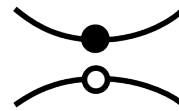


# Steps for Bethe-Salpeter calculation:

0. DFT calculation (pwSCF)



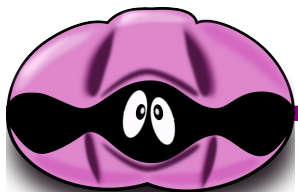
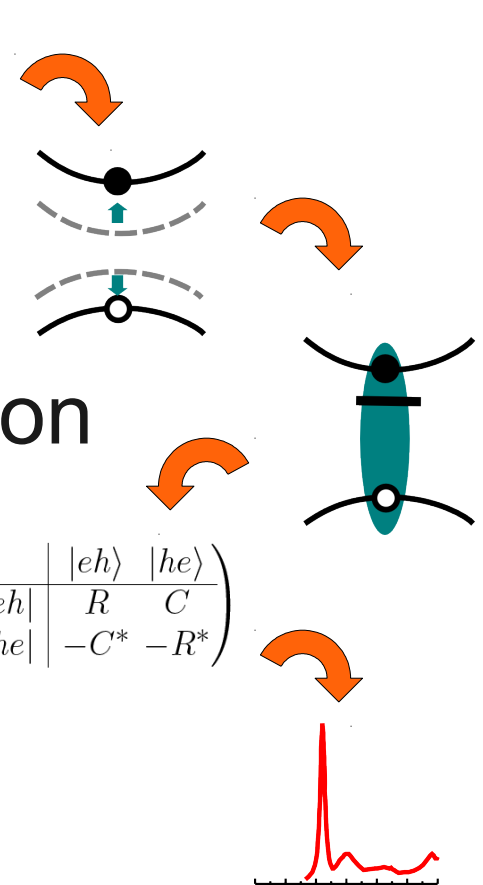
1. Calculation of QP corrections

2. Calculation of the screening function

3. Calculation of the BS matrix

4. Solution of the BS equation

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



# Calculation of the screening:

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

$$\left[ \frac{1}{\omega + \varepsilon_{n\mathbf{k}-\mathbf{q}} - \varepsilon_{n'\mathbf{k}} + i0^+} - \frac{1}{\omega + \varepsilon_{n'\mathbf{k}} - \varepsilon_{n\mathbf{k}-\mathbf{q}} - i0^+} \right].$$

with

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

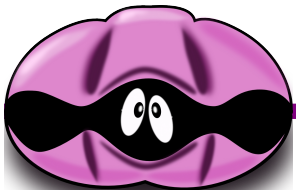
$$\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega) = \left[ \delta_{\mathbf{G}\mathbf{G}'} - v(\mathbf{q} + \mathbf{G}') \chi_{\mathbf{G}\mathbf{G}'}^0(\mathbf{q}, \omega) \right]^{-1} \chi_{\mathbf{G}\mathbf{G}'}^0(\mathbf{q}, \omega).$$

Random-Phase-Approximation

$$\epsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}, \omega) = \delta_{\mathbf{G}\mathbf{G}'} + v(\mathbf{q} + \mathbf{G}') \chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}, \omega). \quad \text{Static: } \omega = 0$$

**[Xs] runlevel: yambo -b, main variables:**

```
% QpntsRXs
  1 |  4 |           # [Xs] Transferred momenta
%
% BndsRnXs
  1 | 60 |          # [Xs] Polarization function bands
%
NGsBlkXs= 51  RL   # [Xs] Response block size
```



# Calculation of the BS matrix:

$$W_{ss'k_1}^{nn'k} = \frac{1}{\Omega N_q} \sum_{\mathbf{G}\mathbf{G}'} \rho_{ns}(\mathbf{k}, \mathbf{q} = \mathbf{k} - \mathbf{k}_1, \mathbf{G}) \rho_{n's'}^*(\mathbf{k}_1, \mathbf{q} = \mathbf{k} - \mathbf{k}_1, \mathbf{G}') \epsilon_{\mathbf{G}\mathbf{G}'}^{-1} v(\mathbf{q} + \mathbf{G}'),$$

$$\bar{V}_{ss'k_1}^{nn'k} = \frac{1}{\Omega N_q} \sum_{\mathbf{G} \neq 0} \rho_{nn'}(\mathbf{k}, \mathbf{q} = 0, \mathbf{G}) \rho_{ss'}^*(\mathbf{k}_1, \mathbf{q} = 0, \mathbf{G}) v(\mathbf{G}).$$

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



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

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

```

KfnQPdb= "none"           # [EXTQP BSK BSS] Database
KfnQP_N= 1                # [EXTQP BSK BSS] Interpolation neighbours
% KfnQP_E
 2.400000 | 1.000000 | 1.000000 |          # [EXTQP BSK BSS] E parameters (c/v)
%
% KfnQP_W
 0.000    | 0.000    | 0.000    | 0.000    |          # [EXTQP BSK BSS] W parameters (c/v)
%
KfnQP_Z= ( 1.000000 , 0.000000 )          # [EXTQP BSK BSS] Z factor (c/v)
BSresKmod= "xc"                # [BSK] Resonant Kernel mode. ('x'; 'c'; 'd')
BSsplKmod= "xc"                # [BSK] Coupling Kernel mode. ('x'; 'c'; 'd'; 'u')
% BSEbands
 5 | 12 |                          # [BSK] Bands range
%
BSENGblk= 5                    RL # [BSK] Screened interaction block size
BSENGexx= 51                   RL # [BSK] Exchange components
    
```



# Solution of the BS equation(1)

Standard diagonalization:

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

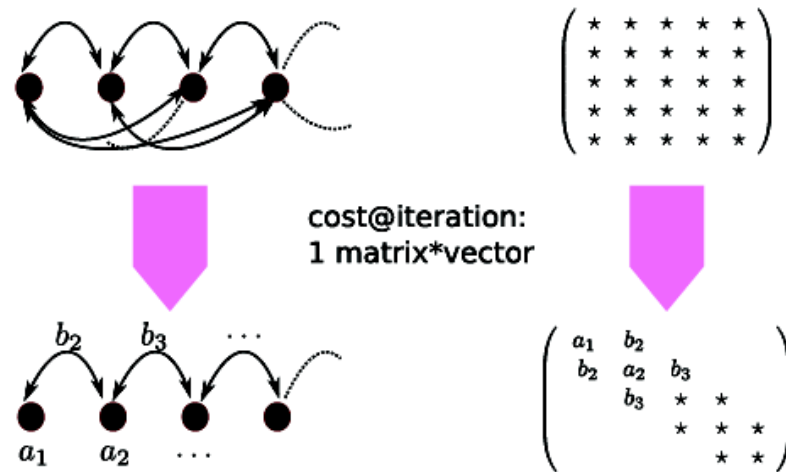
Then the dielectric function:

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



# Solution of the BS equation(2)

Lanczos-Haydock method:



This allows to rewrite the dielectric function as:

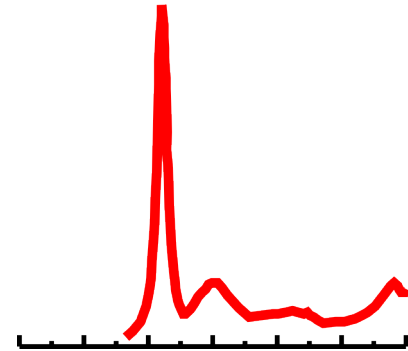
$$\epsilon(\omega) \rightarrow \langle P | (\omega - H)^{-1} | P \rangle = \frac{1}{(\omega - a_1) - \frac{b_2^2}{(\omega - a_2) - \frac{b_3^2}{\dots}}}$$

$$|P\rangle = \lim_{q \rightarrow 0} \frac{1}{|q|} |vck\rangle \langle vk - q | e^{-iq \cdot r} | ck \rangle$$



# Solution of the BS equation(3)

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



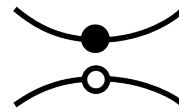
**[BSS] runlevel , yambo -y <opt>, main variables:**

```
%  
BSSmod= "d"                # [BSS] Solvers 'h/d/i/t'  
% BEnRange  
 4.000000 | 8.000000 | eV  # [BSS] Energy range  
%  
% BDmRange  
 0.025000 | 0.025000 | eV  # [BSS] Damping range  
%  
BEnSteps= 400              # [BSS] Energy steps  
% BLongDir  
 1.000000 | 1.000000 | 1.000000 | # [BSS] [cc] Electric Field
```

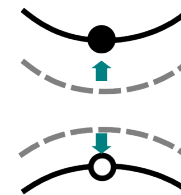


# Steps for Bethe-Salpeter calculation:

0. pwSCF



1. [QP] runlevel: yambo -p p -g n



2. [Xs] runlevel: yambo -b

3. [BSK] runlevel: yambo -o b

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

4. [BSS] runlevel: yambo -y <opt>

