Electron-Phonon Hands-On

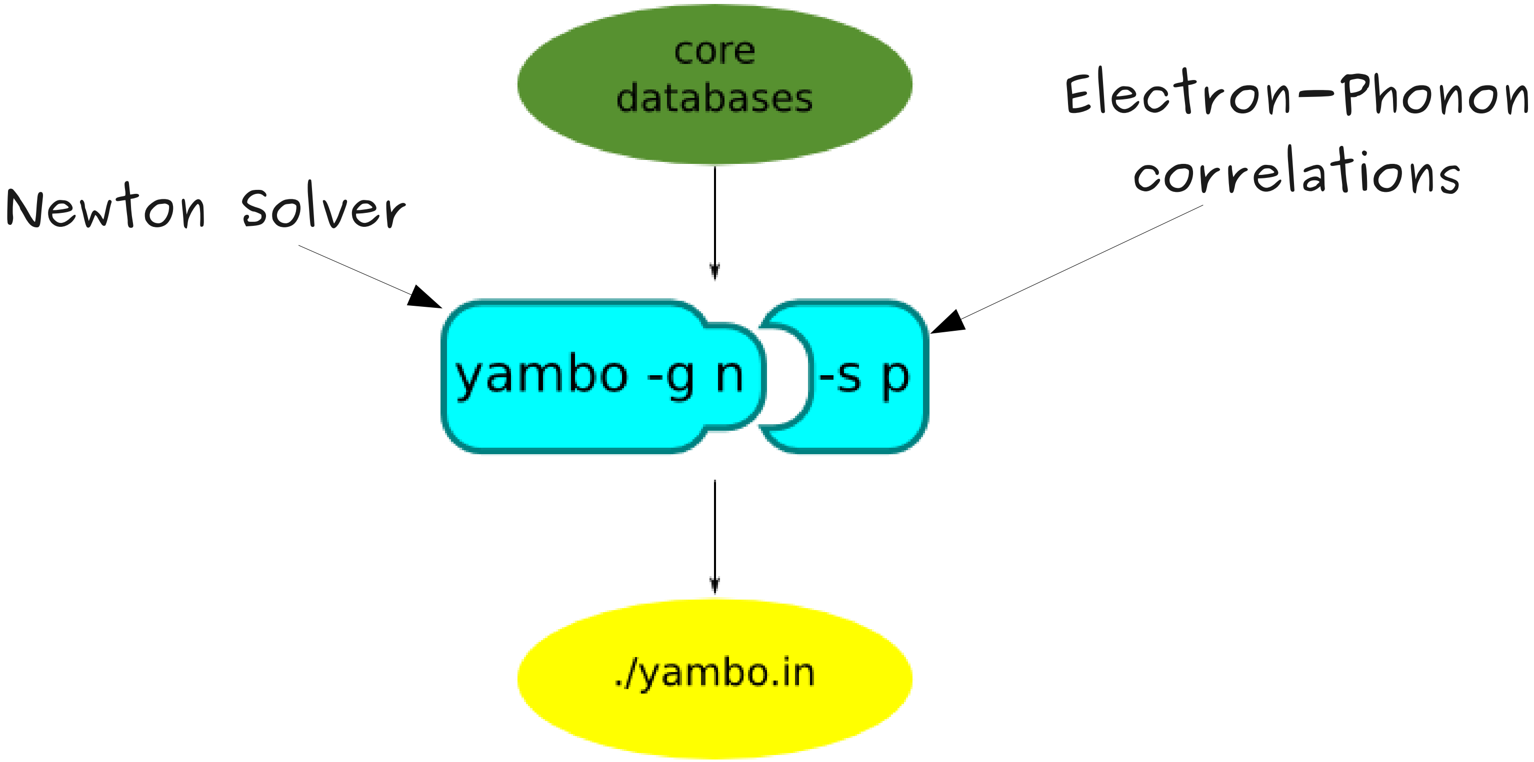
0. (DFT calculation with pwSCF)... Not today!

1. Calculation of Polaronic corrections

2. Calculation of generalized Eliashberg Functions

3. Linewidths & Finite temperature absorption

Inputs & runlevels (Polarons)



[LR] runlevel: yambo_ph -g n -s p

Calculation of the Fan Self-Energy

$$\Sigma^{Fan}_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}\lambda} \frac{1}{N_{\mathbf{q}}} \sum_{n'} \left| g^{\mathbf{q},\lambda}_{n'n\mathbf{k}} \right|^2 \left[\frac{B(\omega_{\mathbf{q}\lambda}) + 1 - f_{n'\mathbf{k}-\mathbf{q}}}{\omega - \epsilon_{n'\mathbf{k}-\mathbf{q}} - \omega_{\mathbf{q}\lambda} - i0^+} + \frac{B(\omega_{\mathbf{q}\lambda}) + f_{n'\mathbf{k}-\mathbf{q}}}{\omega - \epsilon_{n'\mathbf{k}-\mathbf{q}} + \omega_{\mathbf{q}\lambda} - i0^+} \right]$$

$$g^{\mathbf{q}\lambda}_{nn'\mathbf{k}} = \langle n\mathbf{k} | dV^{\mathbf{q}\lambda}_{scf}(\mathbf{r}) | n'\mathbf{k}+\mathbf{q} \rangle$$

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Section_A>ls SAVE/
ndb.elph_gkkp              ndb.elph_gkkp_fragment_2  ndb.elph_gkkp_fragment_4
ndb.elph_gkkp_fragment_6   ndb.elph_gkkp_fragment_8  ns.wf
ndb.elph_gkkp_fragment_1   ndb.elph_gkkp_fragment_3
ndb.elph_gkkp_fragment_5   ndb.elph_gkkp_fragment_7  ns.db1
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$$\Sigma^{DW}_{n\mathbf{k}} = -\sum_{\mathbf{q}\lambda} \frac{1}{N_q} \sum_{n'} \frac{\left| \Lambda^{\mathbf{q}\lambda}_{nn'\mathbf{k}} \right|^2 \left[2B(\omega_{\mathbf{q}\lambda}) + 1 \right]}{\epsilon_{n'\mathbf{k}} - \epsilon_{n\mathbf{k}}}$$

Polarons

On-The-Mass-Shell approx (HAC)

$$\Delta E_{n\mathbf{k}} = \sum_{\mathbf{q}\lambda n'} \left[\frac{|\, g_{n'n\mathbf{k}}^{\mathbf{q},\lambda} \,|^2}{\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}-\mathbf{q}}} - \frac{\Lambda_{n'n\mathbf{k}}^{\mathbf{q}\lambda}}{\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}}} \right] (2B(\omega_{\mathbf{q}\lambda}) + 1)$$

QuasiParticle approximations

$$E_{n\boldsymbol{k}} = \epsilon_{n\boldsymbol{k}} + Z_{n\boldsymbol{k}} \left(\Sigma_{n\boldsymbol{k}}^{Fan}(\epsilon_{nk}) + \Sigma_{n\boldsymbol{k}}^{DW} \right)$$

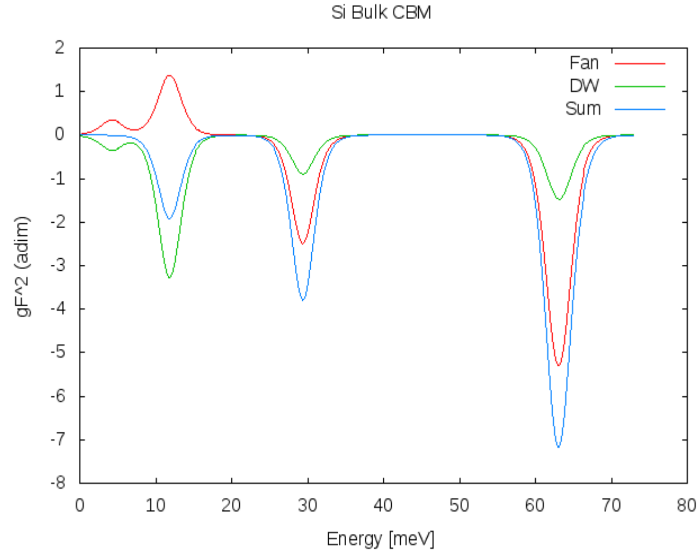
$$Z_{n\mathbf{k}} = \frac{1}{1 - \left.\frac{\partial \Re \Sigma_{n\mathbf{k}}(\omega)}{\partial \omega}\right|_{\omega=\epsilon_{n\mathbf{k}}}}$$

Generalized Eliashberg function

$$\delta E_{n\boldsymbol{k}}(\beta)=\int d\omega\,(g^2F_{FAN}(\omega)+g^2F_{DW}(\omega))(2\mathrm{B}(\omega_{\boldsymbol{q}\lambda})+1)$$

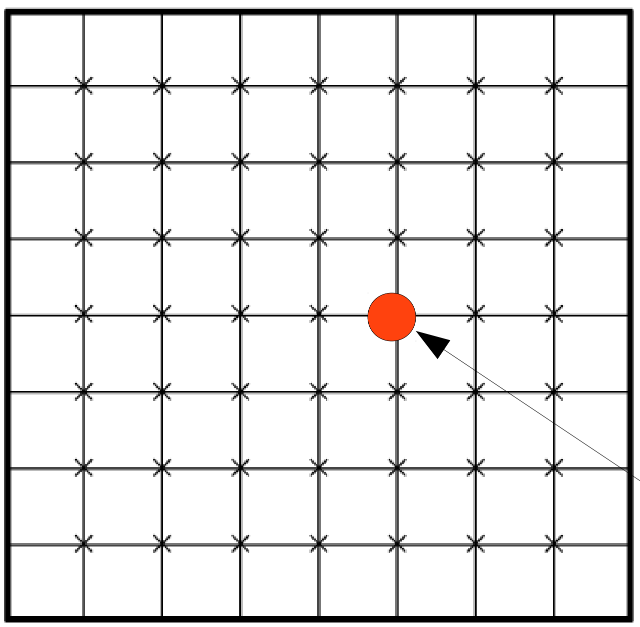
$$g^2F_{FAN}(\omega)=\sum_{\boldsymbol{q}\lambda}\left[\frac{\sum_{n'}|g_{nn'\boldsymbol{k}}^{\boldsymbol{q}\lambda}|^2 N_{\boldsymbol{q}}^{-1}}{\epsilon_{n\boldsymbol{k}}-\epsilon_{n'\boldsymbol{k}'}}\right]\delta(\omega-\omega_{\boldsymbol{q}\lambda})$$

$$g^2F_{DW}(\omega)=\sum_{\boldsymbol{q}\lambda}\left[\frac{\sum_{n'}\Lambda_{nn'\boldsymbol{k}}^{\boldsymbol{q}\lambda}(-2N_{\boldsymbol{q}})^{-1}}{\epsilon_{n\boldsymbol{k}}-\epsilon_{n'\boldsymbol{k}}}\right]\delta(\omega-\omega_{\boldsymbol{q}\lambda})$$

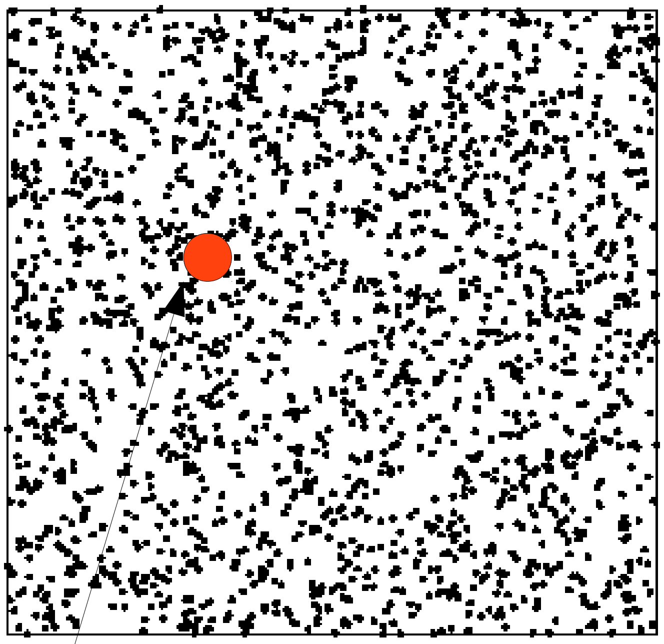


Random Integration Method approach (I)

$$\Delta E_{n\mathbf{k}} = \sum_{\mathbf{q}\lambda n'} \left[\frac{\left| g^{\mathbf{q},\lambda}_{n'n\mathbf{k}} \right|^2}{\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}-\mathbf{q}}} - \frac{\Lambda^{\mathbf{q}\lambda}_{n'n\mathbf{k}}}{\epsilon_{n\mathbf{k}} - \epsilon_{n'\mathbf{k}}} \right] \left(2B(\omega_{\mathbf{q}\lambda}) + 1\right)$$



Uniform Q-grid



Random Q-grid

$$g^{\mathbf{q}\lambda}_{nn'\mathbf{k}} = \langle n\mathbf{k} | dV^{\mathbf{q}\lambda}_{scf}(\mathbf{r}) | n'\mathbf{k}+\mathbf{q} \rangle$$

Random Integration Method approach (II)

$$\Sigma^{Fan}_{n\mathbf{k}}(\omega,T)=\sum_{\mathbf{Q}}\sum_{n'\lambda}\left(\int_{R_{\mathbf{Q}}} d\mathbf{q}\frac{|\,g^{\mathbf{q}\lambda}_{nn'\mathbf{k}}\,|^2}{\Omega_{RL}}\right)\left[\frac{N_{\mathbf{Q}\lambda}(T)+1-f_{n'\mathbf{k}-\mathbf{Q}}}{\omega-\varepsilon_{n'\mathbf{k}-\mathbf{Q}}-\omega_{\mathbf{q}\lambda}-i0^+}+\frac{N_{\mathbf{Q}\lambda}(T)+f_{n'\mathbf{k}-\mathbf{Q}}}{\omega-\varepsilon_{n'\mathbf{k}-\mathbf{Q}}+\omega_{\mathbf{q}\lambda}-i0^+}\right]$$

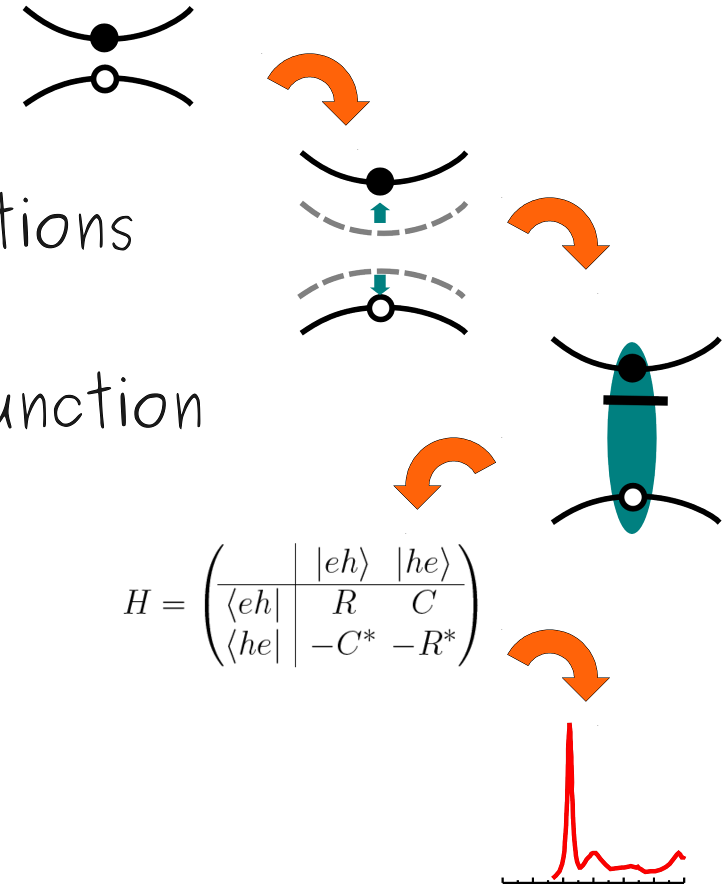
$$\int_{R_{\mathbf{Q}}} d\mathbf{q}\frac{|\,g^{\mathbf{q}\lambda}_{nn'\mathbf{k}}\,|^2}{\Omega_{RL}}\approx\frac{|\,\mathbf{Q}\,|^2\,|\,g^{\mathbf{Q}\lambda}_{nn'\mathbf{k}}\,|^2}{\Omega_{R}L}\left(\int_{R_{\mathbf{Q}}} d\mathbf{q}\mathbf{q}^{-2}\right)$$

Analytical integration of the

ionic potential divergence

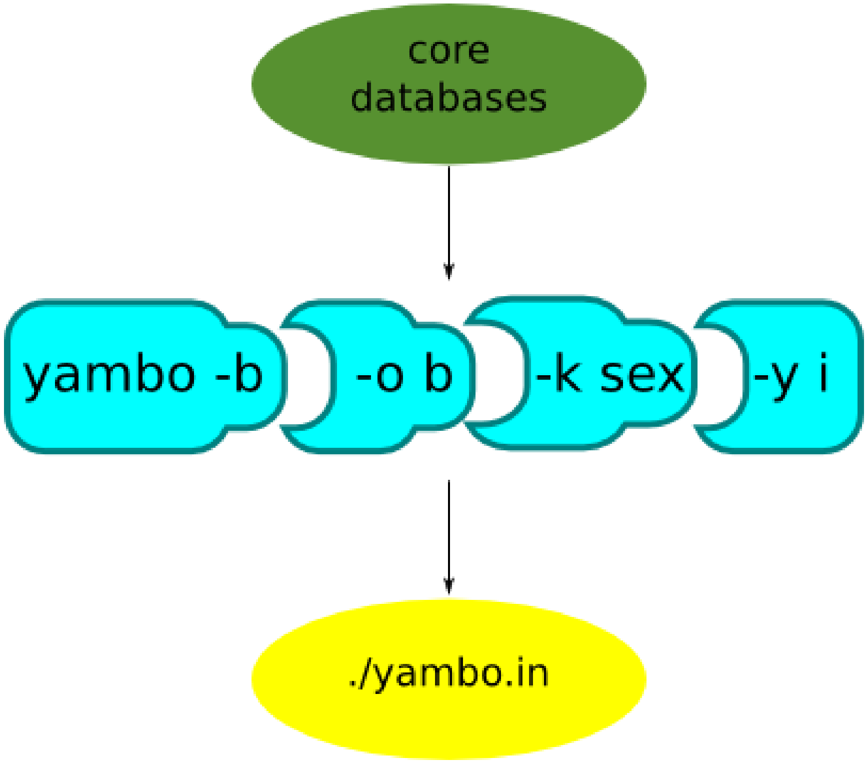
Steps for Finite-Temperature Bethe-Salpeter calculation:

0. DFT calculation (pwSCF)
1. Calculation of Polaronic corrections
2. Calculation of the screening function
3. Calculation of the BS matrix
4. Solution of the BS equation



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

Inputs & runlevels



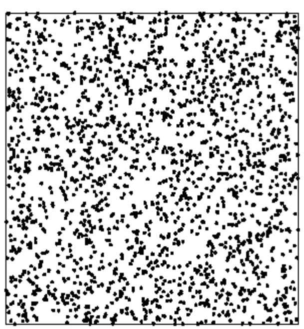
[Xs] runlevel: yambo -b
[BSE/K] runlevel , yambo -o b -k sex
[BSS] runlevel , yambo -y i

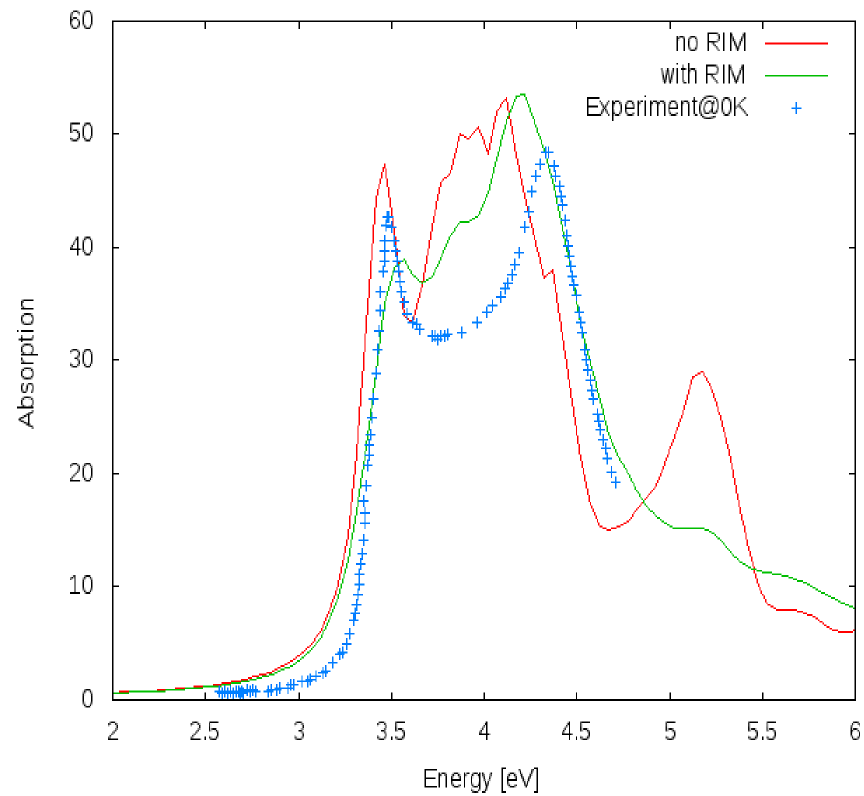
RIM (III): Energy integration

$$\hat{L}(\omega) = \hat{L}^{(0)}(\omega) + i\hat{L}^{(0)}(\omega)\left[\hat{W} - 2\hat{V}\right]\hat{L}(\omega)$$

$$\hat{L}^{(0)}(\omega)\Big|_{cv\mathbf{k},c'v'\mathbf{k}'} \propto \delta_{cc'}\delta_{vv'}\delta_{\mathbf{k}\mathbf{k}'}\frac{1}{\omega - \epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}} + i0^+}$$

$$\hat{L}^{(0,RIM)}(\omega)\Big|_{cv\mathbf{k},c'v'\mathbf{k}'} \propto \delta_{cc'}\delta_{vv'}\delta_{\mathbf{k}\mathbf{k}'}\sum_{p\in R_{\mathbf{k}}}\frac{1}{\omega - \epsilon_{c\mathbf{p}} - \epsilon_{v\mathbf{p}} + i0^+}$$





HOW TO run the Fantastic dimensions tutorial:

Login to ottokar / ssh -X cecampc4.epfl.ch -l tutoXY

0. ssh -X node0XY
   - tuto01 -> node001
   - tuto15 -> node015
   - tuto16 -> node006
   - tuto17 -> node007
   - tuto18 -> node008
   - tuto19 -> node009
   - tuto20 -> node000
1. cd /home/scratch
2. mkdir Yambo-2013
3. cd Yambo-2013
4. cp /nfs_home/tutoadmin/Yambo-2013/Electron_Phonon_NETCDF_databases_and_reference_files.zip
5. unzip Electron_Phonon_NETCDF_databases_and_reference_files.zip
6. cp /nfs_home/tutoadmin/bin/yambo* $HOME/bin/
7. cp /nfs_home/tutoadmin/bin/ypp* $HOME/bin/

8. Follow tutorial on the webpage: www.yambo-code.org/tutorials/Electron_Phonon/index.php