
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 Σ^{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 Σ^{GW} by Σ^{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 Σ^{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 on a mesh in k-space in the full Brillouin zone:

- $\epsilon_m(k)$: The eigenvalues of $H^{DFT}(k)$ in the Wannier basis for all relevant orbitals
- μ : 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
- $\Sigma_{mm'}^{GW}(k, \omega)$: The Selfenergy within GW in the Wannier basis for all relevant orbitals on real frequencies ω .

1.2 The DMFT part

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

The input of the calculation will be the output of the GW calculation. First, one will usually apply a Wannier-interpolation of the GW data to obtain a fine k-mesh since the GW output will be given on a very coarse grid. We then 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 Σ_{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 Σ^{imp}

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

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

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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}

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

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

The Weiss field matrix \mathcal{G} is not explicitly needed, so we do not invert the last equation to obtain \mathcal{G} .

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 τ 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 μ 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 $G_{mm}^{loc}(i\omega_n)$.