ctrlgenM1.py
> Step 3. Make directtory such as Si/ and run lmf, lmfa, mkGWinput.

- Key input files are
  `ctrls.si`,`ctrl.si`
  . See sections below. `rst.si` contains self-consistent electron density. Check iterations with the output file `save.si`. The console output of lmf is in llmf. Not need to know all the console outputs.

- Before QSGW, it is better to confirm the LDA level calculations are fine. In order to do the confirmation, band plot is convenient.
  For band plot we need the symmetry line as `syml.si` which can
  be generated by

  ```
  getsyml si
  ```

  Then run

  ```
  job_band si -np 8
  ```

  results band plots in the gnuplot.

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lmchk

```
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.
(we have to explain how to read space group and so on.)

UsageDetailed

console output

We can see the flow of calculation. We can check band energies, Fermi energies, whether sigm, rst are read.

save.foobar

- Save file record starting history of lmf,lmchk,lmfa. In addition, it give a line of total energies 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 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, we set ctrl.nio for NiO as

PROF

```
SITE    ATOM=Niup POS=  .0   .0   .0
        ATOM=Nidn POS= 1.0  1.0  1.0
        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
      EH=-1 -1 -1 -1  RSMH=1.06 1.06 1.06 1.06
      EH2=-2 -2 -2  RSMH2=1.06 1.06 1.06
      KMXA={kmxa}  LMX=3 LMXA=4 NMCORE=1
    ATOM=Nidn Z=28 R=2.12
      MMOM=0 0 -1.2 0
      EH=-1 -1 -1 -1  RSMH=1.06 1.06 1.06 1.06
      EH2=-2 -2 -2  RSMH2=1.06 1.06 1.06
      KMXA={kmxa}  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 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 O
4 5.380352 -0.000002  1.700000 O
```

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
```

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 set Antiferro symmetry (not yet for SOC=1).
We have README_AF.md and samples at ~/ecalj/Samples/AFsymmetry/
(README_mmtarget.aftest.txt showing 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`

PROF

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
~/ecalj/Samples/GdNldau
~/ecalj/Samples/ReNcub

BoltTrap

--boltztrap option is to generate files required for 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`
now with MaxlocWannier. going to move to MLO

Effective Screening Medium (ESM)

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

lmf and ctrl

See lmf and ctrl

gwsc and GWiput

See gwsc.
For GPU, see ecaljgpu and gwsc for GPU for ISSP together.
See explanation of GWinput.

getsyml: automatic symmetry line and BZ for band plot

See syml

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 getsyml.

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 maitained\dots

ecalj_auto

This is a suit of python script to run thousands of gwsc calculations.
ecalj_auto

background charge and fractional Z

backcround charge

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

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. So, it is better to use your own "simple criterion".
"Not stick to convergence so much. Just stick to Reproducibility."

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4f and 5f

Caution: For 4f and probably also for 5f systems, some special
care is required; just defaults ctrlgenM1 do not work.;
I think this is a little too old--> HowToSet4f_GdQSGW4.pdf
(I will revise this)
Except 4f systems, use default setting (just change k points).

Papers

It is instractive to reproduce samples in Deguchi paper[ecalj/Document/PAPERandPRESENTATION/deguchi2016.pdf].
We can set up templates for your calculations. Ask us.
We have latest paper at https://arxiv.org/abs/2506.03477 for GPU version, but show 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 ctrls.* (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 sigm = Sigma-Vxc^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 calculaiton 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 ...").

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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:
`~/ecalj/TestInstall/bin/diffnum QPU.3run QPU.6run`
is to compare two QPU files which contains QP energies.
(note: QP energies shown are calculated just at the begininig of iteration).

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

Another way is `grep rms lqpe*`. This gives rmsdel. Diffence 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 $V_{\rm xc}^{\rm QSGW}-V_{\rm xc}^{\rm LDA}$.
If sigm exists, lmf read it, and run self-consistent calculations
with adding sigm to the one-body potential.

See TableII 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
```

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This procedure makes self-consistency with keeping the sigm file. This may/(or may not) required. If you expect large obital 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 atteined.

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 `SO={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.