QUANTUMESPRESSO

GWL (GW + Wannier +Lanczos)

GWL hands-on

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Summary

- Calculation general structure (1): finite systems

  METHANE molecule

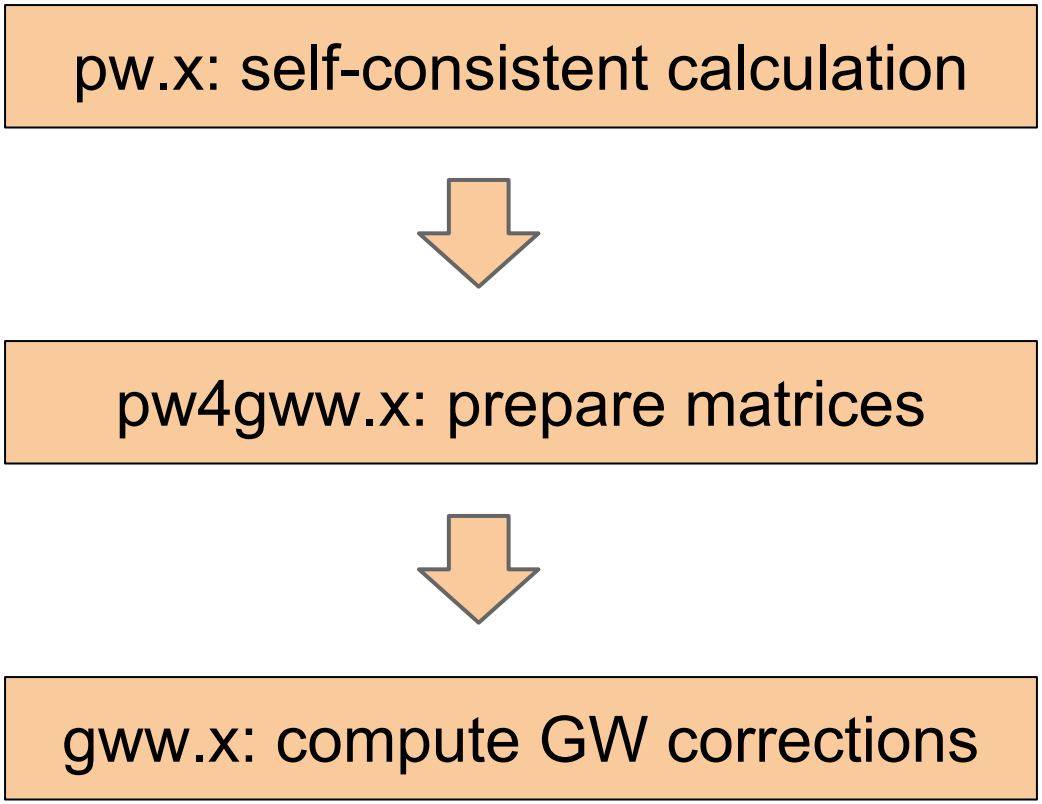
  - minimal example
  - control of the polarizability basis
  - optimal representation of |s> vectors
  - number of lanczos iteration

- Calculation general structure (2): extended systems

  Si bulk

Exercise: CO molecule

Calculation general structure (1): finite systems



Methane
step 1: scf calculation

```
&control
    calculation = 'scf',
    restart_mode='from_scratch',
    prefix='ch4',
    tprnfor = .true.,
    pseudo_dir = '../Pseudo//',
    outdir='.//'
 /
 &system
    ibrav=  1,
    celldm(1) =15.0,
    nat=5,
    ntyp= 2,
    ecutwfc =40.0,
    nbnd=5
 /
 &electrons
    diagonalization='cg'
    mixing_beta = 0.5,
    conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 H  1.0   H.pz-vbc.UPF
 C  12.0  C.pz-vbc.UPF
ATOMIC_POSITIONS {bohr}
H        1.198204546   1.198204546   1.198204546
H       -1.198204546  -1.198204546   1.198204546
H        1.198204546  -1.198204546  -1.198204546
H       -1.198204546   1.198204546  -1.198204546
C        0.000000000   0.000000000   0.000000000
```

Gamma-point calculation

```
./run_scf
```

Methane
step 1: scf calculation

```
&control
    calculation = 'scf',
    restart_mode='from_scratch',
    prefix='ch4',
    tprnfor = .true.,
    pseudo_dir = '../Pseudo//',
    outdir='.//'
 /
 &system
    ibrav=  1,
    celldm(1) =15.0,
    nat=5,
    ntyp= 2,
    ecutwfc =40.0,
    nbnd=5
 /
 &electrons
    diagonalization='cg'
    mixing_beta = 0.5,
    conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 H  1.0   H.pz-vbc.UPF
 C  12.0  C.pz-vbc.UPF
ATOMIC_POSITIONS {bohr}
H        1.198204546   1.198204546   1.198204546
H       -1.198204546  -1.198204546   1.198204546
H        1.198204546  -1.198204546  -1.198204546
H       -1.198204546   1.198204546  -1.198204546
C        0.000000000   0.000000000   0.000000000
```

Gamma-point calculation

```
./run_scf
```

```
> grep 'hest' methane_scf.out

> highest occupied, lowest
> unoccupied level (ev):
> -9.1111    -0.5651
```

Methane
step 2: pw4gww.x

```
./run_pw4gww
```

```
&inputpw4gww
    prefix='ch4'
    num_nbndv(1)=4
    num_nbnds=5
    l_truncated_coulomb=.true.
    truncation_radius=7.5d0
    numw_prod=50
    pseudo_dir = '../Pseudo//',
    outdir='./tmp/'
/
```

Valence band number

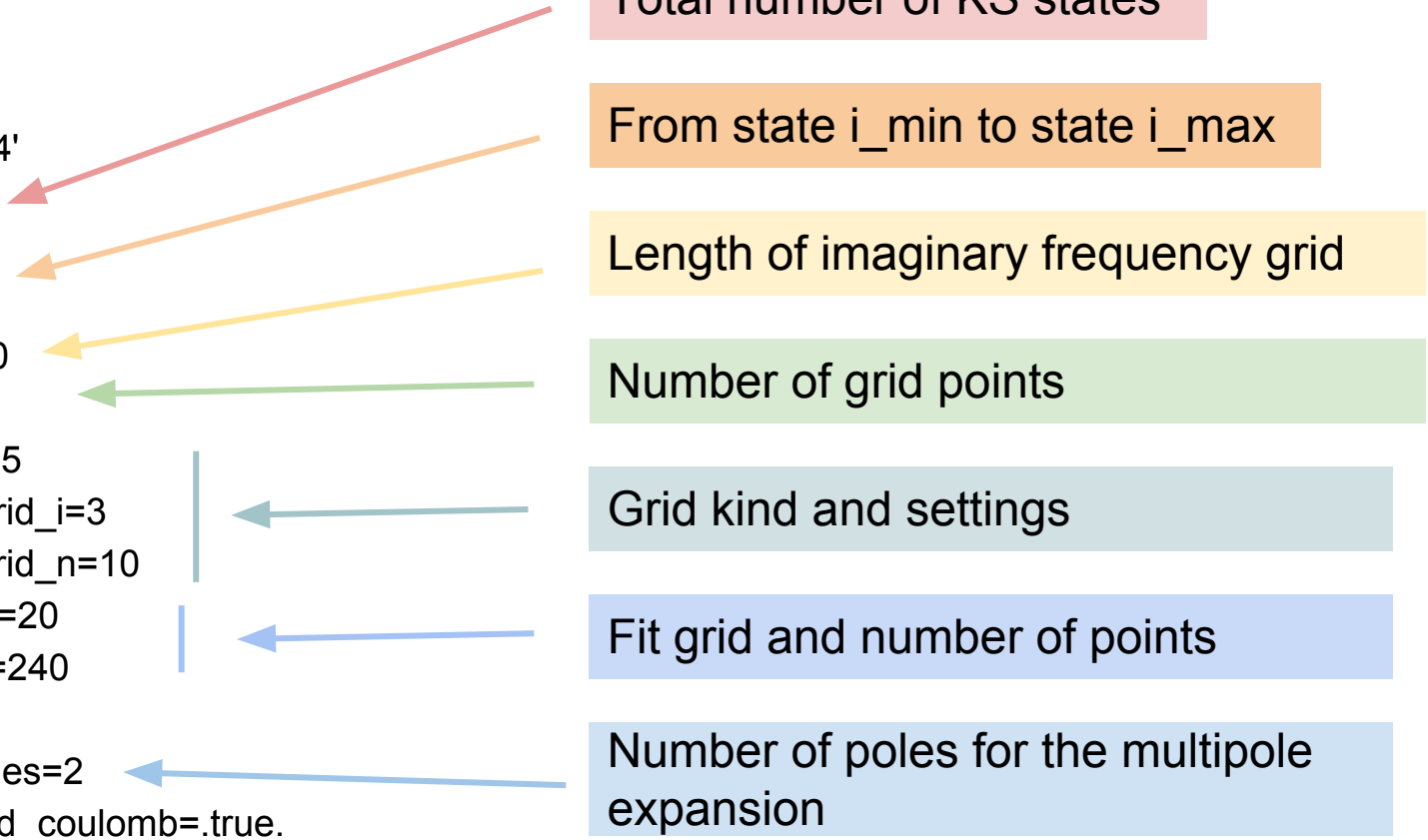
Total number of KS states

Use of truncated Coulomb interaction

Dimension of the polarizability basis

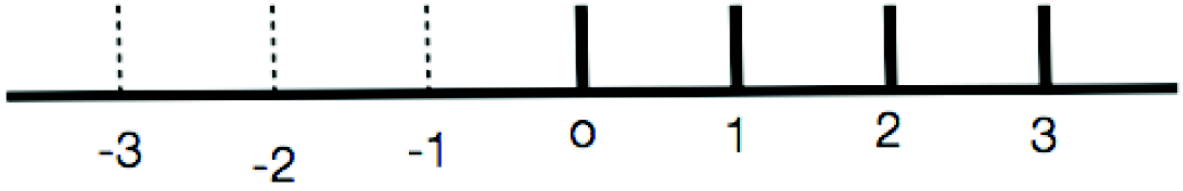
Methane
step 3: gww.x

```
&inputgww
ggwin%prefix='ch4'
ggwin%max_i=5,
ggwin%i_min=1
ggwin%i_max=5
ggwin%omega=20
ggwin%n=118,
ggwin%grid_freq=5
ggwin%second_grid_i=3
ggwin%second_grid_n=10
ggwin%omega_fit=20
ggwin%n_grid_fit=240
ggwin%n_fit=120,
ggwin%n_multipoles=2
ggwin%l_truncated_coulomb=.true.
ggwin%outdir='./tmp'
/
```



gww.x
frequency grids

Equally spaces grid: → ggwin%grid_freq=3



Augmented at low frequencies: → ggwin%grid_freq=5
ggwin%second_grid_i=1
ggwin%second_grid_n=2

gww.x results

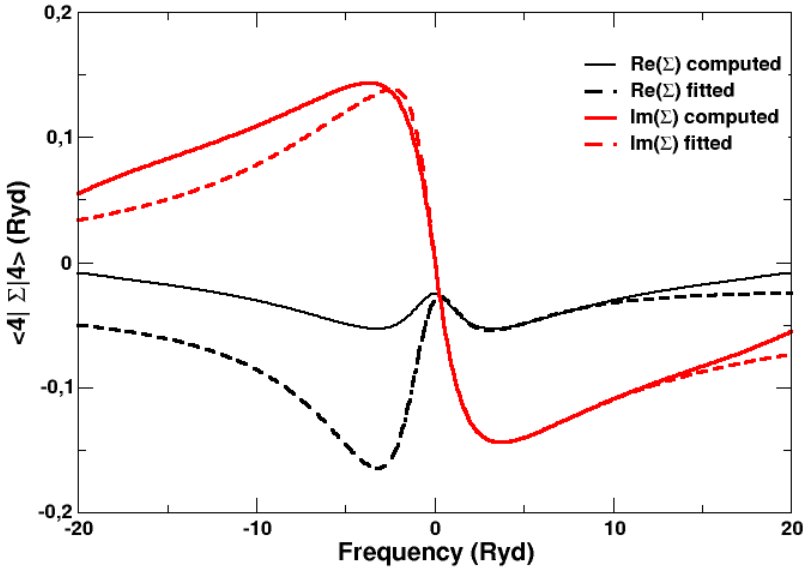
methane_gww.out:

- restart points
- qp corrections

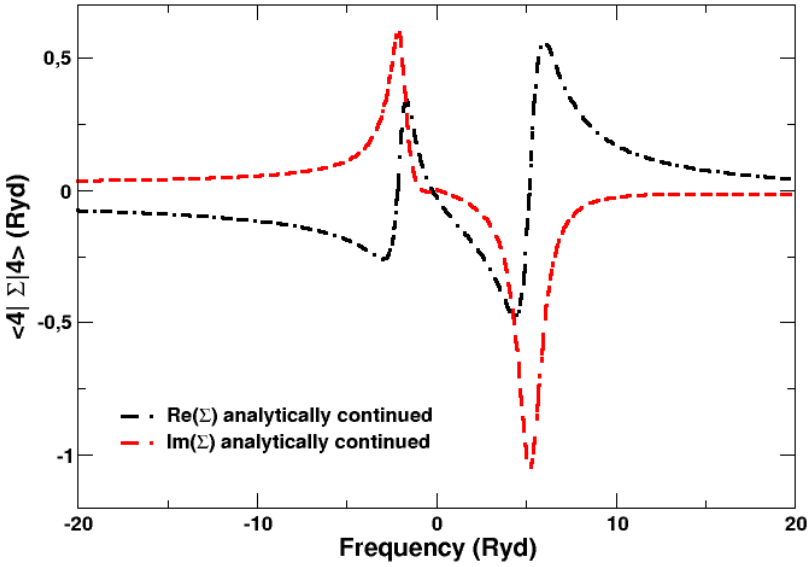
```
QUASI-PARTICLES ENERGIES IN Ev, Spin:          1       1
State:        1DFT  : -16.61262 GW-PERT  : -20.45071 GW  : -20.21650 HF-pert : -25.31702
State:        2DFT  :  -9.11175 GW-PERT  : -13.67373 GW  : -13.58907 HF-pert : -14.42319
State:        3DFT  :  -9.11175 GW-PERT  : -13.67404 GW  : -13.58654 HF-pert : -14.42319
State:        4DFT  :  -9.11175 GW-PERT  : -13.67818 GW  : -13.59240 HF-pert : -14.42319
State:        5DFT  :  -0.56520 GW-PERT  :   0.21353 GW  :   0.21301 HF-pert :   0.90042

 IMAGINARY ENERGIES IN Ev:
State:        1 GW (Im) :   0.48380
State:        2 GW (Im) :  -0.04378
State:        3 GW (Im) :  -0.05230
State:        4 GW (Im) :  -0.04675
State:        5 GW (Im) :   0.02237
```

gww.x
analytic continuation

re_on_imXXXXX and im_on_imXXXXX:
contain the expectation value of the self energy on the imaginary frequency axis (computed and fitted) and on the real axis.



COMPUTED AND FITTED ON IMAGINARY AXIS



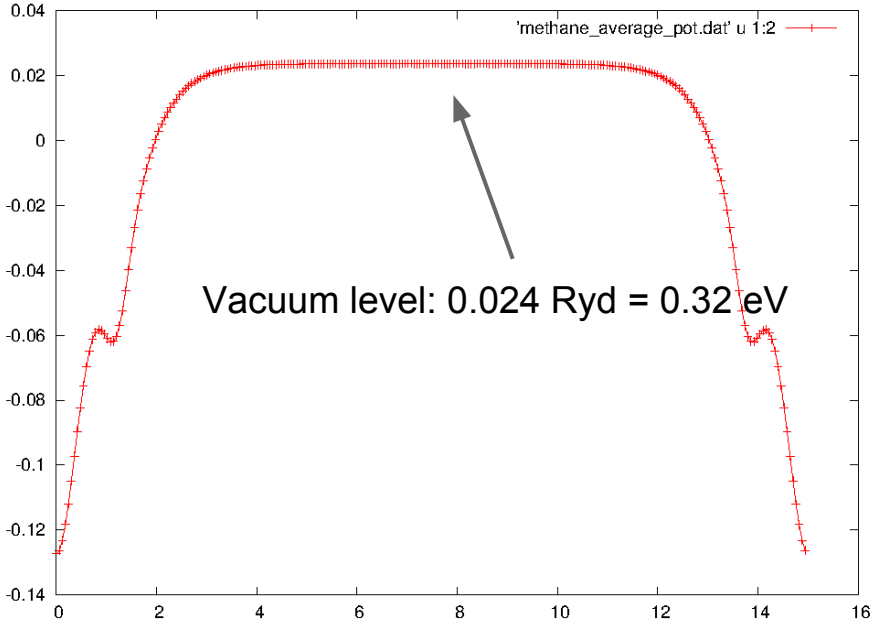
ANALYTICALLY CONTINUED ON REAL AXIS

GWL results: methane ionization potential

1) Get the vacuum level

```
run_vacuum
gnuplot
gnuplot> p 'methane_average_pot.dat' u 1:2 w lp
```

2) Compute the distance between the HOMO level and the vacuum level for the DFT and GW calculations.



IP

EXP: 12.6-13.6 eV
DFT: 9.4 eV
GW: 13.9 eV

GWL convergence (1): polarizability basis

$$P(i\omega) \simeq \sum_{\alpha\beta} \phi_\alpha(r) P_{\alpha\beta}(i\omega) \phi_\beta(r') \qquad \{\phi_\alpha(r)\}$$

1) Consider "fake" conduction states, namely: planewaves below a certain threshold (**pmat_cutoff**) projected onto the conduction manifold.

$$P_0(t=0) = \sum_{vG} |\Psi_v \tilde{G}\rangle\langle \tilde{G}\Psi_v| \qquad |\Psi_v \tilde{G}\rangle \longrightarrow |w_v \tilde{G}\rangle$$

2) Gram-Schmidt orthonormalize $\{|w_v \tilde{G}\rangle\}$ and keep the vectors $\{|f_\mu\rangle\}$ whose norm is above a certain threshold **s_pmat**.

$$P_{\mu\nu} = \sum_{vG} \langle f_\mu|\Psi_v \tilde{G}\rangle\langle \tilde{G}\Psi_v|f_\nu\rangle$$

4) Diagonalize $P_{\mu\nu}$ and keep the **numw_prod** eigenvectors with the largest eigenvalues.

Relevant input variables: **pmat_cutoff**, cutoff for the plane waves; **s_pmat** threshold for the f-states; **numw_prod** dimension of the final basis set.

GWL convergence (1): polarizability basis

```
./run_pol_basis
```

methane_pw4gww.in:

```
&inputpw4gww
      prefix='ch4'
      num_nbndv(1)=4
      num_nbnds=5
      l_truncated_coulomb=.true.
      truncation_radius=7.5d0
      numw_prod= 150
      pmat_cutoff= 5
      pseudo_dir = '../Pseudo//',
      outdir='./tmp/'
/
```

Final dimension of the polarizability basis Np

Cutoff E* for the fake-conduction state

GWL convergence (1): polarizability basis

How is the basis built?

(1) The fake conduction states are built depending on the cutoff E*

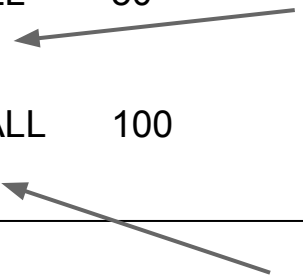
```
grep 'Number of projected orthonormalized plane waves:' *pw*out*
```

```
methane_pw4gww.out_pmc3_nwp100: Number of projected orthonormalized plane waves:    305
methane_pw4gww.out_pmc5_nwp50: Number of projected orthonormalized plane waves:    619
```

(2) the fake conduction states are multiplied by valence bands max. localized wannier functions and the | f > states are built depending on s_pmat.
The total number of | f > states should be 4 times the dimension of the polarizability basis.

```
grep -A1 'NUMW_PROD_ALL' *pw*out*
```

```
methane_pw4gww.out_pmc3_nwp50: NUMW_PROD_ALL       50
methane_pw4gww.out_pmc3_nwp50- ATT1          282
--
methane_pw4gww.out_pmc5_nwp100: NUMW_PROD_ALL      100
methane_pw4gww.out_pmc5_nwp100- ATT1          471
```



GWL convergence (1): polarizability basis

How is the basis accurate?

(1) We keep only the polarizability eigenvectors with Np largest eigenvalues. q* is the value of the smallest eigenvalue under consideration.
To compare calculations on different systems it should be normalized to the cell volume.

```
grep 'POLARIZABILITY eigen:        1' *out*
```

```
pmc3_nwp20: POLARIZABILITY eigen:         1   22.999807219904774
pmc3_nwp50: POLARIZABILITY eigen:         1   2.7577385557053447
pmc3_nwp100: POLARIZABILITY eigen:        1  0.23889032126141180
pmc3_nwp150: POLARIZABILITY eigen:        1   6.1518891131824148E-002

pmc5_nwp20: POLARIZABILITY eigen:         1   51.141601472951244
pmc5_nwp50: POLARIZABILITY eigen:         1   9.1427460621212475
pmc5_nwp100: POLARIZABILITY eigen:        1   1.4549266992868131
pmc5_nwp150: POLARIZABILITY eigen:        1  0.46373813148015497
```

GWL convergence (1): polarizability basis

How is the basis accurate?

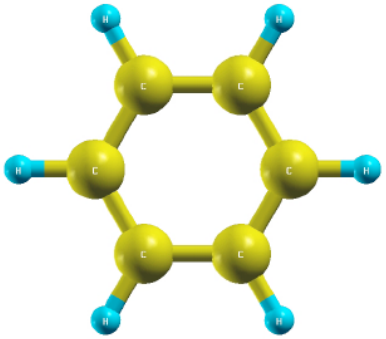
```
grep 'State:  4DFT' *out
```

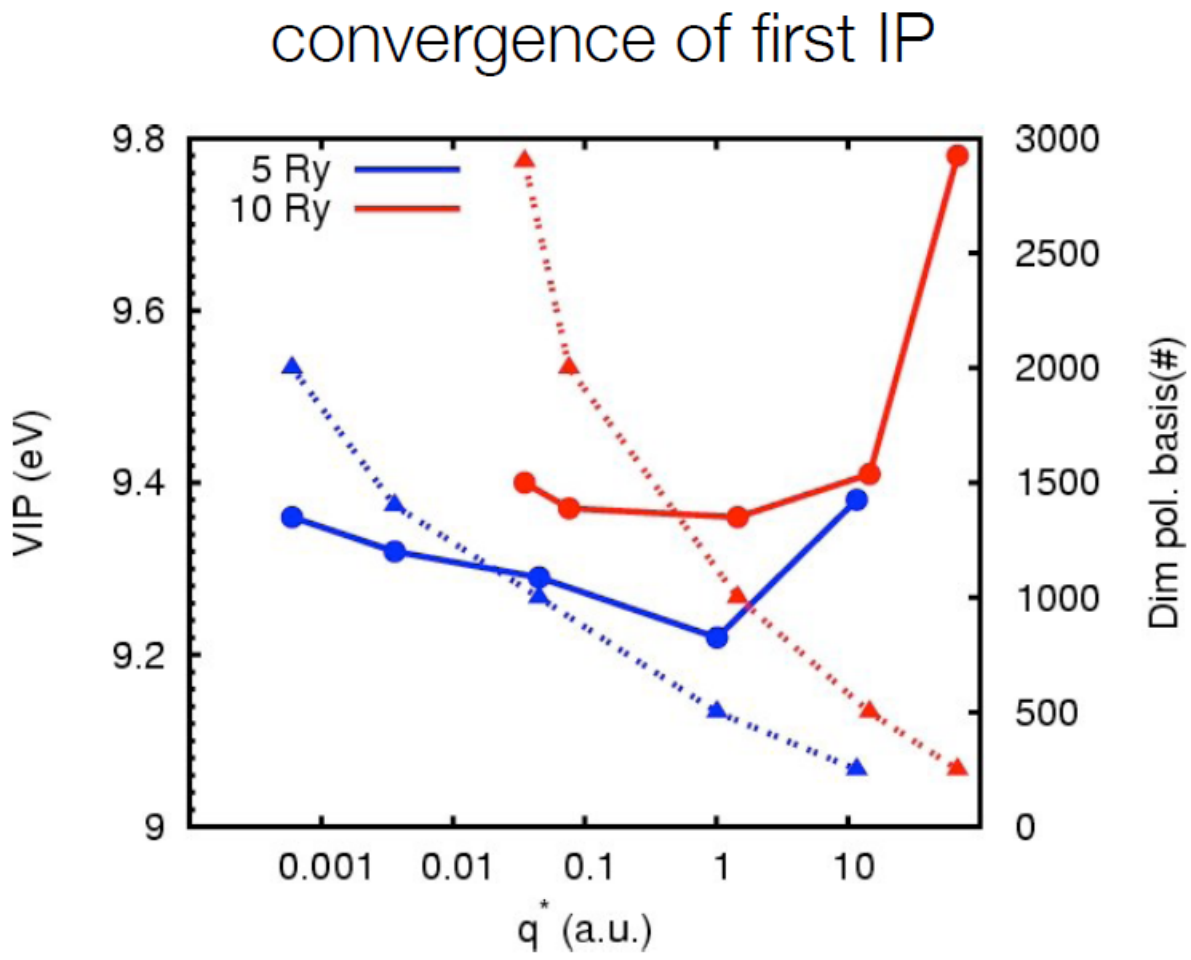
then add 0.32 eV (vacuum level)

IP (eV)	Np=20	Np=50	Np=100	Np=150
E*= 3 Ryd	14.5	13.9	13.6	13.6
E*= 5 Ryd	14.3	14.2	13.9	13.8

EXP. IP
12.6-13.6 eV

GWL convergence (1): polarizability basis -benzene





GWL convergence (2):

optimal representation of large sets of vectors

- The Lanczos chain algorithm is applied twice to large sets of non-orthogonal vectors (to get the dynamical P, and for the calculation of the self-energy matrix elements, where the Green's function appear).

- An optimal representation of these vectors is found by:

(1) 'Locally' diagonalizing the overlap matrix, keeping the eigenvectors with the largest `n_pola_lanczos`, or `n_self_lanczos` eigenvalues.

(2) 'Globally' perform a SVD and keep the eigenvectors with the eigenvalue above `s_pola_lanczos` and `s_self_lanczos`.

In general we find a stronger system dependence for the s parameters.
(For a discussion see the GWL user manual)

GWL convergence (2):

optimal representation of large sets of vectors

```
./run_sself
 grep 'TOTAL NUMBER OF GLOBAL S VECTORS' *out*sself*
```

			IP (eV)
sself0.01:	TOTAL NUMBER OF GLOBAL S VECTORS:	1	14.7
sself0.00001:	TOTAL NUMBER OF GLOBAL S VECTORS:	50	13.8
sself0.000000001:	TOTAL NUMBER OF GLOBAL S VECTORS:	87	13.9
sself1d-12:	TOTAL NUMBER OF GLOBAL S VECTORS:	219	13.9

To notice the effect of n_self_lanczos increase the dimension of the polarizability basis.

```
./run_nself
 grep 'TOTAL NUMBER OF GLOBAL S VECTORS' *out*nself*
```

			IP (eV)
nself10:	TOTAL NUMBER OF GLOBAL S VECTORS:	50	13.1
sself50:	TOTAL NUMBER OF GLOBAL S VECTORS:	250	13.6
sself600:	TOTAL NUMBER OF GLOBAL S VECTORS:	377	13.6

GWL convergence (3): lanczos chain length

```
./run_nlanczos_self
```

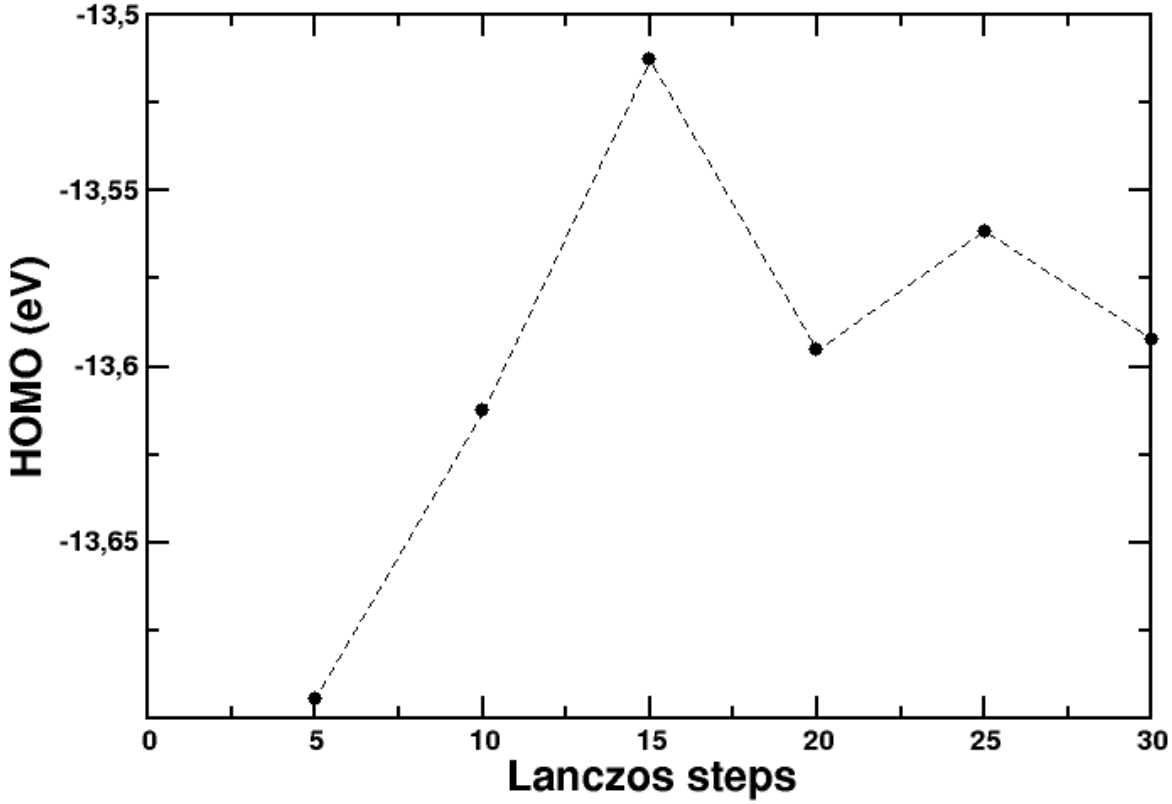
```
&inputpw4gww
        prefix='ch4'
        num_nbndv(1)=4
        num_nbnds=5
        l_truncated_coulomb=.true.
        truncation_radius=7.5d0
        numw_prod= 50
        pmat_cutoff= 3
        pseudo_dir = '$PSEUDO_DIR/',
        outdir='$TMP_DIR/'
        n_pola_lanczos=400
        s_pola_lanczos=0.5d0
        nsteps_lanczos_pola=20
        n_self_lanczos= 600
        s_self_lanczos=1d-12
        nsteps_lanczos_self= $nsteps
        restart_gww=2
        lanczos_restart=3
/
```

The code can be restarted to check the convergence with respect to to lanczos-chain length.

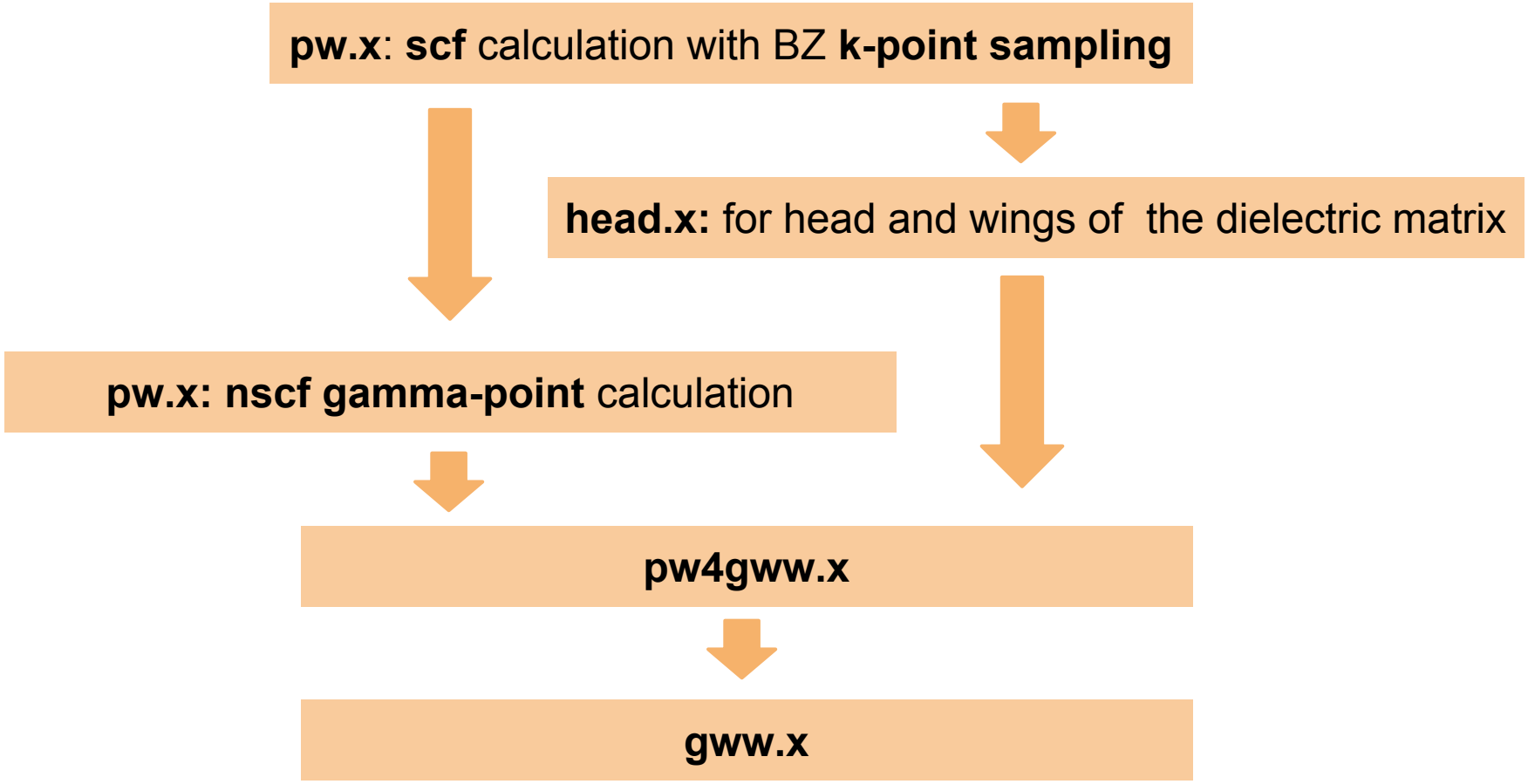
Increasing the number of steps

Restart points

GWL convergence (3): lanczos chain length



Extended Systems
General Scheme (5 calculations)



Si-bulk
step 1 pw.x scf

```
&control
 calculation='scf'
 restart_mode='from_scratch', prefix='si'
 pseudo_dir = '$PSEUDO_DIR/',
 outdir='$TMP_DIR/'
/
&system
 ibrav= 8, celldm(1)= 10.26,celldm(2)= 1, celldm(3)=1,
 nat=  8, ntyp= 1, ecutwfc = 15.0
/
&electrons
 diagonalization='david',
 conv_thr =  1.0d-10,
 mixing_beta = 0.5,
 startingwfc='random',
/
ATOMIC_SPECIES
Si  1. Si.pz-vbc.UPF
ATOMIC_POSITIONS (crystal)
Si 0.00000 0.00000 0.00000
Si 0.50000 0.50000 0.00000
Si 0.00000 0.50000 0.50000
Si 0.50000 0.00000 0.50000
Si 0.25000 0.25000 0.25000
Si 0.75000 0.75000 0.25000
Si 0.75000 0.25000 0.75000
Si 0.25000 0.75000 0.75000
K_POINTS (automatic)
4 4 4 1 1 1
```


8 atom supercell.
THIS IS NOT CONVERGED!!!

BZ K-point sampling

Si-bulk
step 2 head.x

```
calculation of head
 &inputph
  trans=.false.
  l_head=.true.
  tr2_ph=1.d-4,
  prefix='si',
  omega_gauss=20.0
  n_gauss=97
  grid_type=5
  second_grid_i=1
  second_grid_n=10
  niter_ph=1
  nsteps_lanczos=30
  outdir='$TMP_DIR/'
 /
0.0 0.0 0.0
```

Frequency grid parameters
Same as in gww.x input

Lanczos iteration number
Same as in gww.x input

Si-bulk
step 3-4: pw.x (nscf gamma) pw4gww.x

```
&control
 calculation='nscf'
 restart_mode='from_scratch',
 prefix='si'
 pseudo_dir = '$PSEUDO_DIR/',
 outdir='$TMP_DIR/'
/
&system
 ibrav= 8, celldm(1)= 10.26,celldm(2)= 1, celldm(3)=1,
 nat=  8, ntyp= 1, ecutwfc = 15.0,nbnd=32
/
&electrons
 diagonalization='david', conv_thr =  1.0d-10,
 mixing_beta = 0.5,
 startingwfc='random',
/
ATOMIC_SPECIES
Si  1. Si.pz-vbc.UPF
ATOMIC_POSITIONS (crystal)
Si 0.00000 0.00000 0.00000
Si 0.50000 0.50000 0.00000
Si 0.00000 0.50000 0.50000
Si 0.50000 0.00000 0.50000
Si 0.25000 0.25000 0.25000
Si 0.75000 0.75000 0.25000
Si 0.75000 0.25000 0.75000
Si 0.25000 0.75000 0.75000
```

```
&inputpw4gww
      prefix='si'
      num_nbndv(1)=16
      num_nbnds=32
      l_truncated_coulomb=.
false.
      numw_prod=100
      pmat_cutoff=3d0
      s_self_lanczos=1d-8
      outdir='$TMP_DIR'
/
```

Extended system

Si-bulk
step 3-4: pw.x (nscf gamma) pw4gww.x

```
&control
 calculation='nscf'
 restart_mode='from_scratch',
 prefix='si'
 pseudo_dir = '$PSEUDO_DIR/',
 outdir='$TMP_DIR/'
/
&system
 ibrav= 8, celldm(1)= 10.26,celldm(2)= 1, celldm(3)=1,
 nat=  8, ntyp= 1, ecutwfc = 15.0,nbnd=32
/
&electrons
 diagonalization='david', conv_thr =  1.0d-10,
 mixing_beta = 0.5,
 startingwfc='random',
/
ATOMIC_SPECIES
Si  1. Si.pz-vbc.UPF
ATOMIC_POSITIONS (crystal)
Si 0.00000 0.00000 0.00000
Si 0.50000 0.50000 0.00000
Si 0.00000 0.50000 0.50000
Si 0.50000 0.00000 0.50000
Si 0.25000 0.25000 0.25000
Si 0.75000 0.75000 0.25000
Si 0.75000 0.25000 0.75000
Si 0.25000 0.75000 0.75000
```

```
&inputpw4gww
      prefix='si'
      num_nbndv(1)=16
      num_nbnds=32
      l_truncated_coulomb=.
false.
      numw_prod=100
      pmat_cutoff=3d0
      s_self_lanczos=1d-8
      outdir='$TMP_DIR'
/
```

Extended system

You try, now!

Exercise:

-CO molecule

(1) DFT ionization potential

(2) convergence GW

Always check the convergence of your calculations!!

Important information can be found on the user manual, downloadable at the GWL-code web page.