Extended DMFT

DMFT formalism for models with spatially non-local (long-ranged) interactions.

Example: U-V Hubbard model

$$H = -t \underbrace{\sum_{\langle ij\rangle,\sigma}}_{\text{all nn pairs } ij} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_i n_i + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{V}{2} \sum_{\langle ij\rangle} n_i n_j$$

$n_i = n_{i\uparrow} + n_{i\downarrow}$

Action for the lattice model:

$$S = \int_0^\beta d\tau \Big[\sum_{ij,\sigma} c^*_{i\sigma}(\tau)\big((\partial_\tau - \mu)\delta_{ij} + \overset{-t\,\delta_{\langle ij\rangle}}{t_{ij}}\big) c_{j\sigma}(\tau)$$

$$+ \underbrace{U \sum_i n_{i\uparrow}(\tau) n_{i\downarrow}(\tau)}_{\frac{U}{2}\sum_i (n_{i\uparrow}+n_{i\downarrow})^2 - \frac{U}{2}\sum_i (n_{i\uparrow}+n_{i\downarrow})} + \frac{1}{2} \sum_{ij} \underset{V\delta_{\langle ij\rangle}}{v_{ij}} n_i(\tau) n_j(\tau) \Big]$$

$$= \int_0^\beta d\tau \Big[\sum_{ij,\sigma} c^*_{i\sigma}(\tau)\big((\partial_\tau - \underbrace{(\mu + \tfrac{U}{2})}_{=\tilde{\mu}})\big)\delta_{ij} + t_{ij}\big) c_{j\sigma}(\tau) + \frac{1}{2}\sum_{ij} \tilde{v}_{ij} n_i(\tau) n_j(\tau) \Big]$$

$$\tilde{v}_{ij} = U\delta_{ij} + V\delta_{\langle ij\rangle}$$

On a square lattice, the Fourier transforms of t_{ij} and $\tilde{v}_{ij}$ are

$$\varepsilon_k = -2t\,[\cos k_x + \cos k_y]$$

$$\tilde{v}_k = U + 2V\,[\cos k_x + \cos k_y]$$

We next decouple the interaction terms $\frac{1}{2}\tilde{v}_{ij}\, n_i(\tau) n_j(\tau)$ by a Hubbard-Stratonovich transformation. Since $n(\tau)$ is real and β-periodic,

$$e^{-\frac{1}{2}\int_0^\beta d\tau\, n_i(\tau) A_{ij} n_j(\tau)} = \frac{1}{\sqrt{(2\pi)^N \det A}} \int D[\phi_1,\dots,\phi_N]\, e^{\int_0^\beta d\tau \left[-\frac{1}{2}\phi_i(\tau)(A^{-1})_{ij}\phi_j(\tau) - i\phi_i(\tau) n_i(\tau)\right]}$$

also real and β-periodic

Here, $A_{ij} = \tilde{v}_{ij}$

$$\Rightarrow S = \int_0^\beta d\tau \Big[-\sum_{ij,\sigma} c^*_{i\sigma}(\tau) \underbrace{\{(-\partial_\tau + \tilde{\mu})\delta_{ij} - t_{ij}\}}_{=(G_0^{-1})_{ij}} c_{j\sigma}(\tau) + \frac{1}{2}\sum_{ij}\phi_i(\tau)(\tilde{v}^{-1})_{ij}\phi_j(\tau) + i\sum_j \phi_j(\tau) n_j(\tau) \Big]$$

$= (G_0^{-1})_{ij}$, G_0: non-interacting lattice GF

In the EDMFT approximation, we compute the local lattice GF by solving the impurity problem

$$S^{EDMFT} = -\int_0^\beta d\tau d\tau' \sum_\sigma c^*_\sigma(\tau)\,\mathcal{G}^{-1}(\tau-\tau')\,c_\sigma(\tau') + \frac{1}{2}\int_0^\beta d\tau d\tau'\,\phi(\tau)\,\mathcal{U}^{-1}(\tau-\tau')\,\phi(\tau') + i\int_0^\beta d\tau\,\phi(\tau)\,n(\tau)$$

(*)

fermionic Weiss field — "bosonic" Weiss field

to be fixed by a self-consistency condition

$\mathcal{G}(\tau)$: $-\mathcal{U}(\tau)$:

Integrating out the ϕ-field yields an impurity action with retarded interaction:

$$S^{EDMFT} = -\int_0^\beta d\tau d\tau' \sum_\sigma c^*_\sigma(\tau)\,\mathcal{G}^{-1}(\tau-\tau')\,c_\sigma(\tau') - \frac{1}{2}\int_0^\beta d\tau d\tau'\,n(\tau)\,\mathcal{U}(\tau-\tau')\,n(\tau') - \underbrace{\log\sqrt{\det \mathcal{U}}}_{\frac{1}{2}\log \underbrace{\det \mathcal{U}}_{\exp(\mathrm{Tr}\log \mathcal{U})} = \frac{1}{2}\mathrm{Tr}\log\mathcal{U}}$$

(**)

This form of the action is used in actual calculations.

The observables which we need to compute for the self-consistency equations are the Fermionic and Bosonic Green functions

$$G_{imp}(\tau) = -\langle T c(\tau) c^\dagger(0)\rangle$$

$$W_{imp}(\tau) = \langle T \phi(\tau)\phi(0)\rangle$$

From Eq. (*) we get $W_{imp} = 2\dfrac{\delta \ln Z}{\delta \mathcal{U}^{-1}} = 2\dfrac{\delta \ln Z}{\delta \mathcal{U}}\underbrace{\dfrac{\delta \mathcal{U}}{\delta \mathcal{U}^{-1}}}_{-\mathcal{U}^2} = -2\,\mathcal{U}\dfrac{\delta \ln Z}{\delta \mathcal{U}}\,\mathcal{U}$

From Eq (**): $\dfrac{\delta \ln Z}{\delta \mathcal{U}} = \dfrac{1}{2}\langle T n(\tau) n(0)\rangle - \dfrac{1}{2}\dfrac{1}{\mathcal{U}}$

$\Rightarrow$ $W_{imp} = \mathcal{U} - \mathcal{U}\chi_{loc}\mathcal{U}$ with $\chi_{loc} = \langle T n(\tau) n(0)\rangle$

If we define the interaction term as $\bar{n}(\tau)\,\mathcal{U}(\tau-\tau')\,\bar{n}(\tau')$, $\bar{n} = n - \langle n \rangle$

(with corresponding shift in the chemical potential)

$$\Rightarrow \quad W_{imp} = \mathcal{U} - \mathcal{U}\,\bar{\chi}_{loc}\,\mathcal{U} \quad \text{with} \quad \bar{\chi}_{loc} = \langle T\,\bar{n}(\tau)\,\bar{n}(0)\rangle_{S}$$

connected charge-charge correlation function

Fermionic self-consistency (as in usual DMFT):

$$G_{imp} \longrightarrow \Sigma_{imp} = \mathcal{G}^{-1} - G_{imp}^{-1}$$

$$\Sigma(k, i\omega_n) \approx \Sigma_{imp}(i\omega_n)$$

$$G(k, i\omega_n) = \left[G_0^{-1} - \Sigma(k, i\omega_n)\right]^{-1} \approx \left[G_0^{-1} - \Sigma_{imp}(i\omega_n)\right]^{-1}$$

solver

$$G_{loc}(i\omega_n) = \sum_k G(k, i\omega_n)$$

$$(\mathcal{G}^{-1})^{new} = G_{loc}^{-1} + \Sigma_{imp}$$

Bosonic self-consistency (in complete analogy):

$$W_{imp} \longrightarrow \Pi_{imp} = \mathcal{U}^{-1} - W_{imp}^{-1} \qquad (\Pi_{imp} = \text{bosonic self-energy})$$

$$\Pi(k, i\nu_n) \approx \Pi_{imp}(i\nu_n) \qquad \nu_n = \text{bosonic Matsubara frequency}$$

χ_{loc}

$$W(k, i\nu_n) = \left[\tfrac{1}{2}(\tilde{v})^{-1} - \Pi(k, i\nu_n)\right]^{-1} \approx \left(\tfrac{1}{2}(\tilde{v})^{-1} - \Pi_{imp}(i\nu_n)\right]^{-1}$$

$$W_{loc}(i\nu_n) = \sum_k W(k, i\nu_n)$$

solver

$$(\mathcal{U}^{-1})^{new} = W_{loc}^{-1} + \Pi_{imp}$$

($W(k, i\nu_n)$ is the lattice FT of $\langle T\,\phi_i(\tau)\,\phi_j(0)\rangle$

and $\frac{1}{2}(\tilde{v})^{-1}$ is the "non-interacting" GF for the action

without electron-boson coupling, i.e. without the

$i\phi n$ term)

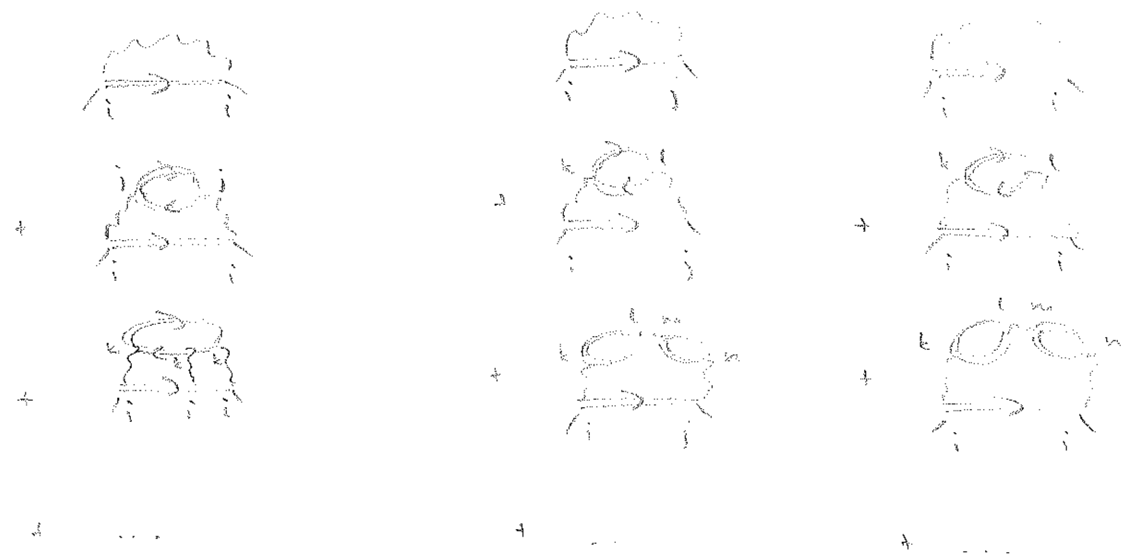
Combining GW and EDMFT

Idea: construct a non-local (momentum-dependent) self-energy by combining the (local) EDMFT self-energy and the non-local part of the GW self-energy

$$\Sigma^{GW+EDMFT}(k,i\omega_n) = \Sigma^{EDMFT}(i\omega_n) + \Sigma^{GW}(k,i\omega_n) - \sum_k \Sigma^{GW}(k,i\omega_n)$$

corresponds to all local diagrams

to avoid a double-counting of local diagrams, subtract



(So, in fact we are missing some local diagrams, e.g.  ?)

Computational scheme for the U-V Hubbard model:

1) Start from the converged EDMFT solution $\rightarrow \Sigma_{imp}, \Pi_{imp}$

$$G(k,i\omega_n) = [G_0^{-1} - \Sigma_{imp}]^{-1}$$

$$W(k,i\nu_n) = [v(k)^{-1} - \Pi_{imp}]^{-1}$$

2) Compute "Weiss fields"

$$G_{loc}(i\omega_n) = \sum_k G(k,i\omega_n) \longrightarrow (\mathcal{G}^{-1})^{new} = G_{loc}^{-1} + \Sigma_{imp}$$

$$W_{loc}(i\nu_n) = \sum_k W(k,i\nu_n) \longrightarrow (\mathcal{U}^{-1})^{new} = W_{loc}^{-1} + \Pi_{imp}$$

3) solve impurity problem $\longrightarrow$ G_{imp}, χ_{imp} $\longrightarrow$ $W_{imp} = \mathcal{U} - \mathcal{U}\chi_{loc}\mathcal{U}$

compute fermionic and bosonic self-energies

$$\Sigma_{imp} = \mathcal{G}^{-1} - G_{imp}^{-1}$$

$$\Pi_{imp} = \mathcal{U}^{-1} - W_{imp}^{-1}$$

4) GW+EDMFT step:

(a) $$\Pi^{GW}(k,\tau) = \sum_q G(q,\tau)G(q-k,-\tau)$$

$$\Sigma^{GW}(k,\tau) = \sum_q G(q,\tau)W(q-k,-\tau)$$

(b) Extract non-local part

$$\Pi^{GW}_{non-local}(k,i\nu_n) = \Pi^{GW}(k,i\nu_n) - \sum_k \Pi^{GW}(k,i\nu_n)$$

$$\Sigma^{GW}_{non-local}(k,i\omega_n) = \Sigma^{GW}(k,i\omega_n) - \sum_k \Sigma^{GW}(k,i\omega_n)$$

(c) Combine GW and EDMFT self-energies

$$\Pi(k,i\nu_n) = \Pi_{imp}(i\nu_n) + \Pi^{GW}_{non-local}(k,i\nu_n)$$

$$\Sigma(k,i\omega_n) = \Sigma_{imp}(i\omega_n) + \Sigma^{GW}_{non-local}(k,i\omega_n)$$

go back to 2) and repeat until convergence is reached