Absorption, Electron Energy Loss (and IXS) with the Yambo code

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G space:

* RPA, RPA with LF and TDDFT

Good description of EELS (and IXSS),
failure of description of absorption

eh space:

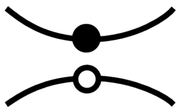
* Casida equation for TDDFT

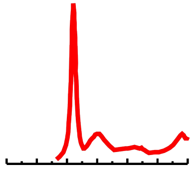
Good approach for isolated systems (?)

* The Bethe-Salpeter equation

The exciting physics of the exciton

Steps for absorption and EELS in G-space

DFT calculation (pwSCF/Abinit) 

Solution of the TDDFT in G space 

Absorption and EELS in G-space the IP-RPA approximation

$$\chi(\mathbf{q},\omega)=\chi^0(\mathbf{q},\omega)+\chi^0(\mathbf{q},\omega)\left(v_{G=0}+v_{G>0}+f_{xc}(\mathbf{q},\omega)\right)\chi(\mathbf{q},\omega)$$

[BSK] runlevel: yambo -o c main variables:

```
optics                        # [R OPT] Optics
chi                          # [R CHI] Dyson equation for Chi.
Chimod= "IP"                       # [X] IP/Hartree/ALDA/LRC/BSfxc
% QpntsRXd
  1 |  8 |                   # [Xd] Transferred momenta
%
% BndsRnXd
  1 |  8 |                   # [Xd] Polarization function bands
%
% EnRngeXd
  0.00000 | 10.00000 | eV    # [Xd] Energy range
%
% DmRngeXd
  0.10000 |  0.10000 | eV    # [Xd] Damping range
%
ETStpsXd= 100                # [Xd] Total Energy steps
% LongDrXd
 1.000000 | 0.000000 | 0.000000 |       # [Xd] [cc] Electric Field
%
```

$$\chi_0(r,r',\omega)=\sum_{ij}\frac{\psi_j(r)\psi_i^*(r)\psi_i(r')\psi_j^*(r')}{\omega-\Delta\epsilon_{ij}+i\eta}$$

$$\epsilon_0^{-1}(q,\omega)=1+\frac{4\pi}{q^2}\int\int dr\,dr'\,e^{iqr}e^{-iqr'}\chi_0(r,r',\omega)$$

$\epsilon_0^{-1}(q\rightarrow 0,\omega)$: *limit direction*

TD-Hatree and TDDFT in G-space

$$\chi(\mathbf{q},\omega)=\chi^0(\mathbf{q},\omega)+\chi^0(\mathbf{q},\omega)\left(v_{G=0}+v_{G>0}+f_{xc}(\mathbf{q},\omega)\right)\chi(\mathbf{q},\omega)$$

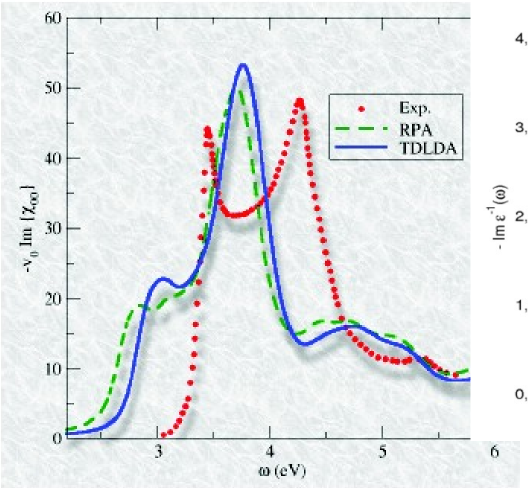
Time-dependent Hartree   Time-dependent ALDA

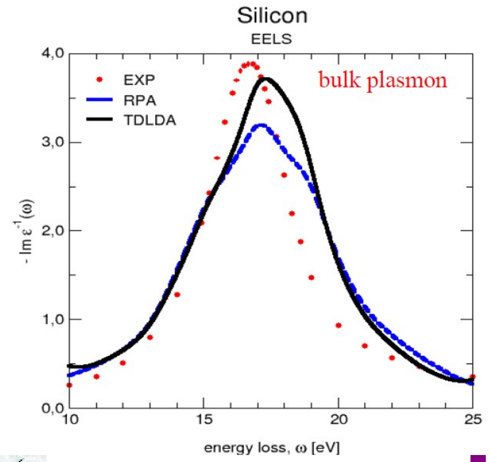
[BSK] runlevel: yambo -o c -k [hartree/alda/lrc], main variables:

```
Chimod= "Hartree"          # [X] IP/Hartree/ALDA/LRC
NGsBlkXd= 1          RL    # [Xd] Response block size

Chimod= "ALDA"             # [X] IP/Hartree/ALDA/LRC
FxcGRLc= 1           RL    # [TDDFT] XC-kernel RL size
NGsBlkXd= 1          RL    # [Xd] Response block size

Chimod= "LRC"              # [X] IP/Hartree/ALDA/LRC/BSfxc
LRC_alpha= 0.000000        # [TDDFT] LRC alpha factor
NGsBlkXd= 1          RL    # [Xd] Response block size
```



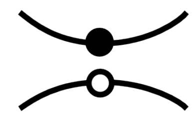


Matrix inversion in G-space :

$$\chi(\mathbf{q},\omega)=\left(\chi_0^{-1}(\mathbf{q},\omega)-v_{G=0}-v_{G>0}-f_{xc}(\mathbf{q},\omega)\right)^{-1}$$

Steps for TDDFT in eh-space calculation:

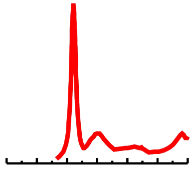
DFT calculation (pwSCF/Abinit)



Calculation of the TDDFT matrix

$$H = \left(\begin{array}{c|cc} & |eh\rangle & |he\rangle \\ \hline \langle eh| & R & C \\ \langle he| & -C^* & -R^* \end{array}\right)$$

Solution of the TDDFT eh equation



TDDFT in the eh space

$$\bar{\chi}^{-1}(\omega)=\chi_0^{-1}(\omega)-v_{G>0}-f_{xc}(\omega)$$

$$H^{2p}_{ij,hk}=(\epsilon_i-\epsilon_j)\delta_{i,h}\delta_{j,k}-(f_j-f_i)K_{ij,hk'}$$

$$H=\left(\begin{array}{c|cc} & |eh\rangle & |he\rangle \\ \hline \langle eh| & R & C \\ \langle he| & -C^* & -R^* \end{array}\right)$$

[BSK] runlevel: yambo -o b, main variables:

$$\chi_0(r,r',\omega)=\sum_{ij}\frac{\psi_j(r)\psi_i^*(r)\psi_i(r')\psi_j^*(r')}{\omega-\Delta\epsilon_{ij}+i\eta}$$

```
optics                    # [R OPT] Optics
bse                       # [R BSE] Bethe Salpeter Equation.
BSEmod= "causal"          # [BSE] resonant/causal/coupling
BSKmod= "IP"              # [BSE] IP/Hartree/HF/ALDA/SEX
% BLongDir
 1.000000 | 0.000000 | 0.000000 |        # [BSS] [cc] Electric Field
%
% BSEBands
  1 |  8 |               # [BSK] Bands range
```

In the IP approx we can Directly construct the dielectric function in the resonant only case:

$$\epsilon_0(q,\omega)=1-\frac{4\pi}{q^2}\int\int dr\,dr'\,e^{iqr}e^{-iqr'}\chi_0(r,r',\omega)$$

$\epsilon_0(q\rightarrow 0,\omega)$: *limit direction*

```
% BEnRange
  0.00000 | 10.00000 | eV    # [BSS] Energy range
%
% BDmRange
  0.10000 |  0.10000 | eV    # [BSS] Damping range
%
BEnSteps= 100               # [BSS] Energy steps
```

TD-DFT, TD-Hartree in the eh space

$$\bar{\chi}^{-1}(\omega)=\chi_0^{-1}(\omega)-v_{G>0}-f_{xc}(\omega)$$

$$H^{2p}_{ij,hk}=(\epsilon_i-\epsilon_j)\delta_{i,h}\delta_{j,k}-(f_j-f_i)K_{ij,hk'}$$

$$H=\left(\begin{array}{c|cc} & |eh\rangle & |he\rangle \\ \hline \langle eh| & R & C \\ \langle he| & -C^* & -R^* \end{array}\right)$$

[BSK] runlevel: yambo -o b -k hartree/alda, main variables:

```
bsk                      # [R BSK] Bethe Salpeter Equation kernel
BSEmod= "causal"            # [BSE] resonant/causal/coupling
BSKmod= "Hartree"           # [BSE] IP/Hartree/HF/ALDA/SEX
```

```
tddft                    # [R   K] Use TDDFT kernel
bsk                      # [R BSK] Bethe Salpeter Equation kernel
BSEmod= "causal"            # [BSE] resonant/causal/coupling
BSKmod= "ALDA"              # [BSE] IP/Hartree/HF/ALDA/SEX
BSENGexx= 2085        RL    # [BSK] Exchange components
```

Solve the eh matrix: diagonalization

Standard diagonalization:

$$H = \left(\begin{array}{c|cc} & |eh\rangle & |he\rangle \\ \hline \langle eh| & R & C \\ \langle he| & -C^* & -R^* \end{array}\right) \Rightarrow \begin{array}{l} \text{eigenstates } |\lambda\rangle \\ \text{eigenvalues } E_\lambda \\ \text{eigenvectors } A^{\lambda}_{n'n\mathbf{k}} = \langle n'n\mathbf{k}|\lambda\rangle \end{array}$$

[BSS] runlevel , yambo -y d

```
bss                # [R BSS] Bethe Salpeter Equation solver
BSSmod= "d"        # [BSS] (h)aydock/(d)iagonalization/(i)nversion`
```

```
% BEnRange
  0.00000 | 10.00000 | eV    # [BSS] Energy range
%
% BDmRange
  0.10000 |  0.10000 | eV    # [BSS] Damping range
%
BEnSteps= 100               # [BSS] Energy steps
```

Then the dielectric function in the resonant only case:

$$\epsilon_M(\omega) \equiv 1 - \lim_{\mathbf{q}\to 0} \frac{8\pi}{|\mathbf{q}|^2 \Omega N_q} \sum_{nn'\mathbf{k}} \sum_{mm'\mathbf{k}'} \rho^*_{n'n\mathbf{k}}(\mathbf{q},\mathbf{G})\, \rho_{m'm\mathbf{k}'}(\mathbf{q},\mathbf{G}') \sum_{\lambda} \frac{A^{\lambda}_{n'n\mathbf{k}} \left(A^{\lambda}_{m'm\mathbf{k}'}\right)^*}{\omega - E_\lambda},$$

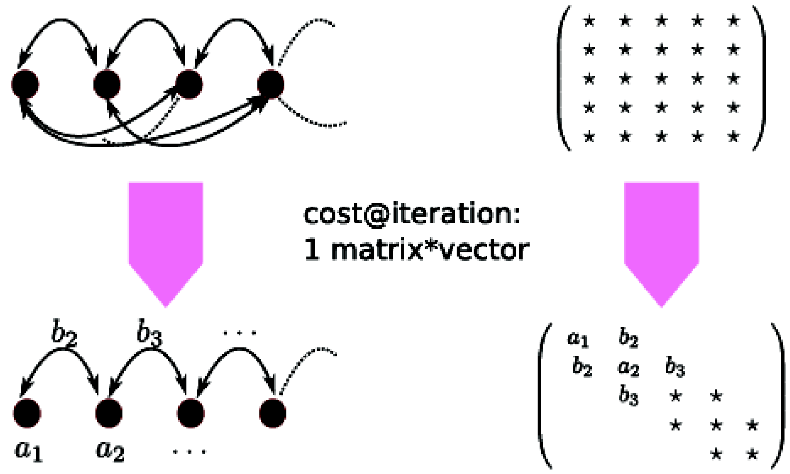
Solve the eh matrix: Lanczo-Haydock method

Lanczos-Haydock method:

[BSS] runlevel , yambo -y h

```
bss                    # [R BSS] Bethe Salpeter Equation solver
BSSmod= "h"            # [BSS] (h)aydock/(d)iagonalization/(i)nversion`
BSHayTrs= -0.02000     # [BSS] [o/o] Haydock treshold.
                         Strict(>0)/Average(<0)

% BEnRange
  0.00000 | 10.00000 | eV    # [BSS] Energy range
%
% BDmRange
  0.10000 |  0.10000 | eV    # [BSS] Damping range
%
BEnSteps= 100                # [BSS] Energy steps
```



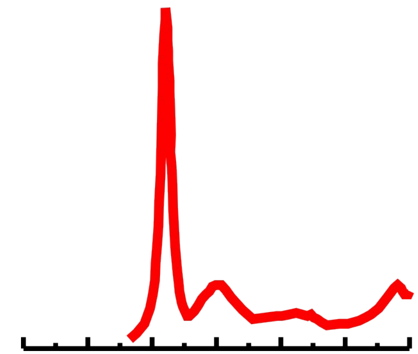
This allows to rewrite the dielectric function as:

$$\epsilon(\omega) \rightarrow \langle P|(\omega - H)^{-1}|P\rangle = \cfrac{1}{(\omega - a_1) - \cfrac{b_2^2}{(\omega - a_2) - \cfrac{b_3^2}{\cdots}}}$$

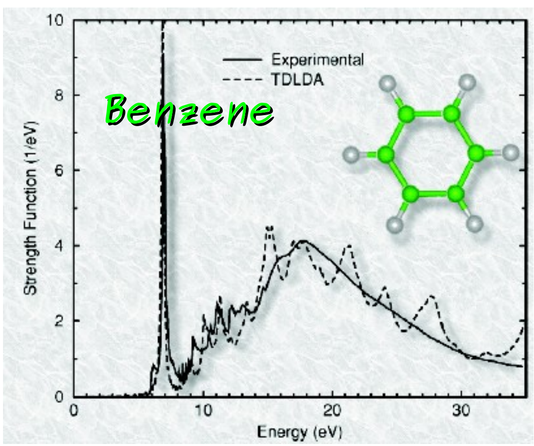
$$|P\rangle = \lim_{\mathbf{q}\to 0} \frac{1}{|\mathbf{q}|} |v c\mathbf{k}\rangle\langle v\mathbf{k}-\mathbf{q}|e^{-i\mathbf{q}\cdot\mathbf{r}}|c\mathbf{k}\rangle$$

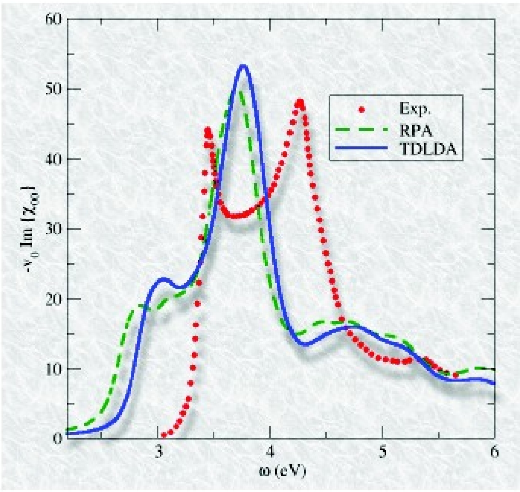
Solve the eh matrix for TDDFT: main variables

$$H = \left(\begin{array}{c|cc} & |eh\rangle & |he\rangle \\ \hline \langle eh| & R & C \\ \langle he| & -C^* & -R^* \end{array}\right)$$



[BSS] runlevel , yambo -y <opt>, main variables:



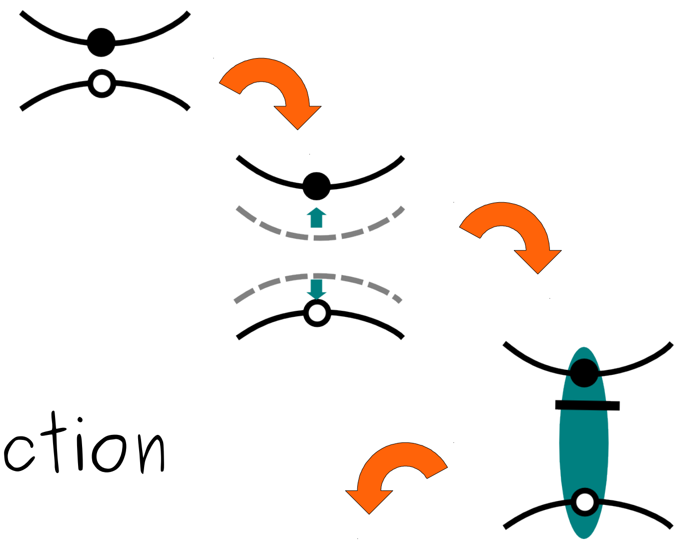


Steps for Bethe-Salpeter calculation:

DFT calculation (pwSCF/Abinit)

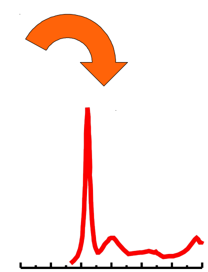
Calculation of QP corrections

Calculation of the screening function



Calculation of the BS matrix

$$H = \left(\begin{array}{c|cc} & |eh\rangle & |he\rangle \\ \hline \langle eh| & R & C \\ \langle he| & -C^{*} & -R^{*} \end{array}\right)$$



Solution of the BS equation

The QP corrections

1 You can compute the quasi-particle corrections as shown yesterday

GW

Screened Coulomb term

$$\Sigma^{GW}(1,2) = iG(12)W(21)$$

⇒ **Standard Bethe-Salpeter equation (Time-Dependent Screened Hartree-Fock)**

[Xd] runlevel: yambo -g n/s

HF

Coulomb term

$$\Sigma_x(1,2) = iG(12)v(21)$$

⇒ **Time-Dependent Hartree-Fock**

[Xd] runlevel: yambo -x

and import them later when you compute the spectrum

KfnQPdb= "E< ndb.QP" **# [EXTQP BSK BSS] Database**

(http://www.yambo-code.org/input_file/vars/var_QPdb.php)

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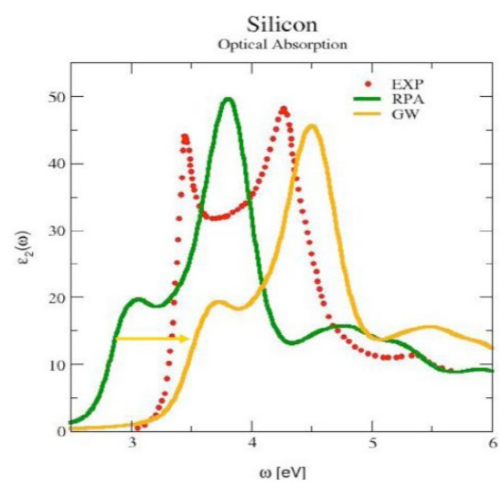
2 Or you can take it from the literature and insert the right parameters in the input file later when you compute the spectrum



% XfnQP_E
0.80000 | 1.000000 | 1.000000 | **# [EXTQP Xd] E parameters (c/v)**
%

Calculation of the static screening:

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

with

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

$$\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) = \left[\delta_{\mathbf{G}\mathbf{G}''} - v(\mathbf{q}+\mathbf{G}'')\chi^0_{\mathbf{G}\mathbf{G}''}(\mathbf{q},\omega)\right]^{-1}\chi^0_{\mathbf{G}''\mathbf{G}'}(\mathbf{q},\omega).$$

Random-Phase-Approximation

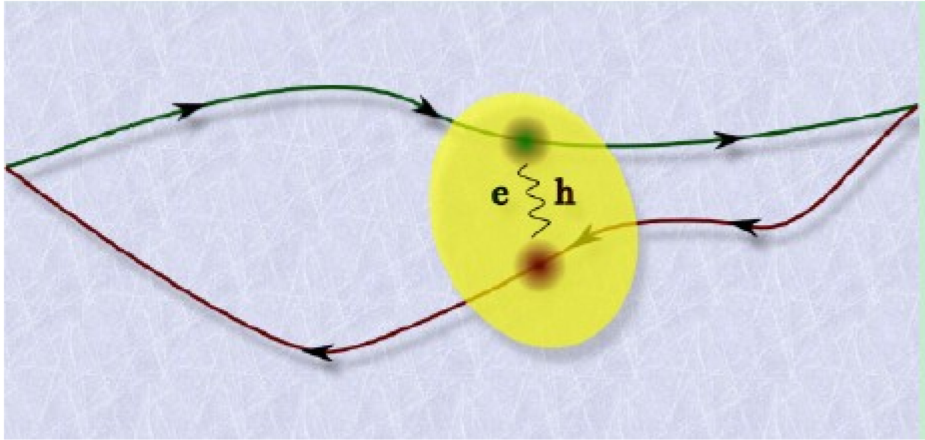
$$\epsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) = \delta_{\mathbf{G}\mathbf{G}'} + v(\mathbf{q}+\mathbf{G})\,\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega).$$

Static : $\omega = 0$

[Xs] runlevel: yambo -b:

```
em1s                       # [R Xs] Static Inverse Dielectric Matrix
Chimod= "hartree"          # [X] IP/Hartree/ALDA/LRC/BSfxc
% BndsRnXs
  1 |  8 |                 # [Xs] Polarization function bands
%
NGsBlkXs= 1          RL    # [Xs] Response block size
% LongDrXs
 1.000000 | 0.000000 | 0.000000 |        # [Xs] [cc] Electric Field
%
```

This will be needed to construct the BSE kernel



Or take the screening from the dynamical screening:

[Xd] runlevel: yambo -d / yambo -d -p p

Maybe you previously calculatade the dynamical dielectric, so you have the ndb.em1d or the ndb.ppa database, and you can use them …

BSE (and TD-HF) in the eh-space

$$\bar{L}^{-1}(\omega) = L_0^{-1}(\omega) - (v_{G>0} - W(\omega=0))$$

$$H = \begin{pmatrix} & |eh\rangle & |he\rangle \\ \langle eh| & R & C \\ \langle he| & -C^* & -R^* \end{pmatrix}$$

$$\bar{L}_{(n_1,n_2)(n_3,n_4)} = [H^{exc} - I\omega]^{-1}_{(n_1,n_2)(n_3,n_4)}(f_{n_4} - f_{n_3})$$

[BSK] runlevel: yambo -o b, main variables:

```
optics                    # [R OPT] Optics
bse                       # [R BSE] Bethe Salpeter Equation.
BSEmod= "causal"          # [BSE] resonant/causal/coupling
BSKmod= "IP"              # [BSE] IP/Hartree/HF/ALDA/SEX
% BLongDir
 1.000000 | 0.000000 | 0.000000 |       # [BSS] [cc] Electric Field
%
% BSEBands
  1 |  8 |                # [BSK] Bands range
```

This are the same as before
… just to remember

$$\epsilon_M(\omega) = 1 - \lim_{\mathbf{q}\to 0}\left[V_{\mathbf{G}=0}(\mathbf{q})\int d\mathbf{r}d\mathbf{r}' e^{-i\mathbf{q}(\mathbf{r}-\mathbf{r}')}\bar{L}(\mathbf{r},\mathbf{r},\mathbf{r}',\mathbf{r}';\omega)\right]$$

$$L^0_{(n_1,n_2)(n_3,n_4)} = \frac{f_{n_1} - f_{n_2}}{\omega - (E_{n_2} - E_{n_1})}\delta_{n_1 n_3}\delta_{n_2 n_4}$$

Calculation of the BS (/TD-HF) matrix:

$$W_{\substack{nn'\mathbf{k}\\ ss'\mathbf{k}_1}} = \frac{1}{\Omega N_q}\sum_{\mathbf{G}\mathbf{G}'} \rho_{ns}\left(\mathbf{k},\mathbf{q}=\mathbf{k}-\mathbf{k}_1,\mathbf{G}\right)\rho^*_{n's'}\left(\mathbf{k}_1,\mathbf{q}=\mathbf{k}-\mathbf{k}_1,\mathbf{G}'\right)\epsilon^{-1}_{\mathbf{G}\mathbf{G}'}v\left(\mathbf{q}+\mathbf{G}'\right),$$

$$\bar{V}_{\substack{nn'\mathbf{k}\\ ss'\mathbf{k}_1}} = \frac{1}{\Omega N_q}\sum_{\mathbf{G}\neq 0} \rho_{nn'}\left(\mathbf{k},\mathbf{q}=0,\mathbf{G}\right)\rho^*_{ss'}\left(\mathbf{k}_1,\mathbf{q}=0,\mathbf{G}\right)v\left(\mathbf{G}\right).$$

$$H_{\substack{nn'\mathbf{k}\\ mm'\mathbf{k}'}} = \left(\varepsilon_{n\mathbf{k}}-\varepsilon_{n'\mathbf{k}}\right)\delta_{nm}\delta_{n'm'}\delta_{\mathbf{k}\mathbf{k}'} + \left(f_{n'\mathbf{k}}-f_{n\mathbf{k}}\right)\left[2\bar{V}_{\substack{nn'\mathbf{k}\\ mm'\mathbf{k}'}} - W_{\substack{nn'\mathbf{k}\\ mm'\mathbf{k}'}}\right].$$

$$H = \begin{pmatrix} & |eh\rangle & |he\rangle \\ \langle eh| & R & C \\ \langle he| & -C^* & -R^* \end{pmatrix}$$

[BSK] runlevel: yambo -o b -k sex/hf, main variables:

```
KfnQPdb= "none"          # [EXTQP BSK BSS] Database
BSEmod= "causal"          # [BSE] resonant/causal/coupling
BSKmod= "SEX"            # [BSE] IP/Hartree/HF/ALDA/SEX
BSENGexx= 2085       RL    # [BSK] Exchange components
BSENGBlk= 1          RL    # [BSK] Screened interaction block size
#WehCpl                  # [BSK] eh interaction included also in coupling
```

or

```
% XfnQP_E
 0.80000 | 1.000000 | 1.000000 |      #
%
```

Screened Coulomb term

$$\Sigma^{GW}(1,2) = iG(12)W(21)$$

⇒ **Standard Bethe-Salpeter equation (Time-Dependent Screened Hartree-Fock)**

Coulomb term

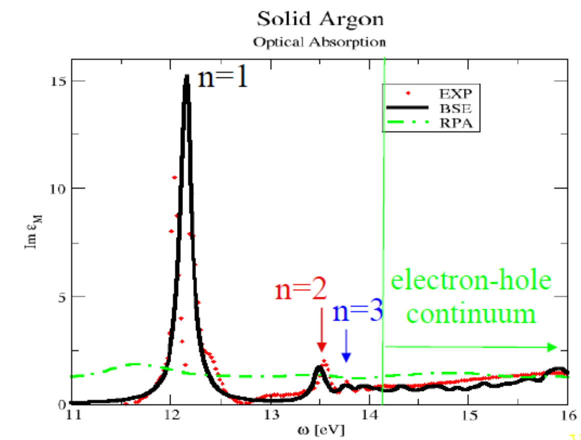
$$\Sigma_x(1,2) = iG(12)v(21)$$

⇒ **Time-Dependent Hartree-Fock**

```
KfnQPdb= "none"          # [EXTQP BSK BSS] Database
BSEmod= "causal"          # [BSE] resonant/causal/coupling
BSKmod= "HF"             # [BSE] IP/Hartree/HF/ALDA/SEX
BSENGexx= 2085       RL    # [BSK] Exchange components
BSENGBlk= 1          RL    # [BSK] Screened interaction block size
```

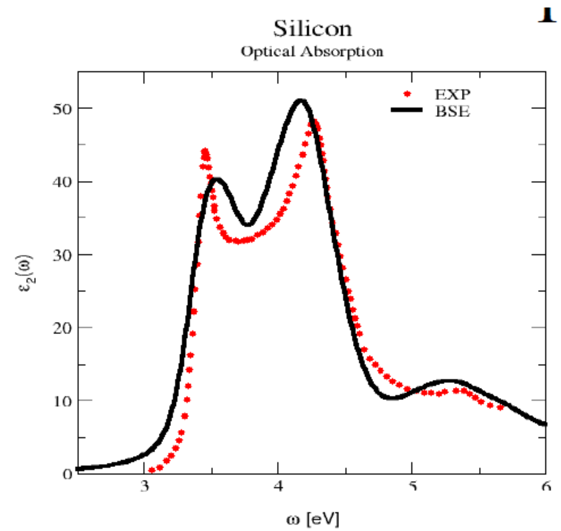
Solve the eh matrix for BSE: main variables

$$H = \left(\begin{array}{c|cc} & |eh\rangle & |he\rangle \\ \hline \langle eh| & R & C \\ \langle he| & -C^* & -R^* \end{array}\right)$$



[BSS] runlevel , yambo -y <opt>, main variables:

As before you can use the diagonalization solver or the Haydock solver (or also the inversion solver)



Thank you for
for your attention!