

# ecalj — Get statrted (aug2013)

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# 1 Introduction

“ecalj package” is for first-principle electronic structure calculations with unique features. Especially, as we explain in the next subsection, a main feature is in the quasiparticle self-consistent GW (QSGW) calculation based on the PMT method (=Linearized APW+MTO method).

## 1.1 Features of the ecalj package.

Generally speaking, central part in any electronic structure packages is the one-body problem solver. That is, how to calculate eigenvalues and eigenfunctions for given one-body potential. In turn, we can calculate one-body potential for given eigenfunctions and eigenvalues based on the density functional theory (DFT) in the LDA or GGA (hereafter LDA means both of LDA and GGA). Then we can make the electron density self-consistent by iterations until converged, and obtain total energy of ground state. We can also calculate atomic forces simultaneously. Based on such a solver, we can implement higher-level approximations such as the QSGW method, where we replace the exchange-correlation potential in DFT with that given by a GW method. In addition, kinds of physical properties, linear responses and so on, can be calculated.

Such one-body problem solvers (in the case of linear methods) are characterized by (i) linear combinations of what basis set give eigenfunctions; (ii) how to represent electron density and one-body potential. In the ecalj, we use the PMT method, which is an all-electron full potential method where we use not only the augmented plane waves (APW), but also the muffintin orbitals (MTO), in addition to the local orbital (lo). Within our knowledge no other methods allow us to use two kinds of augmented waves simultaneously. Thus eigenfunctions are represented by linear combinations of the APWs, MTOs, and the lo's. Then the electron density and the one-body potential are represented by “smooth part + onsite muffin-tin (MT) part - counter parts to remove smooth part within MTs. This part (Soler-Williams formalism) is essentially the same as that of the projected augmented wave method.

With ecalj, we can perform the GW calculation. The usual GW approximation is to obtain quasiparticle energies (QPE) by one-shot calculation starting from LDA; this is so-called “one-shot GW”. Its ability is limited; it can fail when its starting point (eigenfunctions and eigenvalues supplied by LDA) is problematic. Thus T.Kotani with collaborators have developed the QSGW method. The QSGW now becomes popular, performed by other researchers. In principle, results by QSGW do not depend on LDA anymore; the LDA are only used to prepare initial condition for self-consistency cycle of the QSGW calculation (however, exactly speaking, we use LDA to assist efficient implementation of QSGW, e.g. to prepare required radial functions).

Usually the QPEs obtained by QSGW reproduce experiments better than LDA. For example, the band gap by GGA for GaAs is about 0.5 eV in contrast to the experimental value of 1.6eV (If we virtually remove electron-phonon effect from the experimental value, it becomes about 1.7eV). On the other hand, the

QSGW predict about 1.9eV, slightly larger than experiment (for practical use, we sometimes add “scaling correction” on it to have better agreements with experiments). Even in the case of NiO and so on, QSGW gives not so bad results (it tends to give a little larger band gaps than experiments).

From QPEs and eigenfunctions obtained in QSGW, we can calculate dielectric functions and so on. But total energy in QSGW is still in research.

The ecalj package can also do other functions, LDA+U, atomic force and relaxation (in GGA/LDA), spin fluctuation, optical response and so on.

Recent development of dual-based MTO prescription allows us to use very localized MTOs (with damping factors  $\exp(-r/(1\text{a.u.}))$ ), together with APWs of low energy cutoff ( $\sim 3$  Ry). I think this is promising not only for efficient DFT/QSGW scheme, but also for kinds of applications in future. The MTOs can be used instead of the Wannier functions, but not so much research on it yet.

The QSGW calculation requires so much computational time: roughly speaking, it takes 10 or more times expensive than usual one-shot GW (but you can reduce computational time by choosing computational conditions). Thus the size of systems we can treat is about ten atom in a cell; computation requires about a week or so to have reasonable convergence. (heavy atoms require longer computational efforts, light atoms faster; we still have room to accelerate the method, but not yet so much. Minimum MPI parallelization is implemented). The computational effort is  $\propto N^4$ .

The ecalj web site is at

<https://github.com/tkotani/ecalj>

We can download ecalj package from this site. Free to download, modify, and use it, but we need you to clarify acknowledgement to the package in your publications; without it, we can not continue further developments. We also have a web site at <http://pmt.sakura.ne.jp/>, however, most of all are yet in Japanese and not yet well organized. The ecalj is related to lmv7 package at <http://titus.phy.qub.ac.uk/packages/LMTO/fp.html>. The lmv7 and ecalj are branched off at year 2009. After branched, major contributions are due to Takao Kotani and Hiori Kino (NIMS). All codes are now in f90, and we have simplified complications in the lmv7 code.

A manual on lmv7 may be a help to learn ecalj. But it may make you confused, because we have removed confusing parts from it, and simplified. Read this first. Then I show where we should read in the lmv7 manual.

If you have something, let [takaokotani@gmail.com](mailto:takaokotani@gmail.com) know it. With your ideas, we like to have collaborations and newer development on it. Or I may help something on it.

## 1.2 What is in this booklet?

Here we can show minimum on the ecalj package.

- How to perform self-consistent calculations by the density functional theory (DF) in the LDA
- How to perform the QSGW calculations.
- How to plot energy bands (BAND), total density of states (DOS), and the partial density of states (PDOS).
- How to plot dielectric functions, and non-interacting spin susceptibility  $\chi_0^{+-}$ . (not documented yet...)

To perform calculations becomes easier recently. After we prepare a crystal structure file named as `ctrls.*`, we run a script (`ctrlgenM1.py`) to generate `ctrl.*`. Its contains (not so bad) default setting to do calculations. To help writing `ctrls.*`, `ecalj` contains samples and a converter between VASP-POSCAR format and `ecalj-ctrls` format. (Thus we can use tools for VASP).

However, we may need to know a little more to obtain results for publications; some knowledge to judge whether obtained results are reasonable or not. And check convergence by some different conditions. Especially, results by QSGW need to be examined carefully. But, an advantage is that the QSGW code is version controlled and hosted by github, your results can be reproduced by others.

## 2 Install

Look into `ecalj/README`. (or you can see it at <https://github.com/tkotani/ecalj>). The installation is not do difficult (especially for gfortran, and ifort). After finished, we have all required binaries and shell scripts in your `/bin`. (or somewhere else where you specified at the bottom of Makefile.)

## 3 LDA calculations

Calculations are performed by following steps.

- Write `ctrls` file, “crystal structure file”, which contains crystal structure. It can be by hand, or convert it from POSCAR (in vasp). There is a tool to convert between POSCAR and `ctrls`. (`ecalj/StructureTool/README`). There is a checker, `lmchk`, to confirm the crystal structure is read well or not.
- Generate `ctrl` from `ctrls` by a script `ctrlgenM1.py`. `ctrl` is the main control file which contains all required information for calculations; as a part it contains `ctrls`. Then we we edit the generated `ctrl` file for your purpose.
- Do `lmfa` (just calculate atoms (MT sites) placed in the cell). It also calculate core eigenfunctions and valence charge for initial condition. And

start main calculation lmf successively. Then we get self-consistent result of LDA.

- Plot energy band, DOS, PDOS, by running scripts.

These `ctrls` and `ctrl` are with extensions as

```
ctrl.(id)
ctrls.(id)
```

. (id) is extension which we can add (only lower letter allowed). For example, `ctrls.cu`, `ctrls.lagao3`.

### 3.1 Write crystal structure file, `ctrls`

We have a sample of Cu in `~/ecalj/1m7K/TESTsamples/Cu/ctrls.cu`; it is

```
% const da=0 alat=6.798
STRUC  ALAT={alat} DALAT={da}
        PLAT=  0.0 0.5 0.5   0.5 0.0 0.5   0.5 0.5 0.0
SITE    ATOM=Cu POS=0 0 0
```

Another sample at `~/ecalj/1m7K/TESTsamples/GaAs/ctrl.gaas` is

```
#id  = GaAs
%const bohr=0.529177 a=5.65325/bohr
STRUC
        ALAT={a}
        PLAT=0 0.5 0.5   0.5 0 0.5   0.5 0.5 0
SITE
        ATOM=Ga POS=0.0 0.0 0.0
        ATOM=As POS=0.25 0.25 0.25
```

Lines starting from `'#'` are neglected as comment lines. Lines starting from `% const` define variables and set values (in these cases, `da` and `alat bohr`). Then the variable are used as `{alat}`; in the cu case, `{alat}` means 6.798. Lines not start from `"#"` nor `"%"` are main content in the `ctrls` file.

Note that we have two tags of “categories” `"STRUC"` and `"SITE"`. These tags should start from the first column. Thus `ctrls` is divided by multiple “categories”. In a category, we have “tokens” such as `ALAT`, `DLAT`, `PLAT`. These under `STRUC` category. `ALAT+DALAT` specify a unit to measure length in this `ctrl` file. These are in a.u. (= bohr radius=0.529177Å). We use `ALAT+DALAT` as unit to specify primitive vectors to specify unit cell. The unit cell is given by `PLAT` (`ALAT` as unit). In the above example, three primitive cell vectors specified by nine numbers after `PLAT=`; they give three primitive vectors; `PLAT1=(0,0,0.5)`, `PLAT2=(0.5, 0.0, 0.5)`, and `PLAT3=(0.5, 0.5, 0)`. `DALAT` is convenient to change lattice constant; but it is fixed to be zero here; thus no effect in this example.

Note that SITE category can have multiple ATOM tokens. The number of ATOM token under SITE should be the same as atoms in the primitive cell. In the case of GaAs; SITE contain multiple ATOM tokens. POS just next to ATOM is taken as subtokens under ATOM token. (this may looks slightly uncomfortable since the end of range of ATOM token is not so clear; but it is not a problem). In cases, we specify such subtokens as SITE\_ATOM\_POS.

In the SITE category, we place atoms (MT names) in the primitive cell. In these cases we use default atomic symbol (MT names) for ATOM. POS is in the Cartesian coordinate, but in the unit of ALAT+DALAT.

For your test, you may make a test directory and copy a ctrl.\* to your directory. If you have VESTA and ecalj/StructureTool installed, you can see its structure by

```
$ viewvesta ctrl.*
```

(here \$ means command prompt).

NOTE: As written in ecalj/README, you have to install VESTA and viewvesta. Then set VESTA= at the top of ecalj/Structure/viewvesta, and make softlink to it. The command `viewvesta(~/ecalj/StructureTool/viewvesta.py)` generate `POSCAR_cu.vasp` first, then send it to VESTA. `viewvesta` also accept `POSCAR_cu.vasp` directly. Except names starting from `ctrl` and `ctrls`, `viewvesta` sends the name to VESTA directly. VESTA requires extension '.vasp' to identify VASP format. We have samples in `~/ecalj/StructureTool/sample`. A tool `vasp2ctrl` converts `POSCAR.vasp` to `ctrls`. “--help” show a small help.

- ecalj/StructureTool/ is not tested well. Not believe it so much... We will fix it on your request.

Another example with atoms is `~/ecalj/lm7K/TESTsamples/SrTiO3/ctrls.srtio3`. This contains SITE category as

```
SITE
ATOM=Sr POS=1/2 1/2 1/2
ATOM=Ti POS= 0 0 0
ATOM=O POS=1/2 0 0
ATOM=O POS= 0 1/2 0
ATOM=O POS= 0 0 1/2
```

. Note that an expression  $1/2$  can be used for POS. As it show, we can use mathematical expression instead of values. Mathematical expressions such as “+ - \*/ sqrt(...)” are recognized. (instead of  $3 * 2$ , use  $3^2$ . You can use parentheses, but no space for separation). (After ctrl generated, there is a command `lmchk` to check whether atomic structure is correctly given or not.) We can use default atomic symbols (to check default atom name (MT name) type `ctrlgen2.py --showatomlist`). Instead of such default symbols, we can use your own symbol as

```

SITE
  ATOM=M1 POS=1/2 1/2 1/2
  ATOM=M2 POS= 0 0 0
  ATOM=O POS=1/2 0 0
  ATOM=O POS= 0 1/2 0
  ATOM=O POS= 0 0 1/2
SPEC
  ATOM=M1 Z=38
  ATOM=M2 Z=22
  ATOM=O Z=8

```

. Then we have to add extra category SPEC where we set Z number. (You can use Z=37.5 for virtual crystal approximation, however, you can not do it in ctrl. Edit it in ctrl file.)

We can see other samples in `~/ecalj/lm7K/TESTsamples/*/ctrls.*`. (we also have a sample generator. See later section.) Note that ctrl file is just in order to generate default ctrl file in the followings. Not from ctrl but from ctrl, we can start calculations. Thus ctrl is not necessary if we prepare ctrl file directly.

### 3.2 Generate default ctrl from ctrl by ctrlgenM1.py

To run programs of lm7K (lmfa and lmf) in PMT, we need an input file ctrl which contains many other settings. To generate ctrl from ctrl, we have a command "ctrlgenM1.py" (written in python 2.x and call fortran code internally). Two steps required to complete ctrl file: (i) we give reasonable options to invoke ctrlgenM1.py. This generate a ctrl file.; (ii) we need to edit the ctrl file afterwards for your calculation.

At first, try `ctrlgenM1.py` without arguments. It shows help. To generate ctrl from ctrl, type

```
$ ctrlgenM1.py cu --nk1=8
```

Here cu specify ctrl.cu. The option `--nk1=8` means the number of division of the Brillouin zone for integration. It means 8x8x8 division. If we like to use 8x8x4, we have to supply three arguments `--nk1=8 --nk2=8 --nk3=4`. The above command gives following console output.

```

$ ctrlgenM1.py cu --nk1=8
=== INPUT arguments (--help gives default values) ===
--help Not exist
--showatomlist Not exist
--nspin=1
--nk=8
--xcfun=vwn !(bh,vwn,pbe) 1
--systype=bulk !(bulk,molecule)

```



```
--insulator Not exist !(do not set for --systype=molecule)
```

```
...
```

OK! A template of ctrl file, ctrlgen2.ctrl.cu, is generated.

As we see above, options which you specified are shown at the begining of the cosole output (in this case `-nk1=8`). Others such as `-nspin=1` are default settings. If we like to perform spin-polarized calculations, we add other option '`-nspin=2`' as

```
ctrlgenM1.py cu --nspin=2 --nk1=8
```

(NOTE: In the spin-polarized case, we need to set initial condition of size of magnetic moment at each atoms: we have to edit SPEC\_ATOM\_MMOM of ctrl file (MMOM=s p d f ...) to be like MMOM=0 0 2. We will explain this later on). The ctrlgenM1.py generates ctrl file named as ctrlgenM1.ctrl.cu. To do calculations, copy it to ctrl.cu so that lmf recognize it.

```
cp ctrlgenM1.ctrl.cu ctrl.cu
```

### 3.3 crystal structure checker: lmchk

Do lmchk to confirm correct crystal structure is really given or not.

```
lmchk --pr60 cu
```

Then it reads ctrl.cu. `--pr60` is an option of verbose. Bigger number gives more informations.

- Lattice info, Space group symmetry operations (in lmf format), and their generators (these operations can be generated from a few of them.) See <http://titus.phy.qub.ac.uk/packages/LMTO/tokens.html#SYMGRPcat> about how to represent the operations.
- Show atomic positions. If rst.\* (this is generated after DFT calculation and relaxation) exists, it may show a position in rst.\* file (relaxed position). NEED to CHECK.
- Tabulate MT radius and distance between atomic sites.

### 3.4 ctrl file

The ctrl file generated by the ctrlgenM1.py contains explanations. Read it first. This is a head part of ctrl.cu generated by ctrlgenM1.py:

```
### This is generated by ctrlgenM1.py from ctrls
### For tokens, See http://titus.phy.qub.ac.uk/packages/LMTO/tokens.html.
### Do lmf --input to see all effective category and token ###
### It will be not so difficult to edit ctrlge.py for your purpose ###
```

```

VERS    LM=7 FP=7          # version check. Fixed.
IO      SHOW=T VERBOS=35 TIM=2,2
        # SHOW=T shows readin data (and default setting at the begining of
console output)
        # It is useful to check ctrl is read in correctly or not
        (equivalent with --show option).
        # larger VERBOSE gives more detailed console output.
SYMGRP find # 'find' evaluate space-group symmetry automatically.
        # Usually 'find is OK', but lmf may use lower symmetry
...

```

# means comment lines. We can also use lines start from % const ... to define variables and set constant.

We see “categories” such as **VERS** and **IO**, and so on. The begining of categories are starting from the first column. Under categories, we have ”tokens” such as **VERBOSE**. Thus we specify full name of token **VEROSE** under category **IO** as **IO\_VERBOSE**.

The ctrl file generated by ctrlgenM1.py contains explanations. Thus read them first. Here we give some complementary explanations to it.

- **IO\_TIM** is for debugging. It shows which subroutines are called and so on. Bigger number shows deeper subroutines.
- **SYMGRP** is a category without token under it; we set generators of space group (See explanation in previous paragraph). When we set **find**, it automatically calculate symmetry of crystal lattice. If we like to enforce symmetry, set some of generators which are shown by **lmchk**.
- We see **ctrls** is embedded in the **ctrl** by **ctrlgenM1.py**.

```

... (skip) ...
% const da=0 alat=6.798
STRUC  ALAT={alat} DALAT={da}
        PLAT= 0.0 0.5 0.5 0.5 0.0 0.5 0.5 0.5 0.0
        NL=4 NBAS= 1 NSPEC=1
SITE   ATOM=Cu POS=0 0 0
... (skip) ...

```

**NL**, **NBAS**(number of **SITE**) and **NSPEC**(number of **SPEC**) are automatically added by **ctrlgenM1.py**. It is possible to deform unit cell by adding optional tokens (it is possible to rotate **PLAT** for magnetic anisotropy calculation). See <http://titus.phy.qub.ac.uk/packages/LMTO/tokens.html#STRUCcat>. For new calculations, it is better to find some examples first.

- **SITE** category: As for MT sites, we have two categories. (1)**SPEC**(species) and (2)**SITE**(specify centers of atoms(species) in primitive cell) As for **SPEC**, we specify MTs(radius, Z, MTOs on it) appeared in the cell. These are defined subtokens under **SPEC\_ATOM=foobar** (we have multiple

SPEC\_ATOM=foobar). Then we place these SPEC\_ATOM=foobar at SITE sections.

At SITE, we specify atomic sites (What SPEC\_ATOM is placed to positions by POS) in a primitive cell. We set POS= by direct form (cartesian) but with the unit of ALAT+DLAT. Total number of SITE (number of tokens SITE\_ATOM) is the number of atoms in the primitive cell. SITE\_ATOM=foobar means we place foobar defined in SPEC\_ATOM=foobar. We set subtoken SITE\_ATOM\_POS under SITE\_ATOM, to specify atomic positions. In addition, we can set SITE\_ATOM\_RELAX, if you like to find relaxed structure (we simultaneously set DYN category) in LDA. As for relaxation, see LaGa0\_relax/ctrl1.lagao example, and read <http://titus.phy.qub.ac.uk/packages/LMT0/tokens.html#DYNcat>.

The SITE\_ATOM=foobar (with same foobar with different POS) are not necessarily equivalent with respect to the space group operation of a system. Thus SITE\_ATOM=foobar are divided into “classes” which are connected by the operation. The lmf automatically judge “classes” (see also infor by lmchk). Thus not need to specify it, but it may be better to check it. A sample is lmchk lagao at ~/ecalj/lm7K/TESTsamples/LaGa0\_relax

- **SPEC** category: In ctrls, we have not yet specified contents of SPEC; we have just given default symbols or only Z= when we use non-default names (shown by ctrlgenM1.py -showatomlist). The command ctrlgenM1.py adds default SPEC sections.

We have some SPEC\_ATOM, under which we give subtokens such as SPEC\_ATOM\_R(MT radius), SPEC\_ATOM\_Z(nucleus charge), cutoff parameters of angular momentum, and so on. These SPEC\_ATOM is referred to in SITE.

An example of SPEC category is

```
SPEC
  ATOM=Fe Z=26 R=1.70
    KMXA={kmtx} LMX=3 LMXA=4 NMCORE=1
    PZ=0,3.9,4.5
    EH=-1 -1 -1 -1 RSMH=0.85 0.85 0.85 0.85
    EH2=-2 -2 -2 RSMH2=0.85 0.85 0.85
    MMOM=0 0 2 0

  ATOM=... (then the similar block of ATOM= are repeated.)
  ...
```

Under the token ATOM=Fe, we have subtokens SPEC\_ATOM\_Z, SPEC\_ATOM\_R, and so on.

Subtokens Z= is the nucleus charge and R= MT radius. Note that Fe is just a name to distinguish MT sphere in the cell. If you set SPEC\_ATOM\_Z=27, it is recognized as Co (since Z=27). LMX=3 is the maximum l of MTOs.

Thus maximum  $l$  of MTO is  $l=3$ . The maximum of  $l$  to expand electron density and potential within MT is LMXA (in contrast to usual LAPW), we can use quite small LMXA such as LMXA=4. NMCORE=1 means we calculate core density without non magnetically-polarization. This can reduce computational confusion.

PZ is to set local orbital (if not, no local orbitals). EH and RSMH are to specify first set of MTOs. (We can check how local orbitals are set by lmf explained in the next section). EH2 and RSMH2 are to specify second set of MTOs.

After PZ=, we have three numbers. These are numbers for s,p,d,f,g,... channels. Zero means not exist. You can use space or , as delimiter. Here not only the integer part of principle quantum number, but also the fractional part should be supplied (If PZ=0,3,4, it does not work.) Now PZ=3.9 for p and PZ=4.5 for d. This means we use local orbital for 3p, and local orbital for 4d (fractional parts (continuous principle quantum number) are large  $\sim 0.9$  for core like orbital, and smaller for extended orbital  $\sim 0.3$  or something. See Logarithmic Derivative Parameters at <http://titus.phy.qub.ac.uk/packages/LMT0/lmto.html>). This is a little confusing, thus we will explain this in appendix. See Sec.??.

EH(damping factor), and RSMH (where the smooth Hankel function bent) determines MTOs. We now set four numbers for them. Thus we set MTOs s,p,d,f with EH=-1 and RSMH=0.85. Our current test shows that RSMH is one half of R (that is,  $0.85=1.70/2$ , but minimum RSMH is 0.5) and not need to be dependent on s,p,d,f. (If LMX=2, s,p,d are allowed and no f MTOs.) EH is -1; not need to change except test purpose. In a similar manner, EH2 and RSMH2 for second set of MTOs are given. Just three numbers means these for s,p,d.

MMOM=s,p,d,f... gives initial condition of magnetic moment in  $\mu_B$  (number of up-down electron).

In cases such as As, the local orbital given by default ctrl is responsible of rather deep core, and it is not need to be treated as valence electrons. In such a case, we don't need local orbital.

In the case of AntiFerro-II NiO, it contains two NiO in a primitive cell. Thus it is reasonable to have place two SPEC\_ATOM as Ni1 and Ni2, although subtokens under ATOM=Ni1 and ATOM=Ni2 (e.g. SPEC\_ATOM\_EH for them) are the same except initial condition of magnetic moment of MMOM=s,p,d,f... See example of NiO.

The minimum help of call Category\_token\_subtoken are listed with minimum explanation with

```
$ lmf --input
```

It gives a long output. But many of them are experimental and not need to touch them. A part of it is

Token	Input	cast	(size,min)
...	...		
STRUC_ALAT	reqd	r8	1, 1
	Scaling of lattice vectors, in a.u.		
...	...		

This is an minimu explanation of it. "reqd" means "required" (no default). r8 means it read with real number, 1,1 means that ALAT=xxx should contain one number minimum (max is also one) (See also STRUC\_PLAT, and so on).

There are kinds of examples in ecalj packages. Please look into their of ctrls.\* and ctrl.\* These are in lm7K/TESTsample/\* and ecalj/CMDsamples. In addition, ecalj/MATERIALS contain many samples; see a later subsection.

In anyway, we think it is very important to add examples which shows all the functions of ecalj package (not only materials but also to show its functions). It is not yet, but we will do in on your request.

As for what is shown in \$ lmf --input, most of important tokens are already described in the ctrl file generated by ctrlgenM1.py. So, we don't need to care many options shown by it. But we have not explained "STRUC category to defrom crystal, DYN category for dynamics, LDA+U treatment, Adding back-ground charge, Core-Hole treatments" here. We will prepare examples for it if requested.

<http://titus.phy.qub.ac.uk/packages/LMTO/tokens.html#STRUCcat>  
<http://titus.phy.qub.ac.uk/packages/LMTO/tokens.html#DYNcat>

### 3.5 Do LDA/GGA calculations, and get convergence

Here we show how to get converged results from a ctrl file.

At first, we need initial guess of charge density. It can be given by a super position of atomic charge density. To obtain the charge density, we solve atoms first. It is by

```
$ lmf gaas | tee llmfa
```

It takes just a few seconds. Here tee is a command of linux. It divide console output (standard output) to a file, and to console.

Then try

```
$ grep conf llmfa
```

. Then you see a key point that

```
conf:SPEC_ATOM= Ga : --- Table for atomic configuration ---
conf:  isp  1  int(P) int(P)z   Qval   Qcore  CoreConf
conf:    1  0      4  0      2.000   6.000 => 1,2,3,
conf:    1  1      4  0      1.000  12.000 => 2,3,
conf:    1  2      4  3     10.000   0.000 =>
```

```

conf:      1  3      4  0      0.000  0.000 =>
conf:      1  4      5  0      0.000  0.000 =>
conf:-----
conf:SPEC_ATOM= As : --- Table for atomic configuration ---
conf:  isp  1  int(P) int(P)z  Qval  Qcore  CoreConf
conf:      1  0      4  0      2.000  6.000 => 1,2,3,
conf:      1  1      4  0      3.000 12.000 => 2,3,
conf:      1  2      4  3     10.000  0.000 =>
conf:      1  3      4  0      0.000  0.000 =>
conf:      1  4      5  0      0.000  0.000 =>
conf:-----

```

This is an initial electron distribution, and how we divide core and valence. In this case core charge Qcore are (6 electron for s channel=1s,2s,3s and 12 electron for 2s and 3p). Core is not treated separately from valence electrons (frozen core approximation; we superpose rigid core density to make all-electron density). Qval means electrons for each s,p,d channels. The valence channels are 4s,4p,4d,4f (when we set EH=s,p,d,f). The int(P)z column is for local orbital. Thus we have 3d treated as local orbital. (our code can add one local orbital per l)

isp means spin (1 or 2), since -nspin=1 for Ga and As, no isp=2 exist. In summary we have 4s,4p,4d,3d,4f as valence. This means we use corresponding number of MTOs and local orbitals.

After lmf, let us start main calculation.

```
$ lmf cu
```

It might be better to do `$ lmf cu | tee lmf` in order to keep console output to lmf. As it is an iteration calculation, it shows similar output again and again. Then you end up with self-consistent result as

```

.....
it  8  of 30  ehf=  -3304.895853  ehk=  -3304.895853
From last iter  ehf=  -3304.895856  ehk=  -3304.895855
diffe(q)=  0.000003 (0.000007)  tol=  0.000010 (0.000010)  more=F
c ehf=-3304.8958531 ehk=-3304.8958529
Exit 0 LMF
CPU time:    7.024s    Mon Aug 19 02:03:19 2013    on

```

it 8 of 30 means it stops at 8th iteration, although we set maximum number of iteration 30. Note that this number is given by ITER\_NIT=30 in ctrl.cu). ehf and ehk are the ground state energy in Ry. They are calculated in a little different manner. Although they are different during iterations, it finally gets to be almost the same number. (but it can be different like 10 micro Ry per atom even converged. But you don't need to care it so much). ehk: Hohenberg-Kohn energy, ehf: Harris-Foulkner energy.

grep diffe lmf shows how the change of total energy (and charges) during iteration. diffe(q) means changes of energy with previous iteration, q is for

electron density difference as well. See also save.\* file, which only show ehk and ehk.

Thus we do have ground state energy. Although output of lmf is long, most of all are to monitor convergence. As long as it converged well, you don't need to look into it in detail. Eigenvalues are shown as

```
bndfp: kpt 1 of 4, k= 0.00000 0.00000 0.00000 ndimh = 122
-1.2755 -1.2008 -1.2008 -0.2052 -0.2052 -0.2052 -0.0766 -0.0766 -0.0766
-0.0174 -0.0174 -0.0174 0.1094 0.1095 0.1095 0.2864 0.2864 0.4170
0.4170 0.4736 0.6445 0.6445 0.6445
```

This is at  $k = 0.00000 \ 0.00000 \ 0.00000$ . (because of historical reason, two same bndfp: are shown in each iteration; two band path method). At, “lmf cu—grep -A6 BZWTS” shows the fermi energy (for insulator, we see band gap). Deep levels which gives little dependence on  $k$  are core like levels.

rst.\* contains is the main output which contains electron density. mix.\* is a mixing file (which keeps iteration history). When you restart lmf again, it read rst.cu and mix.cu. If you start from lmfa result, please remove them. (or lmf -help show option of -rs=(five numbers), how to read atm file which is the initial atom file by lmfa). We can do parallel calculation with lmf-MPIK, we can invoke it with mpirun -np 8 lmf-MPIK cu. It should give the same answer.

### 3.6 DOS, Band, PDOS plot

We already have script to plot dos and band from the result of lmf self-consistent calculations. At ~/ecalj/lm7K/TESTsmamples/\*, we have

```
job_tdos, job_band_nspin1, job_band_nspin2
```

. Read this script, and then you see how to plot energy bands.

For total DOS plot, it is better to check ctrl file; BZ\_TETRA=1 (this is default; thus make sure that BZ\_TETRA do not exist or BZ\_TETRA=1). In addition, we have to enlarge number of  $k$  point NKABC large enough. Then we do

```
job_tdos cu
```

This shows total DOS as

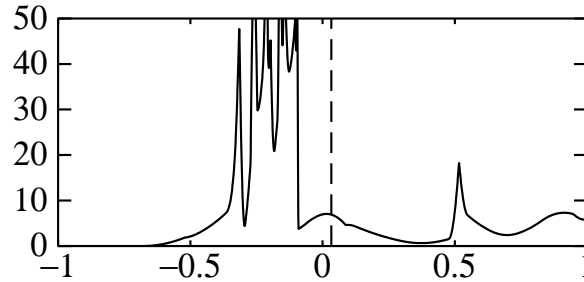


Figure 1: DOS(Cu)

For band plot, we have to set symmetry lines along which we plot eigenvalues. It is given in `syml`. `syml` also must have extension as `syml.cu`. Collections are in `ecalj/MATERIALS/`. Choose and modify one of them and rename it.

Here let us a sample in `syml.cu`.

```
$ cp ~/ecalj/lm7K/TESTsamples/Cu/syml.cu .
```

Thus we have `syml.cu` to your directory.

Look into `syml.cu`; it is

```
21  .5 .5 .5      0 0 0          L to Gamma
21   0 0 0      1 0 0          Gamma to X
0   0 0 0 0 0 0
```

First line means, we calculate eigenvalues for **k** points from **k**=(0.5,0.5,0.5) to **k**=(0,0,0). "L to Gamma" is just a comment since program only read seven numbers for each line. Second line means, we calculate eigenvalues for **k** points from **k**=(0,0,0) to **k**=(1,0,0). 3rd line means calculation just stop here. Units of **k** are in  $2\pi\text{ALAT}$ .

A line starting from '#' is neglected (comment line).

Do

```
job_band_nspin1 cu
```

is for `spin=1`. `job_band_nspin2` is for `spin=2` when it exist. (These scripts try to determine the Fermi energy first. You may skip it in cases.)

For PDOS plot,

```
job_pdos cu
```

It shows many figures in `gnuplot`. It is a little expensive because we use no symmetry to distinguish all `lm` channel in a simple manner. (PDOS is not yet implemented for `SO=1` case; spin-orbit coupling  $L\hat{S}$  is added.) We have to re-organize script of `gnuplot` (`pdos.site*.glt`) for your purpose. In principle, meanings of all data files are shown (see at the bottom of console output about `lm` ordering in a line), thus not so difficult to rewrite `*.glt`. For example, to plot `eg` and `t2g` separaely. (NOTE: site id is shown by `lmchk`).

**WARNING:** Usually `lmf` and so on recognize options such as `-vnspin=2` or something, where `nspin` is defined as `% const nspin=1` in `ctrl` file. The option overlaid `% const nspin=1`; replace it with `=2`; (this is shown as `save.*` file, and top of console output). However, `job_tdos` and so on, do not yet accept these options. Thus you may need to modify these command (we will fix it in future.)

### 3.7 Samples: `ecalj/MATERIAL/`

We have a material database in `ecalj/MATERIALS/`. At the directory, type

```
$ ./job_materials.py
```



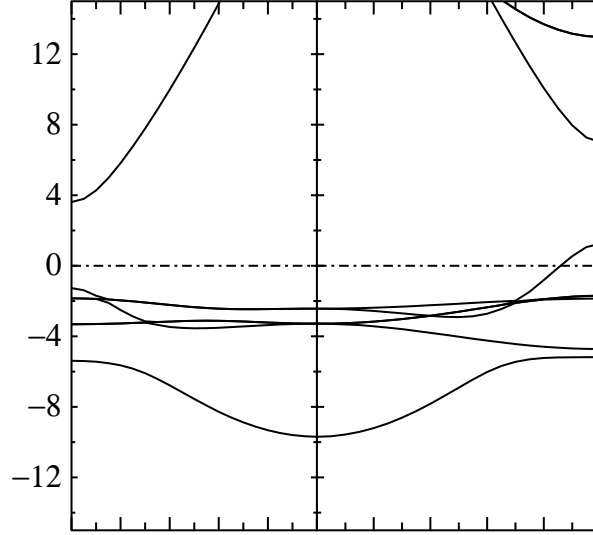


Figure 2: band plot(Cu)

Then it shows a help. You see

```
...
=== Materials in Materials.ctrls.database ===
  2hSiC 3cSiC 4hSiC AlAs AlN AlNzb AlP AlSb Bi2Te3 C
  CdO CdS CdSe CdTe Ce Cu Fe GaAs GaAs_so GaN
  GaNzb GaP GaSb Ge HfO2 HgO HgS HgSe HgTe InAs
  InN InNzb InP InSb LaGaO3 Li MgO MgS MgSe MgTe
  Ni NiO PbS PbTe Si SiO2c Sn SrTiO3 SrVO3 YMn2
...
```

. For these simple materials, input files will be generated. The ctrls are stored in `ecalj/MATERIALS/Materials.ctrls.database` (in addition, options passed to `ctrlgenM1.py` and options to `lmf-MPIK` are included). The command `./job_materials.py` gives `ctrls.*` for these materials based on the description in the `Materials.ctrls.database`. And then it generates ctrl file by calling `ctrlgenM1.py` internally, and run `lmfa lmf-MPIK` successively (when no `-noexec`).

For example, try `./job_materials.py Fe --noexec`. (not `fe` but `Fe` as it shown above). Then it makes a directory `Fe/` and set `ctrl.fe` (also `ctrls.fe`) in the directory. Without `'-noexec'`, it does calculation for `Fe` successively. As for `NiO` and `Fe`, we see that `./job_materials.py` gives `SPEC_ATOM.MMOM` in generated ctrl file.

Try `job_materials.py GaAs Si`.

Then directories `GaAs/` and `Si/` are generated. See `save.*` files containing total energies iteration by iteration. Starting from `ctrl.*` in these directory, the command perform DFT calculations (Console output is stored in `llmf`, `save.*` gives total energies. `rst.*` contains self-consistent density, from which we can calculate energy bands and so on).

`./job_materials --all --noexec` generates `ctrls` and `ctrl` files of these materials. `./job_materials --all` do self-consistent LDA calculations for materials (it takes an hour or more. Change the number of cores for MPIK in the script(search `lmfjob`) if you like).

To make band plot and so on for Fe,

```
$ ./job_materials.py Fe (and need to type return)
```

```
(If you like start over, remove Fe/ under it first).
```

```
$ cd Fe
```

```
$ ./job_materials.py fe
```

(but it might be better to do `--noexec`, and observe `Fe/ctrls.fe` and `Fe/ctrl.fe` first. `grep conf llmf` shows the initial electron distribution).

```
$ cat save.fe (this shows total energies of each iteration. 'c' at  
the first column gives converged result. 'h' is from atm file.)
```

If it does not ends with `'c ...'` line, something strange occurs. see `llmf` (console out put of `lmf` is saved to `llmf`).

```
$ cp ../syml.fe .
```

```
$ job_band_nspin2 fe
```

(As I said, this shell script do not yet accept options to `lmf`. Look into the script).

(This calculate fermi energy first for safe; it takes some time)

```
$ job_tdos fe
```

```
$ job_pdos fe (as I said, this supress space-group symmetry, thus time consuming).
```

Then it shows a help. See `joblmf` file also (it contains options to invoke `lmf`. This is shown in `save.*`. In principle, options in `joblmf` should be passed to band plot and so on. But not yet implemented (it is not so difficult).

## 4 QSGW calculation

The QSGW calculation requires to calculate “non-local exchange-correlation potential  $\Sigma_{xc}$ ” (it may be better to say static version of self-energy), which is calculated by GW calculation. Then  $\Sigma_{xc} - V_{xc}^{LDA}$  is stored into **sigm** file. Then, we calculate one-body calculation by lmf (or lmf-MPIK) where we add sigm to one-body potential. This iteration cycle is performed by a script “gwsc” as we explain later on.

### 4.1 GWinput

Let us start from ctrl.s.i as

In order to perform QSGW, one another input file **GWinput** is necessary in addition to **ctrl**. Thus all input files for QSGW is just two files, **ctrl.\*** and **GWinput**. A template **GWinput** can be generated by a script **mkGWIN\_lmf2**. You may have to modify it in cases for your purpose.

Let us start from ctrl.s.i;

```
#id = Si
%const bohr=0.529177 a= 5.43095/bohr
STRUC
    ALAT={a}
    PLAT=0 0.5 0.5 0.5 0 0.5 0.5 0.5 0
SITE
    ATOM=Si POS=0.0 0.0 0.0
    ATOM=Si POS=0.25 0.25 0.25
```

. Do “ctrlgenM1.py si -tratio=1.0” and rename ctrlgenM1.ctrl.s.i to ctrl.s.i. (-tratio=1.0 means touching MT (check it by lmchk); it is probably slightly advantageous in our version of GW calculation). Let us invoke **mkGWIN\_lmf2** as follows.

```
$ lmfa si (lmfa is needed to do in advance).
$ mkGWIN_lmf2 si
.....
== Type three integers n1 n2 n3 for Brillouin Zone meshing for GW! ==
n1=
```

Then it pause and ask numbers. You have to type three numbers as 2+ return + 2+return+2 return.

```
== Type three integers n1 n2 n3 for Brillouin Zone meshing for GW! ==
n1= 2
n2= 2
n3= 2
2 2 2
```

...(skip)...

OK! GWinput.tmp is generated!

Generated file is GWinput.tmp; you have to copy it to GWinput.

```
$ cp GWinput.tmp GWinput
```

These '2 2 2' you typed is reflected in a section 'n1n2n3 2 2 2' in GWinput. You can edit it, and change it to e.g. 'n1n2n3 4 4 4' if you like to calculate self-energy on dense BZ mesh. (QPNT.chk contains irreducible k point for given n1 n2 n3; KPTKPTin1BZ.gwinit.chk contain all k points in Brillouin Zone). Generally speaking, you don't need to repeat mkGWIN.lmf2 as long as you don't change MTO sections in ctrl file (number of EH,EH2,PZ).

Look into GWinput. Because of historical reason, input system is different from ctrl. Each line is independent; "keyword" followed by some of numbers (or on or off for logical switch of keyword). Except such lines, there are tag sandwiched sections such as <PRODUCT\\_BASIS> ... </PRODUCT\\_BASIS>, no comment lines in the middle allowed. They are read by read(\*,\*) (thus spaces cause no problem).

In the QSGW calculation, we have to set some cutoff parameters for self-energy calculations.

- **emax\_sigm** is the maximum limit of the self-energy (measured from the Fermi energy). I think  $2.5 \sim 5R_y$  is reasonable choice. But in cases, small **emax\_sigm** can give poor dispersion curve (slightly unnatural behavior) because of sudden cutoff by **emax\_sigm**. However, we like to use smaller value to reduce computational time. That is, larger is better, but expensive. Generally speaking, accuracy less than 0.1eV (for bandgap) is allowance of current method. Probably, it may be not impossible to have better accuracy, but it may ask us to repeat many calculations with changing conditions to confirm stability.
- **0.100000D-02 ! =tolopt** controls a number of Product basis to expand the Coulomb interaction. (The product basis is to expand the Coulomb interaction is different from the basis to expand eigenfunction.) In our experience, **0.100000D-02 (=0.001)** is not so bad. If you like to reduce computational time use 0.01 or so, but a little dangerous in cases. With 0.0001, we can check stability on it.
- **QGcut\_psi** is a little (usually 0.5 or so) larger than **QpGcut\_cou**. It becomes accurate if we use large **QpGcut\_cou**. But it enlarge size of IPW(interstitial plane wave) part of Mixed product basis. For test, try 2.7, 3.2, 3.7 for **QGcut\_cou** (and add 0.5 or 1 for **QGcut\_psi**). Larger one is expensive.
- **dw** and **omg\_c** specify real space bins which we accumulate imaginary part weight of polarization functions. **dw** is bin width (in  $R_y$ ) at  $\omega=0$ , then bin width is twiced at **omg\_c**. The bin width is quadratically larger

(become rough). If bins are too wide, dielectric function can be less accurate, but results are not necessarily so much affected. For metal, our code can capture Drude weight numerically. We do not need to be so sensitive to the choice of them usually.

- `n1n2n3`: BZ division for k point integration. We usually take '4 4 4' to '8 8 8' for GaAs. For metal such as Fe, '10 10 10' or more is better.
- `lcutmx(atom)` is the l cutoff of product basis for atoms in the primitive cell (do `lmchk` for atom id). In the case of Oxygen, we can usually use `lcutmx=2` (need check by the diffence when you use `lcutmx=2` or `lcutmx=4`). Then the computational time is reduced well.
- Other part of product basis section in `<PRODUCT\_BASIS> . . . </PRODUCT\_BASIS>` is usually not need to be touched. But if you like to calculate big systems with smaller CPU time, or do very accurate calculations, we may need to touch it. It is described elsewhere.
- `<QPNT>` tag is to specify one-shot GW. At which point, do we calculate QPE, not for QSGW. If you set k point in it not on regular mesh point, you have to set 'Any Q on'; but it is expensive. Since QSGW have ability to plot energy band within full BZ, it should be better to do it.
- `<QforEPS>` and `<QforEPSL>` are to specify at which k point do we calculate susceptibility. It is for `epsPP_lmfh`, `eps_lmfh` (dielectric functions) and `epsPP_chipm` (spin susceptibility).

We need a setting in ctrl file to read sigm file (HAM.SIGP). It is simplified now, and not need to care it so much. As we set `RDSIG=12` in defaults, lmf read sigm file and add it to one-body potential as long as `sigm.*` exist.

**NOTE for old users:** We now set `SIGP[MODE=3 EMAX=9999.]` in ctrl file to read self-energy in lmf (or lmf-MPIK). This is because we use very localized MTOs (similar with the Maxloc Wannier). Our test shows reasonable results and this simplify algolisms. In my previous version, we asked you to use `SIGP[MODE=3 EMAX=2.0]` where EMAX is a little (0.5Ry) less than `emax_sigm`. If something strange occurs, try this setting).

In principle, QSGW result should not depended on the choice of XCFUN. However, it can affect slightly. In our tests, it seems slightly better to use `vwn` (`XCFUN=1`) for QSGW calculations. (BUT need to check more...)

## 4.2 do QSGW calculation

Let us perform QSGW calculation. Fot this purpose, we use a script `gwsc`.

```
gwsc (number of iteration+1) -np (number of nodes) (id of ctrl)
```

If (number of iteration+1)=0, it gives one-shot calculation from LDA. But it is different from the usual one-shot in literatures; since it calculates off-diagonal elements of self-energy also, we can plot energy band dispersion plot. In cases (such as usual semiconductors), it gives rather reasonable results in comparison with experiments from practical point of view.

This is an example of one iteration of QSGW cycle. (now a little different but essentially similar)

```
takao@TT4:~/ecalj/test1$ gwsc 0 -np 2 si
gwsc 0 -np 2 si
### START gwsc: ITER= 0, MPI size= 2, TARGET= si
--- No sigm nor sigm.$TARGET files for starting ---
---- goto sc calculation with given sigma-vxc --- ix=,0
No sigm ---> LDA calculation for eigenfunctions
      Start mpirun -np 2 /home/takao/ecalj/TestInstall/bin/lmf-MPIK si > llmf_lda
OK! --> Start echo 0| /home/takao/ecalj/TestInstall/bin/lmfgw si > llmf_gw0
OK! --> Start echo 1| /home/takao/ecalj/TestInstall/bin/qg4gw > lqg4gw
OK! --> Start echo 1| mpirun -np 2 /home/takao/ecalj/TestInstall/bin/lmfgw-MPIK si> llmf_gw01
OK! --> Start /home/takao/ecalj/TestInstall/bin/lmf2gw > llmf2gw
OK! --> Start echo 0| /home/takao/ecalj/TestInstall/bin/rdata4gw_v2 > lrdata4gw_v2
OK! --> Start echo 1| /home/takao/ecalj/TestInstall/bin/heftet > leftet
OK! --> Start echo 1| /home/takao/ecalj/TestInstall/bin/hchknw > lchknw
OK! --> Start echo 3| /home/takao/ecalj/TestInstall/bin/hbasfp0 > lbasC
OK! --> Start echo 3| mpirun -np 2 /home/takao/ecalj/TestInstall/bin/hvccfp0 > lvccC
OK! --> Start echo 3| mpirun -np 2 /home/takao/ecalj/TestInstall/bin/hsfp0_sc > lsxC
OK! --> Start echo 0| /home/takao/ecalj/TestInstall/bin/hbasfp0 > lbas
OK! --> Start echo 0| mpirun -np 2 /home/takao/ecalj/TestInstall/bin/hvccfp0 > lvcc
OK! --> Start echo 1| mpirun -np 2 /home/takao/ecalj/TestInstall/bin/hsfp0_sc > lsx
OK! --> Start echo 11| mpirun -np 2 /home/takao/ecalj/TestInstall/bin/hx0fp0_sc > lx0
OK! --> Start echo 2| mpirun -np 2 /home/takao/ecalj/TestInstall/bin/hsfp0_sc > lsc
OK! --> Start echo 0| /home/takao/ecalj/TestInstall/bin/hqpe_sc > lqpe
OK! --> == 0 iteration over ==
OK! --> Start mpirun -np 2 /home/takao/ecalj/TestInstall/bin/lmf-MPIK si > llmf_gwscend.0
OK! ==== All calculation finished for gwsc 0 -np 2 si ====
```

Here `echo (integer)` is read in at the beging of the code. To see it, please look into gwsc script (gwsc is at ecalj/fpgw/exec/ and copied to your bin/ by make install2). In anyway, this console output shows calculations finished normally.

Now we get `rst.si` and `sigm.si` file which contains (static version of) self-energy minums  $V_{xc}^{LDA}$ . What we did is the one-shot GW from LDA result; but note that we calculate not only diagonalelements but also off-diagonal elements.

We can write energy dispersion (band plot) in the same manner in LDA. To do it, we need `rst.si`, `sigm.si`, `ctrl.si`, `QGpsi`, and `ESEAVR`. (but `QGpsi` and `ESEAVR` are quickly reproduced). After you have `syml.si` (e.g. in ecalj/MATERIALS/),

Do

```
$ job_band_nspin1 si
```

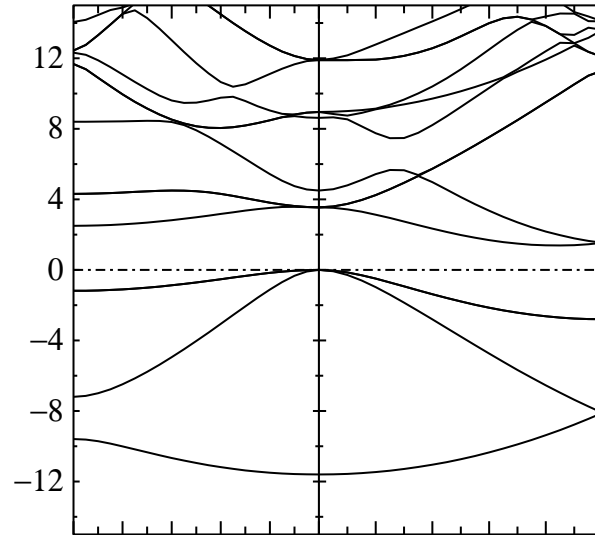


Figure 3: Si, one-shot GW with off-diagonal elements

You can observe large band gap as shown in the Fig.4.2. (To see it again, `gnuplot bnds.gnu.si -p`. All plots are in gnuplot, thus it is easy to replot it as you like).

We have QPU file (and also QPD for spin=2), which contains content of the diagonal part of self-energy. It will be explained elsewhere.

You can make total DOS and PDOS plot by

```
$ job_tdos si
$ job_pdos si
```

CAUTION:pdos plot is not allowed for so=1. (even tdos-*l* ask to t.kotani.)

To get final QSGW results, we have to repeat iteration until eigenvalues are converged. Note that total energy shown by console output `llmf` (and also shown in save file) is not so meaningful in the QSGW; we just take it as an indicator to check convergence. Let us repeat 5 iteration more. "`-np 2`" means one core to use.

```
$ gwsc 5 -np 2 si
### START gwsc: ITER= 5, MPI size= 2, TARGET= si
--- sigm is used. sigm.$TARGET is softlink to it ---
---- goto sc calculation with given sigma-vxc --- ix=,0
we have sigm already, skip iter=0
---- goto sc calculation with given sigma-vxc --- ix=,1
```

...(skeip here) ...

```
mpirun -np 2 /home/takao/bin/hsfp0_sc < _IN_ > lsc
```

OK

```
/home/takao/bin/hqpe_sc < _IN_ > lqpe
```

OK

5 iteration over

```
mpirun -np 2 /home/takao/bin/lmf-MPIK si > llmf_gwscend.5
```

Note that we do skip 0th iteration (it is for one-shot from LDA) since we start from `rst.si` and `sigm.si` given by one-shot LDA. Thus we do just five iterations. Infomation of eigenvalues are in `QPU.(number)run` files. (for magnetic systems with `nspin=2`), wee have `QPD.(number)run` also). Check it by `ls`;

```
$ ls QPU.*run
```

```
QPU0.run  QPU.1run  QPU.2run  QPU.3run  QPU.4run  QPU.5run
```

(These are overwritten when we again repeat `gwsc`; be careful.) Note that `QPU0.run` was old one when you did 1-shot GW from LDA at the begining.

In order to check convergece calculations going well, do

```
$ grep gap llmf*
```

This shows how band gap changes in `llmf.*run` files.

Let us check convergence of the QSGW calculations. For this purpose, it is convenient to take a difference of `QPU(QPD)` files by a script `dqpu`. These files are human readable. To compare `QPU4.run` and `QPU5.run`, do

```
$ dqpu QPU.3run QPU.4run
```

Then we see a list of numbers (these are the differences of values in `QPU` files). Then it shows at the bottom as

```
Error! Difference>2e-2 between:  QPU.4run  and  QPU.5run
:  sum(abs(QPU-QPD))= 0.05736
```

but you don't need to care it so much. You rather need to check the difference of values. I can say most of all difference (especially around the fermi energy are ) are almost 0.00eV or 0.01eV, we can judge QPEs are converged. If not converged well, you may need to repeat `gwsc` again. (when the size of two `QPU` files are different, `dqpu` stops.)

## 5 calculation of dielectric function

eps mode.



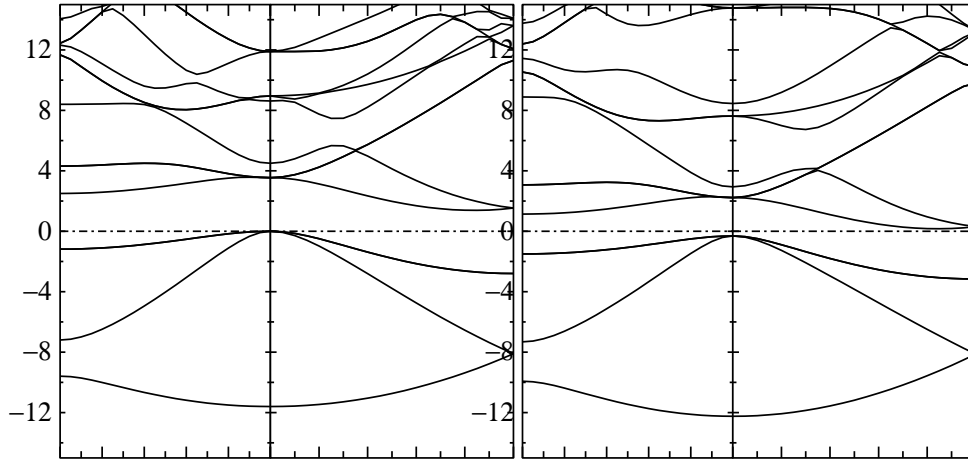


Figure 4: band plot(Si, QSGW one-shot test) and band(Si) (GGA)

## 6 Appendix

### 6.1 appendix 1; How to add spin-orbit coupling

Do LDA and/or QSGW with SO=0 first.

Then apply the spin-orbit coupling by perturbation.

After converged with nspin=1 (or 2), create new directory and copy

ctrl.gas, rst.gas, sigm.gas, QGpsi, ESEAVR

to it. Then we set

nspin=2

METAL=3

SO=1 (this is ldots calculation off-diagonal elements included).

Q=band (we do not change potential.)

in ctrl.gas.

Then run

>lmf gas >& llmf\_SO

You can see "band gap with SO" by

> grep gap llmf\_SO.

Then you can see two same lines.

VBmax = 0.101949 CBmin = 0.236351 gap = 0.134402 Ry = 1.82786 eV

VBmax = 0.101949 CBmin = 0.236351 gap = 0.134402 Ry = 1.82786 eV

(two lines are because of two-band path mechanism,  
which asks less memory usage than a path mehod)

This is the band gap with SO as a first-order perturbation starting on  
top of the "QSGW without SO". When you use ctrl file generated by  
ctrlgenM1.py. You can do the above procedure with

>lmf --rs=1,0 gas -vnit=1 -vso=1 -vnspin=2 -vmetal=3 --quit=band)

(--rs=1,0 read rst.gas but not write rst.gas. Ses lmf --help

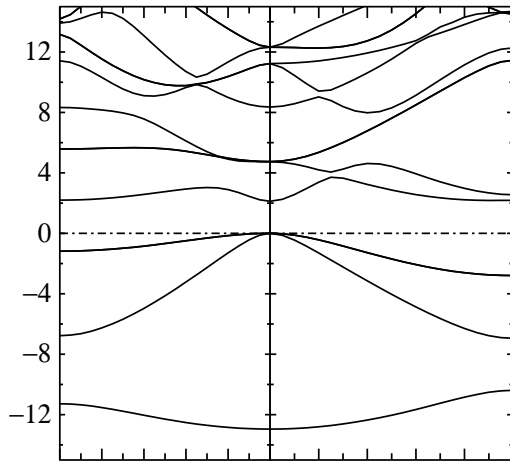


Figure 5: band(GaAs), QSGW (test case)

`-vso=1` replace the setting of `% const so=0` with `so=1`).

For band plot, you can use the same procedure for the case without SO. (Look into the `job_band_nspin1` script. You have to modify it so that `--rs=1,0 gas -vnit=1 -vso=1 -vnspin=2 -vmetal=3 --quit=band` is added as arguments for `>lmf --band:sym1 ...`).

---

For given `sigm` file, it is possible to do full self-consistent SO calculations (then we do not set `Q=band`). However, note that `Vxc` is fixed in QSGW, it is not necessary better than the above procedure.

## 6.2 appendix 2: How to set local orbitals

As we stated, do `"lmfa |grep conf"` to check used MTO basis.

We have to set `SPEC_ATOM_PZ=` (they ordered as `PZ=s,p,d,f,...` ) to set local orbitals.

Continious principle quantum number is defined as

$$P = \text{principleQuantumNumber} + 0.5 - \text{atan}(1/\phi \, d\phi/dr)$$

Its fractionanl part  $0.5 - \text{atan}(1/\phi \, d\phi/dr)$  is closer to unity for core like orbital, but closer to zero for extended orbitals.

There are the free electron value for  $P$

(in the case of constant potential,  $\phi = r^{(l+1)}$ ).

They are shown in 'pfree' in console output. These numbers are  
1.500000

2.250000  
 3.147584 0.147584=0.5-atan(2+1)  
 4.102416  
 5.077979

Examples of choice:

Ga p: in this case, choice 0 or choice 3 is recommended.

We usually use lo for semi-core, or virtually unoccupied level.

(0)no lo (4p as valence is default treatment without lo.)

3p core, 4p valence, no lo: default.

Then we have choice that lo is set to be for 3p,4p,5p.

(1)3p lo ---> 4p val (when 3p is treated as valence)

3d semi core, 4d valence

Set PZ=0,3.9

(P is not required to set. \*.9 for core like state. It is just an initial condition.)

(2)4p lo ---> 5p val (we don't use this usually. this is for test purpose)

4p lo, 5p valence

Set PZ=0,4.5 P=0,5.5 (In this case, set P= simultaneously).

(NOTE: zero for s channel is to use default numbers for s)

(3)5p lo ---> 4p val (PZ>P)

Set PZ=0,5.5

5.5 is just simply given by a guess. If 5.2 or something, it may fails

because of pooriness in linear-dependency. We may need to observe

results should not change so much on the value of PZ.

Ga d: (in this case, choice 0 or choice 1 is recommended).

(0)no lo (3d core, 4d valence, no lo: default.)

Then we have choice that lo is set to be for 3d,4d,5d.

(1) 3d lo ---> 4d val (when 3d is treated as valence)

Set PZ=0,0,3.9 (P is not required to set)

(2) 4d lo ---> 5d val (this is for test purpose)

Set PZ=0,0,5.5 P=0,0,4.5

(NOTE: zero for s,p are to use default numbers )

(3) 5d lo ---> 4d val (PZ>P)

Set PZ=0,0,5.5

If you like to read from atm.ga file instead of rst file(if exist).

You have to do lmf --rs=1,1,0,0,1, for example. See lmf --help

Because rst file keeps the setting of MT0, thus change in ctrl is not reflected without the above option to lmf.

=====

## 7 MEMO random

These are memo randoms. We will detail it. Ask me if you have questions.

xxx underconstruction xxxxxxxxxxxxxxxxx

== not meaningful total energy ==

Total energy shown in QSGW mode in current version is not meaningful.  
(just treat as an indicator to convergence).

== Do we use vwn or gga for QSGW? ==

In principle, QSGW results should not depend on vwn or gga  
(XCFUN=1 or 103 in ctrl). But there is minor dependence, because

1. frozen core density.
2. core eigenfunction.
3. radial basis functions
4. Slight numerical reason

(This is probably because Sigma-interpolation procedure

But not exactly figured out yet

-->affect about 0.02eV as for band gap for GaAs. ).

In anyway, use vwn (HAM\_XCFUN=1) as standard.

And such technical things affects, 0.05 eV level of error for band gap.

== one shot QSGW ==

one-shot QSGW may be useful in cases.

As it contains off-diagonal part, we can resolve band tanglement  
problem in Ge (no band gap).

== Restart calculation in lda ==

lmf(lmf-MPIK) read rst.\* in default.

rst contains electron density.

If rst is already converged, it stops after two iteration.

rst contains atomic positions.

So, in order to read atomic positions change in ctrl,

Use options shown in lmf --help.

== Restart calculation in qsgw ==

To remove mixsigm\* (mixing for sigm), maybe required.

== iteration check ==

First, watch console output of gwsc (do redirect to output file)

Need to check OK! signs arrayed on 1st columns.

gwsc iteration is time consuming,

So we need to check calculations are normally going on or not.

Memory inefficiency.  
 Set 'KeepEigen off' and 'KeepPPOVL' off.  
 In fact, our code is still inefficient for memory usage.

grep gap llmf ---> minimum gap at mesh point.  
 see save.\* , or grep '[xc]' save.\*  
 the end of iteration of lmf is shown as x or c.  
 (if failed, QPU file.  
 dqpu QPU.4run QPU.3run  
 As for usual semi-conductor, accuracy about 0.1 eV is limit of current implementation.  
 Set vwn (xcfun=1) looks better (stable) for GW.

== emax cutoff for APWs. ==  
 We can not use so many APWs in current version,  
 because of overcompleteness (this is because null vector within MTs),  
 In anyway, use pwemax=3 as standard (test it with 4 or 5).  
 To avoid failure of calculation, we may use smaller MT radius for  
 alkali, and alkali-earth elements.

== Check Used MTO  
 Near begining of console output, what MTO you use is shown as: (GaAs case).  
 sugcut: make orbital-dependent reciprocal vector cutoffs for tol= 1.00E-06

spec	l	rsm	eh	gmax	last term	cutoff
Ga	0*	1.13	-1.00	6.579	1.19E-06	1459
Ga	1*	1.13	-1.00	7.028	1.26E-06	1807
Ga	2*	1.13	-1.00	7.475	1.09E-06	2109
Ga	3	1.13	-1.00	7.920	1.06E-06	2637
Ga	0*	1.13	-2.00	6.579	1.19E-06	1459
Ga	1*	1.13	-2.00	7.028	1.26E-06	1807
Ga	2	1.13	-2.00	7.475	1.09E-06	2109
As	0*	1.18	-1.00	6.300	2.13E-06	1243
As	1*	1.18	-1.00	6.720	1.26E-06	1471
As	2*	1.18	-1.00	7.140	1.37E-06	1837
As	3	1.18	-1.00	7.558	1.05E-06	2229
As	0*	1.18	-2.00	6.300	2.13E-06	1243
As	1*	1.18	-2.00	6.720	1.26E-06	1471
As	2	1.18	-2.00	7.140	1.37E-06	1837

== gwsc cause error stop.  
 Have you ever changed MTO setting? Consistent with GWinput?

== QSGW for Fe.  
 It is better to use 3p as core. Furthermore, 3d+4d as valence is better.  
 Thus we need to set PZ=0,3.9,4.5  
 I also got aware that emax\_sigm should be large enough ( $4\sim 5$  Ry)

to have smooth band dispersion.  $n_1n_2n_3$  can be  $10 \times 10 \times 10$ .

== RSRNGE: enlarge RSRNGE ==

Use RSRNGE=10 or so (in cases, RARNGE=20 or more is required),  
for large number of k points. Try and enlarge it if it fails with a  
message "Exit -1 rdsigm: Bloch sum deviates more than allowed tolerance (tol=5e-6)".  
We will have to make it automatic in future.

== QOP check

In cases, it is better to use QOPchoice=2 instead of default QOPchoice=1.  
(For slabs, QOPchoice=2 may be better; need check more. In anyway,  
it is problematic to use unbalanced k points for anisotropic cell).

== EPS mode,

Check Im part of  $\chi_0$  is smoothly damping at high energy (typically  
1Ry or larger energy range). If there is some large Im part remains,  
something strange (usually due to orthogonality problem of  
eigenfunctions when you set low q).

Related source codes are in ecalj/lm7K/ .

A command ecalj/lm7K/ctrlgenM1.py can generate 'standard input file (ctrl file)'  
just from a given crystal structure file called as ctrls file.  
Binaries are lmf and lmf-MPIK (MPI k-parallel version).

Recently, I renewed some part of algorithm of GW/QSGW calculations  
(some ideas are taken from PRB.81,125102(2010)  
and Computer Physics Comm. 176(2007)1-13).

---> this is better than old versions; speed, memory (file size),  
and accuracy for anisotropic systems.

For comparison, you can use old version in .git (gitk --all and check it out).

=== When calculation in LDA level fails ===

when calculation fails in LDA level.

- (1) smaller MT
- (2) fewer PW. smaller pwemax.
- (3) core as semicore.