YAMBO_GW_PWmat

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Introduction

- YAMBO is a open source package for GW, BSE and TDDFT calculations. It is a CPU code.
  http://www.yambo-code.org

  reference: A. Marini, C. Hogan, M. Gruning, D. Varsano, “Yambo: An ab initio tool for excited state calculaitons”, Comp. Phys. Comm. 180, 1392 (2009).

- In this module, we explain how to run YAMBO to get GW quasi-particle energy based on PWmat DFT results.

下载安装

tar zxvf YAMBO.tar.gz
cd YAMBO/yambo-4.3.0
module load intel/2016 #加载intel环境
. yambo.sh
make yambo interfaces

For standard Mstation user, please copy executable: yambo and p2y
To a directory in your path (e.g., /usr/local/bin).

Do: > which yambo, > which p2y
Make sure they can be found in your path

The basic steps to run PWmat-YAMBO:

- (1) Run Pwmat calculations:
  This includes: JOB=SCF calculation with PWSCF_OUTPUT=T
  JOB=NONSCF for larger number of kpoints and band
  with PWSCF_OUTPUT=T (to generate prefix.save).

- (2) Run p2y: to convert the PWscf style file (in prefix.save) to YAMBO file (in a file called SAVE) (quick)

- (3) Run yambo: for initialization (quick)

- (4) Run yambo –F yambo_gw.in: for real yambo run (main yambo run, can be slow)

- (5) Check the results in GW subdirectory

Step 1: PWmat run

This is to generate the DFT wave function and eigen energies for YAMBO GW calculation

(a) First do a SCF PWmat calculation.

```
4                1
IN.ATOM    = atom.config
JOB        = SCF
IN.PSP1    = 31-Ga.LDA.fhi.UPF
IN.PSP2    = 33-As.LDA.fhi.UPF
Ecut       = 40.00
MP_N123    = 6 6 6 0 0 0
PWSCF_OUTPUT = T
```

atom.config

```
        2
Lattice vector
      2.825     2.825     0.00
      2.825     0.0       2.825
      0.0       2.825     2.825
Position, move_x, move_y, move_z
  31    0.000    0.000    0.000  1 1 1
  33    0.250    0.250    0.250  1 1 1
```

(b) Copy out.vr to in.vr, edit etot.input, do a NONSCF PWmat calculation

```
4                1
IN.ATOM    = atom.config
JOB        = NONSCF
IN.PSP1    = 31-Ga.LDA.fhi.UPF
IN.PSP2    = 33-As.LDA.fhi.UPF
Ecut       = 40.0
MP_N123    = 6 6 6 0 0 0
num_band   = 300
IN.VR      = T
PWSCF_OUTPUT = T
```

Important: larger number of num_band
possibly larger MP_N123
PWSCF_OUTPUT=T

It will generate: ./prefix.save diretory

Step 2: run p2y

>cd prefix.save

>copy the xxxx.UPF to prefix.save (>cp ./*.UPF .)

(a) Inside prefix.save, there should be a file called: data-file.xml

(b) Inside prefix.save, run: >p2y -F data-file.xml

it will generate a directory: SAVE

```
31-Ga.LDA.fhi.UPF     gvectors.dat   input.restart  K00005  K00010  K00015     r_setup_03
33-As.LDA.fhi.UPF     gw             K00001         K00006  K00011  K00016     SAVE
charge-density.xml    input.bands    K00002         K00007  K00012  r_setup    yambo_gw.in
data-file.xml         input.dos      K00003         K00008  K00013  r_setup_01 ypp.in
DOC_QE_COMPATABILITY  input.pdos     K00004         K00009  K00014  r_setup_02
[weile@mstation prefix.save]$
```

The prefix.save directory might look like this (without gw)

The screen print out after: >p2y -F data-file.xml

```
<--->  :: Electrons                 : 8.000000
<--->  :: Temperature         [ev]:0.9500E-3
<--->  :: Lattice factors [a.u.]: 5.338476  5.338476  5.338476
<--->  :: K-points                  : 16
<--->  :: Bands                     : 300
<--->  :: Spinor components         : 1
<--->  :: Spin polarizations        : 1
<--->  :: Spin orbit coupling       : no
<--->  :: Symmetries     [spatial]: 24
<--->  ::                  [T-rev]: yes
<--->  :: Max WF components         : 1315
<--->  :: RL vectors          (WF): 1315
<--->  :: RL vectors      (CHARGE):  3695
<--->  :: XC potential              : Slater exchange(X)+Perdew & Zunger(C)
<--->  :: Atomic species            : 2
<--->  :: Max atoms/species         : 1
<---> == DB1 (Gvecs and more) ...
<---> ... Database done
<---> == DB2 (wavefunctions)  ...
<---> [p2y] wfc_io |########################################| [100%] --(E) --(X) done ==
<---> == DB3 (PseudoPotential) ... done ==
<01s>  == P2Y completed ==
<01s>[weile@mstation prefix.save]$
```

Step 3: run yambo (initialization)

>Stay in the prefix.save directory

>Run: >yambo

It will do yambo initialization. Note, in the prefix.save, you cannot have a file called yambo.in, otherwise it will read this file, and cause problem!

```
 ___ ___  _____  ___ ___  _____  _____
|   Y   ||   _  ||   Y   ||   _  \ |  _  |
|   |   ||. |  ||.    ||. |  /  |. |  |
 \_   _/ |. _  ||.\_/ ||. _  \  |. |  |
  |: |   |: |  ||: |  ||: |   \|: |  |
  |::|   |:.|:.||:.|:.||::.    /|::.  |
  `--"   `-- --"`-- --"`-----" `-----"


 <---> [01] CPU structure, Files & I/O Directories
 <---> [02] CORE Variables Setup
 <---> [02.01] Unit cells
 <---> [02.02] Symmetries
 <---> [02.03] RL shells
 <---> Shells finder |########################################| [100%] --(E) --(X)
 <---> [02.04] K-grid lattice
 <---> [02.05] Energies [ev] & Occupations
 <---> [WARNING][X] Metallic system
 <---> [03] Transferred momenta grid
 <---> BZ -> IBZ reduction |########################################| [100%] --(E) --(X)
 <---> X indexes |########################################| [100%] --(E) --(X)
 <---> SE indexes |########################################| [100%] --(E) --(X)
 <---> [04] Timing Overview
 <---> [05] Game Over & Game summary
[weile@mstation prefix.save]$
```

Screen printout after >yambo for initialization

Step 4: run yambo

>Stay in the prefix.save directory >Edit file: yambo_gw.in

```
em1d                                # [R Xd] Dynamical Inverse Dielectric Matrix
ppa                                 # [R Xp] Plasmon Pole Approximation
HF_and_locXC                        # [R XX] Hartree-Fock Self-energy and Vxc
gw0                                 # [R GW] GoWo Quasiparticle energy levels
ElecTemp= 0.000000      eV          # Electronic Temperature
BoseTemp= 0.000000      eV          # Bosonic Temperature
FFTGvecs=  1000         RL          # [FFT] Plane-waves number for wave function
X_Threads = 1                       # [PARALLEL] openMP thread is 1 for HF exchange calc.
DIP_Threads = 1                     # [PARALLEL] openMP thread is 1 for polarization calc.
SE_Threads = 1                      # [PARALLEL] openMP thread is 1 for self-energy calc.
EXXRLvcs= 30            Ry          # [XX] RL components for HF exchange calculation
% BndsRnXp
   1 |  300 |                       # [Xp] Polarization function bands
%
NGsBlkXp= 10             Ry          # [Xp] PW for dielectric, unit Ry, or RL (< FFTGvecs)
% LongDrXp
 1.000 | 0.000  |0.000   |          # [Xp] [cc] Electric Field direction for q=0,k=0 point
%
PPAPntXp= 27.21138      eV          # [Xp] PPA imaginary energy
% GbndRnge
   1 |  300 |                        # [GW] bands range for Green's function
%
GDamping=  0.10000      eV          # [GW] G[W] damping
dScStep=  0.10000       eV          # [GW] Energy step to evaluate Z factors
DysSolver= "n"                      # [GW] Dyson Equation solver ("n","s","g")
%QPkrange                           # [GW] QP generalized Kpoint/Band indices to evaluate the energy
  1| 16|  1|  5|
%
```

Explanation of the yambo_gw.in file

Meaning of the variables can be found in: http://www.yambo-code.org/input_file/vars/
Check that site for more options

- em1d: please keep
- ppa: plasmon pole approximation of the dielectric constant
- HF_and_locXC: please keep
- gw0: g0w0 calculation
- X_threads, DIP_Threads, SE_Threads=1, for openMP calc., please keep
- FFTGvecs: the PW number for wavefunction in G. You can check the PW number in REPORT. FFTGvecs can be smaller (e.g, a factor of 2) than the one in REPORT
- NGsBlkXp: Xp means plasmon pole. The PW cutoff used for dielectric constant calculations. In terms of PW number, should be < FFTGvecs. This Ecut can be significantly smaller than the Ecut in PWmat calc. Suggest: ~ 6-10 Ry.
- BndsRnxp: the band index for polarization calculation (can be large, e.g. a few hundreds)
- GbndRnge: the band index used in the G calculation. (can be smaller than BndsRnxp).
- Qpkrange: “1 | kpt|1 |nband|”: the kpoint and band index for GW energy evaluation

Note: the computer time might steeply depend on: FFTGvecs, NGsBlkXp, BandsRnxp, GbndRnge

Run YAMBO

Run yambo

```
>mpirun -np 4 yambo -F yambo_gw.in -J gw -C gw &
```

- Note, in the directory, there should have no gw directory from previous run.
- The yambo_gw.in is the input file.
- We are using 4 processors for MPI run (in yambo_gw.in, there is no need to write this 4)
- Using >top to check the running of yambo (it is a CPU code).

After the run, it will generate directory: gw.

In gw, we have: o-gw.qp (band file), r-gw_em1d_ppa_HF_and_locXC_gw0 (detail file)

Step 5: Check the result

Check File: r-gw_em1d_ppa_HF_and_locXC_gw0, inside gw directory

```
631   QP [eV] @ K [1] (iku): 0.00      0.00      0.00
632    B=1 Eo=-12.72 E=-12.70 E-Eo=  0.02 Re(Z)=0.44 Im(Z)=0.1293E-2 nlXC=-17.55 lXC=-10.79 So= 6.810
633    B=2 Eo= -0.00 E= -0.47 E-Eo= -0.47 Re(Z)=0.79 Im(Z)=-.1554E-2 nlXC=-12.48 lXC=-11.25 So=0.6336
634    B=3 Eo= -0.00 E= -0.47 E-Eo= -0.47 Re(Z)=0.79 Im(Z)=-.1554E-2 nlXC=-12.48 lXC=-11.25 So=0.6336
635    B=4 Eo=  0.00 E= -0.47 E-Eo= -0.47 Re(Z)=0.79 Im(Z)=-.1554E-2 nlXC=-12.48 lXC=-11.25 So=0.6335
636    B=5 Eo=  0.52 E=  0.70 E-Eo=  0.18 Re(Z)=0.79 Im(Z)=-.1493E-2 nlXC=-6.858 lXC=-10.31 So=-3.224
```

This means, for kpt=0,0,0, for the band 1-5, The LDA energy is Eo, the GW energy is E.
So, in this case, the LDA band gap is 0.52, and the GW band gap is: 0.70-(-0.47)=1.17.
It also give the Z (the GW renormalization factor).

Check File: o-gw.qp, inside gw directory

```
35 #    K-point      Band         Eo          E-Eo         Sc|Eo
36 #
37      1.00000      1.00000   -12.71574      0.01897      6.80999
38      1.000        2.000       -.8110E-6    -.4695       0.6336
39      1.000        3.000       -.5069E-6    -.4695       0.6336
40      1.000000     4.000000     0.000000   -0.469506     0.633550
41      1.000000     5.000000     0.515242    0.181600    -3.223620
42      2.00000      1.00000    -12.42093    -0.03513      6.59294
43      2.000000     2.000000    -2.741699   -0.440705     1.347039
44      2.000000     3.000000    -0.376436   -0.470224     0.730130
45      2.000000     4.000000    -0.376435   -0.470209     0.730141
46      2.000000     5.000000     1.645571    0.144969    -3.457332
```

Note, it only gives E-E0
The same results as in the
Above r-gw_xxxx file.