Cluster Dynamical Mean Field Approximations

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- G. Kotliar, S. Savrasov, G. Palsson, GB PRL V87 186401
- GB, G Kotliar PRB V65 155112

⋮

Outlook

- DMFT (briefly)
- Cluster extensions: why and how?
- CDMFT, DCA, Pair scheme
- Interpretation in terms of generating functional
- Causality
- 2 Applications:
  - (a) Toy model: 1D SU(N) Heisenberg Chain ($N \to \infty$)
  - (b) Hubbard model at half-filling without frustration (MIT, AF, Slater and Mott)

Dynamical Mean Field Theory *

• Hubbard Model

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

• Limit of ∞ dimensions : $t_{ij} \sim \frac{1}{\sqrt{d}}$

$$Z = \int \mathcal{D}c_{i\sigma}^+ \mathcal{D}c_{i\sigma}\, e^{S}$$

$$S = S_0 + \Delta S_{0-out} + S_{out}$$

$$S_0 = \int_0^\beta d\tau\, c_{0\sigma}^+ (\partial_\tau - \mu) c_{0\sigma} + U n_{0\uparrow} n_{0\downarrow}$$

$$\Delta S_{0-out} = -\int_0^\beta d\tau \sum_{i\sigma} t_{i0} \left(c_{i\sigma}^+ c_{0\sigma} + c_{0\sigma}^+ c_{i\sigma}\right)$$

S_{out} : The rest

* Rev. Mod. Phys. V68 (1996) p13
A. Georges, G. Kotliar, W. Krauth, MJ Rozenberg

Integrating out all $c_{i\sigma}^+ c_{i\sigma}$ except 0 $\rightarrow$

$\Rightarrow$ single site effective action : $Z_0 = \int \mathcal{D}c_{0\sigma}^+ \mathcal{D}c_{0\sigma}\, e^{S_0^{eff}}$

$$\boxed{S_0^{eff} = -\int_0^\beta d\tau\, d\tau' \sum_\sigma c_{0\sigma}^+(\tau)\, \mathcal{G}_0^{-1}(\tau-\tau')\, c_{0\sigma}(\tau') + U \int_0^\beta d\tau\, n_{0\uparrow} n_{0\downarrow}}$$

$$\mathcal{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \sum_{ij} t_{0i} t_{0j} G_{ij}^{(0)}(i\omega_n)$$

some computations later....

$$\boxed{G_{00}(i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - t(k) - \Sigma(i\omega_n)} \qquad (1)}$$

$$\boxed{\mathcal{G}_0^{-1}(i\omega_n) = G_{00}^{-1}(i\omega_n) + \Sigma(i\omega_n) \qquad (2)}$$

$\Rightarrow \Sigma_{\text{single site}} \equiv \Sigma_{\text{lattice}}$

Algorithm:

$$\begin{tikzcd} \Sigma \arrow[r, "(1)"] & G_{00} \arrow[d, "(2)"] \\ G_{00} \arrow[u, "(2)"] & \mathcal{G}_0 \arrow[l] \end{tikzcd}$$

solution of the impurity on single site pb.

Extensions of DMFT: Why and How?

Why ?:

→ Description of broken symmetries like D-SC or DDW

→ Include systematically a K-dependence of Σ

→ Capture the effect of SHORT-range fluctuations

How ? 2 possible routes

① Non "Gaussianity" of the cavity field / Renormalization of the 2-particle irreducible vertex

↳ Extended DMFT

② From single site to clusters

↳ Cluster extensions of DMFT

CDMFT

Divide the lattice in clusters

Elementary degrees of freedom: $c\, c^+$ inside a cluster

$$H = -\sum_{nm\alpha\beta} t_{\alpha\beta}(R_n - R_m)\, c^+_{R_n,\alpha}\, c_{R_m,\beta} + \sum_{n\alpha\beta\alpha'\beta'} U_{\alpha\beta\alpha'\beta'}(\{R\})\, c^+_{R_n\alpha}\, c_{R_n\beta}\, c^+_{R_n\alpha'}\, c_{R_n\beta'}$$

$$G_{\alpha\beta}(i\omega_n) = \left(\sum_K \frac{1}{(i\omega_n+\mu)\mathbb{1} - \hat{t}(K) - \hat{\Sigma}(i\omega_n)} \right)_{\alpha\beta} \quad (1)$$

$$\hat{\mathcal{G}}_0^{-1}(i\omega_n) = \hat{G}^{-1}(i\omega_n) + \hat{\Sigma}(i\omega_n) \quad (2)$$

$$\Sigma_{\text{lattice}}(i\omega_n, \vec{x}) = \frac{1}{N_c} \sum_{\alpha\beta:\ \vec{x}_\alpha - \vec{x}_\beta = \vec{x}} \Sigma_{\alpha\beta}(i\omega_n)$$

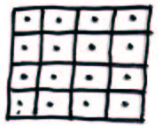
Algorithm:

$$\begin{array}{ccc} \hat{\Sigma} & \xrightarrow{(1)} & \hat{G} \\ \uparrow{\scriptstyle (2)} & & \downarrow{\scriptstyle (2)} \\ \hat{G} & \longleftarrow & \hat{\mathcal{G}}_0 \end{array}$$

solution of a cluster impurity problem

DCA

Σ: piecewise constant in K-space



$\Sigma(K_c; i\omega_n)$

$$G(K_c, i\omega_n) = \sum_{\substack{k \in \\ \text{square } K_c}} \frac{1}{i\omega_n + \mu - t(k) - \Sigma(K_c, i\omega_n)}$$

$$\mathcal{G}_0^{-1}(K_c, i\omega_n) = G^{-1}(K_c, i\omega_n) + \Sigma(K_c, i\omega_n)$$

$$\Sigma_{lattice}(k, i\omega_n) = \Sigma(K_c(k), i\omega_n)$$

where $K_c(k) = K \mod\left(\frac{\pi}{L_c}, \dots, \frac{\pi}{L_c}\right)$

Same algorithm than before

Pair Scheme

$$\Sigma(k, i\omega_n) = \Sigma_{loc}(i\omega_n) + C(k)\Sigma_{NN}(i\omega_n) \quad ; \quad C(k) = \frac{t(k)}{t}$$

In real space $\Sigma_{ij} \neq 0$ if $\begin{matrix} i = j \\ i \text{ n.n. } j \end{matrix}$

2 impurity problems:  , 

$$G_{xx'} = \sum_k \frac{e^{ik(x-x')}}{i\omega_n + \mu - t(k) - \Sigma_{loc}(i\omega_n) - C(k)\Sigma_{NN}(i\omega_n)}$$

$$\mathcal{G}_0^{(1)^{-1}} = G^{-1}_{\substack{loc \\ (xx)}} + \Sigma^{(1)} \qquad \mathcal{G}_{0\,ij}^{(2)^{-1}} = G^{-1}_{ij} + \Sigma^{(2)}_{ij}$$

$$\Sigma_{loc}(i\omega_n) = (1-z)\Sigma^{(1)} + z\,\Sigma^{(2)}_{11}$$

$$\Sigma_{NN} = \Sigma^{(2)}_{12}$$

Algorithm: $\Sigma^{(1)}, \Sigma^{(2)} \to \Sigma_{loc}, \Sigma_{NN} \to G_{loc}, G_{NN}$

$\mathcal{G}_0^{(1)}, \mathcal{G}_0^{(2)} \to G_{loc}, G_{NN}$

solve the one and two impurity problems

Interpretation in terms of generating functional

$$F(G,\Sigma) = -\mathrm{Tr}\ln\left((i\omega_n+\mu)\delta_{ij} - t_{ij} - \Sigma_{ij}\right) - \mathrm{Tr}\,\Sigma\cdot G + \Phi[\{G_{ij}\}]$$

Φ : sum of all 2PI vacuum diagrams with full propagators

$$\frac{\delta F}{\delta \Sigma} = 0 \longrightarrow G_{ij} = \left(\frac{1}{(i\omega_n+\mu) - t - \Sigma}\right)_{ij}$$

$$\frac{\delta F}{\delta G} = 0 \longrightarrow \Sigma_{ij} = \frac{\delta \phi}{\delta G_{ij}}(G)$$

$$\phi_{DMFT} = \sum_i \Phi(\{G_{ij}\})\Big|_{\text{where all } G_{ke}=0 \text{ except } G_{ii}} = \sum_i \Phi_{DMFT}(G_{ii})$$

(Only these terms survive in the $d\to\infty$ limit)

$$\Phi_{DMFT}(G) = \underset{G_0}{\mathrm{extr}}\left[\ln\int Dc^+Dc\, e^{S_{eff}(G_0)} + \mathrm{Tr}\, G_0^{-1}G + \mathrm{Tr}\ln G^{-1}\right]$$

↖ done by the impurity solver

- **CDMFT**

$$\phi_{CDMFT} = \sum_{\underset{\text{cluster index}}{n}} \Phi(\{G_{ij}\})\Big|_{\substack{\text{all } G_{ke}=0 \text{ except the} \\ \text{ones with } K \text{ and } e \\ \text{belonging to the cluster } n}}$$

- **DCA**

In each 2PI diagram replace

$$\delta_{k_1+k_2,\,k_3+k_4} \longrightarrow \delta_{k_1^c+k_2^c,\,k_3^c+k_4^c}$$

$$K^c(k) = K \bmod \left(\frac{\pi}{L_c}, \dots, \frac{\pi}{L_c}\right)$$

- **Pair scheme**

$$\Phi_{PS} = (1-z)\sum_i \Phi_{\substack{\text{single}\\\text{site}}}(G_{ii}) + \sum_{\langle ij\rangle} \Phi_{pair}(G_{ii}, G_{jj}, G_{ij})$$

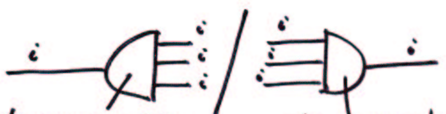
CDMFT : Causal ? Check: Yes

DCA : Causal ? Check: Yes

Pair Scheme: Causal? Check: <u>NO</u>

2 reasons:

① Non-Closure



→ this diagram is not allowed

it may contain G_{is} it may contain G_{ik}

② Σ at II order in U

Σ_{ii} =  Σ_{is} = 

One can choose a G_0 causal that gives a Σ non causal

"Solution" : generalizing the Traveling Cluster Approximation to strongly correlated electrons

Causality of Cluster Schemes

• If Σ causal → $G = (i\omega_n + \mu - t - \Sigma)^{-1}$ is causal (easy)

• If G causal → $\Sigma = \frac{\delta \phi}{\delta G}(G)$ is causal (hard)

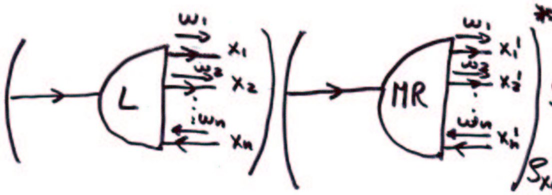
Σ is causal if

$$\frac{1}{2i}\sum_{x x'} w_x \left(\Sigma(x,x',\omega) - \Sigma^*(x',x,\omega)\right) w^*_{x'} \geq 0 \quad \forall \{w_x\}$$

Cutkosky eqs or t'hooft and Veltman cutting eqs

$\Sigma(x,x';\omega) =$ 

$$\frac{1}{i}\left(\Sigma(x,x';\omega) - \Sigma^*(x',x,\omega)\right) =$$

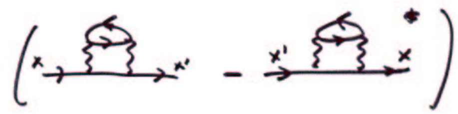
$= \sum_{\substack{\text{All cuts}\\ x_1,x_2,\dots x_n\\ x_1',x_2',\dots x_n'}} \int d\omega_1 \dots d\omega_n$  $\rho_{x_1x_1'}(\omega_1)\theta(\omega_1) \dots \rho_{x_nx_n'}(\omega_n)\theta(-\omega_n)\,\delta(\omega-\omega_1\dots+\omega_n)$

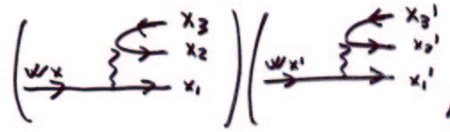
if $\Sigma = \sum_{\text{Diagrams } D} D$

$$\frac{1}{i}\sum_{xx'} w_x\left(\Sigma(x,x',\omega) - \Sigma^*(x',x,\omega)\right) w_{x'}^* = \sum_{\text{Diagrams}} \sum_{\text{cuts}} \int (HL)(MHR)^*$$

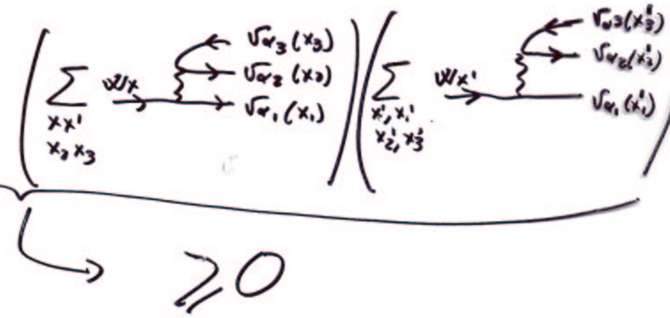
$$= \sum_{\text{type of cuts}} \int \left(\sum_{\text{HL diagrams}} HL\right)\left(\sum_{\text{HL diagrams}} HL\right)^* \geq 0$$

Example : Causality at II order in U

$\sum_{xx'} \frac{w_x}{i}$  $w_{x'}^* =$

$= \int \begin{matrix} d\omega_1 \\ d\omega_2 \\ d\omega_3 \\ \delta(\,) \end{matrix} \sum_{\substack{x x' \\ x_1 x_1' \\ x_2 x_2' \\ x_3 x_3'}}$  $\rho_{x_1,x_1'}(\omega_1)\theta(\omega_1)\;\rho_{x_2x_2'}(\omega_2)\theta(\omega_2)\;\rho_{x_3,x_3'}(\omega_3)\theta(-\omega_3)$

$G_{xx'}$ causal $\longrightarrow \rho_{xx'} = \sum_\alpha v_\alpha(x)\, v_\alpha^*(x')\, \lambda_\alpha ; \quad \lambda_\alpha \geq 0$

$= \sum_{\alpha_1\alpha_2\alpha_3} \int$  $\lambda_{\alpha_1} \lambda_{\alpha_2} \lambda_{\alpha_3}$

Test in a toy model

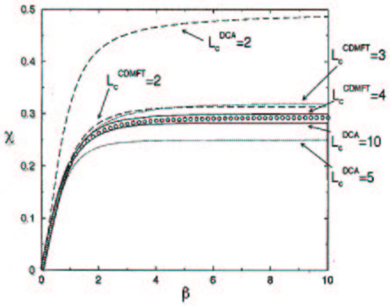
$$H = -t\sum_{i\sigma}\left(c^\dagger_{i\sigma}c_{i+1\sigma} + c^\dagger_{i+1\sigma}c_{i\sigma}\right) + \frac{J}{2N}\sum_{i\sigma\sigma'} c^\dagger_{i\sigma}c_{i\sigma'}c^\dagger_{i+1\sigma'}c_{i+1\sigma}$$

SU(N) 1D Heisenberg Model

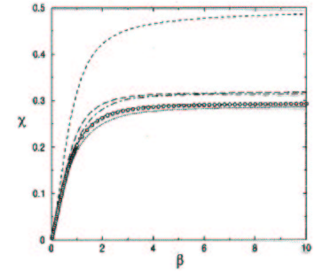
Self-Consistent solution with $\chi = \frac{1}{N}\sum_i \langle c^\dagger_{i\sigma}c_{i+1\sigma}\rangle$

$$t \to (t + \chi J)$$

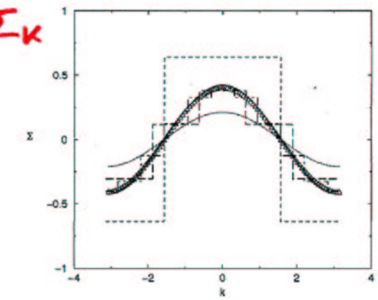
$\chi_{cluster}$



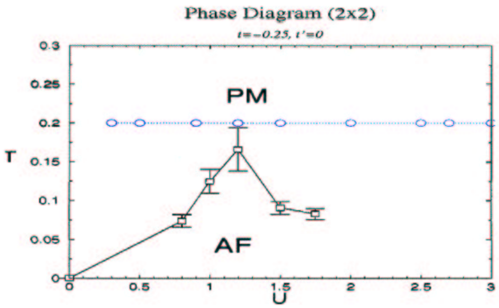
$\chi_{lattice} \neq \chi_{cluster}$

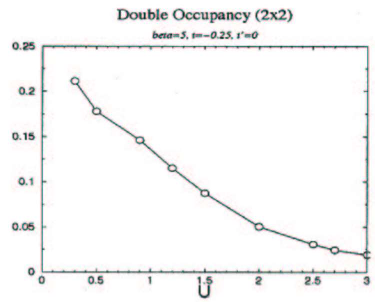


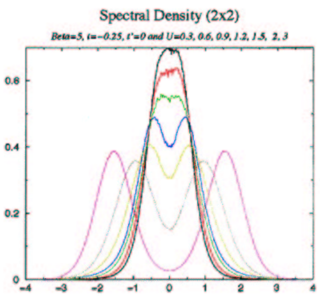
Σ_K



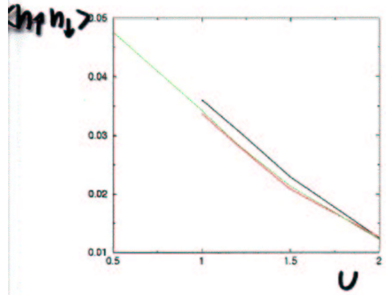
2D Hubbard model at half filling without frustration

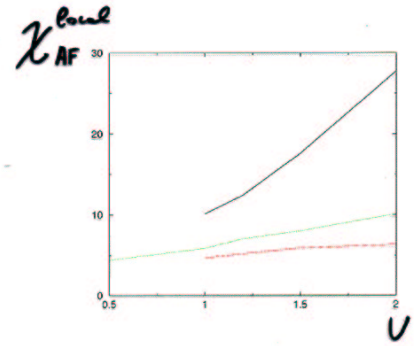


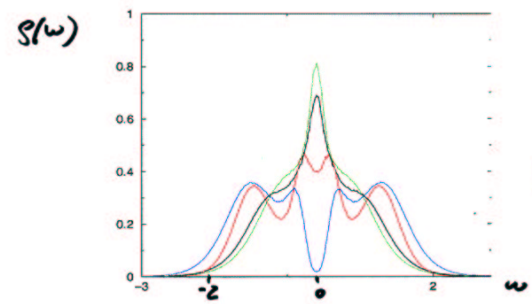




$T = \frac{1}{5}, \frac{1}{7}, \frac{1}{15}$



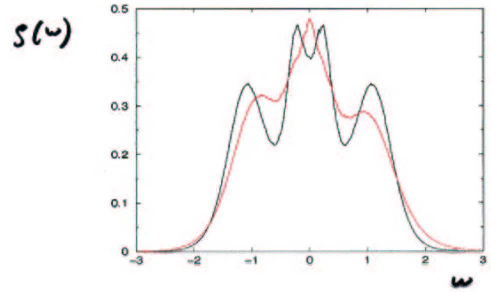




$T = \frac{1}{15}$

$t' = 0$

$U = 1; 1.2; 1.5; 2$



$T = \frac{1}{15}$

$t' = 0.15\,t$

$U = 1.5$