

# gwsc: a script to run QSGW calculation

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gwscがQSGW計算実行スクリプトである。

QSGW計算は、複数のfortran実行ファイル呼び出して実行される。

ファイルGWinputが読み込まれる。

## Usage

**Usage:** gwsc -np NP [-np2 NP2] [--phispinsym] [--gpu] [--mp] nloop extension  
[Options]

-np NP

MPI並列数を指定する。

-np2 NP2

GPU版を使用する場合のみ指定する。GPUで実行される計算のMPI並列数を指定する。

通常は使用できるGPU数を指定する。

--gpu

GPU版を使用する場合のみ指定する。

--mp

GPU-MP版(混合精度)を使用する場合のみ指定する。計算精度に注意すること。

nloop

QSGWのイテレーション数を指定する。

extension

ctrl ファイルの拡張子を指定する。

## Options

追加のオプションを指定する。

追加オプションは、全ての実行ファイルの実行時引数となる。以下追加のオプションのリスト。

またlmfへのオプション-vsoc=1などもここに書く。

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--keepwv

--gpu を指定した場合に自動で付け加わる。

自己エネルギー(関連部分)を計算する際に、遮蔽クーロン相互作用の行列要素をメモリ上に保持する。

GPU計算ではファイルIO, データ転送が特に律速になるが, それを回避するため, ただし十分なGPUおよびCPUメモリが必要となる.

### --nb=X

- Xは整数 --nb=4のように指定する。  
遮蔽クーロン相互作用(W)計算hrcxq or hrcxq\_gpu で使用される。分極関数のMPB基底並列数を指定する。  
GPU計算においてhrcxq(\_gpu)計算でメモリ不足になる場合に使用する。--np2 で指定した並列数を割り切れる値を入れる必要がある。

### --nwpara=X

- Xは整数 --nwpara=2のように指定する。  
相関部分の自己エネルギー計算hsfp0\_sc --job=2 or hsfp0\_sc\_gpu --job=2 で使用される。 $\omega$ 積分の並列数を指定する。  
--keepwv 使用時(GPU版ではデフォルトで使用される) \_\_WVR.X (X=1,...)ファイルがメモリに乗りきらずメモリ不足になる場合に使用する。  
--np2 で指定した並列数を割り切れる値を入れる必要がある。

### --tetwtk

指定すると, 分極関数を計算する際に, 結合状態間の四面体重みをメモリ上に保持しない。 $k$ 点が多い計算でメモリ不足になる場合に使用する。

### --skipGS

lmf --jobgw=1 で使用される。

GW計算ではDFT計算(lmf)で得られた波動関数をlmfとは異なる基底関数で展開しなおす。再展開後の波動関数についてGram-Schmidt正規直行化をしている。その規格直交化をスキップする場合に指定する。

通常は指定する必要はないが, lmf --jobgw=1計算が遅い場合には指定することによって計算の高速化が期待される。

- ecaljでは有限のqで誘電関数が計算できる—このとき分母分子のキャンセレーションが起こるため、波動関数の直行性が正確である必要があり、そのときには--skipGSを使うべきでない。

### --normcheck

lmf --jobgw=1 で使用される。GW計算で使用する波動関数の規格直交性を確認したいときに使用する。

normchk.fobar は

```
> head -20 normchk.si
#      IPW      IPW(diag)  Onsite(tot)  Onsite(phi)  Total
      0.436015    0.805123    0.563972    0.562573    0.999988
      0.339134    0.620353    0.660515    0.656881    0.999649
      0.339133    0.620353    0.660516    0.656882    0.999649
```

0.339133	0.620353	0.660516	0.656882	0.999649
0.507738	0.648515	0.492040	0.487673	0.999778
...				

などとなる。右端の値が、1になっているべきであるが、展開し直しているため従来では高いエネルギー(下の方。ここでは見えてない)でかなり小さくなっていた(0.8などのおおきさ)。最近デフォルトでは、Gram-Schmidt正規直行化をかけているので、正規直行化は8桁程度以上は保たれている。

The first line (corresponding to 1st band of 1st q point) means that total normalization almost unity =  $0.999988 = 0.436015 + 0.563972$ .

--ntqxx

This fix the number of bands to calculate self energy at the first iteration for each  $\mathbf{q}$  point in the IBZ.

In principle, the number is determined by

## Cautions

- QPU.[number]runをチェックして、number回のQSGWイテレーションが終了している、と認識する。  
(初期状態から実行したいときはすべての\*run\*ディレクトリ、ファイルを消すこと)。
- QSGW.[number]runディレクトリには、QSGWのnumber回目の結果rst,sigm(加えて atmpnu,ctrl,GWinput)が格納されており、これを用いてバンドプロットなどができる。

## Other scripts

cleargw: clean up temporary files

gw\_1mfh: The one-shot \GW calculation. Lifetime(impact ionization rate) of QPs.

epsPP0: dielectric function. No local field corrections

(eps\_1mfh : Dielectric function with local-field corrections. computationally expensive. Need some modifications. Old versions)

genMLWF : Wannier function and its matrix elements of the Screened Coulomb interaction.

## Files used in gwsc

Temporary files are with \_\_\*. Thus we can delete \_\_\* (or use cleargw) after you finish gwsc/epsPP0 and so on.

To repeat a small test for gwsc

```
./testecalj.py si_gwsc
```

at ~/ecalj/SRC/TestInstall. This is what contained in InstallTest. Test is running at work/si\_gwsc/. After copy things from si\_gwsc to work/si\_gwsc. You can run followings one by one if you like. Or `ls -rlt` roughly show which generates which files.

```
===== Ititial band structure =====
--> No sigm. LDA caculation for eigenfunctions
0:00:00.990833 mpirun --bind-to core --map-by core -np 1
/home/takao/ecalj/SRC/TestInstall/bin/lmfa si >llmfa
0:00:03.067381 mpirun --bind-to core --map-by core -np 4
/home/takao/ecalj/SRC/TestInstall/bin/lmf si >llmf_lda
===== QSGW iteration start iter 1 ===
0:00:06.584919 mpirun --bind-to core --map-by core -np 1
/home/takao/ecalj/SRC/TestInstall/bin/lmf si --jobgw=0 >llmfgw00
0:00:08.953914 mpirun --bind-to core --map-by core -np 1
/home/takao/ecalj/SRC/TestInstall/bin/qg4gw --job=1 > lqg4gw
0:00:11.026268 mpirun --bind-to core --map-by core -np 4
/home/takao/ecalj/SRC/TestInstall/bin/lmf si --jobgw=1 >llmfgw01
0:00:14.276866 mpirun --bind-to core --map-by core -np 1
/home/takao/ecalj/SRC/TestInstall/bin/heftet --job=1 > leftet
0:00:16.342115 mpirun --bind-to core --map-by core -np 1
/home/takao/ecalj/SRC/TestInstall/bin/hbasfp0 --job=3 >lbasC
0:00:18.457527 mpirun --bind-to core --map-by core -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hvccfp0 --job=3 > lvccC
0:00:20.400344 mpirun --bind-to core --map-by core -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hsfp0_sc --job=3 >lsxC
0:00:22.459518 mpirun --bind-to core --map-by core -np 1
/home/takao/ecalj/SRC/TestInstall/bin/hbasfp0 --job=0 > lbas
0:00:24.614140 mpirun --bind-to core --map-by core -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hvccfp0 --job=0 > lvcc
0:00:26.884440 mpirun --bind-to core --map-by core -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hsfp0_sc --job=1 >lsx
0:00:28.964117 mpirun --bind-to core --map-by core -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hrcxq > lrcxq
0:00:31.358625 mpirun --bind-to core --map-by core -np 4
/home/takao/ecalj/SRC/TestInstall/bin/hsfp0_sc --job=2 > lsc
0:00:33.682640 mpirun --bind-to core --map-by core -np 1
/home/takao/ecalj/SRC/TestInstall/bin/hqpe_sc > lqpe
0:00:35.517672 mpirun --bind-to core --map-by core -np 4
/home/takao/ecalj/SRC/TestInstall/bin/lmf si >llmf
===== QSGW iteration end iter 1 ===
```

## lmfa

atmpnu\*

Logarithmic derivative at MT boundaries generated by lmfa. This is used by lmf when READP=T.

\_\_atm.foobar

This contains electron densities of spherical atoms.

lmf

rst.foobar

This contains self-consistent electron density revised by each iteration of lmf

QPLIST\*.chk

QPLIST.jobgw1.chk (jobgw1 means --jobgw=1 for lmf) is for human, containing q for irr=1.

QPLIST.lmf.chk (no jobgw option) is for human. Irreducible q points for lmf self-consistent calculations.

\_\_HAMindex

q points table and so on for generating Hamiltonian

\_\_mix.foobar

mixing file for lda

lmf --jobgw=0

NLAindx.chk

This is for human. It shows index to expand eigenfunctions in MTs.

\_\_HAMindex0

Generated at L96:main\_lmf.f90 L96: call m\_hamindex0\_init()

Index of MTOs, space-group symmetries and so on.

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QBZ.chk

q points mesh. Just for human reading.

qg4gw

\_\_QGpsi, \_\_QGcou

q+G of the interstitial plane wave (IPW). Type lqg4gw, which shows

```
--- Max number of G for psi, G for Cou= 116 36
  iq=      1 q=  0.000000  0.000000  0.000000 ngp ngc=   111   29
irr.= 1 <--R
  iq=      2 q= -0.250000 -0.250000  0.750000 ngp ngc=   106   34
irr.= 1 <--R
  iq=      3 q= -0.250000  0.750000 -0.250000 ngp ngc=   106   34
```

```

irr.= 0 <--R
  iq=      4 q= -0.500000  0.500000  0.500000 ngp ngc=    116    36
irr.= 1 <--R
  iq=      5 q=  0.750000 -0.250000 -0.250000 ngp ngc=    106    34
irr.= 0 <--R
  iq=      6 q=  0.500000 -0.500000  0.500000 ngp ngc=    116    36
irr.= 0 <--R
  iq=      7 q=  0.500000  0.500000 -0.500000 ngp ngc=    116    36
irr.= 0 <--R
  iq=      8 q=  0.250000  0.250000  0.250000 ngp ngc=    116    36
irr.= 1 <--R
  iq=      9 q= -0.012500 -0.012500  0.037500 ngp ngc=    111    29
irr.= 1 <--Q0P
  iq=     10 q= -0.262500 -0.262500  0.787500 ngp ngc=    106    34
irr.= 1 <--Q0P+R
  iq=     11 q= -0.262500  0.737500 -0.212500 ngp ngc=    106    34
irr.= 1 <--Q0P+R
  iq=     12 q= -0.512500  0.487500  0.537500 ngp ngc=    116    36
irr.= 1 <--Q0P+R
  iq=     13 q=  0.737500 -0.262500 -0.212500 ngp ngc=    106    34
irr.= 0 <--Q0P+R
  iq=     14 q=  0.487500 -0.512500  0.537500 ngp ngc=    116    36
irr.= 0 <--Q0P+R
  iq=     15 q=  0.487500  0.487500 -0.462500 ngp ngc=    116    36
irr.= 1 <--Q0P+R
  iq=     16 q=  0.237500  0.237500  0.287500 ngp ngc=    116    36
irr.= 1 <--Q0P+R
  iq=     17 q= -0.012500  0.012500  0.012500 ngp ngc=    111    29
irr.= 1 <--Q0P
  iq=     18 q= -0.262500 -0.237500  0.762500 ngp ngc=    106    34
irr.= 1 <--Q0P+R
  iq=     19 q= -0.262500  0.762500 -0.237500 ngp ngc=    106    34
irr.= 0 <--Q0P+R
  iq=     20 q= -0.512500  0.512500  0.512500 ngp ngc=    116    36
irr.= 1 <--Q0P+R
  iq=     21 q=  0.737500 -0.237500 -0.237500 ngp ngc=    106    34
irr.= 1 <--Q0P+R
  iq=     22 q=  0.487500 -0.487500  0.512500 ngp ngc=    116    36
irr.= 1 <--Q0P+R
  iq=     23 q=  0.487500  0.512500 -0.487500 ngp ngc=    116    36
irr.= 0 <--Q0P+R
  iq=     24 q=  0.237500  0.262500  0.262500 ngp ngc=    116    36
irr.= 1 <--Q0P+R
  OK! End of qg4gw

```

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Here, we have regular mesh points specified by <- -R. Q0P is the offset Gamma points shown in Q0P. irr=1 shows the irreducible q points at which we have to generate eigenfunctions. ngp is the number of IPW for the expansion of eigenfunctions (controlled by QpGcut\_phi). ngc is for IPW for the MPB (controlled by QpGcut\_cou).

\_\_BZDATA

\_\_BZDATA contains info on regular mesh points, and offset Gamma (Q0P). Data for tetrahedron division.

lmf --jobgw=1

Generate all the following data to perform GW.

See at subroutines/sugw.f90.

@MNLA\_core.chk

human readable: core index

@MNLA\_CPHI

human readable (but program use this):

Eigenfunctions expanded within MT

hbe.d.chk

human readable: size file for check

\_\_PHIVC

radial functions.

\_\_MTOindex

MTO index

\_\_vxcevec\*

Coefficients of eigenfunctions and eigenvalues for  $\langle F_i | H^0 | \psi F_j \rangle$  in the basis of  $PMT\{F_i\}$ .

GEIG,\_\_CPHI,\_\_EValue

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GEIG: Coefficients of eigenfunctions. IPW part

CPHI: Coefficients of eigenfunctions. MT part

EValue: eigenvalue

PPOVLGG, PPOVLI, PPOVLG, PPOVLO

overlap matrix of IPW.

\_\_VXCFP

XC term in LDA (only diagonal part). A part of vxcevec

Used at hsfp0 but not essential (only for convenience of presentation).

heftet --job=1

EFERMI

The Fermi energy in the tetrahedron method

hbasfp0 (we have --job=3 for core and --job=0 for valence)

\_\_BASFP\*

Product basis functions

\_\_PPBRD\*

Radial integrals on each MT, symbolically written as  $\int \phi(r) \phi(r) B(r) dr$

hvccfp0

We call two times one for core, and the other for valence.

\_\_Vcoud\* , \_\_WV.d

the Coulomb matrix (eigenvalues and eigenfunctions of the Coulomb matrix in the expansion of MPB)

hx0fp0

Note that we use a technique to define  $W-v$  at  $\{\mathbf{q}\}=0$  as an average of the Gamma cell.

\_\_WV.d

Size of the dielectric function

\_\_WVR

W-v in the expansion of mixed product basis along the real axis.

\_\_WVI

\_\_\_\_ W-v in the expansion of mixed product basis along the imag axis.

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freq\_r

human readable: energy mesh to accumulate imaginary parts of W-v.

hsfp0\_sc (Core exchange --job=3, valence exchange --job=1, and valence correlation --job=2)

These are moved to SEBK at the end of gwsc iteration cycle.

SEXcoreU,SEXcore2U :

core exchange --job=3 . SEXcoreU is diagonal part for human check but not used so much.

We have \*D for down spin (isp=2) as well.

SEU,SEX2U



valence exchange --job=1 . SECU is diagonal part for human check but not used so much.

SECU,SEC2U:

valence correlation --job=2 . SECU is diagonal part for human check but not used so much.

XCU

LDA exchange correlation

lqpe

QPU, QPD

human readable format.

decomposition of self-energy for diagonal elements.QPD is for isp=2.

An example of one-shot GW by gw\_lmfh si (small size calculation in TestInstall) is:

...

q			state			SEx	SExcore	SEc	vxc	dSE
dSEnoZ	eLDA	eQP	eQPnoZ	eHF	Z	FWHM=2Z*Simg	ReS(elda)			
0.00000	0.00000	0.00000	1	-16.91		-1.85	6.62	-12.47	0.22	
0.33	-12.24	-12.03	-11.92	-18.54	0.66	1.25708		-12.14031		
0.00000	0.00000	0.00000	2	-13.87		-1.96	2.81	-13.61	0.47	
0.59	-0.31	0.16	0.28	-2.53	0.80	0.00000		-13.02308		
0.00000	0.00000	0.00000	3	-13.87		-1.96	2.81	-13.61	0.47	
0.59	-0.31	0.16	0.28	-2.53	0.80	0.00000		-13.02308		
0.00000	0.00000	0.00000	4	-13.87		-1.96	2.81	-13.61	0.47	
0.59	-0.31	0.16	0.28	-2.53	0.80	0.00000		-13.02308		
0.00000	0.00000	0.00000	5	-4.60		-1.41	-4.27	-11.81	1.19	
1.52	2.23	3.42	3.75	8.03	0.78	-0.02515		-10.28546		
0.00000	0.00000	0.00000	6	-4.60		-1.41	-4.27	-11.81	1.19	
1.52	2.23	3.42	3.75	8.03	0.78	-0.02515		-10.28546		
0.00000	0.00000	0.00000	7	-4.60		-1.41	-4.27	-11.81	1.19	
1.52	2.23	3.42	3.75	8.03	0.78	-0.02515		-10.28546		
0.00000	0.00000	0.00000	8	-5.11		-3.79	-5.14	-15.23	0.91	
1.20	2.95	3.86	4.14	9.28	0.76	-0.07397		-14.03341		
0.50000	0.00000	0.00000	1	-16.80		-1.91	5.97	-12.64	-0.06	
-0.10	-11.18	-11.24	-11.27	-17.25	0.67	0.84187		-12.73584		
0.50000	0.00000	0.00000	2	-13.77		-2.37	2.91	-13.84	0.47	
0.60	-3.84	-3.37	-3.24	-6.14	0.78	0.04107		-13.24015		
0.50000	0.00000	0.00000	3	-13.57		-1.74	3.01	-12.76	0.37	
0.47	-2.20	-1.84	-1.74	-4.75	0.78	0.00000		-12.29249		
0.50000	0.00000	0.00000	4	-13.57		-1.74	3.01	-12.76	0.37	
0.47	-2.20	-1.84	-1.74	-4.75	0.78	0.00000		-12.29249		
0.50000	0.00000	0.00000	5	-4.27		-1.19	-4.08	-10.97	1.17	
1.43	0.76	1.92	2.19	6.27	0.81	-0.00000		-9.53378		
0.50000	0.00000	0.00000	6	-3.83		-1.10	-4.38	-10.98	1.33	
1.68	2.98	4.31	4.65	9.03	0.79	-0.01203		-9.30307		

0.50000	0.00000	0.00000	7	-4.73	-1.66	-4.56	-12.65	1.34
1.70	5.45	6.79	7.14	11.70	0.79	-0.08743	-10.95431	
0.50000	0.00000	0.00000	8	-4.73	-1.66	-4.56	-12.65	1.34
1.70	5.45	6.79	7.14	11.70	0.79	-0.08743	-10.95431	
1.00000	0.00000	0.00000	1	-15.60	-2.13	4.43	-13.20	-0.08
-0.11	-8.13	-8.21	-8.24	-12.67	0.78	0.61936	-13.30329	
1.00000	0.00000	0.00000	2	-15.60	-2.13	4.43	-13.20	-0.08
-0.11	-8.13	-8.21	-8.24	-12.67	0.78	0.61936	-13.30329	
1.00000	0.00000	0.00000	3	-13.66	-1.70	3.17	-12.58	0.30
0.39	-3.16	-2.86	-2.77	-5.94	0.77	0.07961	-12.19216	
1.00000	0.00000	0.00000	4	-13.66	-1.70	3.17	-12.58	0.30
0.39	-3.16	-2.86	-2.77	-5.94	0.77	0.07961	-12.19216	
1.00000	0.00000	0.00000	5	-3.97	-0.91	-3.95	-10.33	1.22
1.50	0.31	1.53	1.81	5.76	0.81	-0.00000	-8.82976	
1.00000	0.00000	0.00000	6	-3.97	-0.91	-3.95	-10.33	1.22
1.50	0.31	1.53	1.81	5.76	0.81	-0.00000	-8.82976	
1.00000	0.00000	0.00000	7	-3.59	-2.37	-5.91	-13.53	1.20
1.66	9.81	11.01	11.47	17.37	0.72	-0.40499	-11.86796	
1.00000	0.00000	0.00000	8	-3.59	-2.37	-5.91	-13.53	1.20
1.66	9.81	11.01	11.47	17.37	0.72	-0.40499	-11.86796	

All of the unit of energy is in eV. Detailed value of eLDA is in {TOTE.UP}.

For insulators, the Fermi energy is at the middle of band. For metals, one shot GW can be problematic if we consider the self-consistency of the Fermi energy.

q : q vector

state: Band index n for valence.

SEx:  $\langle \Psi_{\{\mathbf{k}\}n} | \Sigma_{\mathbf{x}}^{\text{valence}}(\mathbf{r}, \mathbf{r}') | \Psi_{\{\mathbf{k}\}n} \rangle$

SExcore:  $\langle \Psi_{\{\mathbf{k}\}n} | \Sigma_{\mathbf{x}}^{\text{core}}(\mathbf{r}, \mathbf{r}') | \Psi_{\{\mathbf{k}\}n} \rangle$

SEc:  $\langle \Psi_{\{\mathbf{k}\}n} | \Sigma_{\mathbf{c}}^{\text{valence}}(\mathbf{r}, \mathbf{r}', \epsilon_n(\mathbf{k})) | \Psi_{\{\mathbf{k}\}n} \rangle$

vxc: LDA exchange correlation energy.  $\langle \Psi_{\{\mathbf{k}\}n} | V_{\mathbf{xc}}^{\text{LDA}}([n_{\text{total}}], \mathbf{r}) | \Psi_{\{\mathbf{k}\}n} \rangle$

dSE:  $Z_n \times \text{dSEnoZ}$

dSEnoZ:  $\langle \Psi_{\{\mathbf{k}\}n} | \Sigma_{\mathbf{x}}^{\text{core}}(\mathbf{r}, \mathbf{r}') + \Sigma_{\mathbf{xc}}^{\text{valence}}(\mathbf{r}, \mathbf{r}', \epsilon_n(\mathbf{k})) | \Psi_{\{\mathbf{k}\}n} \rangle - \langle \Psi_{\{\mathbf{k}\}n} | V_{\mathbf{xc}}^{\text{LDA}}([n_{\text{total}}], \mathbf{r}) | \Psi_{\{\mathbf{k}\}n} \rangle = \text{SEx} + \text{SExcore} + \text{SEc} - \text{vxc}$

eLDA: LDA eigenvalues.  $\epsilon_n(\mathbf{k})$

eQP: QP energy.  $\epsilon_n(\mathbf{k}) + \text{dSE}$

eQPnoZ: QP energy without  $Z$ .  $\epsilon_n(\mathbf{k}) + \text{dSEnoZ}$

eHF: HF energy of 1st iteration.  $\epsilon_n(\mathbf{k}) + \text{SE} + \text{SEcore} - v_{xc}$

Z: Z factor.  $Z_n(\mathbf{k})$

FWHM=2Z\*S<sub>img</sub>: Quasi-particle life time.  $2 Z_n(\mathbf{k}) \times \langle \Psi_{\mathbf{k}n} | \Sigma_{\text{c}}^{\text{valence}}(\mathbf{r}, \mathbf{r}') \epsilon_n(\mathbf{k}) | \Psi_{\mathbf{k}n} \rangle$

ReS(elda) 😞  $\langle \text{Re} | \langle \Psi_{\mathbf{k}n} | \Sigma_{\text{x}}^{\text{core}}(\mathbf{r}, \mathbf{r}') + \Sigma_{\text{xc}}^{\text{valence}}(\mathbf{r}, \mathbf{r}') \epsilon_n(\mathbf{k}) | \Psi_{\mathbf{k}n} \rangle$

- NOTE: QPU for **gwsc** is a little different. No Z and no life time shown.  
Shown eQP is just the eigenvalues of starting point of lmf.

## TOTE.UP

numerical detailed values of QPU. TOTE.DN for QPD

In one-shot GW **gw\_lmfh**, TOTE.UP contains LDA and QP energies.

It contains two kind of QP energies {QP QPnoZ}.

\_\_mixsig

mixing file for sigm.foobar

sigm

self-energy file in the expansion of eigenfunctions of  $H^0$ .

## Product basis

The product basis section in GWinput is given as follows. Recall that the product basis is made of the product basis within MT and the interstitial plane waves (IPWs).

From the **<PRODUCT\_BASIS>** table, we generate possible product basis of atomic functions within MTs.

Product basis is originally given by F.Aryasetiawan and O.Gunnarsson at

<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.49.16214>

The mixed product basis [https://doi.org/10.1016/S0038-1098\(02\)00028-5](https://doi.org/10.1016/S0038-1098(02)00028-5) is the successor of original.

```
<PRODUCT_BASIS>
  tolerance to remove products due to poor linear-independency
  1d-3 ! =tolopt; larger gives smaller num. of product basis. See lbas
  and lbasC, which are output of hbasfp0.
  lcutmx(atom) = maximum l-cutoff for the product basis. =4 is required
  for atoms with valence d, like Ni Ga
  4 4
  atom 1 nnvv nnc ! Do not touch. nnvv: num. of radial functions
  (valence) on the augmentation-waves. nnc: num. for core.
    1 0 2 3
    1 1 2 2
    1 2 3 0
```

```

1      3      2      0
1      4      2      0
2      0      2      3
2      1      2      2
2      2      2      1
2      3      2      0
2      4      2      0
atom   l      n  occ unocc ! Valence(1=yes,0=no) ! You can set 0 or 1
to give the groups 'occ' and 'unocc'
1      0      1      1      1 ! 4s_phi -----
1      0      2      0      0 ! 4s_phidot
1      1      1      1      1 ! 4p_phi
1      1      2      0      0 ! 4p_phidot
1      2      1      0      1 ! 4d_phi
1      2      2      0      0 ! 4d_phidot
1      2      3      1      0 ! 3d_phiz
1      3      1      0      1 ! 4f_phi
1      3      2      0      0 ! 4f_phidot
1      4      1      0      0 ! 5g_phi
1      4      2      0      0 ! 5g_phidot
2      0      1      1      1 ! 4s_phi -----
2      0      2      0      0 ! 4s_phidot
2      1      1      1      1 ! 4p_phi
2      1      2      0      0 ! 4p_phidot
2      2      1      0      1 ! 4d_phi
2      2      2      0      0 ! 4d_phidot
2      3      1      0      1 ! 4f_phi
2      3      2      0      0 ! 4f_phidot
2      4      1      0      0 ! 5g_phi
2      4      2      0      0 ! 5g_phidot
atom   l      n  occ unocc ForX0 ForSxc ! Core (1=yes, 0=no) <--
Obsolate from here on. But do not change.
1      0      1      0      0      0      0 ! 1S -----
1      0      2      0      0      0      0 ! 2S
1      0      3      0      0      0      0 ! 3S
1      1      1      0      0      0      0 ! 2P
1      1      2      0      0      0      0 ! 3P
2      0      1      0      0      0      0 ! 1S -----
2      0      2      0      0      0      0 ! 2S
2      0      3      0      0      0      0 ! 3S
2      1      1      0      0      0      0 ! 2P
2      1      2      0      0      0      0 ! 3P
2      2      1      0      0      0      0 ! 3D
</PRODUCT_BASIS>

```

PROF

- **tolerance**: cut off of linear-dependency of product basis. If we like to reduce computational size 1d-2 is a possibility.`
- **lcutmx**: The integers next to **lcutmx(atom)**.... This is \$l\$ cutoff for product basis for each atomic sites. The integers give the maximum angular momentum \$l\$ for the product basis for atomic sites.

In our experience, lcutmx=4 is required when the valence  $3d$  electrons exist.

For oxygen 2 is fine. For 4f/5f atoms we need 6. SiteInfo.lmchk shows atom order (SITE order in ctrl file).

- Keep a blocks as it is.

"atom l nnvv nnc ..." shows how many radial functions for cores and valence electrons for each atom and l.

nnvv=2 in the case of  $\phi$  and  $\dot{\phi}$ ; nnvv=3 in the case to add the local orbital in addition.

- There are two blocks after the line

atom 1 n occ unocc :Valence(1=yes, 0=no)

and after

atom 1 n occ unocc ForX0 ForSxc ! Core (1=yes, 0=no)

These are used to choose atomic functions to construct the product basis.

The product basis are generated from the products of two atomic basis.

- n=1 with the comment 4p\_phi indicates  $\phi_{4p}$  (n=1), n=2 with 4p\_phidot for  $\dot{\phi}_{4p}$ , and n=3 for 3d\_phiz

with the local orbital  $\phi^{\text{local}}_{3d}$  (n=3).

- The switches for columns occ and unocc can take 0 (not included) or 1 (included). With the switch, we can construct two groups of orbitals, occ and unocc. With the switches, we see the group  $\text{occ} = \{\phi_{4s}, \phi_{4p}, \phi^{\text{local}}_{3d}\}$  for atom 1. The group  $\text{unocc} = \{\phi_{4s}, \phi_{4p}, \phi_{4d}, \phi_{4f}\}$ . occ and unocc roughly corresponds to occupied and unoccupied orbitals. Usually we don't include  $\dot{\phi}$  for calculations to have smaller number of product basis. But it should be better to be included.  
Then any product of combinations  $\text{occ} \times \text{unocc} = \{\phi_{4s}, \phi_{4p}, \phi^{\text{local}}_{3d}\} \times \{\phi_{4s}, \phi_{4p}, \phi_{4d}, \phi_{4f}\}$  are included as for the basis of the product basis. But we reduce the number of products with the linear dependency. We have to consider not only the product of radial parts, but also synthesis of  $Y_{lm} \times Y_{l'm'}$ .

- Last section is obsolete. Each line of the last section are

atom	1	n	occ	unocc	ForX0	ForSxc	:CoreState(1=yes, 0=no)
1	2	1	A	x	B	C	

We generally set A=B=C=0.

This setting was for the concept of CORE1 and CORE2 in EQ.35 in 2007 paper.

In our recent calculations, we do not use CORE2. Thus these lines are obsolete (keep them as they are).

## MEMO

- We need to explain how to set Gamma-cell averaged  $\tilde{W}(\mathbf{q}=0, \omega)$ .

- [ecaljdetails](#) Details of ecalj algorithm. This should be revised.