An introduction to Dynamical mean field theory

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Outline

- Some backgrouds.
- The main idea of DMFT, derivation of self-consistent equations.
- Conclusions

Why DMFT?

Strongly correlated fermion systems

Perturbation

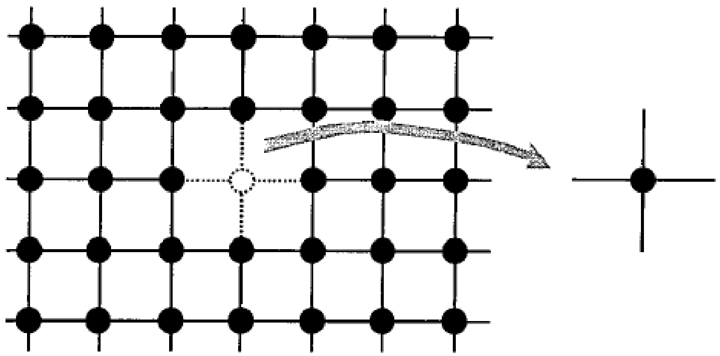
Mean field approach:

Hartree-Fock: Attempts to parametrize the whole mean-field function by a single number. This amounts to freezing local quantum fluctuation , which is only reasonble when a single low-energy scale is important.

DMFT: Use engery-dependent mean field function to replace a single number ,which can take into account local quantum fuctuation.

Classical case

$$\sum_{S_i, i\neq o} e^{-\beta H} \equiv e^{-\beta H_{\text{eff}}[S_o]}.$$



$$H = -h_o S_o - \Sigma_i J_{io} S_o S_i + H^{(o)}$$

$$J_{io} S_o \equiv \eta_i$$

$$H_{\text{eff}} = \text{const} + \sum_{n=1}^{\infty} \sum_{i_1 \cdots i_n} \frac{1}{n!} \eta_{i_1} \cdots \eta_{i_n} \langle S_{i_1} \cdots S_{i_n} \rangle_c^{(o)}$$

For a ferromagnetic system, with $J_{ij} > 0$ scaled as $1/d^{|i-j|}$

$$H_{\text{eff}} = -h_{\text{eff}} S_o; \qquad d \to \infty$$

Dimensionality depress fluctuation correlation

$$h_{\text{eff}} = h + \sum_i J_{oi} \langle S_i \rangle^{(o)}$$

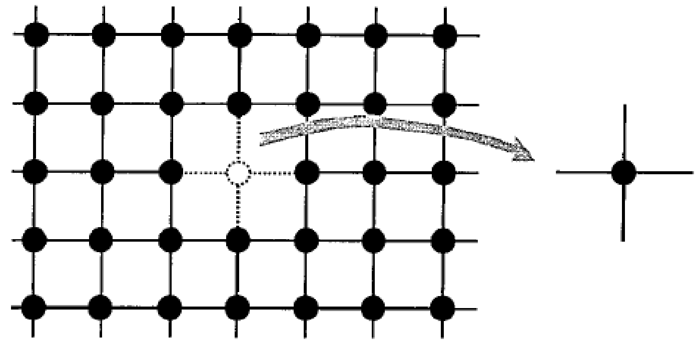
Weiss field

$$m = \tanh(\beta h_{\text{eff}})$$

$\langle S_i \rangle^{(o)} \rightarrow \langle S_i \rangle$

$$\left\{ \begin{array}{l} \langle S_i \rangle = \langle S_o \rangle \equiv m \\ h_{\text{eff}} = h + zJm \\ m = \tanh \beta h_{\text{eff}} \end{array} \right\}$$

Quantum case



A closed set of functional equations for on-site Green's function and Weiss function

$$S_{\rm eff}=-\int_0^\beta d\tau\int_0^\beta d\tau'\sum_\sigma c_{o\sigma}^+(\tau)\mathscr{G}_0^{-1}(\tau-\tau')c_{o\sigma}(\tau')+U\int_0^\beta d\tau\, n_{o\uparrow}(\tau)n_{o\downarrow}(\tau).$$

$$\mathscr{G}_0^{-1}=\Sigma+1/\tilde{D}(i\omega_n+\mu-\Sigma)$$

$$G(\tau-\tau')\equiv-\langle Tc(\tau)c^+(\tau')\rangle_{S_{\rm eff}},$$

$$G(i\omega_n)=\int_0^\beta d\tau\, G(\tau)e^{i\omega_n\tau},\quad \omega_n\equiv\frac{(2n+1)\pi}{\beta}$$

$$G(\mathbf{k},i\omega_n)=\frac{1}{i\omega_n+\mu-\epsilon_{\mathbf{k}}-\Sigma(i\omega_n)}$$

$$G_{ii}(i\omega_n)=\Sigma_{\mathbf{k}}G(\mathbf{k},i\omega_n)$$

$$\Sigma(i\omega_n)=\mathscr{G}_0^{-1}(i\omega_n)-G^{-1}(i\omega_n).$$

$$D(\epsilon)=\sum_{\mathbf{k}}\delta(\epsilon-\epsilon_{\mathbf{k}}),\quad \epsilon_{\mathbf{k}}\equiv\sum_{ij}t_{ij}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)},$$

$$\tilde{D}(\zeta)\equiv\int_{-\infty}^{+\infty}d\epsilon\,\frac{D(\epsilon)}{\zeta-\epsilon}$$

Hold on paramagnetic phase only! We use translation invariance! ($G_\uparrow(i\omega_n)$ $G_\downarrow(i\omega_n)$ **)**

$$D(\epsilon)=\frac{1}{t\sqrt{2\pi}}\exp\left(-\frac{\epsilon^2}{2t^2}\right).$$

Cubic lattice in infinite dimension

Coherent path integral

Bosonic

$$a_i|\phi\rangle = \phi_i|\phi\rangle$$

$$\boxed{|\phi\rangle \equiv \exp[\textstyle\sum_i \phi_i a_i^\dagger]|0\rangle}$$

$$\boxed{\int \prod_i \frac{d\bar{\phi}_i d\phi_i}{\pi} e^{-\sum_i \bar{\phi}_i \phi_i} |\phi\rangle\langle\phi| = \mathbf{1}_{\mathcal{F}}}$$

fermionic

$$a_i|\eta\rangle = \eta_i|\eta\rangle$$

$$\boxed{|\eta\rangle = \exp[-\textstyle\sum_i \eta_i a_i^\dagger]|0\rangle}$$

$$\boxed{\int \prod_i d\bar{\eta}_i d\eta_i e^{-\sum_i \bar{\eta}_i \eta_i} |\eta\rangle\langle\eta| = \mathbf{1}_F}$$

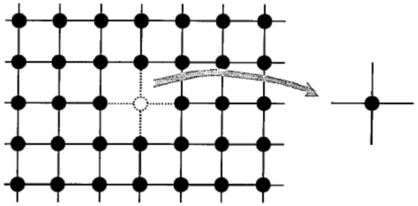
$$\mathcal{Z} = \sum \langle n|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle$$

$$\mathcal{Z} = \int_{\bar{\psi}_N=-\zeta\bar{\psi}_0,\,\psi_N=-\zeta\psi_0} \prod_{n=0}^{N} d[\bar{\psi}_n, \psi_n] e^{-\sum_{n=1}^{N}\left[\bar{\psi}_n\cdot(\psi_n-\psi_{n-1})+\Delta\beta(H(\bar{\psi}_n,\psi_{n-1})-\mu N(\bar{\psi}_n,\psi_{n-1}))\right]}$$

$$\Delta\beta\sum_{n=0}^{N} \to \int_0^\beta d\tau, \qquad \frac{\psi_n-\psi_{n-1}}{\Delta\beta} \to \partial_\tau\psi\Big|_{\tau=n\Delta\beta}, \qquad \prod_{n=0}^{N} d[\bar{\psi}_n, \psi_n] \to D(\bar{\psi}, \psi)$$

$$\boxed{\mathcal{Z} = \int_{\substack{\bar{\psi}(\beta)=-\zeta\bar{\psi}(0)\\ \psi(\beta)=-\zeta\psi(0)}} D(\bar{\psi}, \psi) e^{-S[\bar{\psi},\psi]}, \qquad S[\bar{\psi}, \psi] = \int_0^\beta d\tau \left(\bar{\psi}\cdot\partial_\tau\psi + H(\bar{\psi}, \psi) - \mu N(\bar{\psi}, \psi)\right)}$$

Derivations of the DMFT equations



Hubbard model:

$$H=-\sum_{\langle ij\rangle,\sigma} t_{ij}(c_{i\sigma}^{+}c_{j\sigma}+c_{j\sigma}^{+}c_{i\sigma})+U\sum_{i} n_{i\uparrow}n_{i\downarrow}\,.$$

$$Z=\int\prod_{i} Dc_{i\sigma}^{+}Dc_{i\sigma}e^{-S}$$

$$S=\int_{o}^{\beta}d\tau\left(\sum_{i\sigma} c_{i\sigma}^{+}\partial_{\tau}c_{i\sigma}-\sum_{ij,\sigma} t_{ij}c_{i\sigma}^{+}c_{j\sigma}-\mu\sum_{i\sigma} c_{i\sigma}^{+}c_{i\sigma}+U\sum_{i} n_{i\uparrow}n_{i\downarrow}\right). \qquad ($$

Effective action of site o:

$$\frac{1}{Z_{\text{eff}}}e^{-S_{\text{eff}}[c_{o\sigma}^{+},c_{o\sigma}]}\equiv\frac{1}{Z}\int\prod_{i\neq o,\sigma} Dc_{i\sigma}^{+}Dc_{i\sigma}e^{-S}.$$

$$S=S^{(o)}+S_{o}+\Delta S$$

$$S_{o}=\int_{0}^{\beta}d\tau\left(\sum_{\sigma} c_{o\sigma}^{+}(\partial_{\tau}-\mu)c_{o\sigma}+Un_{o\uparrow}n_{o\downarrow}\right)$$

$$\Delta S=-\int_{0}^{\beta}d\tau\sum_{i\sigma} t_{io}(c_{i\sigma}^{+}c_{o\sigma}+c_{o\sigma}^{+}c_{i\sigma})$$

$$\eta_{i}\equiv t_{io}c_{o\sigma}$$

Plays the role of a source coupled to $c_{i\sigma}^{+}$

$$\frac{1}{Z_{\text{eff}}} e^{-S_{\text{eff}}[c^+_{o\sigma}, c_{o\sigma}]} \equiv \frac{1}{Z} \int \prod_{i \neq o, \sigma} Dc^+_{i\sigma} Dc_{i\sigma} e^{-S}.$$

The integration over fermions for $i \neq o$ Brings in the generating function of the connected Green's function $G^{(o)}$ of the cavity Hamiltonian.

$$S_{\text{eff}} = \sum_{n=1}^{\infty} \sum_{i_1 \cdots j_n} \int \eta^+_{i_1}(\tau_{i_1}) \cdots \eta^+_{i_n}(\tau_{i_n}) \eta_{j_1}(\tau_{j_1}) \times \cdots \eta_{j_n}(\tau_{j_n}) G^{(o)}_{i_1 \cdots j_n}(\tau_{i_1} \cdots \tau_{i_n}, \tau_{j_1} \cdots \tau_{j_n}) + S_o + \text{const.}$$

The scaling of the hopping amplitude :

$$\epsilon_{\mathbf{k}} = -2t \sum_{j=1}^{d} \cos k_j$$

$$t = t^* / (2d)^{1/2}$$

$$S_{\text{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c^+_{o\sigma}(\tau) \mathscr{G}_0^{-1}(\tau - \tau') c_{o\sigma}(\tau') + U \int_0^\beta d\tau\, n_{o\uparrow}(\tau) n_{o\downarrow}(\tau).$$

$d \rightarrow \infty$

$$G(\tau - \tau') \equiv -\langle T c(\tau) c^+(\tau') \rangle_{S_{\text{eff}}},$$

$$G(i\omega_n) = \int_0^\beta d\tau\, G(\tau) e^{i\omega_n \tau}, \quad \omega_n \equiv \frac{(2n+1)\pi}{\beta}$$

$$\mathscr{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \sum_{ij} t_{oi} t_{oj} G^{(o)}_{ij}(i\omega_n)$$

$$G^{(o)}_{ij} = G_{ij} - \frac{G_{io} G_{oj}}{G_{oo}}$$

$$\mathscr{G}_0^{-1} = \Sigma + 1/\tilde{D}(i\omega_n + \mu - \Sigma)$$

Self consistent relation:
the relation between field and local observble.

Some coments

- We can interpret $\mathscr{G}_0(\tau-\tau')$ as the quantum generalisation of the Weiss effective field in the classical case. The main difference with the classical case is that this “dynamical mean-field” is a *function of energy (or time) instead of a single number.* $\mathscr{G}_0(\tau-\tau')$ also plays the role of a bare Green’s function for the effective action .
- This is required in order to take full account of local quantum fluctuations, which is the main purpose of DMFT.

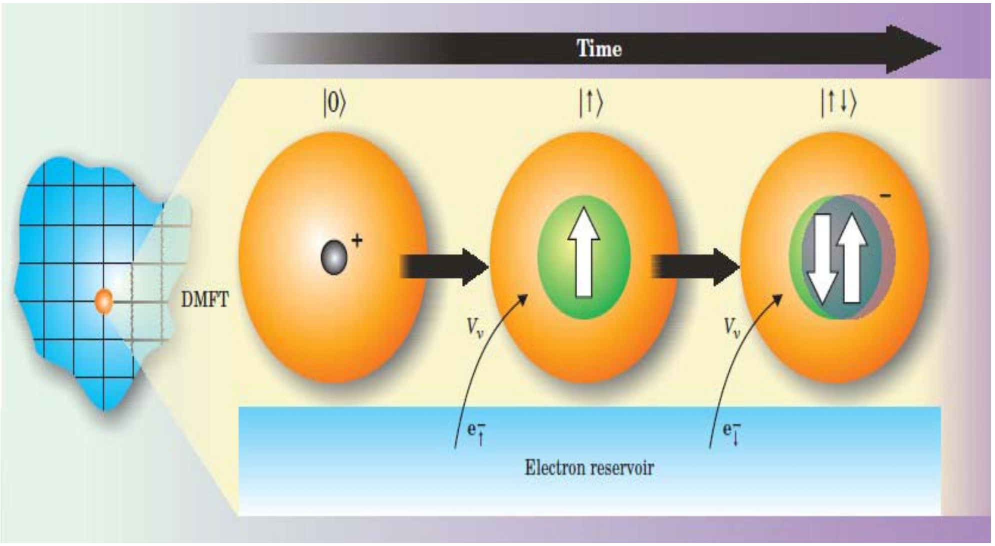
TABLE I. Correspondence between the mean-field theory of a classical system and the (dynamical) mean-field theory of a quantum system.

Quantum case	Classical case	
$-\sum_{\langle ij\rangle\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + U\sum_i n_{i\uparrow} n_{i\downarrow}$	$H = -\sum_{\langle ij\rangle} J_{ij} S_i S_j - h\sum_i S_i$	Hamiltonian
$t_{ij} \sim (1/\sqrt{d})^{\lvert i-j\rvert}$	$J_{ij} \sim (1/d)^{\lvert i-j\rvert}$ (ferromagnet)	Scaling
$G_{ij}(i\omega_n) = -\langle c^{+}_i(i\omega_n) c_j(i\omega_n)\rangle$	$\langle S_i S_j\rangle$	Correlation function
$G_{ii}(i\omega_n) = -\langle c^{+}_i(i\omega_n) c_i(i\omega_n)\rangle$	$m_i = \langle S_i\rangle$	Local observable
$-\int\int c^{+}_\sigma(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_\sigma(\tau') + \int U n_\uparrow n_\downarrow$ $H_{\mathrm{eff}} = \sum_{l\sigma}\tilde{\epsilon}_l a^{+}_{l\sigma} a_{l\sigma} + \sum_{l\sigma} V_l (a^{+}_{l\sigma} c_\sigma + \text{H.c.})$ $-\mu\sum_\sigma c^{+}_\sigma c_\sigma + U n_\uparrow n_\downarrow$	$H_{\mathrm{eff}} = -h_{\mathrm{eff}} S_0$	Single-site Hamiltonian
$\mathcal{G}_0(i\omega_n)$	h_{eff}	Weiss field/function
$\mathcal{G}_0^{-1}(i\omega_n) = \omega_n + \mu + G(i\omega_n)^{-1}$ $-R[G(i\omega_n)]$	$h_{\mathrm{eff}} = z\ J\ m + h$	Relation between Weiss field and local observable

Mapping it to Anderson impurity model

The impurity model offers an intuitive picture of the local dynamics of a quantum many-body system. (if we identify some quantities, the scenario above is the same as Anderson impurity model)

$$H_{AIM} = H_{atom} + H_{bath} + H_{coupling}$$



$$H_{atom} = U n^c_\uparrow n^c_\downarrow + (\varepsilon_0 - \mu)(n^c_\uparrow + n^c_\downarrow)$$

$$H_{bath} = \sum_{l\sigma} \widetilde{\varepsilon}_l a^\dagger_{l\sigma} a_{l\sigma}$$

$$H_{coupling} = \sum_{l\sigma} V_l (a^\dagger_{l\sigma} c_\sigma + c^\dagger_\sigma a_{l\sigma})$$

The $\widetilde{\varepsilon}_l$ *and* V_l's *are parameters which should be chosen in such a way that the* impurity Green's function of coincides with the local Green's function of the lattice Hubbard model under consideration

The essential idea is to replace a lattice model by a single-site quantum impurity problem embedded in an effective medium determined self-consistently.

$$S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\sigma^+(\tau)\mathscr{G}_0^{-1}(\tau-\tau')c_\sigma(\tau') + U\int_0^\beta d\tau\, n_\uparrow(\tau)n_\downarrow(\tau)$$

$$\mathscr{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \varepsilon_0 - \Delta(i\omega_n) \qquad \Delta(i\omega_n) = \sum_l \frac{|V_l|^2}{i\omega_n - \widetilde{\varepsilon}_l}$$

$$\begin{aligned}\Sigma_{imp}(i\omega_n) &\equiv \mathscr{G}_0^{-1}(i\omega_n) - G^{-1}(i\omega_n) \\ &= i\omega_n + \mu - \varepsilon_0 - \Delta(i\omega_n) - G^{-1}(i\omega_n)\end{aligned}$$

Original lattice :

$$G(\tau-\tau') \equiv -< Tc(\tau)c^+(\tau') >_{S_{eff}}$$

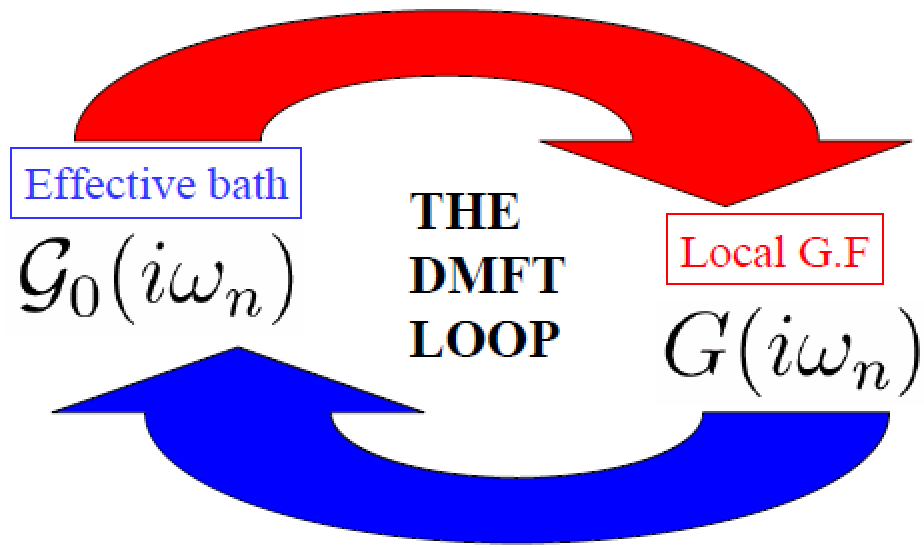
$$G(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \varepsilon_0 - \varepsilon_\mathbf{k} - \Sigma(\mathbf{k}, i\omega_n)}$$

$$\Sigma_{ii} \simeq \Sigma_{imp}$$

$$\sum_\mathbf{k} \frac{1}{\Delta(i\omega_n) + G(i\omega_n)^{-1} - \varepsilon_\mathbf{k}} = G(i\omega_n)$$

$$\int d\varepsilon \frac{D(\varepsilon)}{\Delta(i\omega_n) + G(i\omega_n)^{-1} - \varepsilon} = G(i\omega_n)$$

EFFECTIVE LOCAL IMPURITY PROBLEM



SELF-CONSISTENCY CONDITION

$$S_{\text{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_{o\sigma}^+(\tau)\mathscr{G}_0^{-1}(\tau-\tau')c_{o\sigma}(\tau') + U\int_0^\beta d\tau\, n_{o\uparrow}(\tau)n_{o\downarrow}(\tau).$$

$$G(\tau-\tau') \equiv -\langle Tc(\tau)c^+(\tau')\rangle_{S_{\text{eff}}},$$

$$G(i\omega_n) = \int_0^\beta d\tau\, G(\tau)e^{i\omega_n\tau}, \quad \omega_n \equiv \frac{(2n+1)\pi}{\beta}$$

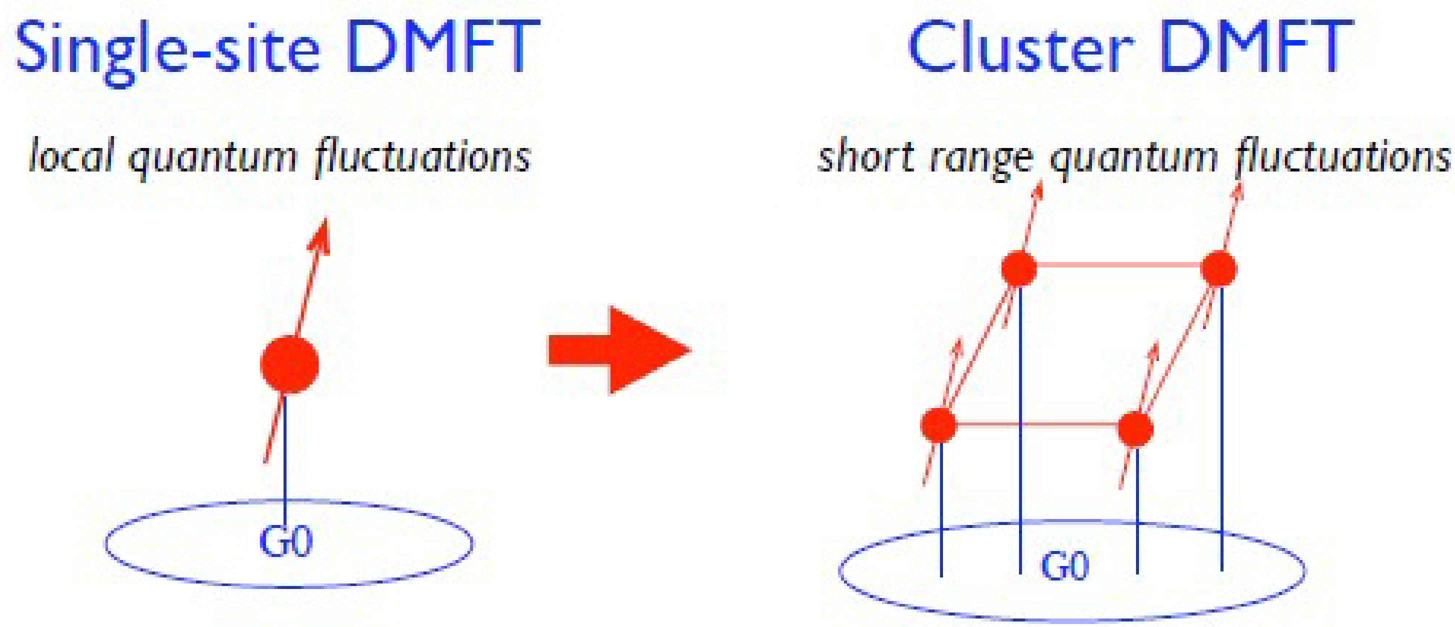
$$\Sigma(i\omega_n) = \mathscr{G}_0^{-1}(i\omega_n) - G^{-1}(i\omega_n).$$

$$\mathscr{G}_0^{-1} = \Sigma + 1/\tilde{D}(i\omega_n + \mu - \Sigma)$$

Conclusions:

- DMFT is a theory which can fully take into account local quantum fluctuation self-consistently.
- The DMFT equations can easily be extended to study phases with long-range order, calculate critical temperatures for ordering as well as phase diagrams.
- Thermodynamic quantities for the original model can all be simply related to their single-site model counterparts: energy, free energy,dynamic response function ,transport properties.
- Successful applications:Hubbard model,Mott metal –insulator transition)

Beyond DMFT(Cluster DMFT)



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