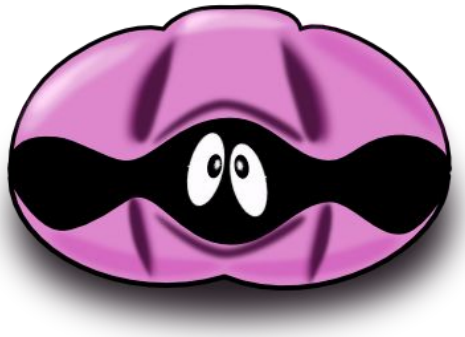
Yambo©



Cheatsheet

For yambo 5.0

MAX

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
 -nompi                             :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
$ yambo -F RPA_optics.in
```

⇒ Generate RPA_optics.in input file (-F)

⇒ Run yambo. Parameters are loaded from RPA_optics.in (-F)

Advanced

```
$ yambo -F Screening.in -X s -V RL
$ yambo -F Screening.in -J EM1S -C EM1S_out
```

⇒ Generate static Screening.in input file

⇒ 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
$ yambo -F BSE.in -J "BSE,EM1S" -C BSE_out
```

⇒ Generate BSE.in input file

⇒ 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
$ yambo -F BSE.in -optics b -kernel sex -Ksolver h -X s
$ yambo -F BSE.in -J "BSE,EM1S" -C BSE_out
```

⇒ You could also use KERNEL in place of BSE and use it later

⇒ Notice that we always use BSE and BSE_out

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

See (2)

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

```
% 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
%
ETStpsXd = 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 ($q \to 0$)

$$\langle n\mathbf{k}|\mathbf{p} + i[V^{\mathrm{NL}}, \mathbf{r}]|m\mathbf{k}\rangle$$

Screening matrix elements (FFT)

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

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`

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

Hartree ALDA/LRC

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

See (2)

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

```
% 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

`% EhEngyXd (-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`

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

Hartree — ALDA/LRC

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

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(G,G')

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

Connection with experiment:

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

$$\mathrm{Abs}(\omega) = \mathrm{Im}\,\epsilon_M(\omega) \qquad \mathrm{EELS}(\omega) = -\mathrm{Im}\,\frac{1}{\epsilon_M(\omega)}$$

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

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

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

A better approximation is given by:

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

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

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

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`

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

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

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

S: interactting region:

CUTGeo= "box Z" X/Y/Z 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

- 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

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

(7) Exchange self energy - Vxc : $\Sigma^x_{n\mathbf{k}} - V^{xc}_{n\mathbf{k}}$ yambo -hf

$$\Sigma^x_{n\mathbf{k}} = \langle n\mathbf{k}|\Sigma^x(\mathbf{r}_1,\mathbf{r}_2)|n\mathbf{k}\rangle = -\sum_m \int_{BZ} \frac{d\mathbf{q}}{(2\pi)^3} \sum_{\mathbf{G}} v(\mathbf{q}+\mathbf{G}) \left|\rho_{nm}(\mathbf{k},\mathbf{q},\mathbf{G})\right|^2 f_{m(\mathbf{k}-\mathbf{q})}$$

See (6) — See (2)

occupied bands only

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

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

```
EXXRLvcs= 2487001 RL
VXCRLvcs= 2487001 RL
```

```
%QPkrange
  1|  5| 20|  59|
  4|  8| 60|  80|
%
%QPerange (-V qp)
  1| 32| 0.0|-1.0|
%
```

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`

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

```
%QPkrange
  1|  5| 20|  59|
  4|  8| 60|  80|
%
%QPerange (-V qp)
  1| 32| 0.0|-1.0|
%
```

```
% 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)

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

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

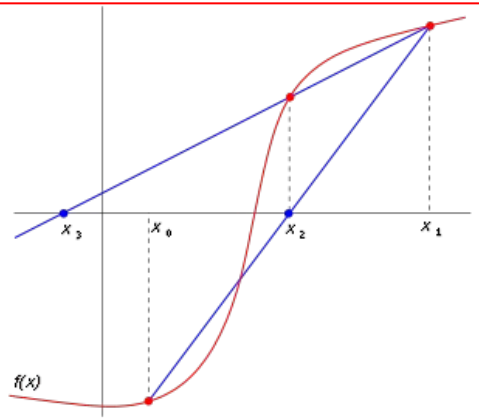
$$Z_{nk} = \left[1 - \frac{d\Sigma_{nk}(\omega)}{d\omega} \Big|_{\omega=\epsilon_{nk}} \right]^{-1}$$

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:

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

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 ω = 0 and ω = iE_{PPA} with E_{PPA} being a suitable user-defined parameter.

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

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

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 x N_c x K_{BZ}] x [N_v x N_c x K_{BZ}]

$$H^{exc}_{\substack{vc\mathbf{k}\\ v'c'\mathbf{k}'}} = (\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}})\delta_{c,c'}\delta_{v,v'}\delta_{\mathbf{k}\mathbf{k}'} + (f_{c\mathbf{k}} - f_{v\mathbf{k}})[2\bar{V}_{\substack{vc\mathbf{k}\\ v'c'\mathbf{k}'}} - W_{\substack{vc\mathbf{k}\\ v'c'\mathbf{k}'}}]$$

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):

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

BSENGexx = 30 Ry
Components of Hartree potential

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

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

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:

$$\epsilon_M(\omega) \equiv 1 - \lim_{\mathbf{q}\to 0} \frac{8\pi}{|\mathbf{q}|^2\Omega} \sum_{vc\mathbf{k}} \sum_{v'c'\mathbf{k}'} \langle v\mathbf{k}-\mathbf{q}|e^{-i\mathbf{qr}}|c\mathbf{k}\rangle\langle c'\mathbf{k}'|e^{i\mathbf{qr}}|v'\mathbf{k}'-\mathbf{q}\rangle \sum_{\lambda} \frac{A^{\lambda}_{cv\mathbf{k}} \left(A^{\lambda}_{c'v'\mathbf{k}'}\right)^*}{\omega - E_{\lambda}}$$

```
% 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:

$$\epsilon_M(\omega) \equiv 1 - \lim_{\mathbf{q}\to 0} \frac{8\pi}{|\mathbf{q}|^2\Omega} \sum_{vc\mathbf{k}} \left|\langle v\mathbf{k}-\mathbf{q}|e^{-i\mathbf{q}\mathbf{r}}|c\mathbf{k}\rangle\right|^2 \cfrac{1}{(\omega-a_1)-\cfrac{b_2^2}{(\omega-a_2)-\cfrac{b_3^2}{\cdots}}}.$$

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`

Store eigenvectors to disk for post-processing

Not possible !

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

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

```
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)

`WRbsWF`
Store eigenvectors to disk for post-processing

Advanced (optional) parameters

```
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

$$\chi^0_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) = 2\sum_{c,v}\int_{BZ}\frac{d\mathbf{k}}{(2\pi)^3}\rho^*_{cv\mathbf{k}}(\mathbf{q},\mathbf{G})\rho_{cv\mathbf{k}}(\mathbf{q},\mathbf{G}')f_{v\mathbf{k}-\mathbf{q}}(1-f_{c\mathbf{k}})\times\left[\frac{1}{\omega+\epsilon_{v\mathbf{k}-\mathbf{q}}-\epsilon_{c\mathbf{k}}+i0^+}-\frac{1}{\omega+\epsilon_{c\mathbf{k}}-\epsilon_{v\mathbf{k}-\mathbf{q}}-i0^+}\right]$$

Q momenta (MPI q)

Xo bands (MPI c,v)

k momenta (MPI k)

Space DoF

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

```
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

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

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.

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.

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

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 -exiton 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