Non-Local Correlation Effects in Solids: Beyond DMFT

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In collaboration with

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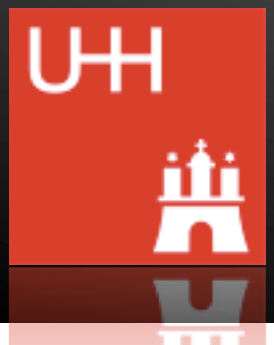
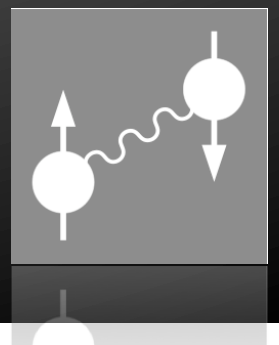




Outline

QM-Language

1-Q

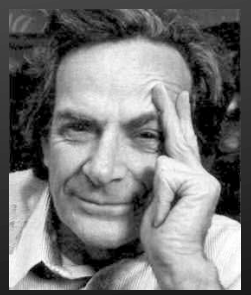
$$\left(-\frac{1}{2}\Delta + V_{eff}(\vec{r})\right)\psi(\vec{r}) = \varepsilon\psi(\vec{r})$$

2-Q

$$\hat{H} = \sum_{ij\sigma} t_{ij}\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} + \sum_{i} U\hat{n}_{\uparrow}\hat{n}_{\downarrow}$$

3-PI

$$Z = Sp(e^{-\beta\hat{H}}) = \int D[c^*,c]e^{-\int_0^\beta d\tau\left[c^*_\tau\partial_\tau c_\tau + H(c^*_\tau,c_\tau)\right]}$$



Path Integral: quick reference

http://www.physnet.uni-hamburg.de/hp/group_magno/pim_10.php

Literature:

1. J.W. Negele and H. Orland "Quantum Many-Particle Systems" (Addison-Wesley, 1988)
2. N. Nagaosa "Quantum Field Theory in Condensed Matter Physics" (Springer, 1999)
3. A. Atland and B. Simons "Condensed Matter Field Theory" (Cambridge University Press 2006)

http://www.tcm.phy.cam.ac.uk/~bds10/

4. E. Fradkin "Field Theory of Condensed Matter Systems" (Addison Wesley, 1991)
5. P. Coleman "Many Body Physics"

http://www.physics.rutgers.edu/~coleman/pdf/bk.pdf

Summary: $\zeta = \begin{cases} +1 & \text{Boson} \\ -1 & \text{Fermion} \end{cases}$ $\quad [\hat{c}_i, \hat{c}_j^\dagger] = \delta_{ij}^\zeta$

$\hat{c}_i |c\rangle = c_i |c\rangle$ with $|c\rangle = e^{\zeta \sum_i c_i \hat{c}_i^\dagger} |0\rangle$

$\langle c| \hat{c}_i^\dagger = \langle c| c_i^*$ with $\langle c| = \langle 0| e^{\zeta \sum_i \hat{c}_i c_i^*}$

$\hat{c}_i^\dagger |c\rangle = \zeta \partial_{c_i} |c\rangle$ and $\langle c| \hat{c}_i = \partial_{c_i^*} \langle c|$

Overlap: $\langle \bar{c} | c \rangle = e^{\sum_i \bar{c}_i^* c_i}$

Completeness: $\int dc^* dc \, e^{-\sum_i c_i^* c_i} |c\rangle\langle c| = \hat{\mathbb{1}}_{\mathcal{F}}$

Trace $\forall \hat{H}$: $\mathrm{Tr}\, \hat{H} = \sum_n \langle n| \hat{H} |n\rangle = \int dc^* dc \, e^{-\sum_i c_i^* c_i} \langle \zeta c| \hat{H} |c\rangle$

P.I. measure: $\mathcal{D}[c^*, c] \equiv \lim_{N\to\infty} \prod_i \frac{dc_i^* dc_i}{(2\pi i)^{(1+\zeta)/2}}$

3.2 Fermion coherent state: $\{\hat{c}_i, \hat{c}_j^+\} = \delta_{ij}$

$$\hat{c}_i |c\rangle = c_i |c\rangle$$

Anticommutivity of $\{\hat{c}_i, \hat{c}_j\} = 0$ implies that eigenvalues c_i anticommute $c_i c_j + c_j c_i = 0$

$$\rightarrow \quad c_i c_j = -c_j c_i$$ is not ordinary number!

Grassmann Algebra: $\{c_i\}$

1) Anticommuting number: $c_i c_j + c_j c_i = 0$
2) $c_i^2 = 0$
3) Anticommute with Fermi-operators: $c\hat{c}^+ + \hat{c}^+ c = 0$
4) Can be add to and multiply by complex numbers (!)
   Functions: $F(c_i) = c_i + \sum_j f_j c_j$
5) Differentiation! $\partial_{c_i} c_j = \delta_{ij}$

   N.B. ordering! $\partial_{c_i} c_j c_i = -c_j$

6) Integration:

$$\left.\begin{aligned} \int dc\, 1 &= 0 \\ \int dc\, c &= 1 \end{aligned}\right\} \quad \int \equiv \partial$$

General Path-Integral representation:

$$Z = \int_{c(\beta)=\zeta c(0)} \mathcal{D}[c^*, c]\, e^{-\int_0^\beta d\tau \left[c^* \frac{\partial}{\partial \tau} c + H(c^*, c) - \mu N(c^*, c) \right]}$$

analogy: Feynman: $\int dp\, dq\, e^{i \int_1^2 dt (p \partial_t q - H(p,q))}$

Coherent state: $\int dc^*\, dc\, e^{i \int_1^2 dt (c^* \partial_t c - H(c^*, c))}$

$\Rightarrow$ c^* ← conjugate → c

1 ⇝ 2

with boundary condition!

Boson	Fermion
$c(\beta) = c(0)$	$c(\beta) = -c(0)$
$c^*(\beta) = c^*(0)$	$c^*(\beta) = -c^*(0)$

For our Hamiltonian: $Z = \int \mathcal{D}[c^*, c]\, e^{-S[c^*, c]}$

with Action:

$$S[c^*, c] = \int_0^\beta d\tau \left\{ \sum_{ij} c_i^*(\tau) \left[\left(\frac{\partial}{\partial \tau} - \mu \right) \delta_{ij} + h_{ij} \right] c_j(\tau) + \frac{1}{2} \sum_{ijkl} V_{ijkl}\, c_i^*(\tau) c_j^*(\tau) c_l(\tau) c_k(\tau) \right\}$$

Hubbard-Stratonovich Transformation

Reminder! Gauß: $\int_{-\infty}^{\infty} dx\, e^{-ax^2+bx} = \sqrt{\frac{\pi}{a}}\, e^{\frac{b^2}{4a}}$

$$\int \mathcal{D}[c^*, c] \exp\left(-\sum_{i,j} c_i^* M_{ij} c_j + \sum_i (J_i^* c_i + c_i^* J_i)\right) = (\det M)^{-\zeta} \exp\left(\sum_{i,j} J_i^* (M^{-1})_{ij} J_j\right)$$

1) One-bosonic field - ϕ (Un^2 - interaction)

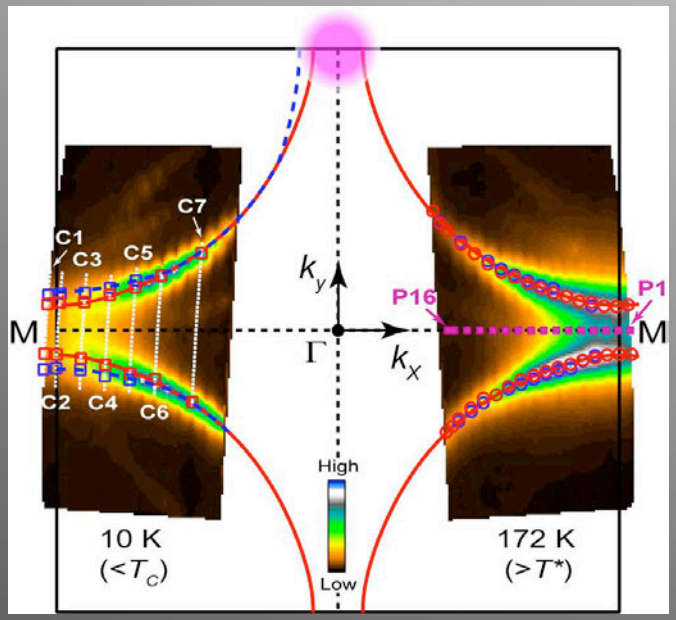
$$e^{-n_m U_{ml} n_l} = \int \mathcal{D}[\phi]\, e^{-\frac{1}{4}\phi_m U^{-1}_{ml} \phi_l - i\phi_m n_m}$$

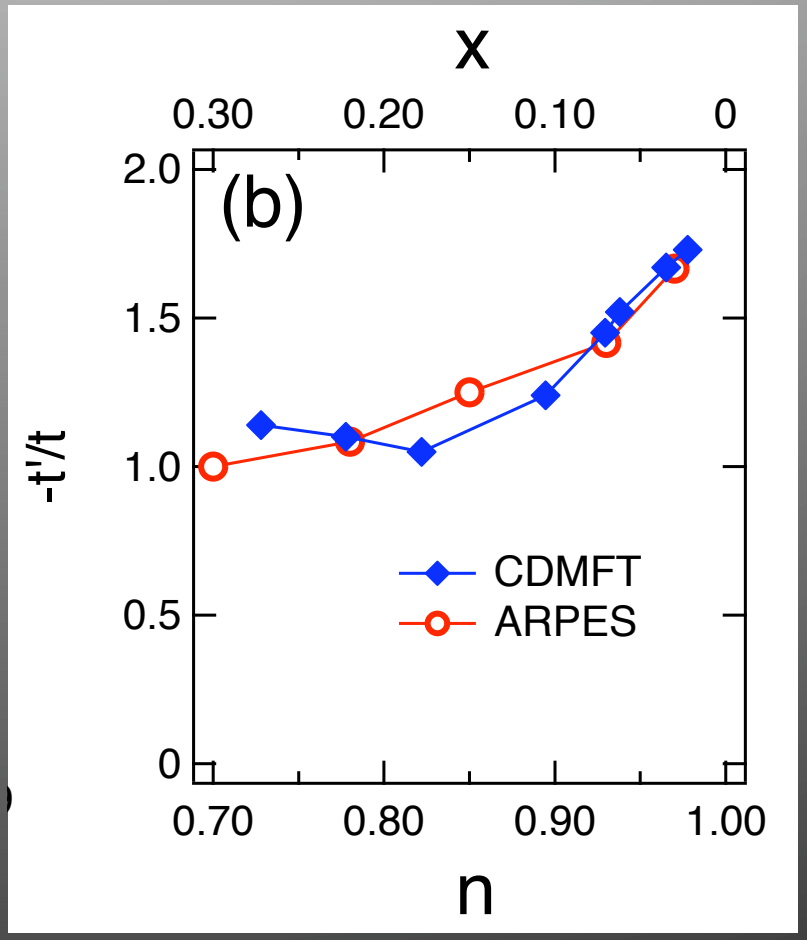
2) Fermionic transformation: $(c^*, c) \longrightarrow (f^*, f)$ (Grassmann, Grassmann)

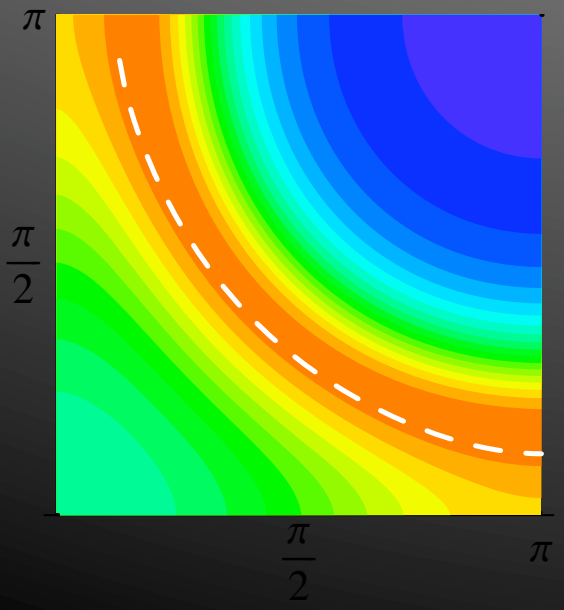
$$e^{c_i^* G_{ij} c_j} = \det(G) \int \mathcal{D}[f^*, f]\, e^{-f_i^* G^{-1}_{ij} f_j + f_i^* c_i + c_i^* f_i}$$

ARPES of HTSC

Z.X. Shen (Stanford)



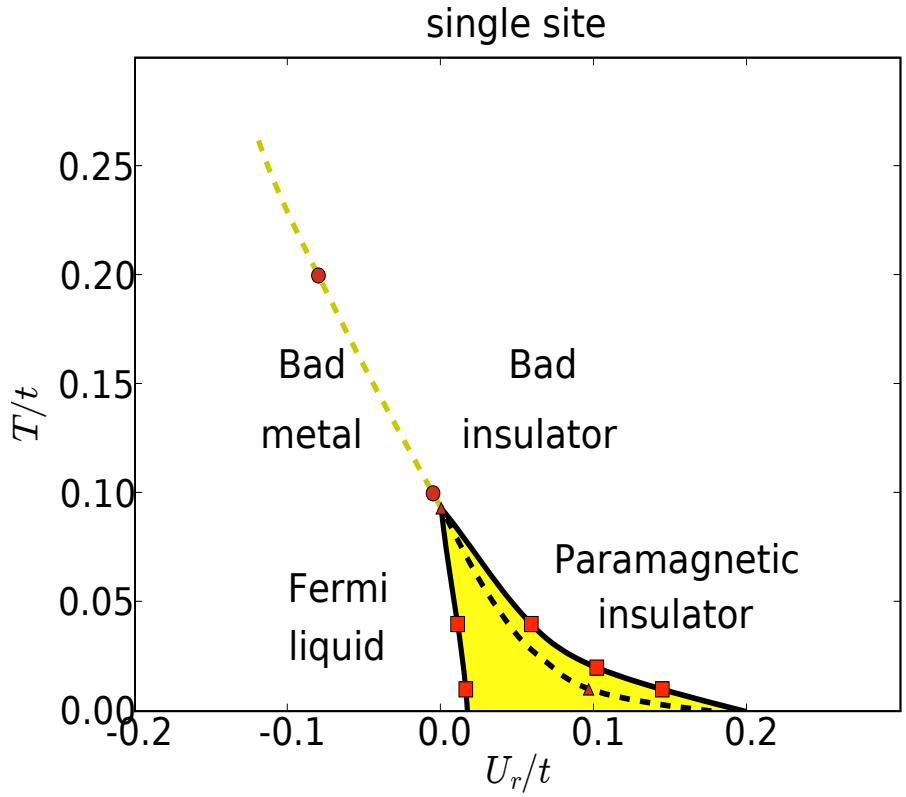




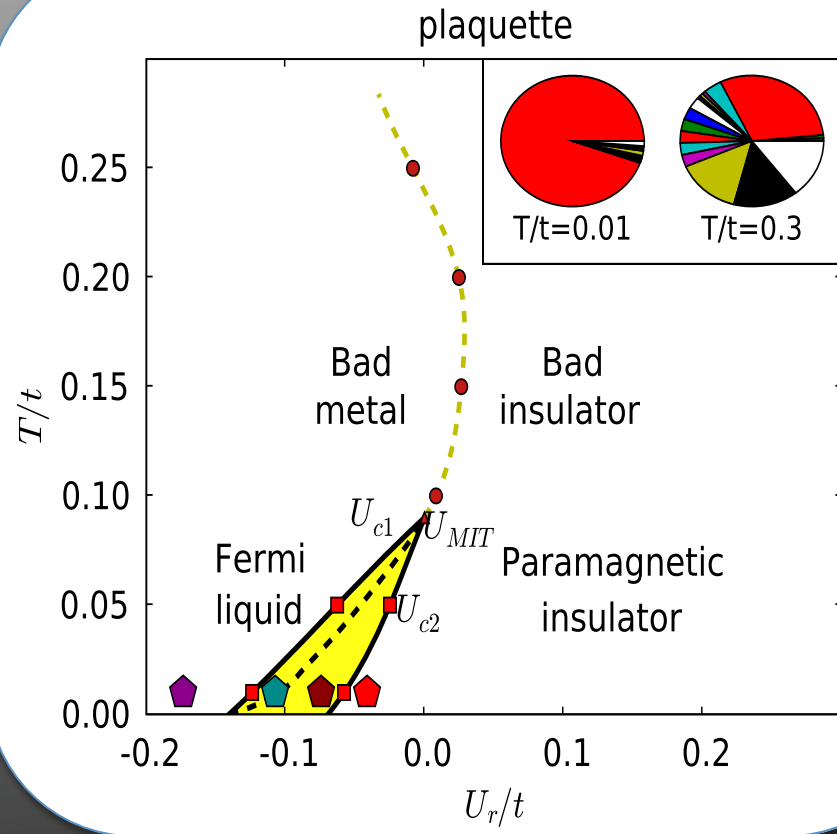
M. Civelli et al PRL (2005) CDMFT

Phase diagram of Hubbard model

Uc=9.35t

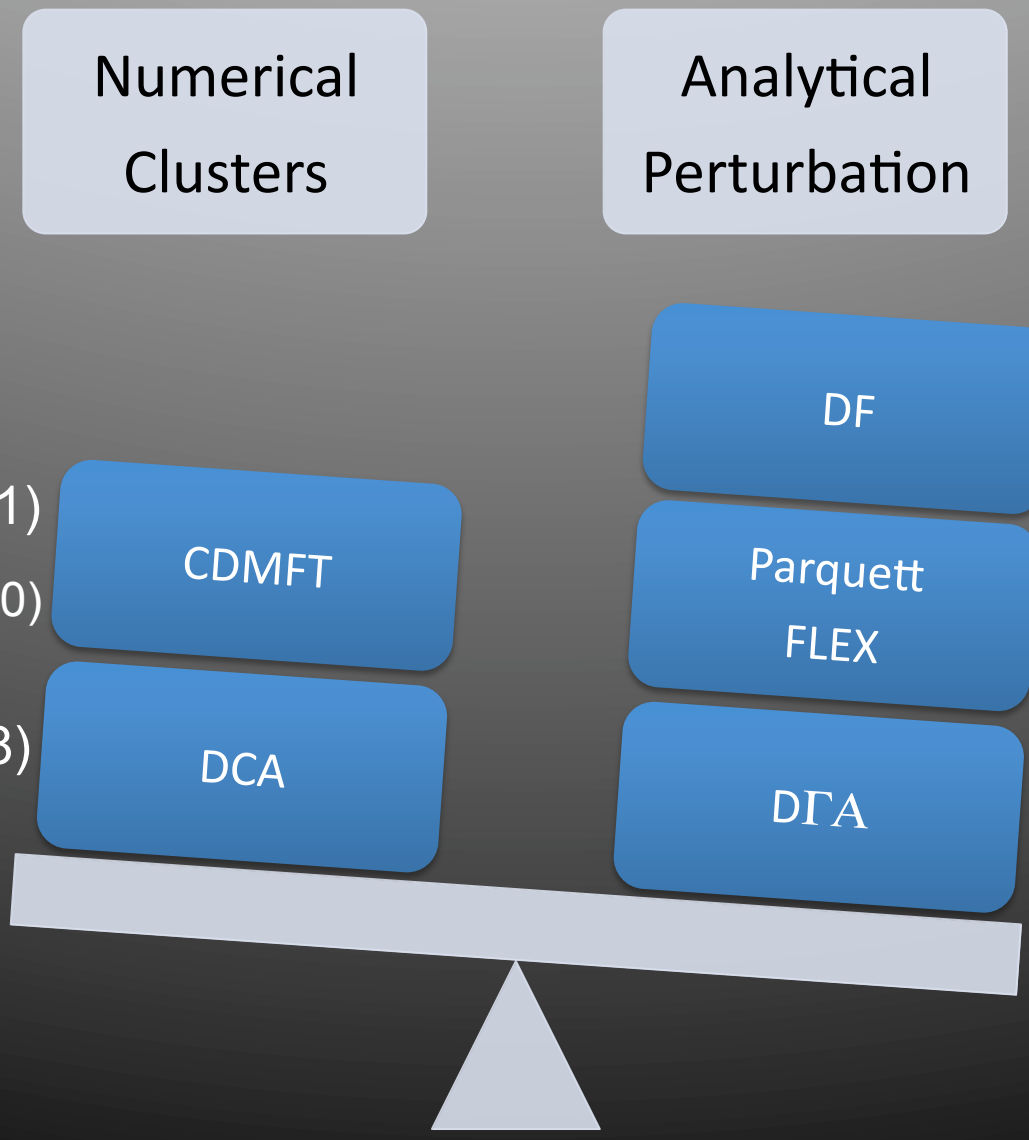


Uc=6.05t



H. Park et al PRL (2008)
C-DMFT with CT-QMC

Beyond DMFT



A. Rubtsov et al (2008)

G. Kotliar et al (2001)

A.L.,M. Katsnelson (2000)

C. Slezak et al (2009)

H. Kusunose (2006)

M. Hettler, et al (1998)

A. Toschi et al (2007)

General Cluster Idea

One-band Habbard model on Lattice

$$H = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

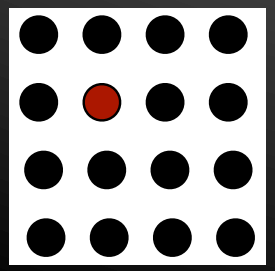
Exact solurion:

$$G(\mathbf{k}, i\omega) = (i\omega + \mu - t(\mathbf{k}) - \Sigma(\mathbf{k}, i\omega))^{-1}$$

Approximate self-energy:

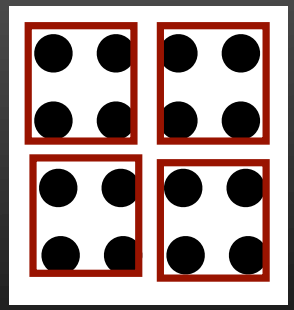
$$\Sigma(\mathbf{k}, i\omega) \approx \sum_{i=1}^{N} \phi_i(\mathbf{k}) \Sigma_i(\omega)$$

N=1 ⇔ single-site DMFT



MIT
Mott Transition
Paramagnetic Insulator

N=4 ⇔ plaquette CDMFT



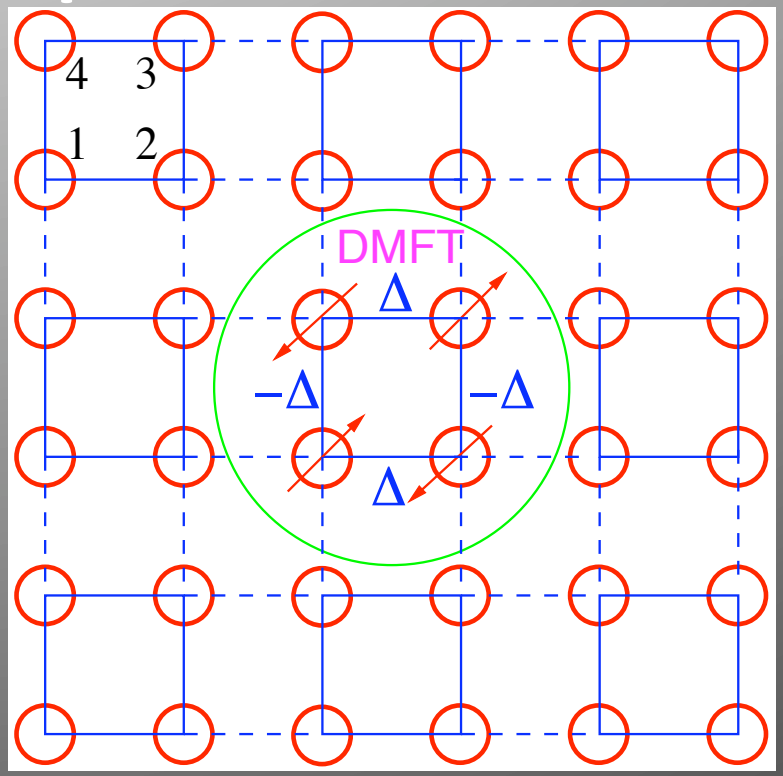
d-wave HTSC
Antiferromagnetism
CDW

Cluster-DMFT

Plaquette hopping matrix

$$T_{I,J}(\mathbf{K}) = \begin{pmatrix} 0 & t_x K_x^+ & 0 & t_y K_y^+ \\ t_x K_x^- & 0 & t_y K_y^+ & 0 \\ 0 & t_y K_y^- & 0 & t_x K_x^- \\ t_y K_y^- & 0 & t_x K_x^+ & 0 \end{pmatrix}$$

where $K_{x(y)}^{\pm} \equiv 1 + \exp\left(\pm i K_{x(y)} a\right)$



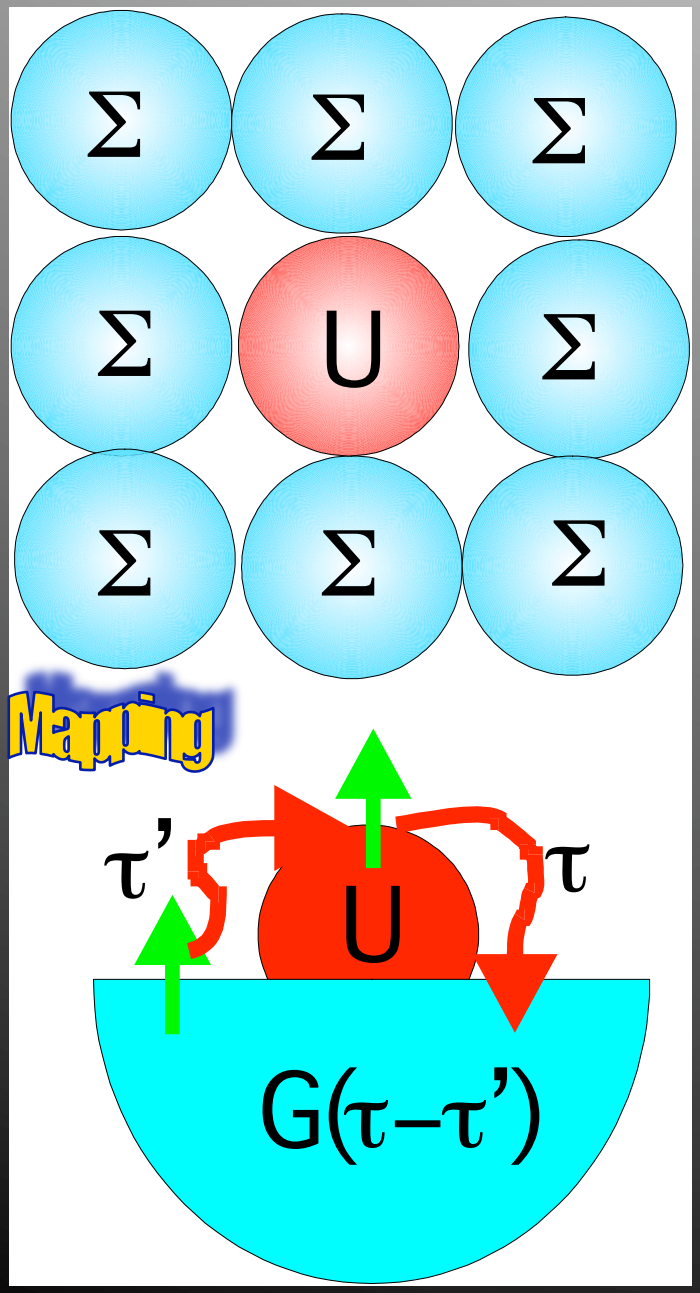
Supercell Green Function

$$G(\mathbf{K}, i\omega) = \left[(i\omega + \mu)\mathbf{1} - T(\mathbf{K}) - \Sigma(i\omega)\right]^{-1}$$

Where Self-energy matrix for plaquette has the form:

$$\Sigma_{I,J}(i\omega) = \begin{pmatrix} \Sigma_0 & \Sigma_x & \Sigma_{xy} & \Sigma_y \\ \Sigma_x & \Sigma_0 & \Sigma_y & \Sigma_{xy} \\ \Sigma_{xy} & \Sigma_y & \Sigma_0 & \Sigma_x \\ \Sigma_y & \Sigma_{xy} & \Sigma_x & \Sigma_0 \end{pmatrix}$$

Dynamical Mean Field Theory



$$\hat{G}(i\omega_n) = \frac{1}{\Omega}\sum_{\vec{k}}^{BZ}\left[\hat{I}(\mu + i\omega_n) - \hat{H}_0(\vec{k}) - \hat{\Sigma}(i\omega_n)\right]^{-1}$$

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

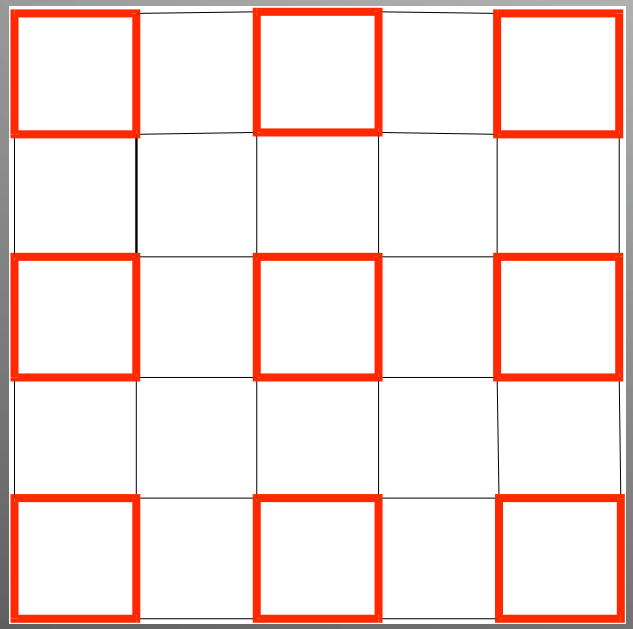
$$S_{eff} = -\int\int d\tau d\tau' c_\sigma^+(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_\sigma(\tau') + \int d\tau U n^\uparrow(\tau)n^\downarrow(\tau)$$

$$\hat{G}(\tau-\tau') = -\frac{1}{Z}\int D[c,c^+]c(\tau)c^+(\tau')e^{-S_{eff}}$$

$$\hat{\Sigma}_{new}(i\omega_n) = \hat{\mathcal{G}}_0^{-1}(i\omega_n) - \hat{G}^{-1}(i\omega_n)$$

W. Metzner and D. Vollhardt, PRL(1989)
A. Georges et al., RMP 68, 13 (1996)

Cluster DMFT scheme



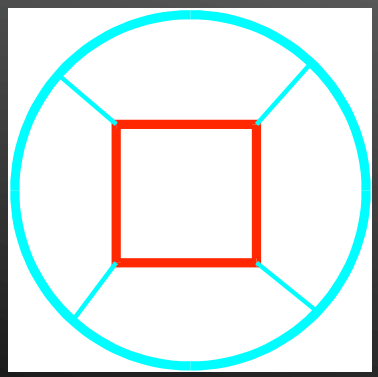
$$\hat{G}(i\omega_n) = \frac{1}{\Omega}\sum_{k}^{BZ}\left[\hat{I}(\mu + i\omega_n) - \hat{H}_0(\vec{k}) - \hat{\Sigma}(i\omega_n)\right]^{-1}$$

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

$$S_{eff} = -\iint d\tau d\tau' c_{I\sigma}^{+}(\tau)\mathcal{G}_{IJ}^{-1}(\tau-\tau')c_{J\sigma}(\tau') + \int d\tau U n_{I\uparrow}(\tau)n_{J\downarrow}(\tau)$$

Mapping

$$\hat{G}_{IJ}(\tau-\tau') = -\frac{1}{Z}\int D[c,c^{+}]c_I(\tau)c_J^{+}(\tau')e^{-S_{eff}}$$



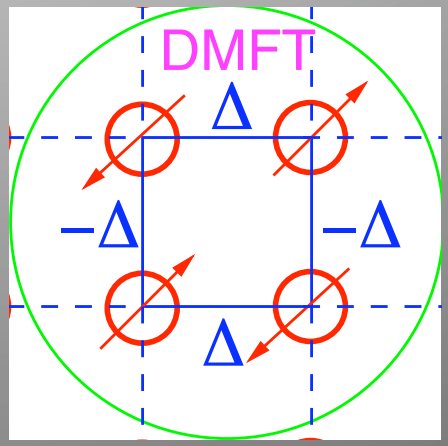
$$\hat{\Sigma}_{new}(i\omega_n) = \hat{\mathcal{G}}_0^{-1}(i\omega_n) - \hat{G}^{-1}(i\omega_n)$$

*A.L., M. Katsnelson, PRB **62**, R928368, (2000)*
*G. Kotliar, et al RMP **78**, 865 (2006)*

Cluster Impurity Problem

Super-impurity partition function:

$$Z = \int \mathcal{D}[c^*, c] e^{-S_{simp}}$$



$$\Psi_I^+(\tau) = \left(c_{I\uparrow}^\dagger, c_{I\downarrow}^\dagger, c_{I\uparrow}, c_{I\downarrow} \right)$$ I=(1,2,3,4)

$$S_{simp} = -\sum_{I,J=0}^{N} \int_0^\beta d\tau \int_0^\beta d\tau' \, c_{I\sigma}^*(\tau) \left[\mathcal{G}_\sigma^{-1}(\tau - \tau') \right]_{IJ} c_{J\sigma}(\tau') + \sum_{I=1}^{N} \int_0^\beta d\tau U n_{I,\uparrow}(\tau) n_{I,\downarrow}(\tau)$$

Local plaquette Green-function:

$$G_{IJ}(i\omega) = \sum_{\mathbf{K}} G_{IJ}(\mathbf{K}, i\omega)$$

Bath Green-fanction matrix:

$$\mathcal{G}^{-1}(i\omega) = G^{-1}(i\omega) + \Sigma(i\omega)$$

CTQMC: Exact solution of S-imp:

$$G_{IJ}^{simp}(\tau) = -\langle c_{I\sigma}(\tau) c_{J\sigma}^\dagger(0) \rangle_{simp}$$

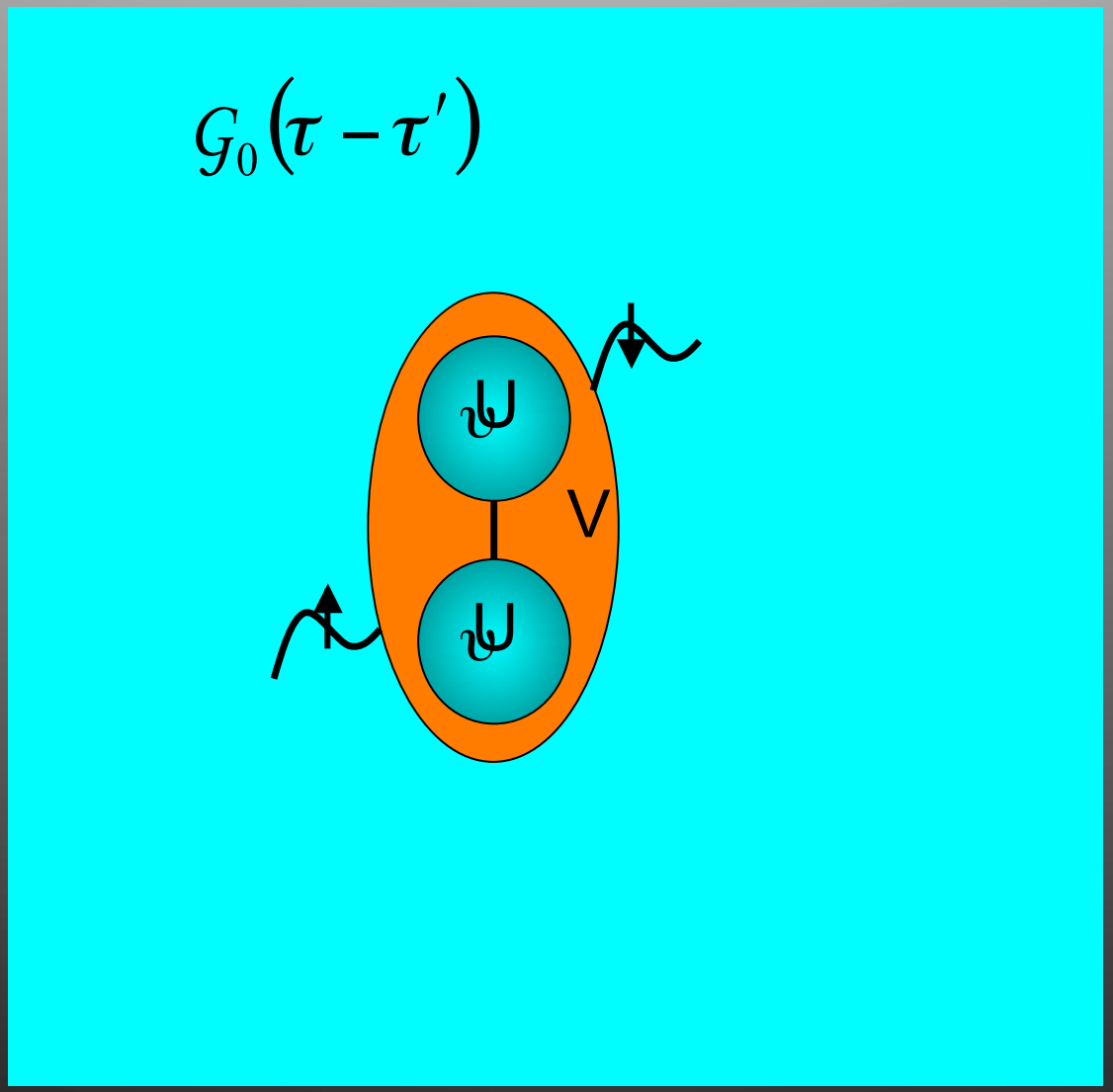
New self-energy matrix:

$$\Sigma_{new}(i\omega) = \mathcal{G}^{-1}(i\omega) - G_{simp}^{-1}(i\omega)$$

CDMFT: Self-consistent condition:

$$G_{IJ}^{simp}(i\omega) = G_{IJ}(i\omega)$$

Cluster DMFT: Self-Consistent Set of Equations



Dynamical Cluster Approximation

T. Maier, M. Jarrell, T. Pruschke, and M.H. Hettler, RMP 77, 1027 (2005)

Cluster (L_c) in Reciprocal space

Position vector:

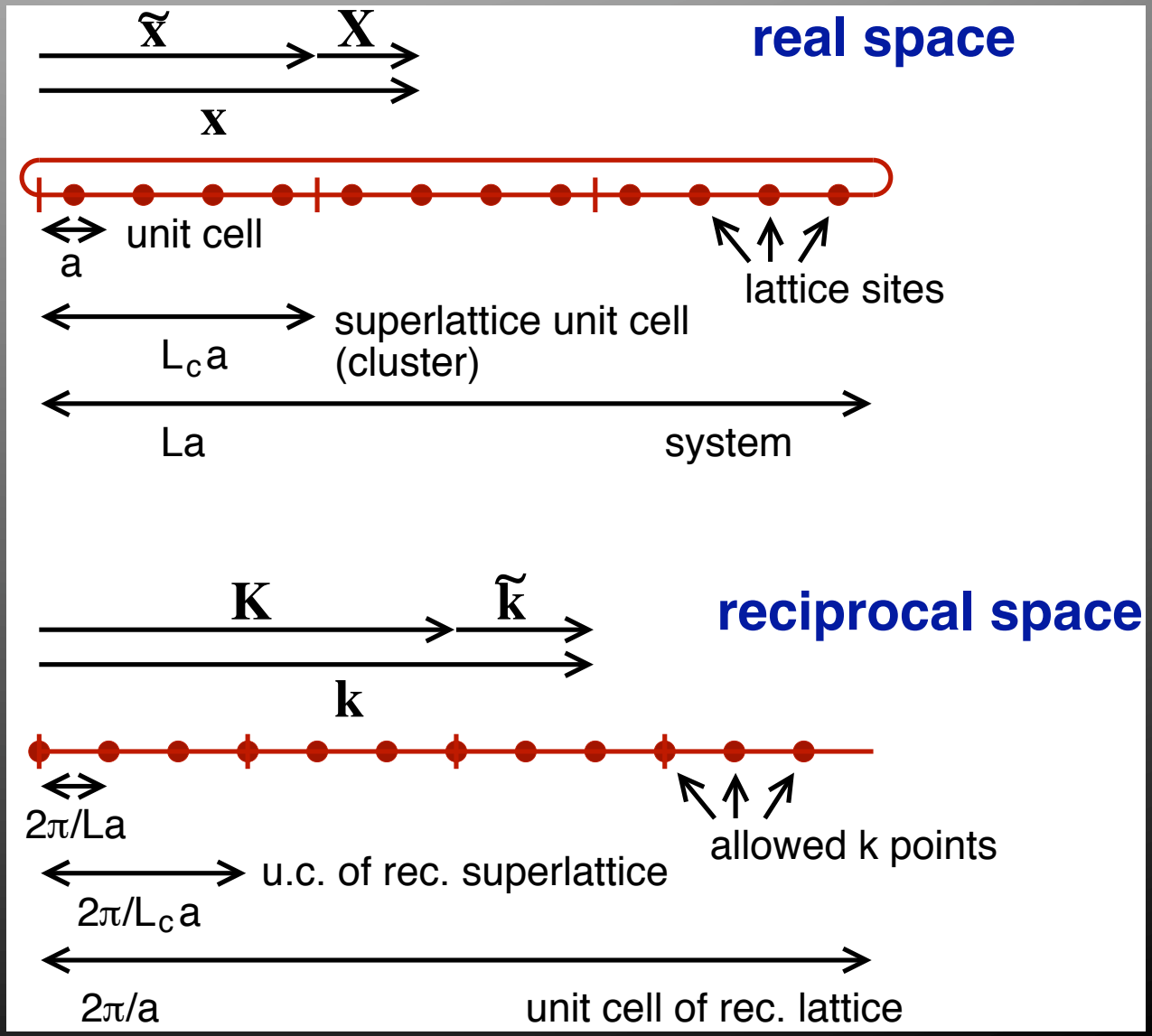
$$\boldsymbol{x} = \boldsymbol{X} + \tilde{\boldsymbol{x}}$$

Reciprocal vector:

$$\boldsymbol{k} = \tilde{\boldsymbol{k}} + \boldsymbol{K}$$

Superlattice vector K:

$$\exp(i\boldsymbol{K}\tilde{\boldsymbol{x}}) = 1$$



M. Potthoff et al PRB (2007)

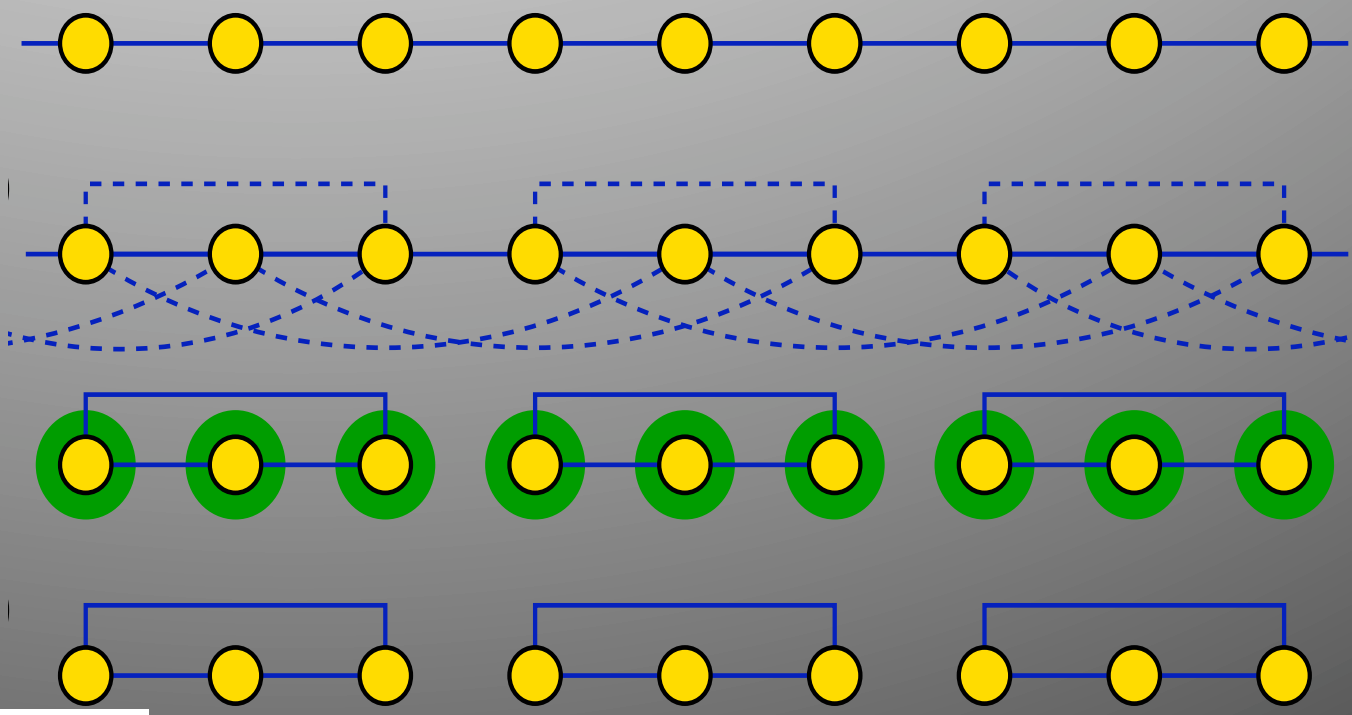
DCA-transformation

Different transformations:

$$U_{\boldsymbol{x},\boldsymbol{k}} = \frac{1}{\sqrt{L}} e^{i\boldsymbol{k}\boldsymbol{x}}$$

$$V_{\tilde{\boldsymbol{x}},\tilde{\boldsymbol{k}}} = \frac{1}{\sqrt{L/L_c}} e^{i\tilde{\boldsymbol{k}}\tilde{\boldsymbol{x}}}$$

$$W_{\boldsymbol{X},\boldsymbol{K}} = \frac{1}{\sqrt{L_c}} e^{i\boldsymbol{K}\boldsymbol{X}}$$



Main Problem: $\boldsymbol{U \neq VW = WV}$

M. Potthoff et al PRB (2007)

$$U_{\boldsymbol{x},\boldsymbol{k}} = \frac{1}{\sqrt{L}} e^{i\boldsymbol{k}\boldsymbol{x}} = \frac{1}{\sqrt{L}} e^{i(\tilde{\boldsymbol{k}}\boldsymbol{X}+\tilde{\boldsymbol{k}}\tilde{\boldsymbol{x}}+\boldsymbol{K}\boldsymbol{X})} \neq \frac{1}{\sqrt{L}} e^{i(\tilde{\boldsymbol{k}}\tilde{\boldsymbol{x}}+\boldsymbol{K}\boldsymbol{X})} = V_{\tilde{\boldsymbol{x}},\tilde{\boldsymbol{k}}} W_{\boldsymbol{X},\boldsymbol{K}}$$

Lattice invarince: $t_{\boldsymbol{x}+\boldsymbol{x}_0,\boldsymbol{x}'+\boldsymbol{x}_0} = t_{\boldsymbol{x},\boldsymbol{x}'}$ $\Leftrightarrow$ $(\boldsymbol{U}^\dagger \boldsymbol{t} \boldsymbol{U})_{\boldsymbol{k}\boldsymbol{k}'} = t(\boldsymbol{k})\delta_{\boldsymbol{k},\boldsymbol{k}'}$

Superlattice invarince: $T_{\boldsymbol{x}+\tilde{\boldsymbol{x}}_0,\boldsymbol{x}'+\tilde{\boldsymbol{x}}_0} = T_{\boldsymbol{x}+\boldsymbol{X}_0,\boldsymbol{x}'+\boldsymbol{X}_0} = T_{\boldsymbol{x},\boldsymbol{x}'}$ $\Leftrightarrow$

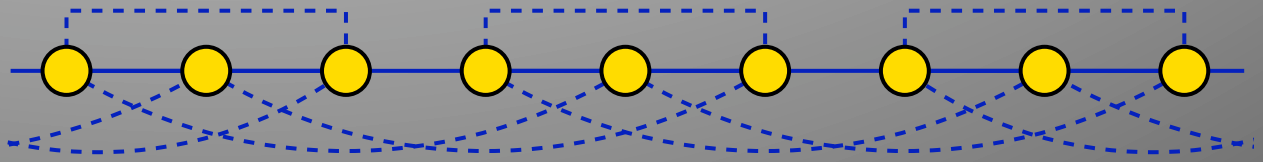
$$(\boldsymbol{W}^\dagger \boldsymbol{V}^\dagger \boldsymbol{T} \boldsymbol{V} \boldsymbol{W})_{\tilde{\boldsymbol{k}}\boldsymbol{K},\tilde{\boldsymbol{k}}'\boldsymbol{K}'} = T(\tilde{\boldsymbol{k}},\boldsymbol{K})\delta_{\tilde{\boldsymbol{k}},\tilde{\boldsymbol{k}}'}\delta_{\boldsymbol{K},\boldsymbol{K}'}$$

Real-space DCA

Effective DCA-hopping: $\bar{\boldsymbol{t}} = (\boldsymbol{V}\boldsymbol{W})\boldsymbol{U}^\dagger\, \boldsymbol{t}\, \boldsymbol{U}(\boldsymbol{V}\boldsymbol{W})^\dagger$

Band-structure spectrum: $\varepsilon(\boldsymbol{k}) = (\boldsymbol{U}^\dagger \boldsymbol{t} \boldsymbol{U})(\boldsymbol{k})$

DCA long-range hopping:



$$\bar{t}_{\boldsymbol{x}\boldsymbol{x}'} = \frac{1}{L_c}\sum_{\boldsymbol{K}} e^{i\boldsymbol{K}(\boldsymbol{X}-\boldsymbol{X}')} \frac{L_c}{L}\sum_{\tilde{\boldsymbol{k}}} e^{i\tilde{\boldsymbol{k}}(\tilde{\boldsymbol{x}}-\tilde{\boldsymbol{x}}')}\varepsilon(\tilde{\boldsymbol{k}}+\boldsymbol{K})$$

Comparison of real and DCA hopping:

$$\bar{t}_{\boldsymbol{X}\boldsymbol{X}'}(\tilde{\boldsymbol{k}}) = \frac{1}{L_c}\sum_{\boldsymbol{K}} e^{i\boldsymbol{K}(\boldsymbol{X}-\boldsymbol{X}')}\varepsilon(\tilde{\boldsymbol{k}}+\boldsymbol{K}) = \frac{L_c}{L}\sum_{\tilde{\boldsymbol{x}}\tilde{\boldsymbol{x}}'} e^{-i\tilde{\boldsymbol{k}}(\tilde{\boldsymbol{x}}+\boldsymbol{X}-\tilde{\boldsymbol{x}}'-\boldsymbol{X}')} t_{\tilde{\boldsymbol{x}}+\boldsymbol{X},\tilde{\boldsymbol{x}}'+\boldsymbol{X}'} = e^{-i\tilde{\boldsymbol{k}}(\boldsymbol{X}-\boldsymbol{X}')} t_{\boldsymbol{X}\boldsymbol{X}'}(\tilde{\boldsymbol{k}})$$

DCA Green function: $$G(\mathbf{K}+\tilde{\mathbf{k}}, i\omega) = \frac{1}{i\omega + \mu - \varepsilon(\mathbf{K}+\tilde{\mathbf{k}}) - \Sigma(\mathbf{K}, i\omega)}$$

Self-consistent condition: $$G^{imp}(\mathbf{K}, i\omega) = G(\mathbf{K}, i\omega) \equiv \sum_{\tilde{\mathbf{k}}} G(\mathbf{K}+\tilde{\mathbf{k}}, i\omega)$$

Periodization of CDMFT

Double Fourier Transform:

$$\Sigma(\mathbf{k},\mathbf{k}',i\omega)=\frac{1}{L_{\mathrm{c}}}\sum_{\mathbf{Q}}\sum_{\mathbf{X},\mathbf{X}'}e^{i\mathbf{k}\mathbf{X}}\Sigma_{\mathrm{c}}(\mathbf{X},\mathbf{X}',i\omega)e^{-i\mathbf{k}'\mathbf{X}'}\delta(\mathbf{k}-\mathbf{k}'-\mathbf{Q})$$

Translational invariant solution: Q=0

$$\Sigma(\mathbf{k},i\omega)=\frac{1}{L_{\mathrm{c}}}\sum_{\mathbf{X},\mathbf{X}'}=e^{i\mathbf{k}(\mathbf{X}-\mathbf{X}')}\Sigma_{\mathrm{c}}(\mathbf{X},\mathbf{X}',i\omega)$$

Real space periodic self-energy:

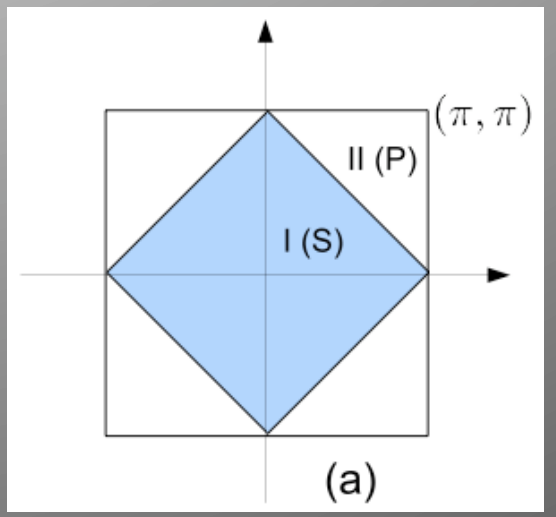
$$\Sigma(\mathbf{x}-\mathbf{x}',i\omega)=\frac{1}{L_{\mathrm{c}}}\sum_{\mathbf{X},\mathbf{X}'}\Sigma_{\mathrm{c}}(\mathbf{X},\mathbf{X}',i\omega)\,\delta_{\mathbf{X}-\mathbf{X}',\mathbf{x}-\mathbf{x}'}$$

M-Periodization - cumulant (G. Kotliar et al):

$$\Sigma^{(M)}_{\mathrm{latt}}(\mathbf{k},\omega)=\omega+\mu-M_{\mathrm{latt}}(\mathbf{k},\omega)^{-1}$$

DCA: symmetry of 2-site cluster

$$\hat{G}^{imp} = \begin{pmatrix} G_0 & G_1 \\ G_1 & G_0 \end{pmatrix} \quad \hat{\Sigma}^{imp} = \begin{pmatrix} \Sigma_0 & \Sigma_1 \\ \Sigma_1 & \Sigma_0 \end{pmatrix}$$



C. Lin and A. Millis PRB (2009)

$$\Sigma_{DCA}(\vec{k},\omega) = \begin{cases} \Sigma_S^{imp} = \Sigma_0 + \Sigma_1 & \text{for } \mathbf{k} \in \text{Region } I(S) \\ \Sigma_P^{imp} = \Sigma_0 - \Sigma_1 & \text{for } \mathbf{k} \in \text{Region } II(P) \end{cases}$$

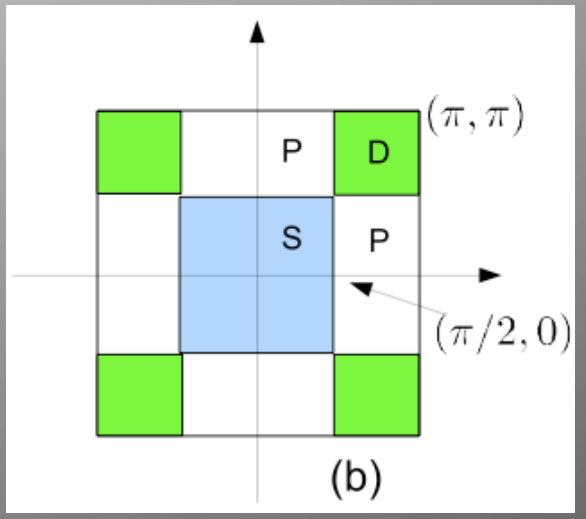
$$G_0 = (G_S + G_P)/2$$
$$G_1 = (G_S - G_P)/2$$

$$D_{S(P)}(\epsilon) = 2 \times \int_{\mathbf{k} \in I(II)} d\mathbf{k}\ \delta(\epsilon - \epsilon_{\mathbf{k}})$$

$$G_{S(P)} = \int \frac{D_{S(P)}(\epsilon)\ d\epsilon}{\omega + \mu - \epsilon_{\mathbf{k}} - (\Sigma_0 \pm \Sigma_1)}$$

DCA: symmetry of 4-site cluster

$$\hat{G}^{imp} = \begin{pmatrix} G_0 & G_1 & G_2 & G_1 \\ G_1 & G_0 & G_1 & G_2 \\ G_2 & G_1 & G_0 & G_1 \\ G_1 & G_2 & G_1 & G_0 \end{pmatrix} \quad \hat{\Sigma}^{imp} = \begin{pmatrix} \Sigma_0 & \Sigma_1 & \Sigma_2 & \Sigma_1 \\ \Sigma_1 & \Sigma_0 & \Sigma_1 & \Sigma_2 \\ \Sigma_2 & \Sigma_1 & \Sigma_0 & \Sigma_1 \\ \Sigma_1 & \Sigma_2 & \Sigma_1 & \Sigma_0 \end{pmatrix}$$



C. Lin and A. Millis PRB (2009)

$$\begin{aligned} \Sigma_S &= \Sigma_0 + 2\Sigma_1 + \Sigma_2 \\ \Sigma_P &= \Sigma_0 - \Sigma_2 \\ \Sigma_D &= \Sigma_0 - 2\Sigma_1 + \Sigma_2 \end{aligned}$$

$$\begin{aligned} G_0 &= (G_S + 2G_P + G_D)/4 \\ G_1 &= (G_S - G_D)/4 \\ G_2 &= (G_S - 2G_P + G_D)/4 \end{aligned}$$

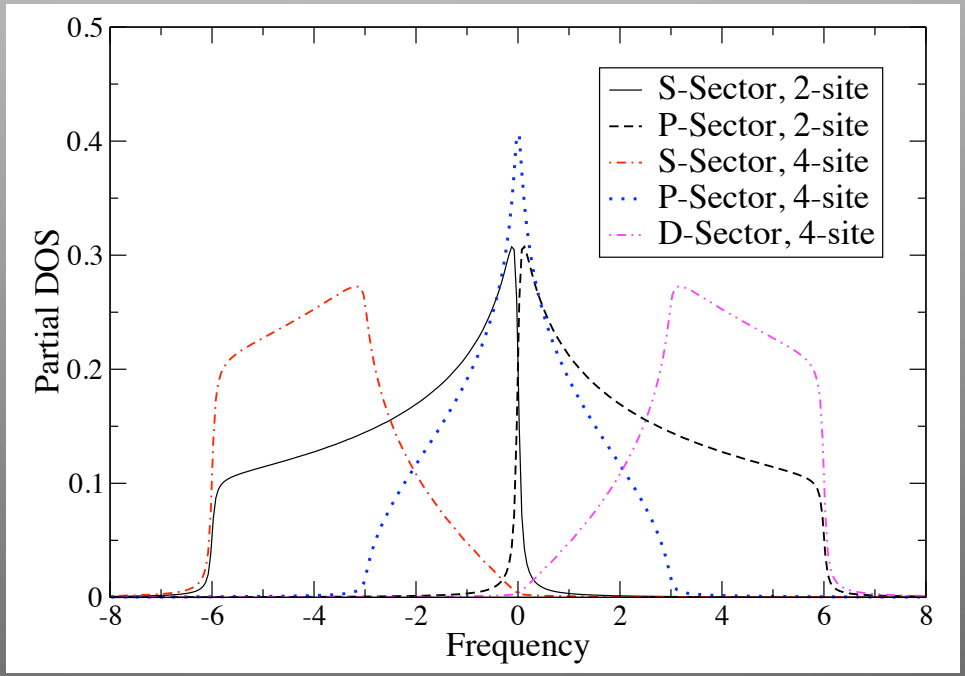
$$D^{(4)}_{S(P,D)}(\epsilon) = 4 \times \int_{\mathbf{k} \in S(P,D)} d\mathbf{k}\ \delta(\epsilon - \epsilon_{\mathbf{k}})$$

$$G_{S(P,D)} = \int \frac{D_{S(P,D)}(\epsilon) d\epsilon}{i\omega_n + \mu - \epsilon - \Sigma_{S(P,D)}}$$

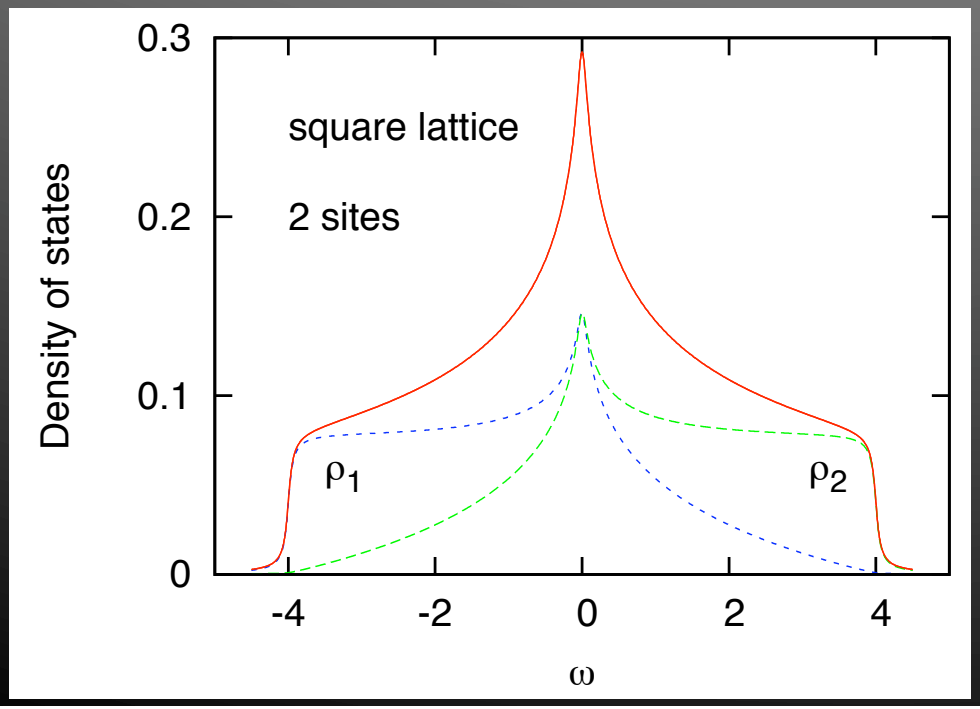
CDMFT vs. DCA

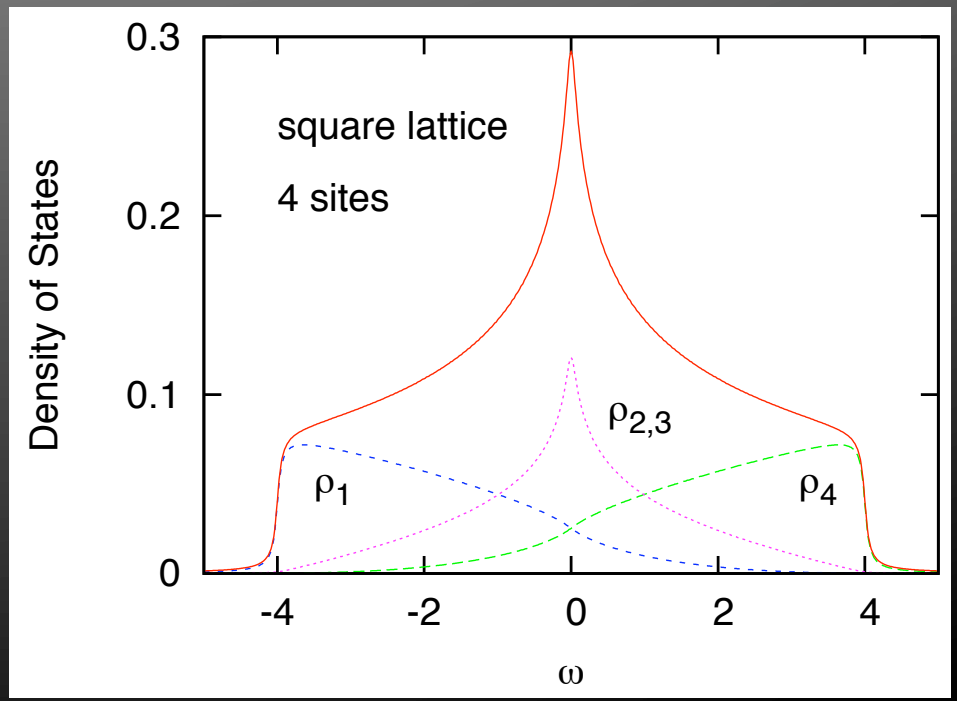
DOS comparison:

DCA:
C. Lin and A. Millis PRB (2009)

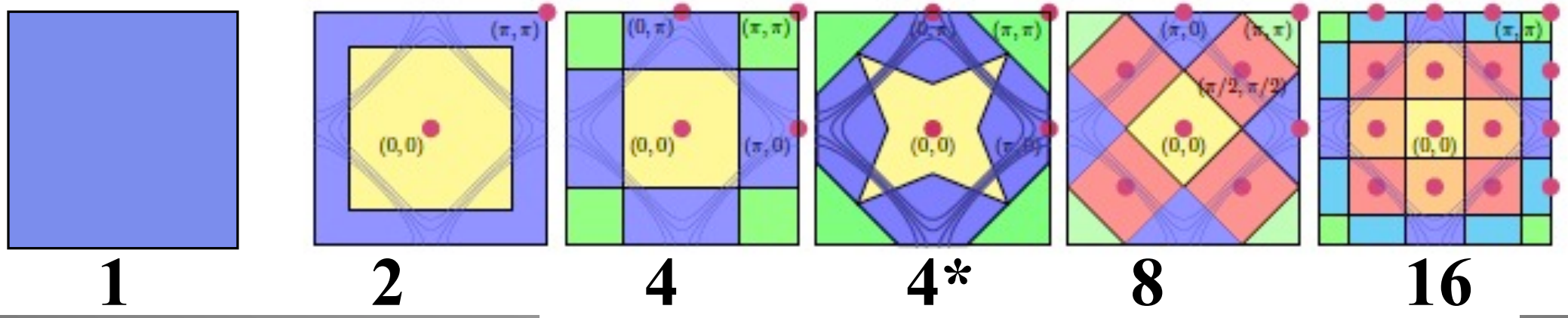


CDMFT:
A. Liebsch et al, PRB (2009)

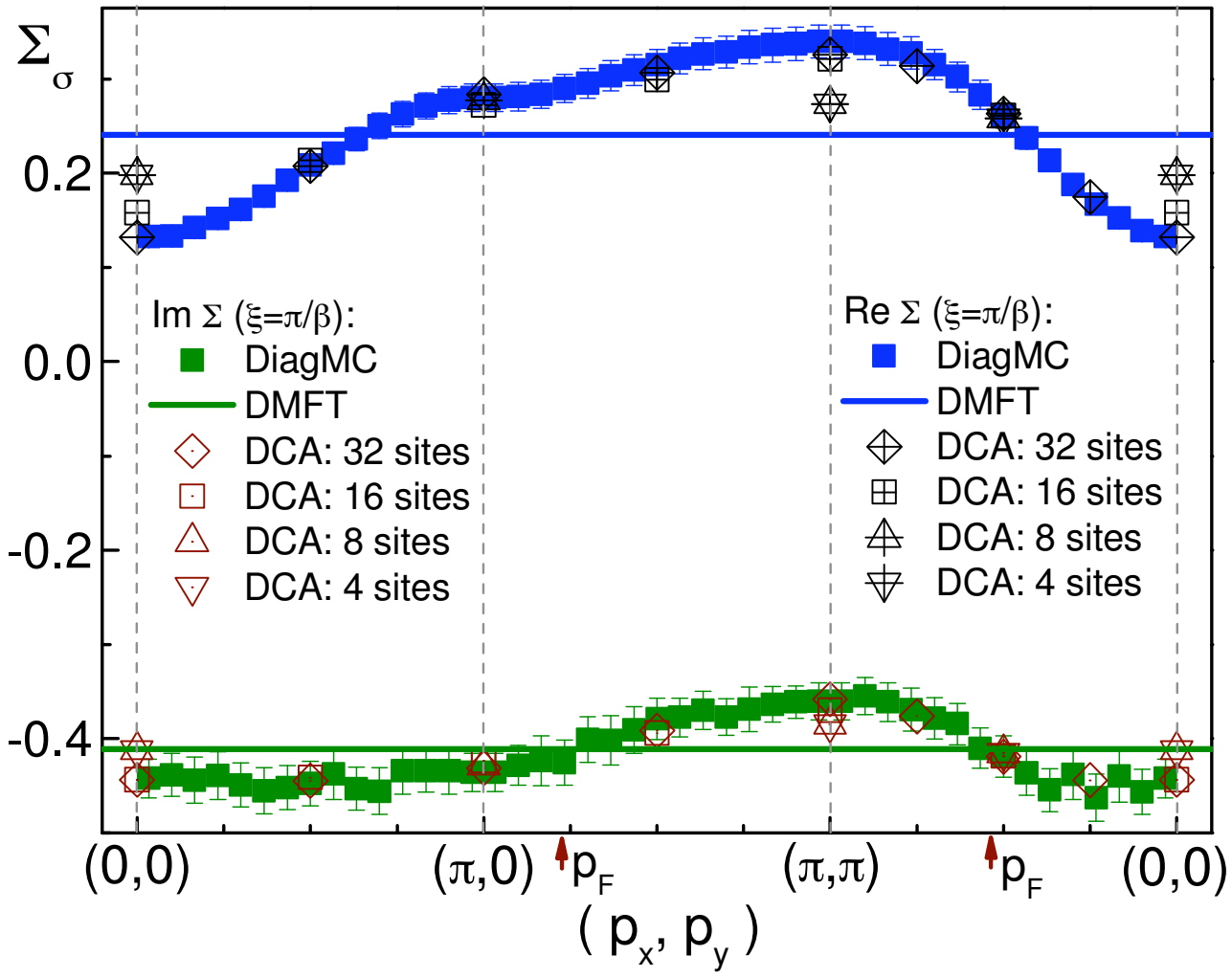




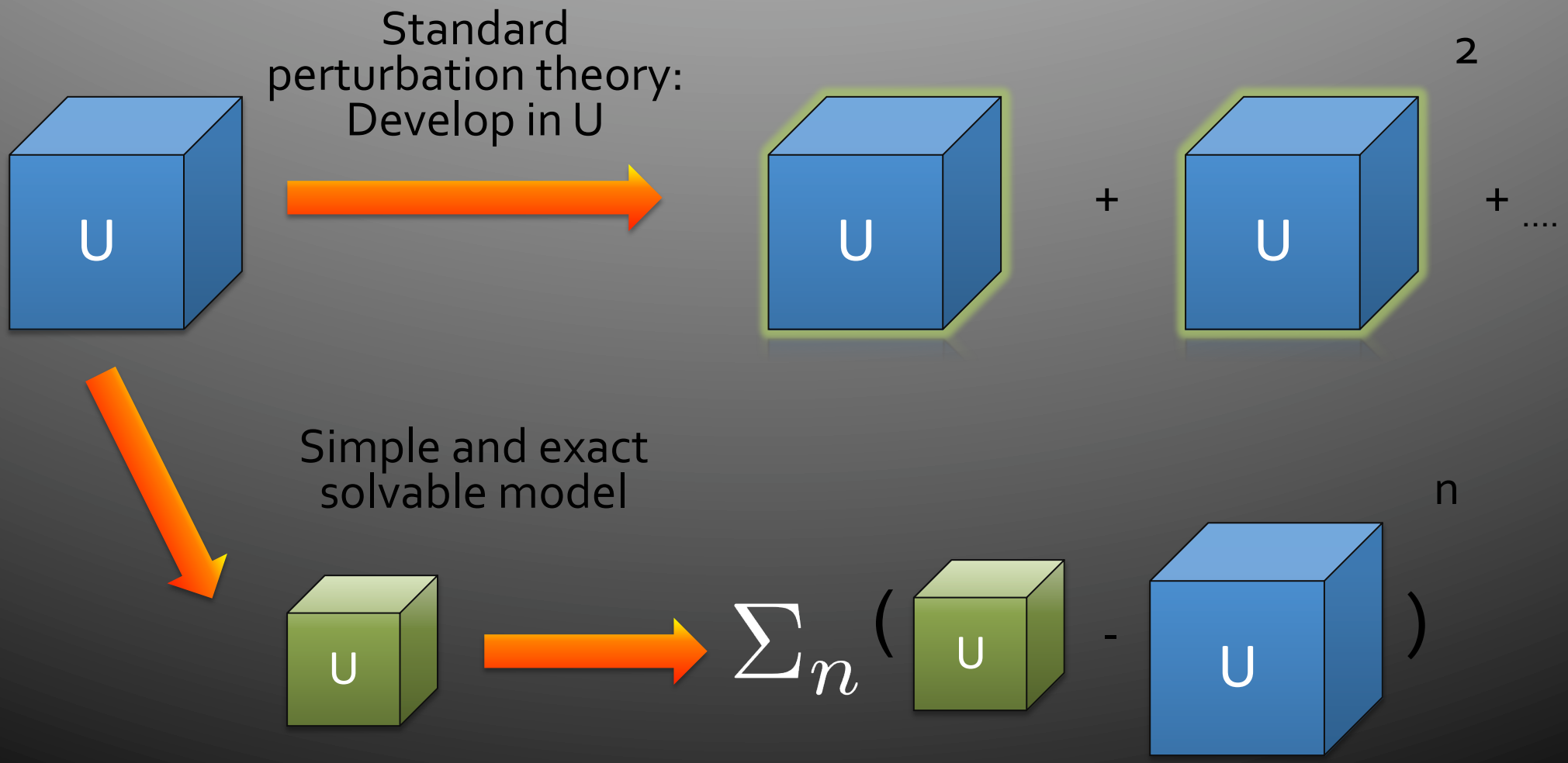
DCA in practice



E. Kozik,
E. Gull et all
EPL (2010)

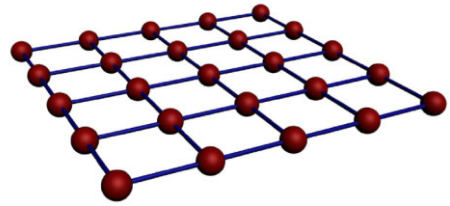


Beyond DMFT: Superperturbation



Beyond DMFT: Dual Fermion scheme

General Lattice Action $H = h + U$

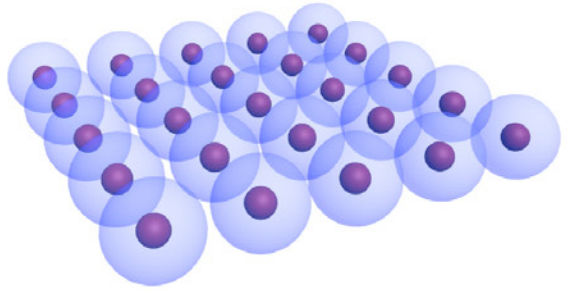


$$S[c^*,c] = \sum_{\omega k m m' \sigma} \left[h_k^{mm'} - (i\omega+\mu)1\right] c^*_{\omega k m \sigma} c_{\omega k m' \sigma} + \frac{1}{4} \sum_{i\{m,\sigma\}} \int_0^\beta U_{1234} c_1^* c_2^* c_3 c_4 d\tau$$

Reference system: Local Action with hybridization Δ_ω

$$S_{loc} = \sum_{\omega m m' \sigma} \left[\Delta_\omega^{mm'} - (i\omega+\mu)1\right] c^*_{\omega m \sigma} c_{\omega m' \sigma} + \frac{1}{4} \sum_{i\{m,\sigma\}} \int_0^\beta U_{1234} c_1^* c_2^* c_3 c_4 d\tau$$

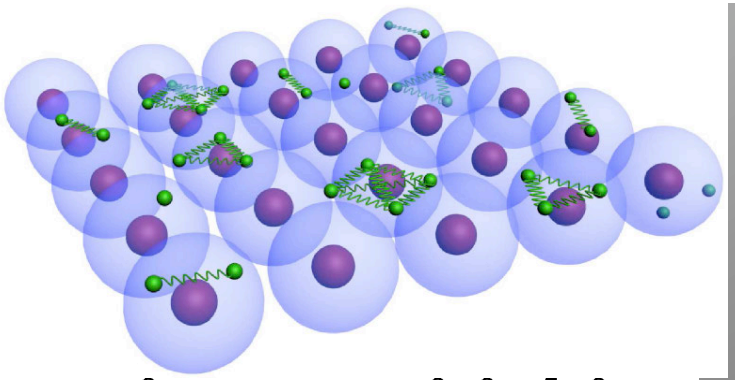
Lattice-Impurity connection:



$$S[c^*,c] = \sum_i S_{loc}[c_i^*, c_i] + \sum_{\omega k m m' \sigma} \left(h_k^{mm'} - \Delta_\omega^{mm'}\right) c^*_{\omega k m \sigma} c_{\omega k m' \sigma}$$

A. Rubtsov, et al, PRB **77**, 033101 (2008)

Dual Fermions



Gaussian path-integral

$$\int D[\vec{f}^*,\vec{f}]\exp(-\vec{f}^*\hat{A}\vec{f}+\vec{f}^*\hat{B}\vec{c}+\vec{c}^*\hat{B}\vec{f})=\det(\hat{A})\exp(\vec{c}^*\hat{B}\hat{A}^{-1}\hat{B}\vec{c})$$

With

$$\begin{aligned} A &= g_\omega^{-1}(\Delta_\omega - h_k)g_\omega^{-1} \\ B &= g_\omega^{-1} \end{aligned}$$

new Action:

$$S_d[f^*,f]=-\sum_{k\omega}\mathcal{G}^{-1}_{k\omega}f^*_{k\omega}f_{k\omega}+\frac{1}{4}\sum_{1234}\gamma^{(4)}_{1234}f^*_1f^*_2f_4f_3+\ldots$$

Diagrammatic:

→ $\mathcal{G}_{k\omega}=G^{DMFT}_{k\omega}-g_\omega$

□ $\gamma^{(4)}_{1234} = g^{-1}_{11'}g^{-1}_{22'}\left(\chi_{1'2'3'4'}-\chi^0_{1'2'3'4'}\right)g^{-1}_{3'3}g^{-1}_{4'4}$

g_ω and $\chi_{\nu,\nu',\omega}$ from DMFT impurity solver

Dual Fermion Action: Details

Lattice - dual action

$$S[c^*, c, f^*, f] = \sum_i S_{\text{site},i} + \sum_{\omega \mathbf{k}\, \alpha\beta} f^*_{\omega \mathbf{k}\alpha} [g_\omega^{-1} \left(\Delta_\omega - t_{\mathbf{k}}\right)^{-1} g_\omega^{-1}]_{\alpha\beta} f_{\omega \mathbf{k}\beta}$$

$$S_{\text{site},i}[c_i^*, c_i, f_i^*, f_i] = S_{\text{loc}}[c_i^*, c_i] + \sum_{\alpha\beta} f^*_{\omega i\alpha}\, g^{-1}_{\omega\,\alpha\beta} c_{\omega i\beta} + c^*_{\omega i\alpha}\, g^{-1}_{\omega\,\alpha\beta} f_{\omega i\beta}$$

For each site I integrate-out c-Fermions:

$$\int \mathcal{D}[c^*, c] \exp\left(-S_{\text{site}}[c_i^*, c_i, f_i^*, f_i]\right) =$$

$$\mathcal{Z}_{\text{loc}} \exp\left(- \sum_{\omega\, \alpha\beta} f^*_{\omega i\alpha}\, g^{-1}_{\omega\,\alpha\beta} f_{\omega i\beta} - V_i[f_i^*, f_i]\right)$$

Dual potential:

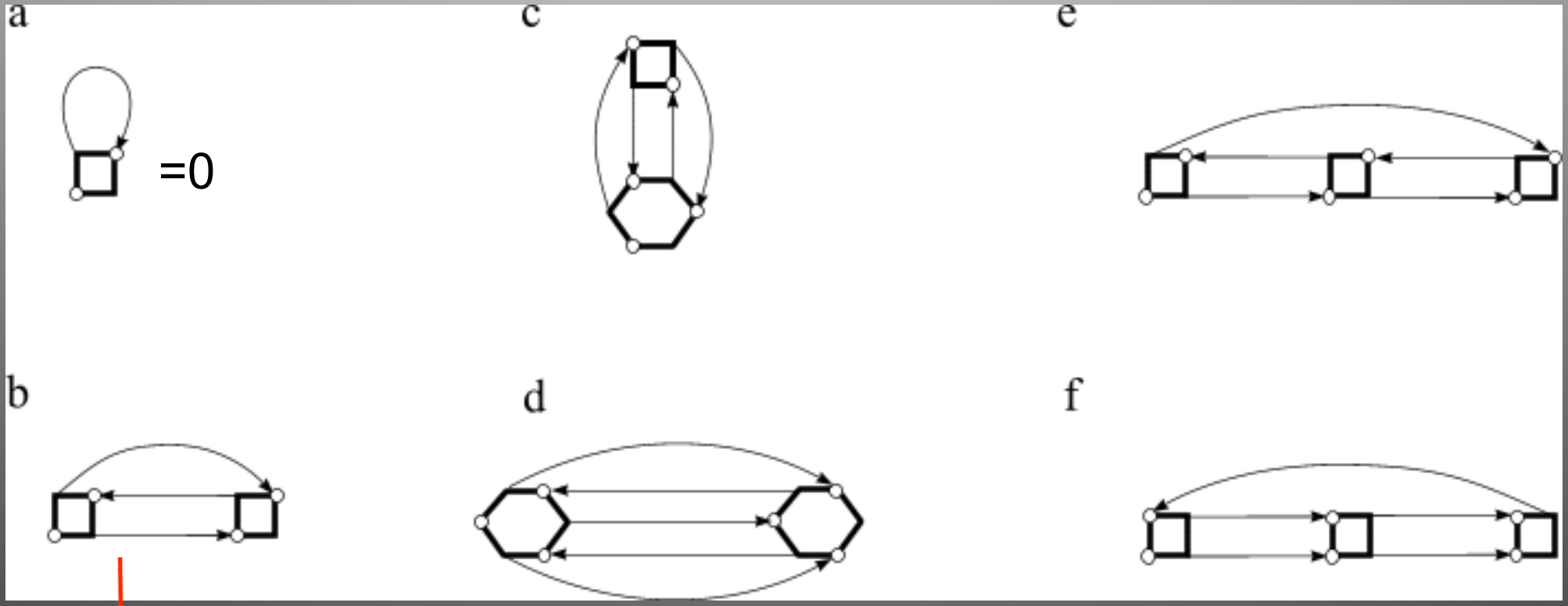
$$V[f^*, f] = \frac{1}{4} \gamma_{1234} f_1^* f_2^* f_4 f_3 \; + \ldots$$

$$\gamma_{1234} = g^{-1}_{11'} g^{-1}_{22'} \left[\chi_{1'2'3'4'} - \chi^0_{1'2'3'4'}\right] g^{-1}_{3'3} g^{-1}_{4'4}$$

$$\chi^0_{1234} = g_{14} g_{23} - g_{13} g_{24}$$

$$\chi^{1234} = \langle c_1 c_2 c_3^* c_4^* \rangle_{\text{loc}} = \frac{1}{\mathcal{Z}_{\text{loc}}} \int \mathcal{D}[c^*, c] c_1 c_2 c_3^* c_4^* \exp\left(- S_{\text{loc}}[c^*, c]\right)$$

Basic diagrams for dual self-energy



Lines - dual Green's function.

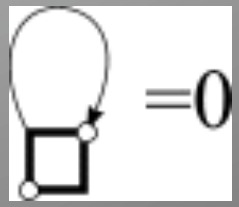
$$\tilde{G}^0_\omega(\mathbf{k}) = \left[g_\omega^{-1} + \Delta_\omega - t_{\mathbf{k}}\right]^{-1} - g_\omega$$

$$\tilde{\Sigma}^{(b)}_{12}(\mathbf{k}) = -\frac{1}{2}\left(\frac{T}{N}\right)^2 \sum_{\mathbf{k}_1\mathbf{k}_2} \sum_{345678} \gamma_{1345}\tilde{G}_{57}(\mathbf{k}_1)\tilde{G}_{83}(\mathbf{k}_2)\tilde{G}_{46}(\mathbf{k}+\mathbf{k}_2-\mathbf{k}_1)\gamma_{6728}$$

Condition for Δ and relation with DMFT

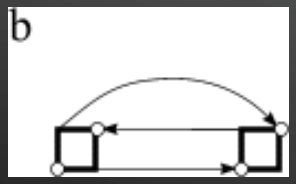
$G^d = G^{DMFT} - g$

To determine Δ, we require
that Hartree correction in dual variables vanishes.
If no higher diagrams are taken into account, one obtains DMFT:



$$\frac{1}{N}\sum_{\mathbf{k}} \tilde{G}^0_\omega(\mathbf{k}) = 0 \quad \Longleftrightarrow \quad \frac{1}{N}\sum_{\mathbf{k}} G^{\mathrm{DMFT}}_\omega(\mathbf{k}) = g_\omega$$

Higher-order diagrams give corrections to the DMFT self-energy,
and already the leading-order correction is nonlocal.



$$\Sigma(k,\omega) = \Sigma_{\mathrm{DMFT}}(\omega) + \Sigma_d(k,\omega)/[1 + g\Sigma_d(k,\omega)]$$

Dual and Lattice Green's Functions

Two equivalent Eqs for partition function:

$$F[J^*, J; L^*, L] = \ln \mathcal{Z}_f \int \mathcal{D}[c^*, c; f^*, f] \exp\left(-S[c^*, c; f^*, f] + J_1^* c_1 + c_2^* J_2 + L_1^* f_1 + f_2^* L_2\right)$$

$$F[L^*, L] = \ln \tilde{\mathcal{Z}}_f \int \mathcal{D}[f^*, f] \exp\left(-S_{\mathrm{d}}[f^*, f] + L_1^* f_1 + f_2^* L_2\right)$$

Hubbard-Stratanovich transformation:

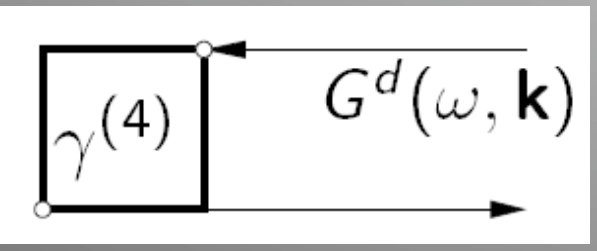
$$F[J^*, J; L^*, L] = L_1^*[g(\Delta - h)g]_{12} L_2 + \ln \int \mathcal{D}[c^*, c] \exp\Big(- S[c^*, c] + \\ + J_1^* c_1 + c_2^* J_2 + L_1^*[g(\Delta - t)]_{12} c_2 + c_1^*[(\Delta - t)g]_{12} L_2\Big)$$

Relation between Green functions:

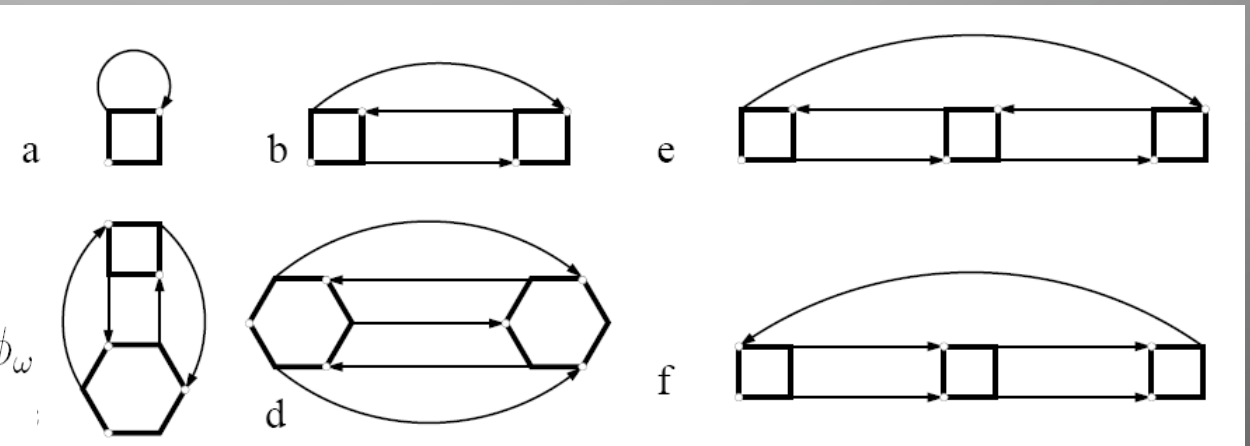
$$\tilde{G}_{12} = -\frac{\delta^2 F}{\delta L_2 \delta L_1^*}\bigg|_{L^* = L = 0}$$

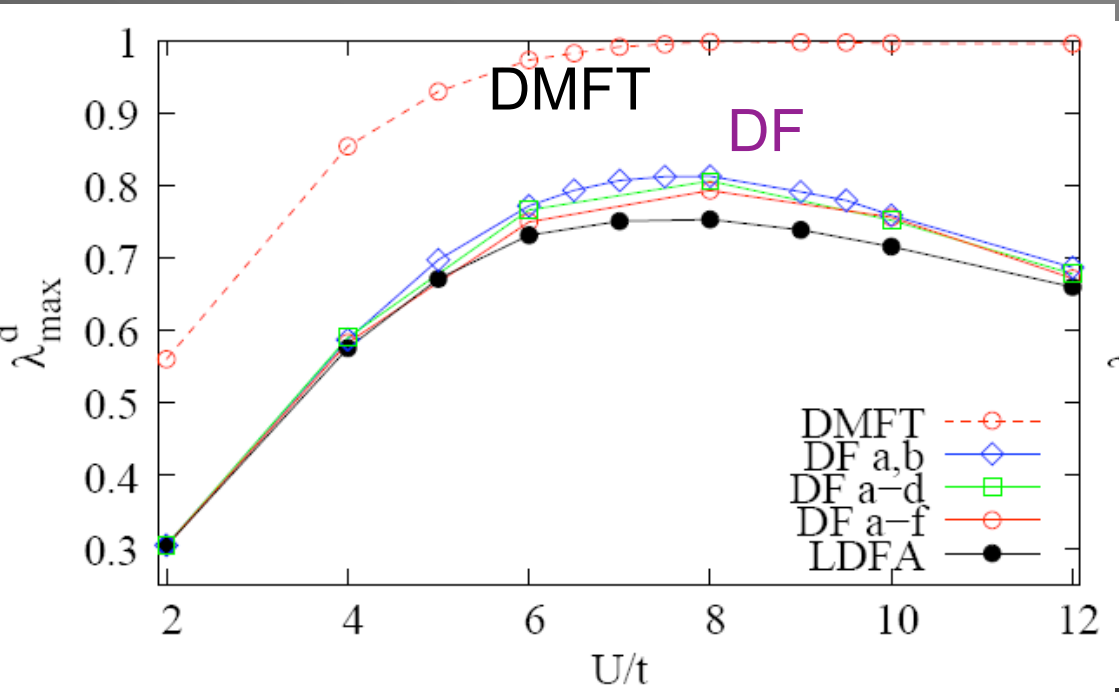
$$\tilde{G}_{12} = -[g(\Delta - t)g]_{12} + [g(\Delta - t)]_{11'} G_{1'2'} [(\Delta - t)g]_{2'2}$$

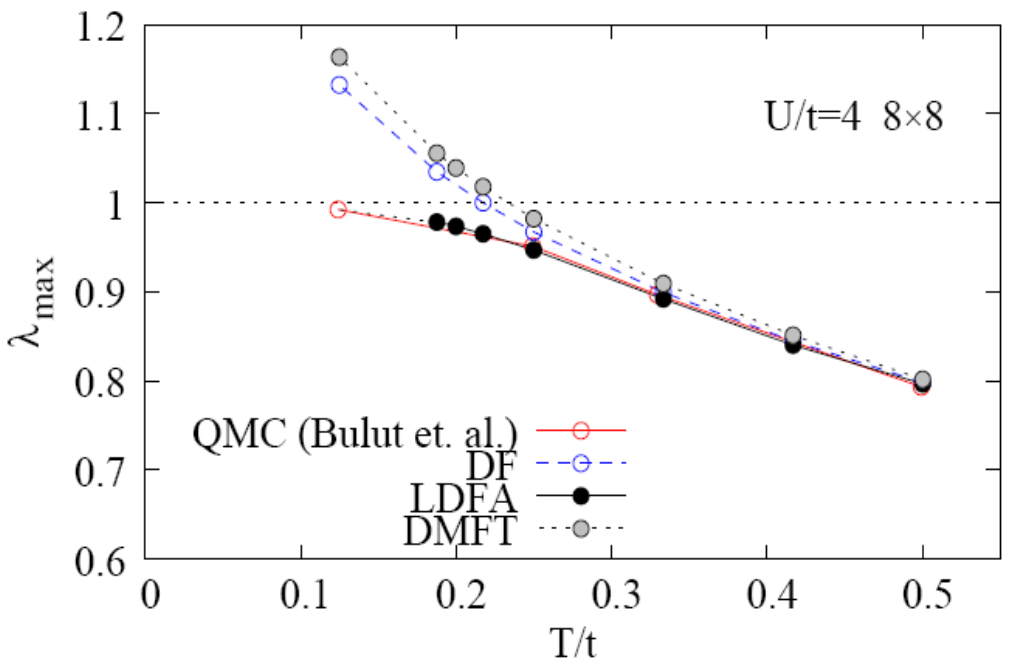
Convergence of Dual Fermions: 2d



$$-\frac{T}{N}\sum_{w'\mathbf{k}'}\Gamma^{d\,\mathrm{irr},s}_{\omega\omega'\Omega}\,G^d_{\omega'}(\mathbf{k}')\,G^d_{\omega'+\Omega}(\mathbf{k}'+\mathbf{q})\phi_{\omega'}=\lambda\phi_\omega$$

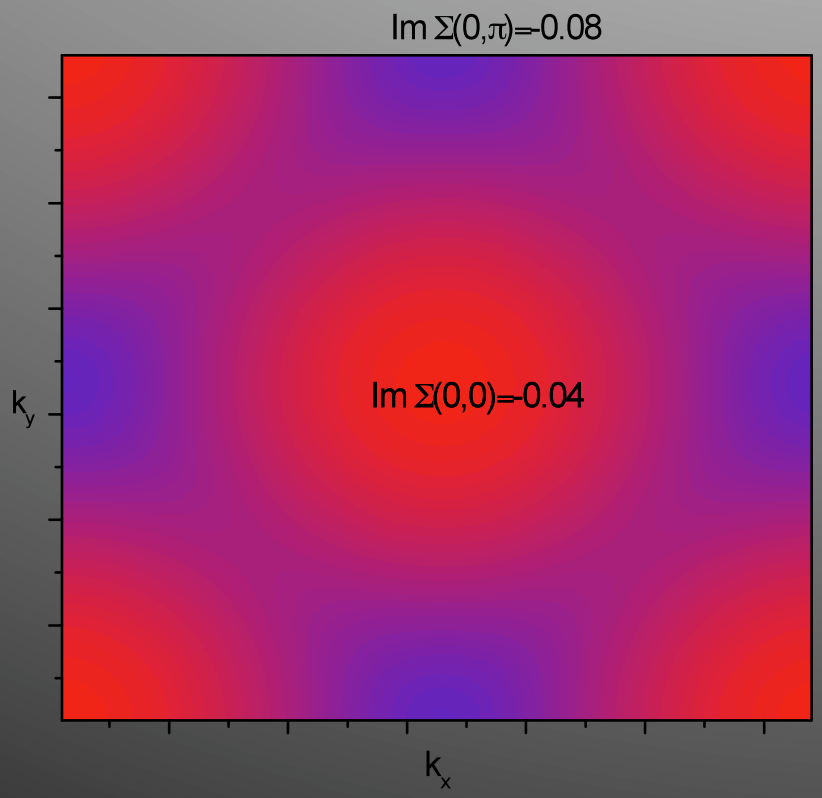




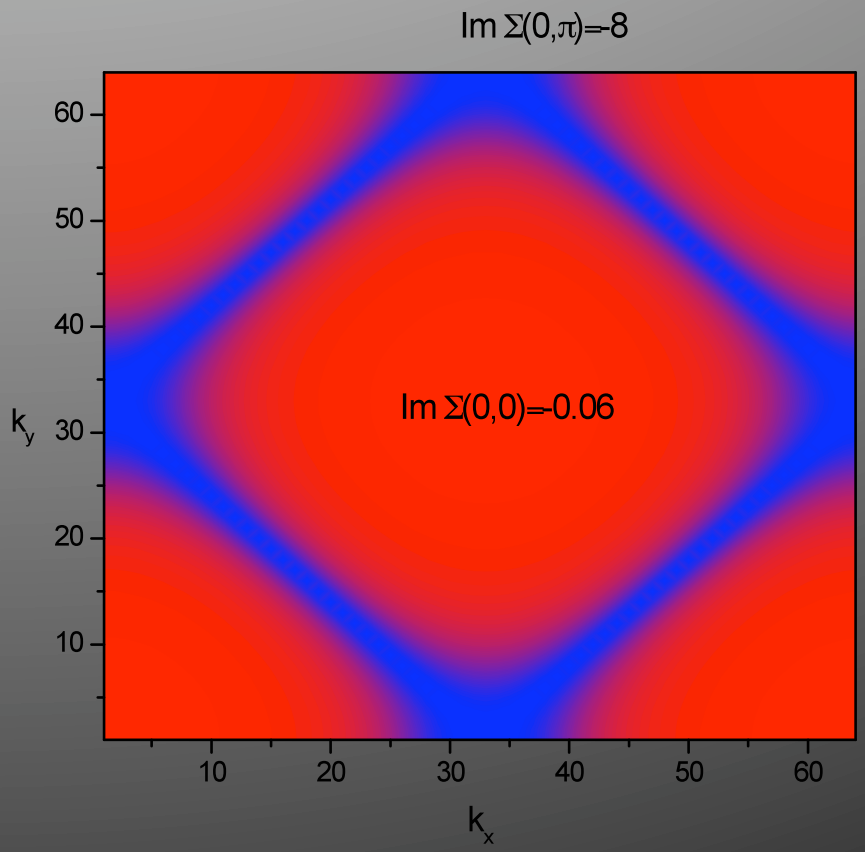


H. Hafermann, et al. PRL**102**, 206401 (2009)

ARPES: Im $\Sigma(k, \omega=0)$



U=1



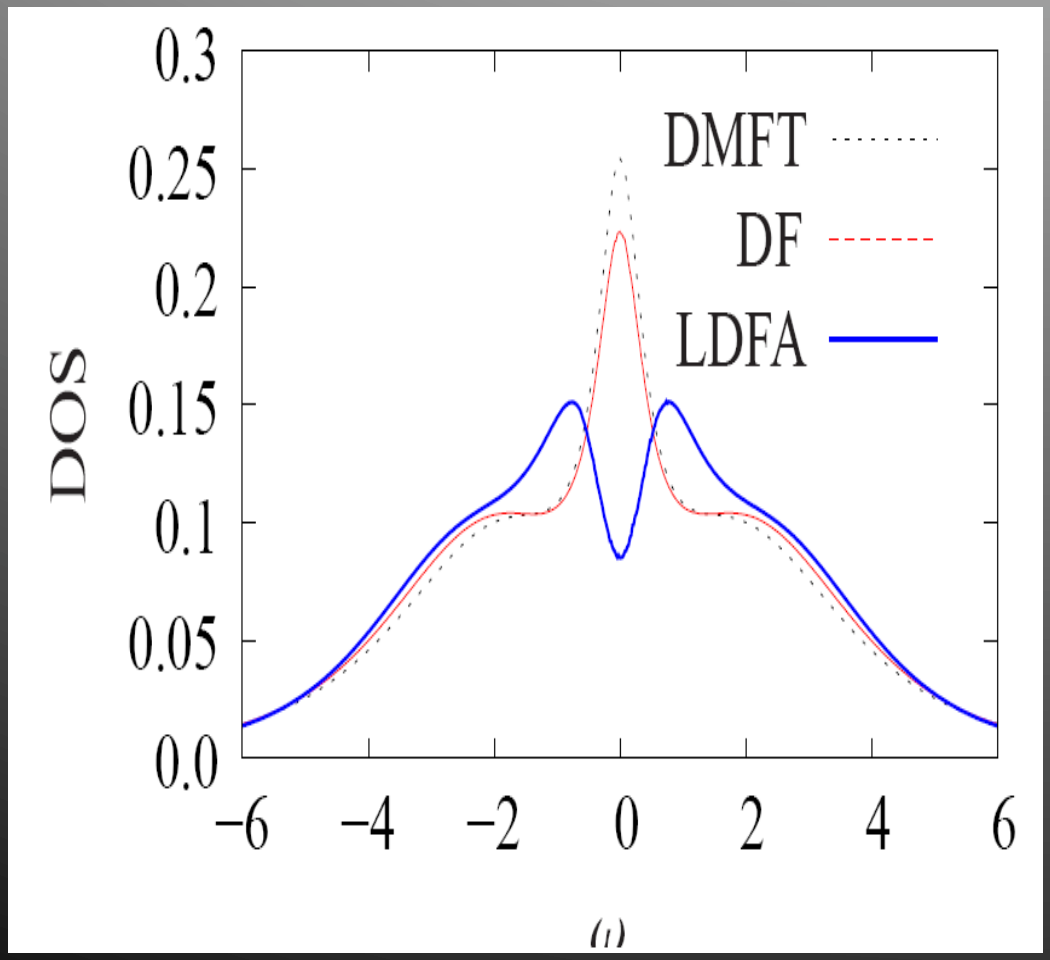
U=2

Hubbard model with $8t = 2, \beta = 20$ at half-filling.
Data for Im Σ_k at $\omega = 0$.

A. Rubtsov, et al, PRB **79**, 045133 (2009)

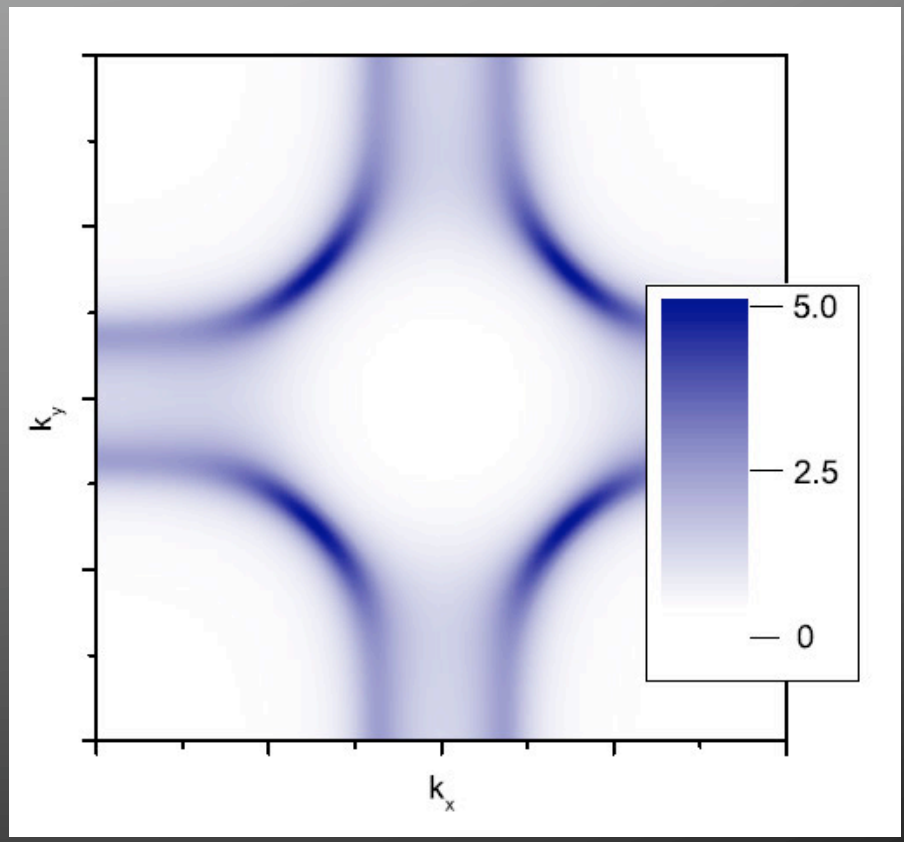
Pseudogap in HTSC: dual fermions

$$S[f,f^*] = \sum_{\omega k \sigma} g_\omega^{-2} \left((\Delta_\omega - \epsilon_k)^{-1} + g_\omega \right) f^*_{\omega k \sigma} f_{\omega k \sigma} + \sum_i V_i$$



n=1

H. Hafermann (Ladder-DF)



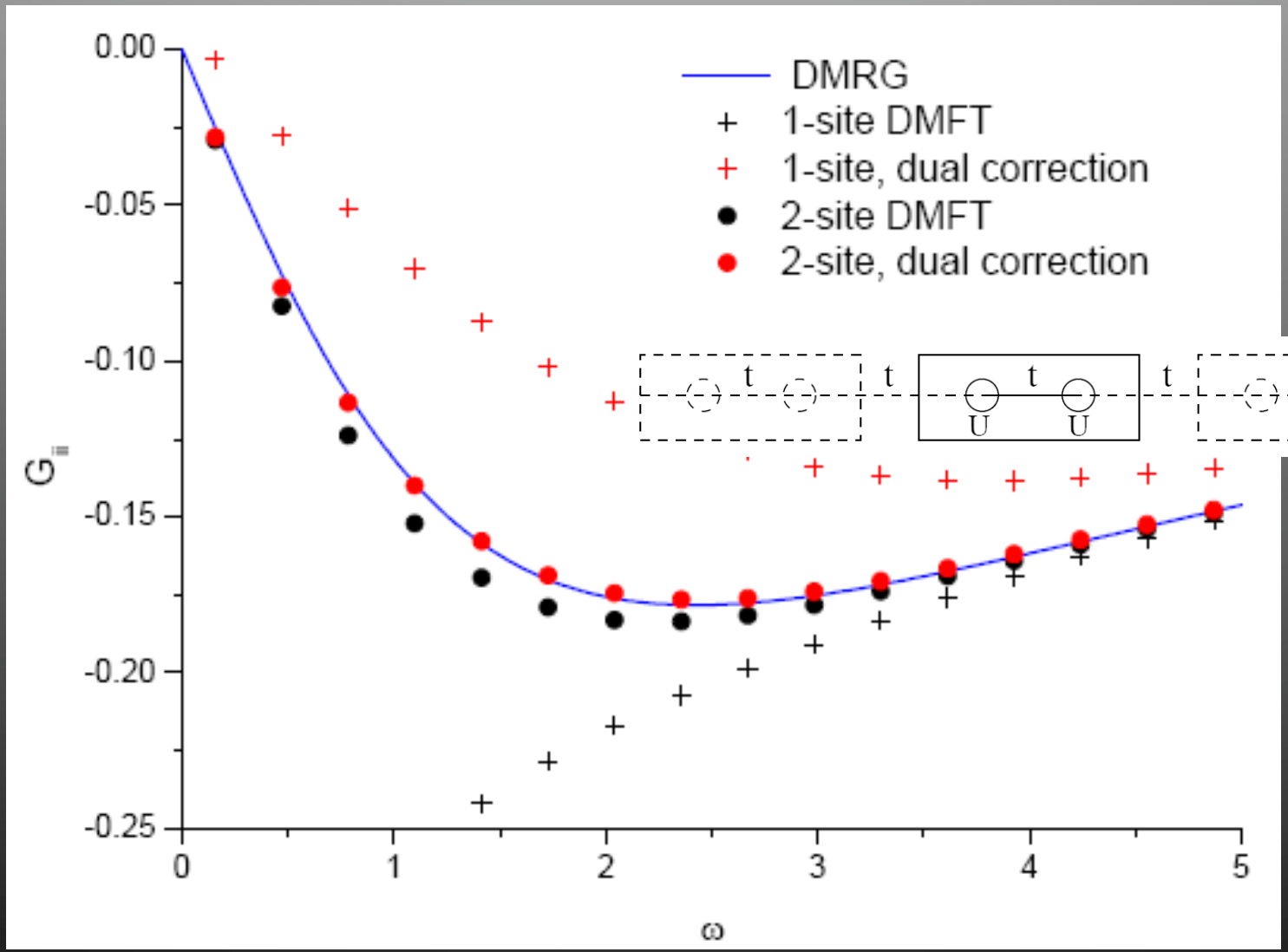
FS, n=0.85

A. Rubtsov (DF)

2d: U=W=2

Cluster Dual Fermions: 1d-test, n=1

1D Hubbard chain $U/t = 6$, $\beta = 10$, $\epsilon(\mathbf{k}) = -2t\cos(ka)$



H. Hafermann, et al. JETP Lett (2007), arXiv:0707.4022

Two-particle Green-Functions

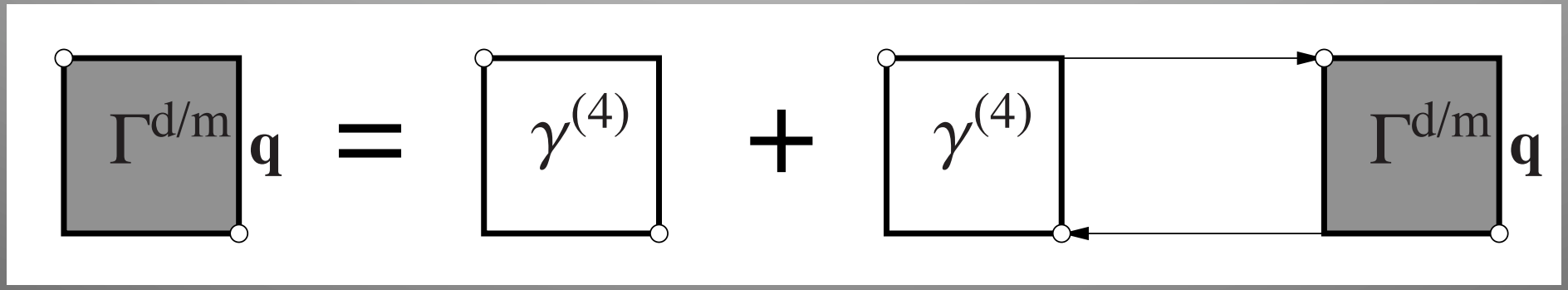
Exact relation between TPGF in real and dual space:

$$\left[\tilde{X} - \tilde{G} \otimes \tilde{G}\right]_{1234} = \left. \frac{\delta^4 F}{\delta L_4 \delta L_3 \delta L_2^* \delta L_1^*} \right|_{L^* = L = 0}$$

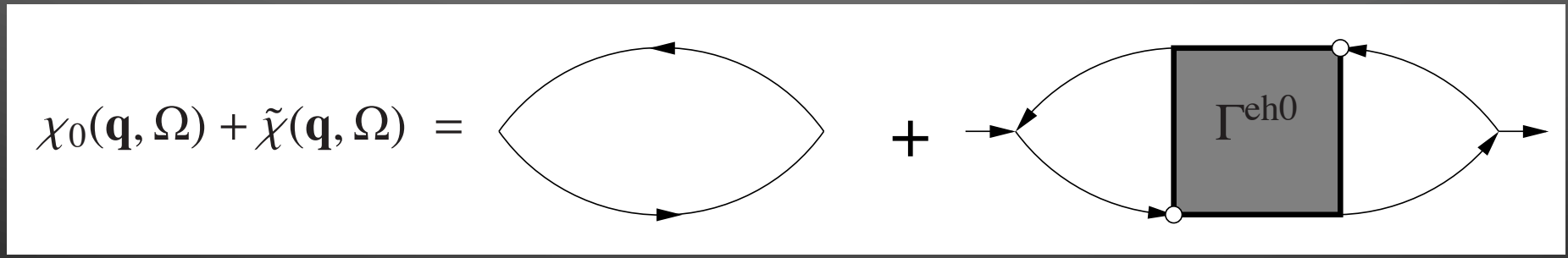
$$\left[\tilde{X} - \tilde{G} \otimes \tilde{G}\right]_{1234} =$$

$$[g(\Delta - t)]_{11'} [g(\Delta - t)]_{22'} [X - G \otimes G]_{1'2'3'4'} [(\Delta - t)g]_{3'3} [(\Delta - t)g]_{4'4}$$

TPGF: Bethe-Salpeter Equations

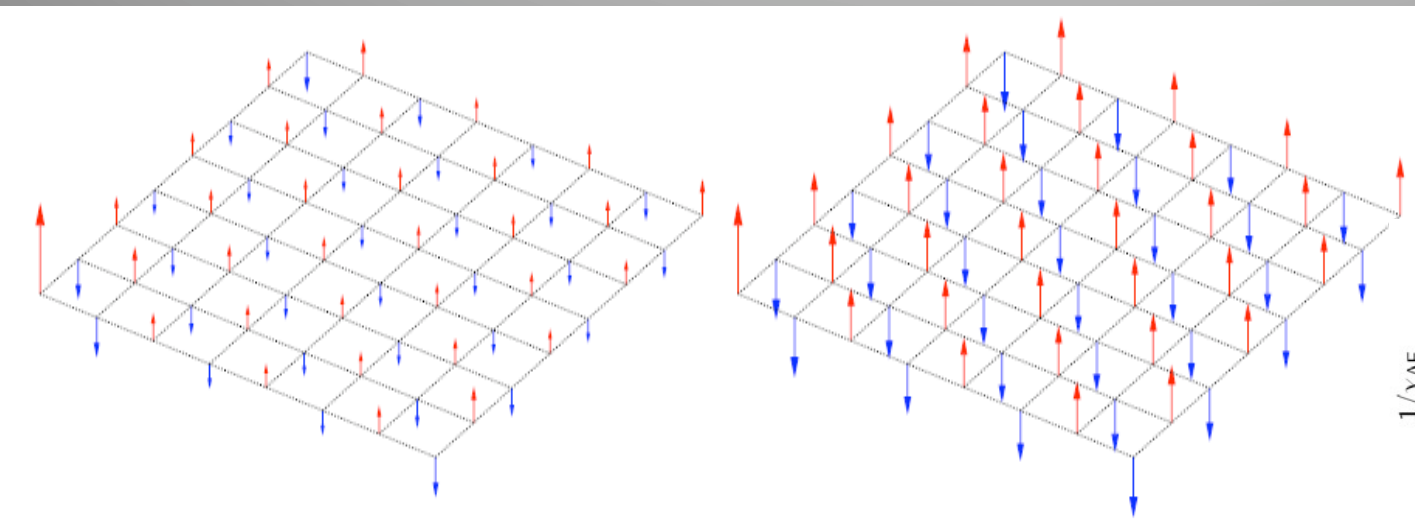


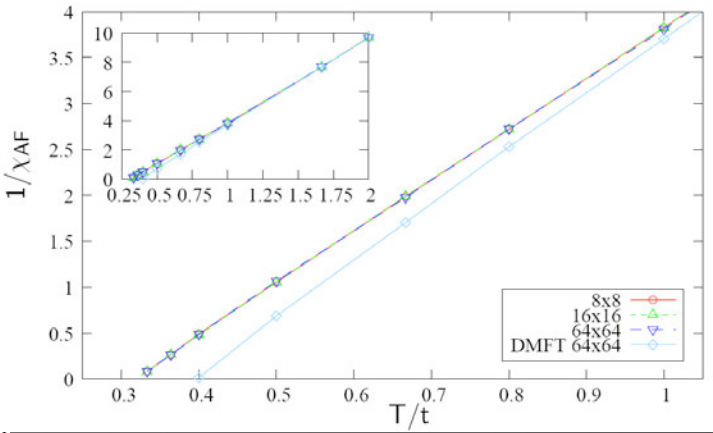
Non-local susceptibility with vertex corrections

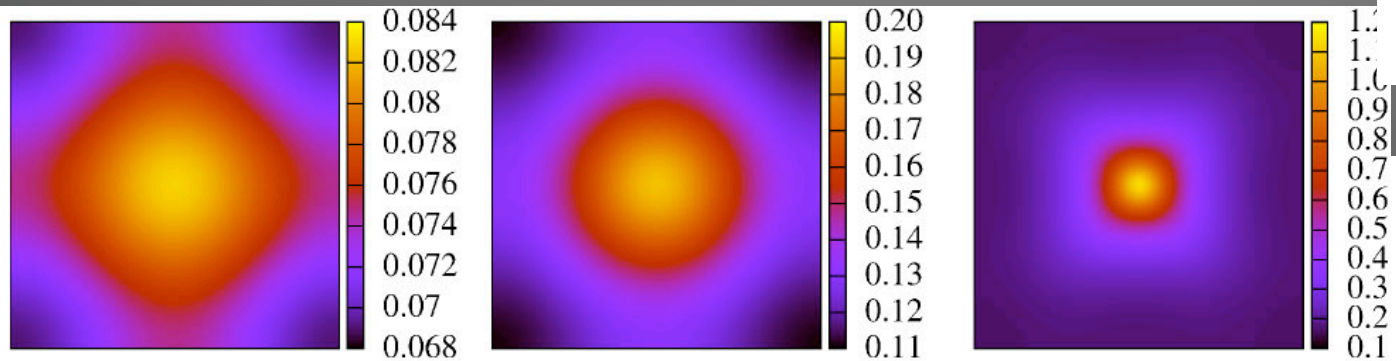


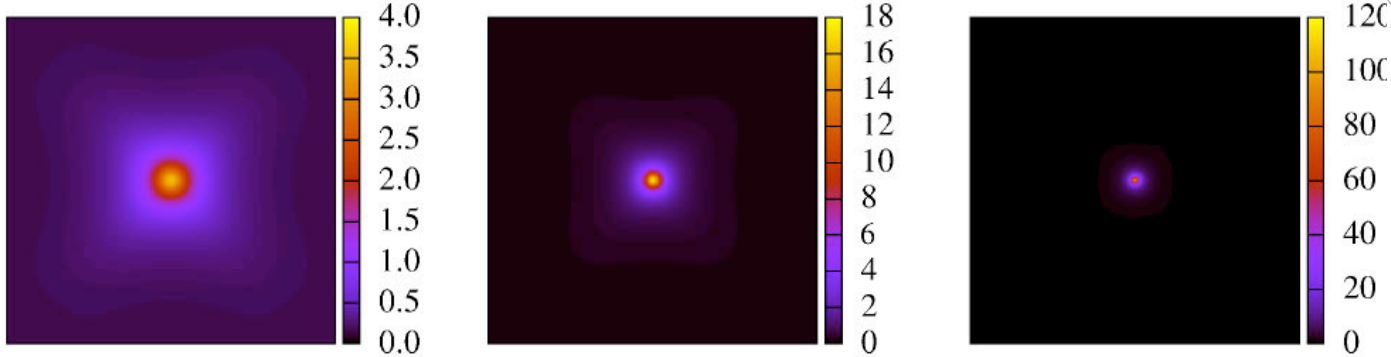
Susceptibility: 2d – Hubbard model

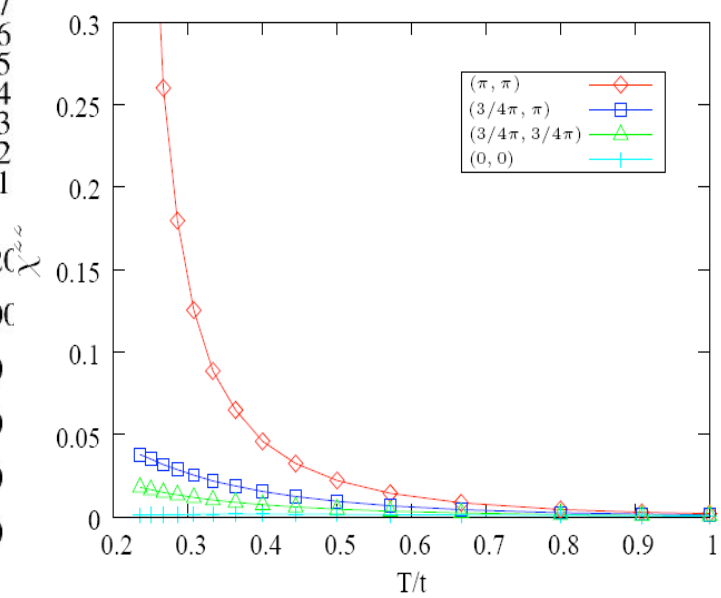
H. Hafermann











Summary

- Cluster DMFT can treat well short-range non-local correlations
- DF is an efficient scheme to describe long-range non-local correlation effects in solids