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# 1 GW (oneshot) + DMFT documentation

This document provides the prescription of the combination of a GW calculation for correlated materials with DMFT applied only to a subset of correlated orbitals. At this level, the GW calculation will be performed only once at the beginning (one-shot) based on a DFT Hamiltonian  $H^{DFT}$ , to obtain a Selfenergy  $\Sigma^{GW}$  for all states. Based on the new Hamiltonian  $H^{GW}$ , DMFT will be used to selfconsistently generate a non-perturbative Selfenergy for a set of correlated local orbitals, and replaces the local component of the Selfenergy  $\Sigma^{GW}$  by  $\Sigma^{DMFT}$ .

No further selfconsistency will be performed, *i.e.* no update of the single-particle spectra of  $H^{GW}$  will be done. By this, the final interacting system will be described by a Green's function with the non-interacting DFT dispersion, corrected by a non-local Selfenergy where the non-local components correspond to  $\Sigma^{GW} = G_0 W_0$ , while the local components of the correlated orbitals correspond to  $\Sigma^{DMFT}$ .

Extensions to a full GW+DMFT selfconsistency will be discussed elsewhere.

## 1.1 The GW part

On the basis of  $H^{DFT}$  a  $G_0 W_0$  calculation has to be performed on the full system. By this, the Selfenergy in the Kohn-Sham basis is obtained for all states

$$\Sigma_{\nu\nu'}(k, \omega) = [G_0 W_0]_{\nu\nu'}(k, \omega). \quad (1.1.1)$$

By this, the GW estimate for the full interacting Green's function is given by

$$G_{\nu\nu'}^{GW}(k, \omega) = [\mathbb{1}(\omega + \mu + i\delta) - H^{DFT}(k) + v^{XC}(k) - \Sigma^{GW}(k, \omega)]_{\nu\nu'}^{-1}. \quad (1.1.2)$$

### 1.1.1 Output

At this point the basis transformation to the local Wannier basis will be performed on the GW side. For the next step of the DMFT calculation one needs

- $\epsilon_m(k)$ : The eigenvalues of  $H^{DFT}(k)$  in the Wannier basis for all relevant orbitals
- $\mu$ : The chemical potential that yields the correct physical number of electrons  $N_e$  for  $H^{DFT}$
- $v_{mm'}^{XC}(k)$ : The value of the exchange-correlation potential in the Wannier basis for all relevant orbitals
- $\Sigma_{mm'}(k, \omega)$ : The Selfenergy in the Wannier basis for all relevant orbitals on real frequencies  $\omega$ .

## 1.2 The DMFT part

Within DMFT we then calculate a local correction  $\Sigma^{DMFT}$  for a subset of correlated Wannier orbitals.

The input of the calculation will be the output of the GW calculation. We proceed as follows:

1. Transform the Selfenergy from GW to the imaginary Matsubara axis by

$$\Sigma_{mm'}^{GW}(k, i\omega_n) = \frac{1}{2\pi i} \int \frac{\Sigma_{mm'}^{GW}(k, \omega)}{\omega - i\omega_n} d\omega, \quad \text{or} \quad (1.2.1)$$

$$= \frac{1}{\pi} \int \frac{\text{Im}[\Sigma_{mm'}^{GW}(k, \omega)]}{\omega - i\omega_n} d\omega, \quad \text{or} \quad (1.2.2)$$

$$= \frac{1}{\pi i} \int \frac{\text{Re}[\Sigma_{mm'}^{GW}(k, \omega)]}{\omega - i\omega_n} d\omega. \quad (1.2.3)$$

2. Calculate the local diagonal part of the GW Selfenergy ONLY for the correlated subset of orbitals  $f$

$$\Sigma_f^{GW,loc}(i\omega_n) = \frac{1}{N_k} \sum_k \Sigma_{ff}^{GW}(k, i\omega_n). \quad (1.2.4)$$

3. (This step can be omitted if the correct physical number of electrons  $N_e$  is already known)

Construct the initial non-interacting Green's function on the imaginary Matsubara axis via

$$G_{0,mm'}(k, i\omega_n) = [\mathbb{1}(i\omega_n + \mu) - H^{DFT}(k)]_{mm'}^{-1}, \quad (1.2.5)$$

and calculate the total number of electrons

$$N_e = \lim_{\tau \rightarrow 0^-} \frac{1}{\beta N_k} \sum_{i\omega_n} \sum_{k,m} G_{0,mm}(k, i\omega_n) e^{-i\omega_n \tau}. \quad (1.2.6)$$

4. Make a first guess for the local impurity Selfenergy of the correlated orbitals  $\Sigma_{ff}^{imp}$ , for example one can use the GW result

$$\Sigma_{ff}^{imp}(i\omega_n) = \Sigma_f^{GW,loc}(i\omega_n). \quad (1.2.7)$$

5. Set up the interacting Green's function, where the local component of the GW Selfenergy for the correlated orbitals  $f$  is replaced by  $\Sigma^{imp}$

$$G_{mm'}(k, i\omega_n) = [\mathbb{1}(i\omega_n + \mu) - H^{DFT}(k) + v^{XC}(k)] \quad (1.2.8)$$

$$- \Sigma^{GW}(k, i\omega_n) + \Sigma_f^{GW,loc}(i\omega_n) - \Sigma_{ff}^{imp}(i\omega_n)]_{mm'}^{-1}. \quad (1.2.9)$$

6. Calculate the local Green's function (for all orbitals) then and Weiss field  $\mathcal{G}$  ONLY on the subset of correlated orbitals  $f$ . Neglecting offdiagonal components in the hybridization we are also only interested in the diagonal components of  $\mathcal{G}$

$$G_{mm'}^{loc}(i\omega_n) = \frac{1}{N_k} \sum_k G_{mm'}(k, i\omega_n), \quad (1.2.10)$$

$$\Rightarrow \mathcal{G}_{ff}^{-1}(i\omega_n) = [G_{ff}^{loc}]_{ff}^{-1}(i\omega_n) + \Sigma_{ff}^{imp}(i\omega_n). \quad (1.2.11)$$

(Matsubara frequencies are suppressed in the last equation for clarity) The Weiss field matrix  $\mathcal{G}$  is not explicitly needed, so we do not invert the last equation to obtain  $\mathcal{G}$ .

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7. Calculate the Hybridization function

$$\Delta_{ff}(i\omega_n) = i\omega_n + \tilde{\mu}_f - \mathcal{G}_{ff}^{-1}(i\omega_n), \quad (1.2.12)$$

where the local chemical potential  $\tilde{\mu}_f$  is given by

$$\tilde{\mu}_f = \lim_{\omega_n \rightarrow \infty} \text{Re} [\mathcal{G}_{ff}^{-1}(i\omega_n)] \quad (1.2.13)$$

and transform  $\Delta(i\omega_n)$  to the imaginary time axis  $t$  by a Fourier transform

$$\Delta_{ff}(\tau) = \frac{1}{\beta} \sum_{i\omega_n} \Delta_{ff}(i\omega_n) e^{-i\omega_n \tau} \quad (1.2.14)$$

and solve the impurity model for the correlated  $f$  orbitals.

8. Obtain the new local Selfenergy  $\Sigma_{ff}^{imp}(i\omega_n)$  from the impurity model and calculate the updated full Green's function

$$G_{mm'}(k, i\omega_n) = [\mathbb{1}(i\omega_n + \mu) - H^{DFT}(k) + v_{mm'}^{XC}(k) \quad (1.2.15)$$

$$- \Sigma^{GW}(k, i\omega_n) + \Sigma_f^{GW,loc}(i\omega_n) - \Sigma^{imp}(i\omega_n)]_{mm'}^{-1}. \quad (1.2.16)$$

Adjust the chemical potential  $\mu$  in such a way that the number of electrons  $N_e$  is preserved. Then go back to step 5. Repeat until convergence is reached.

### 1.2.1 Output

After convergence, *e.g.* the local spectral function  $A_m(\omega)$  can be obtained by analytic continuation of  $G_{mm}^{loc}(i\omega_n)$ .