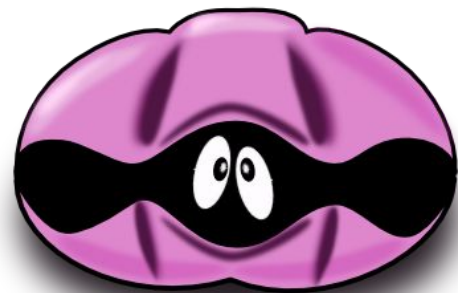


Yambo[®]



Cheatsheet

For yambo 5.0



DRIVING THE EXASCALE TRANSITION

Input file generation and command line interface (yambo -h)

Initializations:

-setup (-i) :Initialization
-coulomb (-r) :Coulomb potential

Response Functions:

-optics (-o) <string> :Linear Response optical properties (more with -h optics)
-X (-d) <string> :Inverse Dielectric Matrix (more with -h X)
-dipoles (-q) :Oscillator strenghts (or dipoles)
-kernel (-k) <string> :Kernel (more with -h kernel)

Self-Energy:

-hf (-x) :Hartree-Fock
-gw0 (-p) <string> :GW approximation (more with -h gw0)
-dyson (-g) <string> :Dyson Equation solver (more with -h dyson)
-lifetimes (-l) :GoWo Quasiparticle lifetimes

Bethe-Salpeter Equation:

-Ksolver (-y) <string> :BSE solver (more with -h Ksolver)

Total Energy:

-acfdt :ACFDT Total Energy

Input file generation and command line interface (**yambo -h xxxxx**)

yambo -h optics Description :Linear Response optical properties
<string>=c Reciprocal-Space
<string>=b for Transition-Space Bethe-Salpeter

yambo -h X Description :Inverse Dielectric Matrix
<string>=(s) static/(p) PA/(f) ull

yambo -h kernel Description :Kernel
<string>=hartree/alda/lrc/hf/sex/bsfxc
hf/sex only eh-space; lrc only G-space

yambo -h Ksolver Description :BSE solver
<string>=h/d/s/(p/f) i
(h) aydock/(d) iagonalization/(s) lepc/(i) nversion

yambo -h gw0 Description :GW approximation
<string>=(p) PA/(c) HOSEX/(r) eal-axis

yambo -h dyson Description :Dyson Equation solver
<string>=(n) ewton/(s) ecant/(g) reen

Input file generation and command line interface (yambo -h)

Help & version:

-help (-h) <string> :<string> can be an option (e.g. -h optics)
-version :Code version & libraries

Input file & Directories:

-Input (-F) <string> :Input file
-Verbosity (-V) <string> :Input file variables verbosity (more with -h Verbosity)
-Job (-J) <string> :Job string
-Idir (-I) <string> :Input directory
-Odir (-O) <string> :I/O directory
-Cdir (-C) <string> :Communication directory

Parallel Control:

-parenv (-E) <string> :Environment Parallel Variables file
-nomp :Switch off MPI support
-noopenmp :Switch off OPENMP support

Utilites:

-Quiet (-Q) :Quiet input file creation
-fatlog :Verbose (fatter) log(s)
-DBlist (-D) :Databases properties
-walltime <int> :Walltime (more with -h walltime)
-slktest :ScaLapack test

Example of practical use

Simple

```
$ yambo -F RPA_optics.in -optics c -kernel hartree ⇒ Generate RPA_optics.in input file (-F)
$ yambo -F RPA_optics.in ⇒ Run yambo. Parameters are loaded from RPA_optics.in (-F)
```

Advanced

```
$ yambo -F Screening.in -X s -V RL ⇒ Generate static Screening.in input file
$ yambo -F Screening.in -J EM1S -C EM1S_out ⇒ Run yambo to compute screening.
```

- Human readable files are stored inside EM1S_out folder (-C)
- To all human readable file-names is appended the EM1S string (-J)
- Binary files are stored inside EM1S folder (-J)

```
$ yambo -F BSE.in -optics b -kernel sex -Ksolver h -X s ⇒ Generate BSE.in input file
$ yambo -F BSE.in -J "BSE,EM1S" -C BSE_out ⇒ Do a BSE simulation loading the screening from
EM1S folder. The parameters inside BSE.in for screening must match the Screening.in input file
```

You can even split the last simulation in two steps (this needs to store the BSE matrix on disk)

```
$ yambo -F BSE_kernel.in -optics b -kernel sex
$ yambo -F BSE.in -J "BSE,EM1S" -C BSE_out ⇒ You could also use KERNEL in place of BSE and use it later
$ yambo -F BSE.in -optics b -kernel sex -Ksolver h -X s
$ yambo -F BSE.in -J "BSE,EM1S" -C BSE_out ⇒ Notice that we always use BSE and BSE_out
```

(1) Linear response (IP/RPA-NLF): `yambo -optics c`

$$\epsilon_{\alpha,\alpha}(\omega) = 1 + \frac{16\pi}{\Omega} \sum_{c,v} \sum_{\mathbf{k}} \frac{1}{E_{c\mathbf{k}} - E_{v\mathbf{k}}} \frac{|\langle v\mathbf{k} | \mathbf{p}_{\alpha} + i[V^{\text{NL}}, \mathbf{r}_{\alpha}] | c\mathbf{k} \rangle|^2}{(E_{c\mathbf{k}} - E_{v\mathbf{k}})^2 - (\omega + i\gamma)^2}$$

See (2)

```
% LongDrXd  
1.000 | 0.000 | 0.000 |  
%  
E-field direction (for q=0)  
Vector (cartesian coordinate)  
Refers to first q-point (QpntsRXd)
```

DFT
k-grid

```
% EnRngeXd  
0.000 | 10.000 | eV  
%  
ETStepsXd = 100  
Energy grid in output  
Range from 0 to 10 in 100 steps
```

```
% BndsRnXd  
1 | 100 |  
Bands used (empty & filled)  
Range from 1 to nbnd  
Reduce range to lower memory. In metals, includes  
partially filled bands. See also EhEngyXd (-V all)
```

```
% DmRngeXd  
0.1000 | 0.100 | eV  
%  
Broadening of spectra  
Either a fixed value, or linearly  
changing between 2 values
```

(2) FFT and oscillators: `yambo -optics c -V RL` (several runlevels)

Dipole/momentum matrix elements ($q \rightarrow 0$) $\langle n\mathbf{k} | \mathbf{p} + i[V^{\text{NL}}, \mathbf{r}] | m\mathbf{k} \rangle$

Screening matrix elements (FFT) $\rho_{nm}(\mathbf{k}, \mathbf{q}, \mathbf{G}) = \langle n\mathbf{k} | e^{i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{r}} | m\mathbf{k} - \mathbf{q} \rangle$

where the wavefunction is expanded over reciprocal lattice (G) vectors: $\phi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{G}} e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}} c_{n\mathbf{k}}(\mathbf{G})$

`FFTGvecs = 1 RL`

Number of G-vectors (or energy cutoff) for expanding wavefunctions in transition matrix elements and FFT operations

Units: number of G-vectors (RL), or energy unit (Ry, mHa, eV)

Determines size (memory) of calculation. Corresponds to cutoff in DFT calculation; can be much less than geometry cutoff

Non-local commutator term

Can greatly increase CPU time. Remove by hiding the `SAVE/ns.kb_pp_pwscf` file.

(3) With local fields (RPA-LFE): `yambo -optics c -kernel hartree`

$$\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \chi_{\mathbf{G},\mathbf{G}'}^0(\mathbf{q},\omega) + \sum_{\mathbf{G}_1,\mathbf{G}_2} \chi_{\mathbf{G},\mathbf{G}_1}^0(\mathbf{q},\omega) [v_{\mathbf{G}_1}(\mathbf{q})\delta_{\mathbf{G}_1,\mathbf{G}_2} + f_{\mathbf{G}_1,\mathbf{G}_2}^{xc}] \chi_{\mathbf{G}_2,\mathbf{G}'}(\mathbf{q},\omega)$$

$$\chi_{\mathbf{G}\mathbf{G}'}^0(\mathbf{q},\omega) = 2 \sum_{c,v} \int_{BZ} \frac{d\mathbf{k}}{(2\pi)^3} \rho_{cv\mathbf{k}}^*(\mathbf{q},\mathbf{G}) \rho_{cv\mathbf{k}}(\mathbf{q},\mathbf{G}') f_{v\mathbf{k}-\mathbf{q}}(1 - f_{c\mathbf{k}}) \times$$

$$\times \left[\frac{1}{\omega + \epsilon_{v\mathbf{k}-\mathbf{q}} - \epsilon_{c\mathbf{k}} + i0^+} - \frac{1}{\omega + \epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}-\mathbf{q}} - i0^+} \right]$$

`% QpntsRXd`

`1 | 6 |`

`%`

Transferred momenta

Range from 1:nqpt (1 = q→0)

`NGsBlkXd=1`

Response block size

Depends on inhomogeneity; needs convergence study, but much less than FFTGvecs

`% EhEnergyXd (-V resp)`

`-1.000 | -1.000 | eV`

Electron-hole energy

range An alternative way to BndsRnXd to restrict transitions, but will not reduce memory

`Chimod="Hartree"`

Kernel: set with -k <opt>

Hartree/ALDA/LRC

`GrFnTpXd="T" (-V resp)`

Green's function: T/R/r/Ta/Ra

"R" = resonant gives the causal response function

(4) Linear response TDDFT: `yambo -optics c -kernel ALDA/LRC`

$$\chi_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \chi_{\mathbf{G},\mathbf{G}'}^0(\mathbf{q},\omega) + \sum_{\mathbf{G}_1,\mathbf{G}_2} \chi_{\mathbf{G},\mathbf{G}_1}^0(\mathbf{q},\omega) \left[v_{\mathbf{G}_1}(\mathbf{q})\delta_{\mathbf{G}_1,\mathbf{G}_2} + f_{\mathbf{G}_1,\mathbf{G}_2}^{xc} \right] \chi_{\mathbf{G}_2,\mathbf{G}'}(\mathbf{q},\omega)$$

Hartree
ALDA/LRC

$$\chi_{\mathbf{G}\mathbf{G}'}^0(\mathbf{q},\omega) = 2 \sum_{c,v} \int_{BZ} \frac{d\mathbf{k}}{(2\pi)^3} \rho_{cv\mathbf{k}}^*(\mathbf{q},\mathbf{G}) \rho_{cv\mathbf{k}}(\mathbf{q},\mathbf{G}') f_{v\mathbf{k}-\mathbf{q}}(1-f_{c\mathbf{k}}) \times$$

See (2)

$$\times \left[\frac{1}{\omega + \epsilon_{v\mathbf{k}-\mathbf{q}} - \epsilon_{c\mathbf{k}} + i0^+} - \frac{1}{\omega + \epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}-\mathbf{q}} - i0^+} \right]$$

`NGsBlkXd=1`

Response block size

*Depends on inhomogeneity;
needs convergence study, but
much less than FFTGvecs*

`FxcGRLc=1`

XC-kernel size

*Needs convergence study.
Much less than FFTGvecs*

`LRC_alpha=1`

LRC fitting parameter

*Long-range tail of the f_{xc}
kernel. Depends on the
system: the larger the
screening the smaller this
parameter.*

`Chimod="ALDA"`

Kernel: set with `-k <opt>`

`<opt>=ALDA`

`<opt>=LRC: semi-empirical kernel
with proper long-range behaviour. It
needs a fitting parameter!`

(5) Screening (RPA): `yambo -x d`

See sheet (3): this runlevel computes the inverse dielectric matrix from $X(\mathbf{G}, \mathbf{G}')$

$$\epsilon_{\mathbf{G}, \mathbf{G}'}^{-1}(\mathbf{q}, \omega) = \delta_{\mathbf{G}, \mathbf{G}'} + v_{\mathbf{G}}(\mathbf{q}) \chi_{\mathbf{G}, \mathbf{G}'}(\mathbf{q}, \omega)$$

Connection with experiment:

$$\epsilon_M(\omega) = \lim_{\mathbf{q} \rightarrow 0} \frac{1}{\epsilon_{\mathbf{G}=0, \mathbf{G}'=0}^{-1}(\mathbf{q}, \omega)}$$

$$\text{Abs}(\omega) = \text{Im} \epsilon_M(\omega) \quad \text{EELS}(\omega) = -\text{Im} \frac{1}{\epsilon_M(\omega)}$$

(6a) Coulomb integrals RIM (Random Integration Method): `yambo -coulomb`

$$v(\mathbf{q} + \mathbf{G}) = \frac{4\pi}{|\mathbf{q} + \mathbf{G}|^2}$$

$$\int_{Bz} \frac{d^3q}{2\pi^3} f(\mathbf{q}, G) v(\mathbf{q} + G) \approx \sum_{q_i} f(q_i, G) v(q_i + G) \Omega_{q_i} \quad \text{Discretization of Bz for integrals}$$

A better approximation is given by:

$$\int_{Bz} \frac{d^3q}{2\pi^3} f(\mathbf{q}, G) v(\mathbf{q} + G) \approx \sum_{q_i} f(q_i, G) I_{q_i}(G)$$

Monte Carlo integral of the Coulomb potential in each region the Bz has been dissected by the q point sampling

$$I_{q_i}(G) = \int_{R_\Gamma} \frac{d^3q'}{(2\pi)^3} v(\mathbf{q} + \mathbf{q}' + G)$$

- Tip: 1. **Needed** for non 3D system to avoid divergences for small q. Suggested also for 3D system to accelerate Sx convergences.
2. **Needed** to build cutoff potential with box shape

Random Integration Method

`RandQpts=1000000`

Number of q points to perform Monte Carlo Integration,

`RandGvec= 1 RL`

Number of G vectors the RIM is calculated

Tip: `RandGvec=1` (gamma) is usually enough. 1 or 2

Million q points is usually accurate.

(6b) Coulomb cutoff :

`yambo -coulomb`

$$v(\mathbf{q} + \mathbf{G}) = \frac{4\pi}{|\mathbf{q} + \mathbf{G}|^2}$$

Truncation of the Coulomb potential for non 3D system to speed up convergence with respect the vacuum

$$V_c(\mathbf{r}) = \begin{cases} \frac{1}{|\mathbf{r}|}, & \text{if } \mathbf{r} \in \mathbf{S}. \\ 0, & \text{otherwise.} \end{cases}$$

- Sphere XYZ: assign: `CUTRadius= 10.0 a.u`
- Cylinder Z: assign `CUTRadius` and `CUTCylLen` (`CUTCylLen=0` indicates infinite cylinder)
- Box Z: assign `CUTBox`

% `CUTBox`

0.00 | 0.00 | 32.00 | # [CUT] [au]

Box sides

%

Box side=0 means do not cut in that direction

S: interacting region:

`CUTGeo= "box Z" XY/YZ or XY/XZ/YZ or XYZ`

- Possible region:
- sphere (0D for molecules),
- cylinder (1D for polymers, tubes, etc),
- box (0D, 1D, 2D).

XYZ: cut in all directions

Box: XY: cut in XY only, etc...

Cylinder X/Y/Z indicates cylinder axis

Tip: When using Box shapes, the RIM is also needed to calculate the potential. In Box for large enough boxes assigns Box side slightly smaller than the cell box

(7) Exchange self energy - Vxc : $\sum_{nk}^x - V_{nk}^{xc}$ **yambo -hf**

$$\Sigma_{nk}^x = \langle nk | \Sigma^x(\mathbf{r}_1, \mathbf{r}_2) | nk \rangle = - \sum_m \int_{BZ} \frac{d\mathbf{q}}{(2\pi)^3} \sum_{\mathbf{G}} v(\mathbf{q} + \mathbf{G}) \|\rho_{nm}(\mathbf{k}, \mathbf{q}, \mathbf{G})\|^2 f_m(\mathbf{k} - \mathbf{q})$$

occupied
bands only

DFT k-grid
{q} = {k-k'}

See (6)

See (2)

`EXXRLvcs= 2487001 RL`

`VXCRLvcs= 2487001 RL`

`%QPkrange`

`1 | 5 | 20 | 59 |`

`4 | 8 | 60 | 80 |`

`%`

`%QPerange (-V qp)`

`1 | 32 | 0.0 | -1.0 |`

`%`

G-vectors in the exchange and xc-potential

Number of RL vectors, or energy in Ry / mHa / etc

Tip : to be converged, possibly leave the maximum value

nk, n'k' ranges where GW/ Σ_x elements are calculated

first k-point | last k-point | lower band | upper band

This can be split over several lines for multiple groups

Tip: careful use of fewer k-points and bands reduces the calculation time; yambo will interpolate the rest

nk,nk' ranges (alternative method)

first k-point | last k-point | lower energy | upper energy

(8) Correlation part of self energy:

yambo -gw0 ppa

$$\Sigma_{n\mathbf{k}}^c(\omega) = \langle n\mathbf{k} | \Sigma^c | n\mathbf{k} \rangle = i \sum_m \int_{BZ} \frac{d\mathbf{q}}{(2\pi)^3} \sum_{\mathbf{G}, \mathbf{G}'} \frac{4\pi}{|\mathbf{q} + \mathbf{G}|^2} \rho_{nm}(\mathbf{k}, \mathbf{q}, \mathbf{G}) \rho_{nm}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}') \times \int d\omega' G_{m\mathbf{k}-\mathbf{q}}^0(\omega - \omega') \epsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}, \omega')$$

```
% GbndRnge  
1 | 50 |  
%
```

Bands used in the GW summation

QP energies usually shows slow convergence

Tip: If you are interested in gaps, energy differences converge faster

```
NGsBlkXp= 100 RL  
Response block size  
See (9)
```

%QPkrange

```
1 | 5 | 20 | 59 |  
4 | 8 | 60 | 80 |
```

%

%QPenergy (-V qp)

```
1 | 32 | 0.0 | -1.0 |
```

%

nk, n'k' ranges where GW/ Σ_c elements are calculated
first k-point | last k-point | lower band | upper band
This can be split over several lines for multiple groups
Tip: careful use of fewer k-points and bands reduces the calculation time; yambo will interpolate the rest

(8a) Dyson Solver: `yambo -dyson n/s`

$$E_{nk}^{QP} = \epsilon_{nk} + \langle \psi_{nk} | \Sigma(E_{nk}^{QP}) - V_{xc} | \psi_{nk} \rangle$$

DysSolver= "n" First order expansion around KS eigenvalue

$$E_{nk}^{QP} = \epsilon_{nk} + Z_{nk} \langle \psi_{nk} | \Sigma(\epsilon_{nk}) - V_{xc} | \psi_{nk} \rangle$$

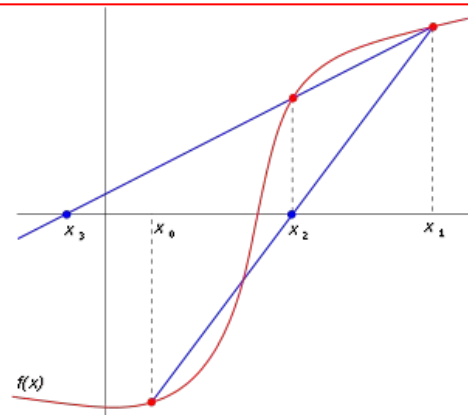
$$Z_{nk} = \left[1 - \frac{d\Sigma_{nk}(\omega)}{d\omega} \Big|_{\omega=\epsilon_{nk}} \right]^{-1}$$

dScStep= 0.10000 eV # [GW] Energy step to evaluate Z

DysSolver= "s" Secant iterative method

https://en.wikipedia.org/wiki/Secant_method

$$x_n = x_{n-1} - f(x_{n-1}) \frac{x_{n-1} - x_{n-2}}{f(x_{n-1}) - f(x_{n-2})} = \frac{x_{n-2} f(x_{n-1}) - x_{n-1} f(x_{n-2})}{f(x_{n-1}) - f(x_{n-2})}$$



(9) Plasmon Pole approximation (PPA):

yambo -X p

Components of the Dielectric matrix approximated has a single pole functions:

$$\epsilon_{\mathbf{G},\mathbf{G}'}^{-1}(\mathbf{q}, \omega) \sim \delta_{\mathbf{G},\mathbf{G}'} + \mathbf{R}_{\mathbf{G},\mathbf{G}'}(\mathbf{q})[(\omega - \Omega_{\mathbf{G},\mathbf{G}'}(\mathbf{q}) + i0^+)^{-1} - (\omega + \Omega_{\mathbf{G},\mathbf{G}'}(\mathbf{q}) - i0^+)^{-1}]$$

Residuals $R_{\mathbf{G},\mathbf{G}'}(\mathbf{q})$ and energies $\Omega_{\mathbf{G},\mathbf{G}'}(\mathbf{q})$ are found by imposing the PPA to reproduce the exact ϵ^{-1} function at $\omega = 0$ and $\omega = iE_{PPA}$ with E_{PPA} being a suitable user-defined parameter.

$$R_{\mathbf{G},\mathbf{G}'}(\mathbf{q}) = \frac{\epsilon_{\mathbf{G},\mathbf{G}'}^{-1}(\mathbf{q}, \omega=0) \Omega_{\mathbf{G},\mathbf{G}'}}{2}$$

$$\Omega_{\mathbf{G},\mathbf{G}'} = E_{PPA} \sqrt{\frac{\epsilon_{\mathbf{G},\mathbf{G}'}^{-1}(\mathbf{q}, \omega=E_{PPA})}{\epsilon_{\mathbf{G},\mathbf{G}'}^{-1}(\mathbf{q}, \omega=0) - \epsilon_{\mathbf{G},\mathbf{G}'}^{-1}(\mathbf{q}, \omega=E_{PPA})}}$$

The QP energies should not depend too much on the choice of imaginary plasmon frequency. **Tip:** Choose a value higher in energy than the plasmon peak (EELS spectrum)

```
% BndsRnXp
```

```
1 | 100 |
```

Bands used (empty & filled)

Range from 1 to nbnd

Reduce range to lower memory.

```
NGsBlkXp= 100      RL
```

Response block size

```
PPAPntXp= 27.21138  eV
```

PPA imaginary energy

(10a) BSE Hamiltonian: `yambo -optics b -kernel sex -X s`

BSE is rewritten as an eigenvalue problem for the 2 particle Hamiltonian:
size of matrix $[N_v \times N_c \times K_{BZ}] \times [N_v \times N_c \times K_{BZ}]$

$$H_{v'c'k'}^{exc\ vck} = (\epsilon_{ck} - \epsilon_{vk}) \delta_{c,c'} \delta_{v,v'} \delta_{\mathbf{k}\mathbf{k}'} + (f_{ck} - f_{vk}) \left[2\bar{V}_{v'c'k'}^{vck} - W_{v'c'k'}^{vck} \right]$$

Difference of quasiparticle energies:
From DFT + QP corrections:

Kernel part: see next slide

KfnQPdb= " E < ./SAVE/ndb.QP"
Location of QP corrections database
From previous GW calculation

OR

% KfnQP_E
1.4000 | 1.200 | 0.900 |
QP corrections parameters
scissor | stretch conduction | stretch valence

% BSEBands
2 | 8 |
Bands Range
lower band | upper band |

(10b) BSE kernel: `yambo -optics b -kernel sex -X s`

Electron-hole exchange part (from Hartree potential - local field effects):

$$K_{vc\mathbf{k},v'c'\mathbf{k}'}^x = \bar{V}_{vc\mathbf{k},v'c'\mathbf{k}'} = \frac{1}{\Omega} \sum_{\mathbf{G} \neq 0} v(\mathbf{G}) \langle c\mathbf{k} | e^{i\mathbf{G}\mathbf{r}} | v\mathbf{k} \rangle \langle v'\mathbf{k}' | e^{-i\mathbf{G}\mathbf{r}} | c'\mathbf{k}' \rangle$$

BSENGexx = 30 Ry
Components of Hartree potential

Electron-hole attraction part (from screened exchange potential - excitonic effects):

$$K_{vc\mathbf{k},v'c'\mathbf{k}'}^c = W_{vc\mathbf{k},v'c'\mathbf{k}'} = \frac{1}{\Omega} \sum_{\mathbf{G}, \mathbf{G}'} v(\mathbf{q} + \mathbf{G}) \epsilon_{\mathbf{G}, \mathbf{G}'}^{-1}(\mathbf{q}) \langle c\mathbf{k} | e^{i(\mathbf{q} + \mathbf{G})\mathbf{r}} | c'\mathbf{k}' \rangle \langle v'\mathbf{k}' | e^{-i(\mathbf{q} + \mathbf{G}')\mathbf{r}} | v\mathbf{k} \rangle \delta_{\mathbf{q}\mathbf{k} - \mathbf{k}'}$$

BSENGblk = 2 Ry
Screened interaction block size

%BandsRnXs
1 | 20 |
NGsBlkXs = 2 Ry
% LongDrXS
1.000 | 1.000 | 1.000|

See (3)

(11a) BSE solver (diagonalisation):

yambo -Ksolver d

The macroscopic dielectric function is obtained as:

$$\epsilon_M(\omega) \equiv 1 - \lim_{\mathbf{q} \rightarrow 0} \frac{8\pi}{|\mathbf{q}|^2 \Omega} \sum_{v\mathbf{k}} \sum_{v'\mathbf{k}'} \langle v\mathbf{k} - \mathbf{q} | e^{-i\mathbf{q}\mathbf{r}} | c\mathbf{k} \rangle \langle c'\mathbf{k}' | e^{i\mathbf{q}\mathbf{r}} | v'\mathbf{k}' - \mathbf{q} \rangle \sum_{\lambda} \frac{A_{cv\mathbf{k}}^{\lambda} (A_{c'v'\mathbf{k}'}^{\lambda})^*}{\omega - E_{\lambda}}$$

```
% BLongDir
1.000000 | 1.000000 | 0.000000
|
%
Direction of the longitudinal perturbation
```

```
% BEnRange
2.00000 | 8.00000 | eV
%
min | max energy range
```

```
BEnSteps= 200
Number of evenly spaced energy points
```

```
% BDmRange
0.10000 | 0.10000 | eV
%
Lorentzian broadening changes linearly
broad@min energy | broad@max energy
```

```
WRbsWF
Store eigenvectors to disk for post-processing
```

Very demanding, gives spectrum,
excitonic energies and wave-functions

(11b) BSE solver (Lanczos-Haydock): `yambo -Ksolver h`

The macroscopic dielectric function is obtained as:

$$\epsilon_M(\omega) \equiv 1 - \lim_{\mathbf{q} \rightarrow 0} \frac{8\pi}{|\mathbf{q}|^2 \Omega} \sum_{v\mathbf{k}} |\langle v\mathbf{k} - \mathbf{q} | e^{-i\mathbf{q}\mathbf{r}} | c\mathbf{k} \rangle|^2 \frac{1}{(\omega - a_1) - \frac{b_2^2}{(\omega - a_2) - \frac{b_3^2}{\dots}}}$$

The a's and b's are obtained iteratively from Lanczos algorithm

`BShayTrs= -0.02000`

Threshold for accuracy of the iterative process of two consecutive approximations to the spectrum

Negative sign: average difference over the energy range

Positive sign: maximum difference over the energy range

In addition to input parameters defined in (11a)

Very efficient, only the spectrum is obtained in output

~~`WRbsWF`~~

~~Not possible !~~

~~Store eigenvectors to disk for post-processing~~

(11b) BSE solver (Slepc library): `yambo -Ksolver s`

$$\epsilon_M(\omega) \equiv 1 - \lim_{q \rightarrow 0} \frac{8\pi}{|q|^2 \Omega} \sum_{vck} \sum_{v'c'k'} \langle vk - q | e^{-iqr} | ck \rangle \langle c'k' | e^{iqr} | v'k' - q \rangle \sum_{\lambda} \frac{A_{cvk}^{\lambda} (A_{c'v'k'}^{\lambda})^*}{\omega - E_{\lambda}}$$

`BSSNEig=20`

Number of eigenvalues to compute

`BSSEnTarget=2.00 eV`

Algorithm looks for the N eigen closest to Target energy

`BSSSlepcMaxIt=500`

Maximum number of iterations (if 0 automatically set by PETSC)

In addition to input parameters defined in (11a)

Advanced (optional) parameters

`WRbsWF`

Store eigenvectors to disk for post-processing

`BSSSlepcApproach="Krylov-Schur"`

(Krylov-Schur, Generalized-Davidson, Jacob-Davidson)

`BSSSlepcPrecondition="bcgs+jacobi"`

Precondition technique (none|preonly+jacobi|bcgs+jacobi)

`BSSSlepcExtrac="harmonic"`

Extraction method

`BSSSlepcTol=1.E-6`

Threshold for iterative schemes

`#BSSSlepcMatrix`

Use faster algorithm which does not use memory distribution

`BSSSlepcNCV= 300`

Dimension of subspace for iterate approaches

Quite efficient. Computational load depends on the number of eigenvalues requested. Gives spectrum, excitonic energies and wave-functions for such eigenvalues.

(13a) Parallelism: Linear Response

$$\chi_{\mathbf{G}\mathbf{G}'}^0(\mathbf{q}, \omega) = 2 \sum_{c,v} \int_{BZ} \frac{d\mathbf{k}}{(2\pi)^3} \rho_{c\nu\mathbf{k}}^*(\mathbf{q}, \mathbf{G}) \rho_{c\nu\mathbf{k}}(\mathbf{q}, \mathbf{G}') f_{\nu\mathbf{k}-\mathbf{q}} (1 - f_{c\mathbf{k}}) \times$$

$$\times \left[\frac{1}{\omega + \epsilon_{\nu\mathbf{k}-\mathbf{q}} - \epsilon_{c\mathbf{k}} + i0^+} - \frac{1}{\omega + \epsilon_{c\mathbf{k}} - \epsilon_{\nu\mathbf{k}-\mathbf{q}} - i0^+} \right]$$

$$\chi(\mathbf{q}, \omega) = [I - \chi^0(\mathbf{q}, \omega)v]^{-1} \chi^0(\mathbf{q}, \omega)$$

`X_all_q_ROLES= "q k c v"` # [PARALLEL] CPUs roles (q,k,c,v)
`X_all_q_CPU= "1 2 4 2"` # [PARALLEL] CPUs for each role
`X_Threads= 4` # [OPENMP/GW] Number of threads
 # for response functions
`X_all_q_LinAlg_INV = 32` # [PARALLEL] CPUs for matrix inv

num MPI tasks = 1 * 2 * 4 * 2
 num threads/MPI-tasks = 4
 Total num threads = 4 * (1 * 2 * 4 * 2)
 MPI-c,v best memory distribution
 MPI-k efficient, some mem repl
 MPI-q may lead to load unbalance
 OpenMP efficient, need extra mem

(13b) Parallelism: Correlation part of self energy

$$\Sigma_{n\mathbf{k}}^c(\omega) = \langle n\mathbf{k} | \Sigma^c | n\mathbf{k} \rangle = i \sum_m \int_{BZ} \frac{d\mathbf{q}}{(2\pi)^3} \sum_{\mathbf{G}, \mathbf{G}'} \frac{4\pi}{|\mathbf{q} + \mathbf{G}|^2} \rho_{nm}(\mathbf{k}, \mathbf{q}, \mathbf{G}) \rho_{nm}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}') \times \int d\omega' G_{m\mathbf{k}-\mathbf{q}}^0(\omega - \omega') \epsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}, \omega')$$

QP states (MPI qp)

G bands (MPI b)

Q transferred momenta (MPI q)

Space DoF (OMP SE_Threads)

SE_ROLES= "q qp b" # [PARALLEL] CPUs roles (q,qp,b)
 SE_CPU= "1 2 8" # [PARALLEL] CPUs for each role
 SE_Threads= 4 # [OPENMP/GW] Number of threads
 # for self-energy

num MPI tasks = 1 x 2 x 8
 num threads/MPI-tasks = 4
 Total num threads = 4 x (1 x 2 x 8)
 MPI-b best memory distribution
 MPI-qp no communication
 MPI-q leads to load unbalance
 OpenMP very efficient

(14) IO: `yambo -V io`

`StdoHash= 40`

`# [IO] Live-timing Hashes`

`DBsIOoff= "none"`

`# [IO] Space-separated list of DB with NO I/O.`

`DB=(DIP,X,HF,COLLS,J,GF,CARRIERS,W,SC,BS,ALL)`

`DBsFRAGpm= "none"`

`# [IO] Space-separated list of +DB to be FRAG and -DB NOT to be FRAG.`

`DB=(DIP,X,W,HF,COLLS,K,BS,QINDX,`

`#WFbuffIO`

`# [IO] Wave-functions buffered I/O`

Parts of the WFs are stored by the node. Nodes communicate when these elements are needed. Memory heavy.

Fragments the database. Smaller files (e.g. `ndb.em1s_fragment_*`) are created instead of a large one (e.g. `ndb.em1s`).

No `ndb.*` file is written. Example: `DBsIOoff= "DIP"` - `ndb.dip_iR_and_P_fragment_*` is not written, but stored in memory if Yambo needs it.

Faster read/write operations in parallel runs

Input file generation and command line interface (ypp -h)

Brillouin Zone:

-grid (-k) <string> :BZ Grid generator (more with -h grid)
-map (-m) :Fine to coarse grid Map

Conversions:

-wf (-w) <string> :WFs (more with -h wf)
-fixsym (-y) :Remove symmetries not consistent with an external perturbation
-qpdb <string> :Quasiparticle Databases (more with -h qpdb)

Plots:

-BSiq (-b) <int> :Excitonic State Momentum
-electron (-s) <string> :Electronic properties (more with -h electron)
-exciton (-e) <string> :Excitonic properties (more with -h exciton)
-freehole :Free hole position in the excitonic plot
-avehole :Average hole/electron wavefunction

Wannier:

-wannier :Wannier 90 interface

Input file generation and command line interface (**ypp -h xxxxx**)

`ypp -h grid` `Description :BZ Grid generator`
`<string>=(k)pt, (q)pt, (s)hifted, (h)igh symmetry, (r)andom, r(e)gular`

`ypp -h wf` `Description :WFs`
`<string>=(p)erturbative SOC mapping, (c)onversion`

`ypp -h qpdb` `Description :Quasiparticle Databases`
`<string>=(g)enerate-modify/ (m)erge/ (e)xpand`
`(e)xpand uses the symmetries to generate a BZ-expanded QP database`

`ypp -h electron` `Description :Electronic properties`
`<string>=(w)ave, (d)ensity, (m)ag, do(s), (b)ands, (c)urrent`

`ypp -h exciton` `Description :Excitonic properties`
`<string>=(s)ort, (sp)in, (a)mplitude, (w)ave, (i)nterpolate`

(YPP 1) Postprocessing - exciton plot:

`ypp -exciton w qindx`

```
excitons          # [R] Excitons
wavefunction      # [R] Wavefunction
Format= "x"       # Output format [(c)ube/(g)nuplot/(x)crysden]
Direction= "123"  # [rlu] [1/2/3] for 1d or [12/13/23] for 2d [123] for 3D
FFTGvecs= 30 Ry  # [FFT] Plane-waves
States= "1 - 3"   # Index of the BS state(s)
Degen_Step= 0.0100 eV # Maximum energy separation of two degenerate states
% Cells
5 | 5 | 1 |      # Number of cell repetitions in each direction (odd or 1)
%
% Hole
0.00 | 3.44      | 0.00 | # [cc] Hole position in unit cell
```

Excitonic wavefunction does not have the periodicity of the e and h wavefunctions but is generally more extended, with a fictitious periodicity due to the k-points sampling