The Dynamic Cluster Approximation and its DCA$^+$ extension

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Outline

The dynamic cluster approximation

The DCA$^+$ method

Applications to the 2D Hubbard model

Discussion and concluding remarks

Brief (and incomplete) history

- 1989: Dynamical mean-field theory (DMFT)

  Metzner & Vollhardt, Müller-Hartmann

- 1998—2000: Dynamical cluster approximation

  Jarrell et al.

- 2001: Cellular DMFT

  Kotliar et al.

- 2000: Cluster perturbation theory (CPT)

  Sénéchal et al., Gros & Valenti '93

References

- Original DCA papers

  *Hettler, Tahvildar-Zadeh, Jarrell, Pruschke, Krishnamurthy, Phys. Rev. B **58**, R7475 (1998)*

  *Hettler, M. Mukherjee, Jarrell, Krishnamurthy, Phys. Rev. B **61**, 12739 (2000)*

- Quantum cluster theories (DCA and other cluster dynamical mean-field theories)

  *TAM, Jarrell, Pruschke, Hettler, Rev. Mod. Phys. **77**, 1027 (2005)*

- Continuous time QMC cluster/impurity solvers

  *Gull, Millis, Liechtenstein, Rubtsov, Troyer, Werner, Rev. Mod. Phys. **83**, 349 (2011).*

- The DCA$^+$ extension

  *Staar, TAM, Schulthess, Phys. Rev. B **88**, 115101 (2013)*
  *Staar, TAM, Schulthess, Phys. Rev. B **89**, 195133 (2014)*

Preliminaries

- Hubbard model

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

- Dispersion

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$$

Preliminaries

- Thermodynamic Green's function

$$G_{ij,\sigma} = -\langle T_\tau c_{i\sigma}(\tau) c^\dagger_{j\sigma} \rangle$$

$$G_{ij,\sigma}(i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n \tau} G_{ij,\sigma}(\tau)\,, \;\; \omega_n = (2n+1)\pi T$$

$$G_\sigma(\mathbf{k}, i\omega_n) = \frac{1}{N} \sum_{ij} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} G_{ij,\sigma}(i\omega_n)$$

Matsubara frequencies

Preliminaries

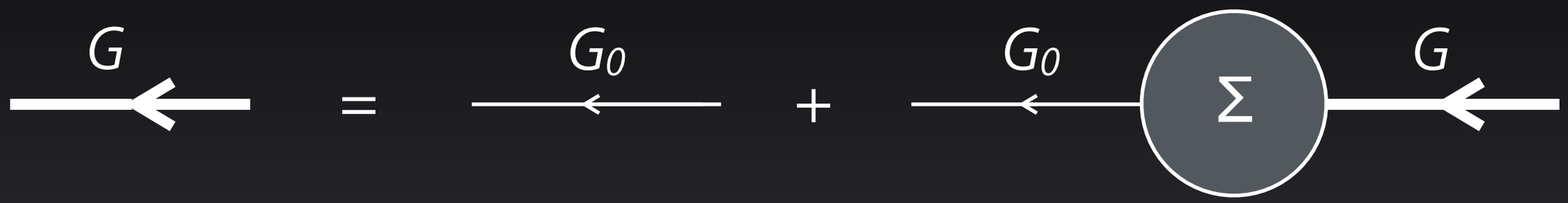
- Non-interacting (bare) Green's function

$$G_0(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \varepsilon_{\mathbf{k}}}$$

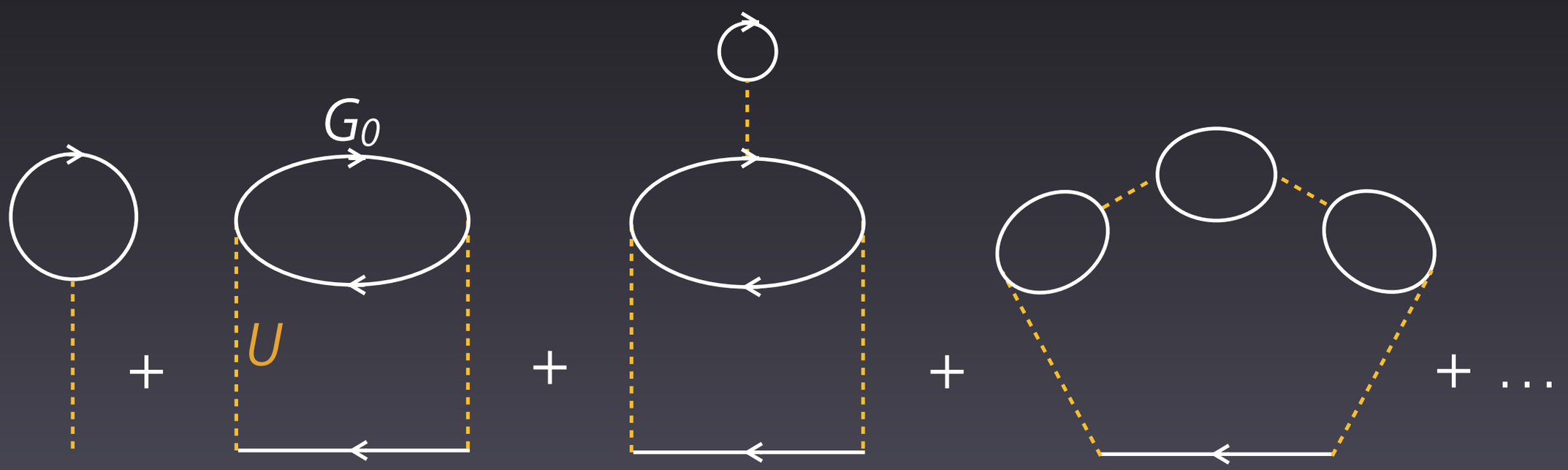
- Interacting Green's function and Dyson equation

$$\begin{aligned} G(\mathbf{k}, i\omega_n) &= G_0(\mathbf{k}, i\omega_n) + G_0(\mathbf{k}, i\omega_n)\Sigma(\mathbf{k}, i\omega_n)G(\mathbf{k}, i\omega_n) \\ &= \frac{1}{G_0^{-1}(\mathbf{k}, i\omega_n) - \Sigma(\mathbf{k}, i\omega_n)} \end{aligned}$$

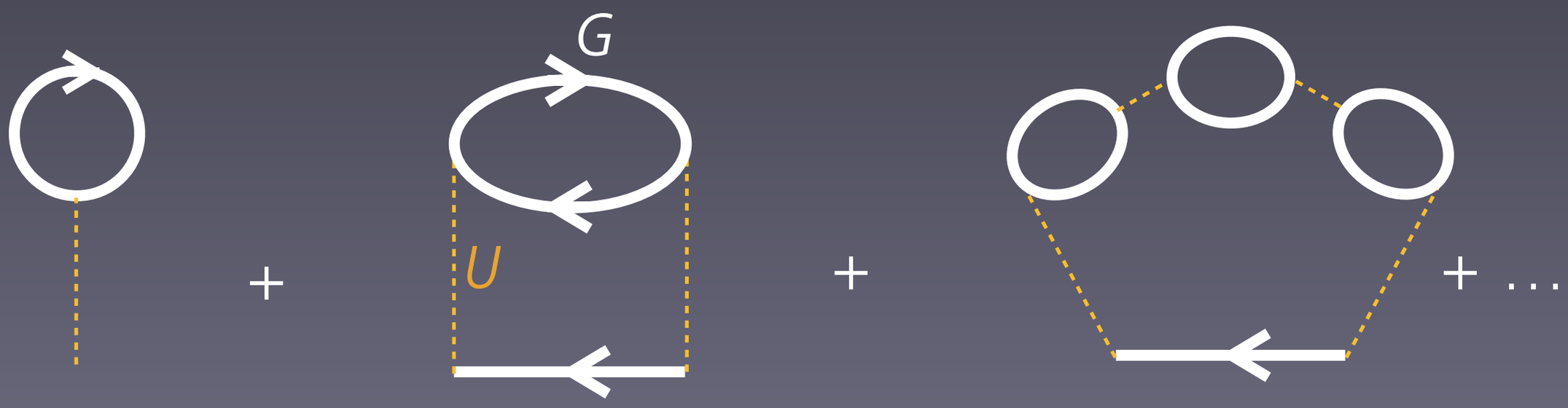
Self-energy



$\Sigma[G_0, U] =$



$\Sigma[G, U] =$



Preliminaries

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

- Action

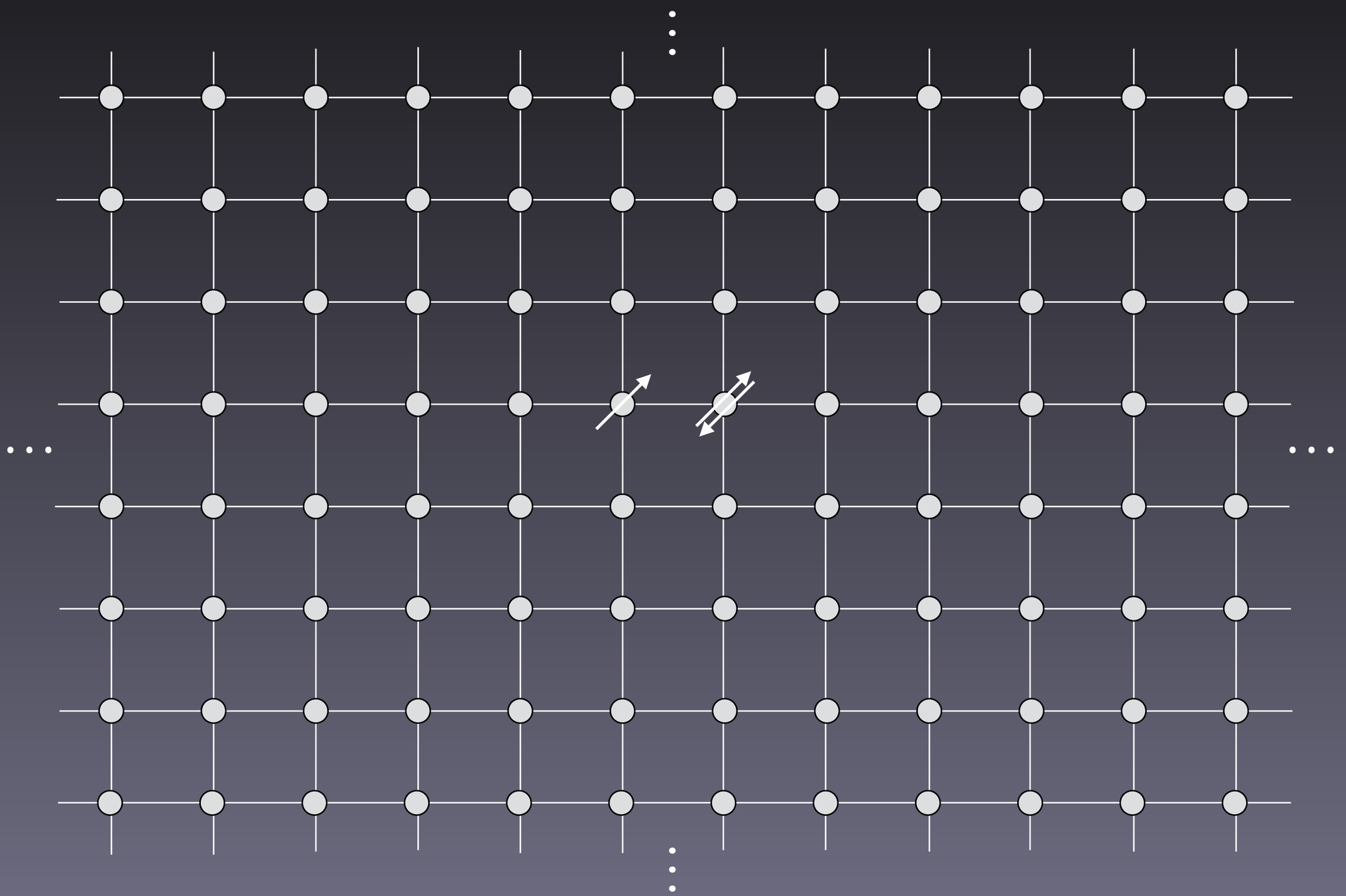
$$S[\phi^*, \phi] = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{k},\sigma} \phi^*_{\mathbf{k}\sigma}(\tau) G^{-1}_{0,\sigma}(\mathbf{k}, \tau - \tau') \phi_{\mathbf{k}\sigma}(\tau) + \\ + \int_0^\beta d\tau \sum_i U \phi^*_{i\uparrow}(\tau) \phi_{i\uparrow} \phi^*_{i\downarrow}(\tau) \phi_{i\downarrow}(\tau)$$

- Interacting Green's function

$$G_{c,\sigma}(\mathbf{k}, \tau - \tau') = \frac{1}{Z} \int \mathcal{D}[\phi^* \phi] \phi_{\mathbf{k}\sigma}(\tau) \phi^*_{\mathbf{k}\sigma}(\tau') e^{-S[\phi^*, \phi]}$$

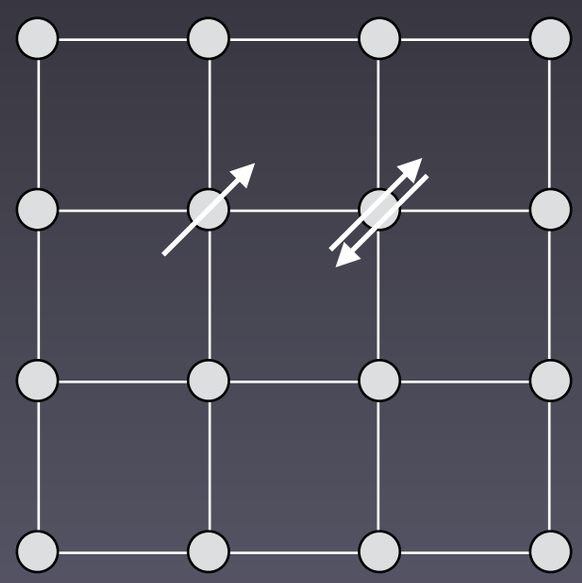
The Problem

4^N states



The finite size solution

4^{16} states



Determine exact Green's function/self-energy of *L* x *L* cluster

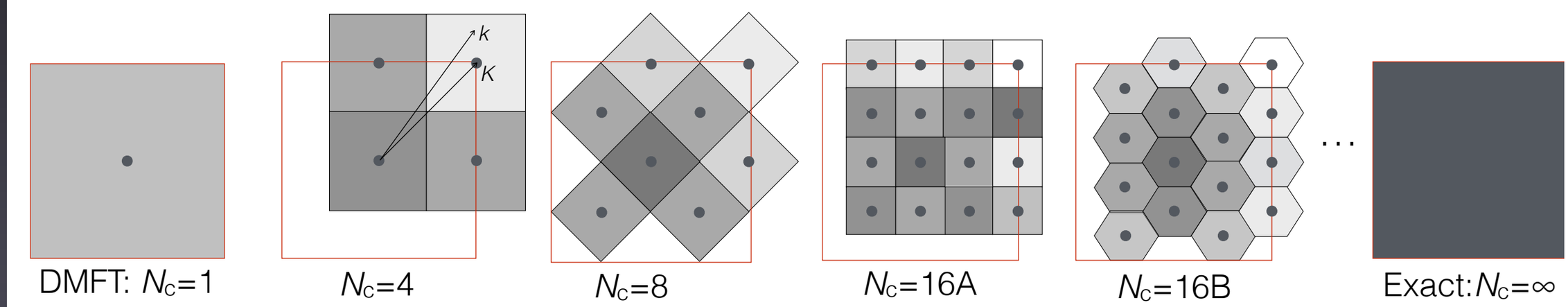
Dynamic Cluster Approximation (DCA)

Dynamic cluster approximation

General idea:

Represent bulk system by a reduced number of cluster degrees of freedom, and use coarse-graining to retain information about remaining degrees of freedom.

Coarse-graining of momentum space



$$\phi_{\mathbf{K}}(\mathbf{k}) = \begin{cases} 1, & \text{if } \mathbf{k} \text{ in patch } \mathbf{K}. \\ 0, & \text{otherwise.} \end{cases}$$

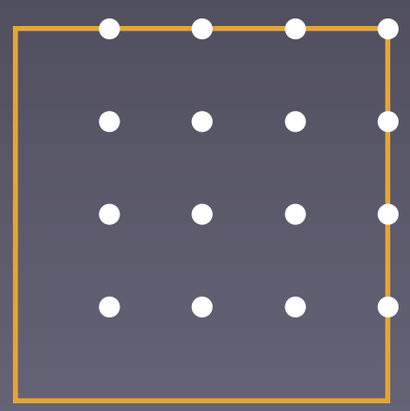
Momentum sums: $\sum_{\mathbf{k}} \rightarrow \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k})$

Basic assumption

Self-energy is short-ranged/weakly momentum dependent

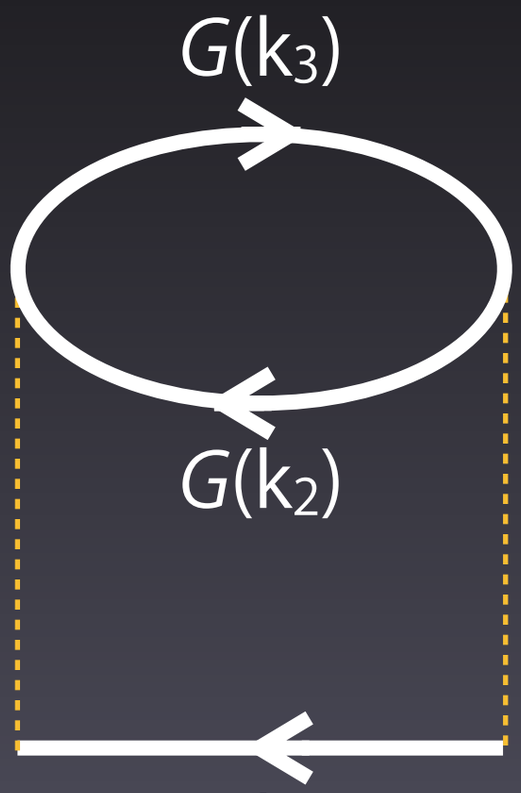
$$\Sigma(\mathbf{k}, i\omega_n) \simeq \Sigma_c(\mathbf{K}, i\omega_n)$$

and thus is well approximated on a coarse-grid of cluster ***K*** momenta



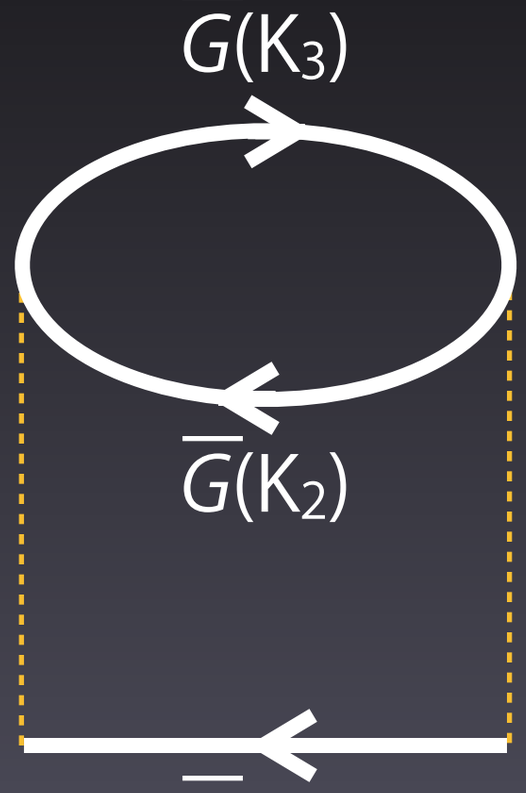
$$\Sigma^{DCA}(\mathbf{k}, i\omega_n) = \sum_{\mathbf{K}} \phi_{\mathbf{K}}(\mathbf{k}) \Sigma_c(\mathbf{K}, i\omega_n)$$

Coarse-graining



$$\delta(k_1 + k_2, k_3 + k) \rightarrow$$

$$\phi_{K_1}(k_1)\phi_{K_2}(k_2)\phi_{K_3}(k_3)\delta(K_1 + K_2, K_3 + K)$$



$$\bar{G}(\mathbf{K}) = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) G(\mathbf{k})$$

$$\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} G(\mathbf{k}_1)G(\mathbf{k}_2)G(\mathbf{k}_3)\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}} \longrightarrow \sum_{\mathbf{K}_1,\mathbf{K}_2,\mathbf{K}_3} \bar{G}(\mathbf{K}_1)\bar{G}(\mathbf{K}_2)\bar{G}(\mathbf{K}_3)\delta_{K_1+K_2,K_3+K}$$

$$\Sigma(\mathbf{k}) = \Sigma[G(\mathbf{k}), U] \longrightarrow \Sigma(\mathbf{k}) = \Sigma[\bar{G}(\mathbf{k}), U]$$

DCA self-consistency

$$\Sigma^{DCA}(\mathbf{k}, i\omega_n) = \sum_{\mathbf{K}} \phi_{\mathbf{K}}(\mathbf{k}) \Sigma_c(\mathbf{K}, i\omega_n)$$

$$\bar{G}(\mathbf{K}, i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) G(\mathbf{k}, i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) \frac{1}{i\omega_n - \varepsilon_{\mathbf{k}} + \mu - \Sigma^{DCA}(\mathbf{k}, i\omega_n)}$$

$$\Sigma_c(\mathbf{K}, i\omega_n) = \Sigma[\bar{G}(\mathbf{K}, i\omega_n), U]$$

DCA algorithm

(2) Coarse-graining

$$\bar{G}(\mathbf{K}, i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) \frac{1}{i\omega_n - \varepsilon_{\mathbf{k}} + \mu - \Sigma^{DCA}(\mathbf{k}, i\omega_n)}$$

(1) DCA self-energy

$$\Sigma^{DCA}(\mathbf{k}, i\omega_n) = \sum_{\mathbf{K}} \phi_{\mathbf{K}}(\mathbf{k}) \Sigma_c(\mathbf{K}, i\omega_n)$$

Iterate to self-consistency:

$$\Sigma_c^{\text{new}} = \Sigma_c^{\text{old}}$$

(3) Bare cluster propagator

$$\mathcal{G}_0(\mathbf{K}, i\omega_n) = \left[\bar{G}^{-1}(\mathbf{K}, i\omega_n) + \Sigma_c(\mathbf{K}, i\omega_n)\right]^{-1}$$

(4) Cluster solver

$$S_c[\phi^*, \phi] = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{K},\sigma} \phi^*_{\mathbf{K}\sigma}(\tau) \mathcal{G}^{-1}_{0,\sigma}(\mathbf{K}, \tau - \tau') \phi_{\mathbf{K}\sigma}(\tau) + \int_0^\beta d\tau \sum_i U \phi^*_{i\uparrow}(\tau) \phi_{i\uparrow} \phi^*_{i\downarrow}(\tau) \phi_{i\downarrow}(\tau)$$

$$\Sigma_c(\mathbf{K}, i\omega_n) = \Sigma[\mathcal{G}_0(\mathbf{K}, i\omega_n), U]$$

DCA vs. finite size

$$\Sigma_c(\mathbf{K}, i\omega_n) = \Sigma[\mathcal{G}_0(\mathbf{K}, i\omega_n), U]$$

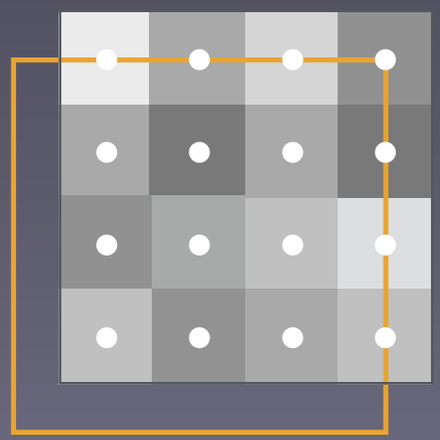
$$\mathcal{G}_0(\mathbf{K}, i\omega_n) = \frac{1}{i\omega_n - \bar{\varepsilon}_{\mathbf{K}} + \mu - \Gamma(\mathbf{K}, i\omega_n)}$$

$$\bar{\varepsilon}_{\mathbf{K}} = N_c/N \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) \varepsilon_{\mathbf{k}}$$

$$\Gamma(\mathbf{K}, i\omega_n) = \frac{\frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) \delta t^2_{\mathbf{K}}(\mathbf{k}) G(\mathbf{k}, i\omega_n)}{1 + \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) \delta t_{\mathbf{K}}(\mathbf{k}) G(\mathbf{k}, i\omega_n)}$$

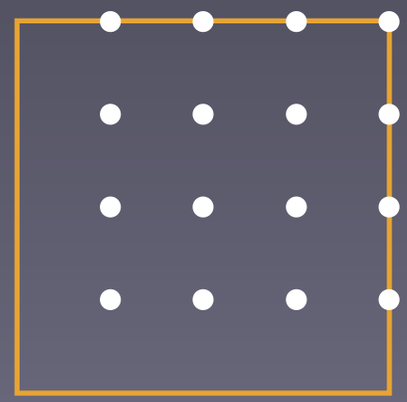
$$\delta t_{\mathbf{K}}(\mathbf{k}) = \varepsilon_{\mathbf{k}} - \bar{\varepsilon}_{\mathbf{K}}$$

Embedded cluster



$$\mathcal{G}_0(\mathbf{K}, i\omega_n) = \frac{1}{i\omega_n - \varepsilon_{\mathbf{K}} + \mu}$$

Isolated cluster



QMC cluster solver

- Excellent review of continuous-time QMC solvers

  E. Gull et al., Continuous-time Monte Carlo methods for quantum impurity models. Rev. Mod. Phys. 83, 349–404 (2011).

- Interaction expansion, hybridization expansion and auxiliary field algorithms

- Continuous-time auxiliary field (CT-AUX) QMC

  Employs auxiliary field decoupling of interaction term, then performs Monte Carlo sampling of expansion in interaction

CT-AUX QMC

- Auxiliary field decomposition

$$1-\frac{\beta U}{K}\sum_i\left[n_{i\uparrow}n_{i\downarrow}-\frac{1}{2}(n_{i\uparrow}+n_{i\downarrow})\right]=\frac{1}{2N_c}\sum_{i,s_i=\pm1}e^{\gamma s_i(n_{i\uparrow}-n_{i\downarrow})}\;;\quad\cosh(\gamma)=1+\frac{U\beta N_c}{2K}$$

- Partition function

$$Z=\sum_{k=0}^{\infty}\sum_{s_1\ldots s_k=\pm1}\int_0^\beta d\tau_1\ldots\int_{\tau_{k-1}}^\beta d\tau_k\left(\frac{K}{2\beta N_c}\right)^k Z_k(\{x,\tau,s\}_k)$$

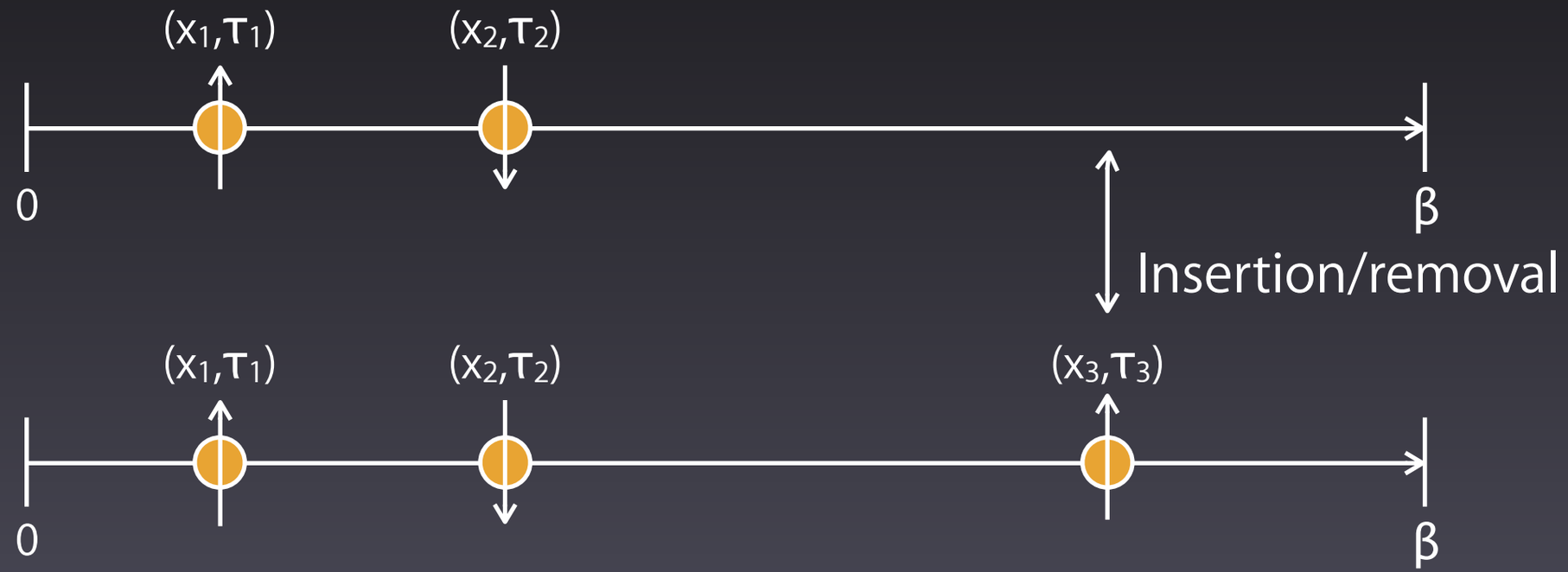
- Sum over expansion orders

$$Z_k(\{x,\tau,s\}_k)=Z_0\prod_\sigma\det N_\sigma^{-1}(\{x,\tau,s\}_k)\;;\;[N_\sigma^{-1}]_{ij}=e^{\gamma(-1)^\sigma s_i}\delta_{ij}-\mathcal{G}_{0,\sigma}(x_i,\tau_i;x_j,\tau_j)(e^{\gamma(-1)^\sigma s_i}-\delta_{ij})$$

- Monte Carlo sampling space

QMC updates

Insertion and removal updates



Probability for updating configuration x to x'

$$R_{x\to x'} = \min(1, R)\,;\; R = \frac{K}{k+1}\prod_{\sigma}\frac{\det \mathbf{N}_{\sigma}^{-1}(\{x',\tau',s'\})}{\det \mathbf{N}_{\sigma}^{-1}(\{x,\tau,s\})}$$

Measurement of Green's function

$$G_{pq}(\tau,\tau') = \frac{1}{Z}\sum_{k=0}^{\infty}\sum_{s_1\ldots s_k=\pm 1}\int_0^{\beta} d\tau_1 \ldots \int_{\tau_{k-1}}^{\beta} d\tau_k \left(\frac{K}{2\beta N_c}\right)^k Z_k(\{x,\tau,s\}_k)\tilde{G}_{pq}^{\{x,\tau,s\}_k}(\tau,\tau')$$

$$\tilde{G}_{pq}(\tau,\tau') = [\mathbf{N}\mathcal{G}_0]_{pq}$$

Sign problem

- Weights of configurations can be negative

$$A = \frac{1}{Z}\int dx\, A(x)p(x) = \frac{1}{Z}\frac{\int dx\, A(x)|p(x)|sgn(x)}{\int dx\, sgn(x)|p(x)|} = \frac{\langle A\rangle_{|p|}}{\langle sgn\rangle_{|p|}}$$

- Average sign

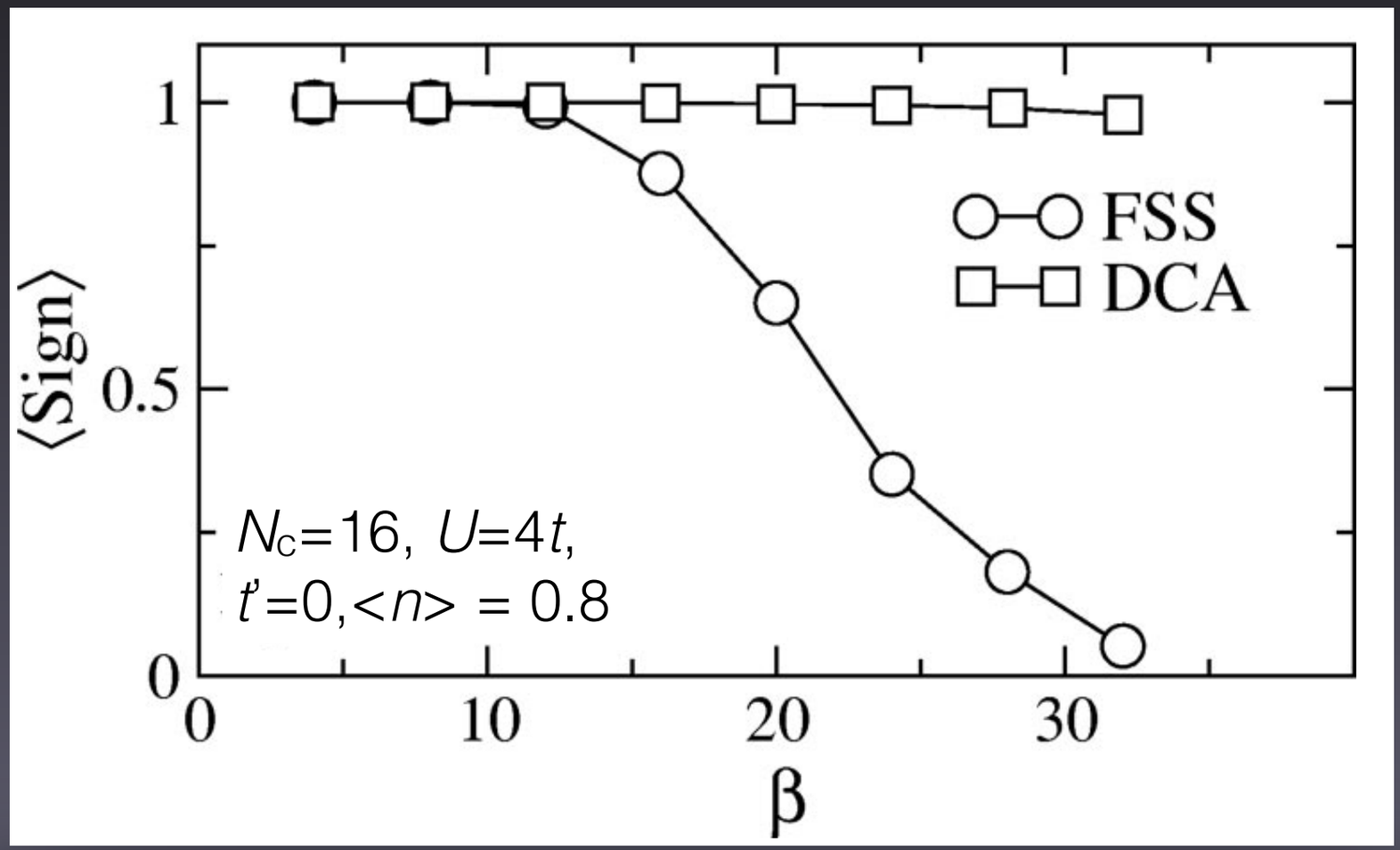
$$\langle sgn\rangle = \frac{\int dx\, sgn(x)|p(x)|}{\int dx\, |p(x)|} = \frac{Z}{Z_{|p|}}$$

- Ratio of Z and $Z_{|p|}$ of "bosonic" system with positive weights

$$\frac{Z}{Z_{|p|}} = \exp(-\beta\Delta F)$$

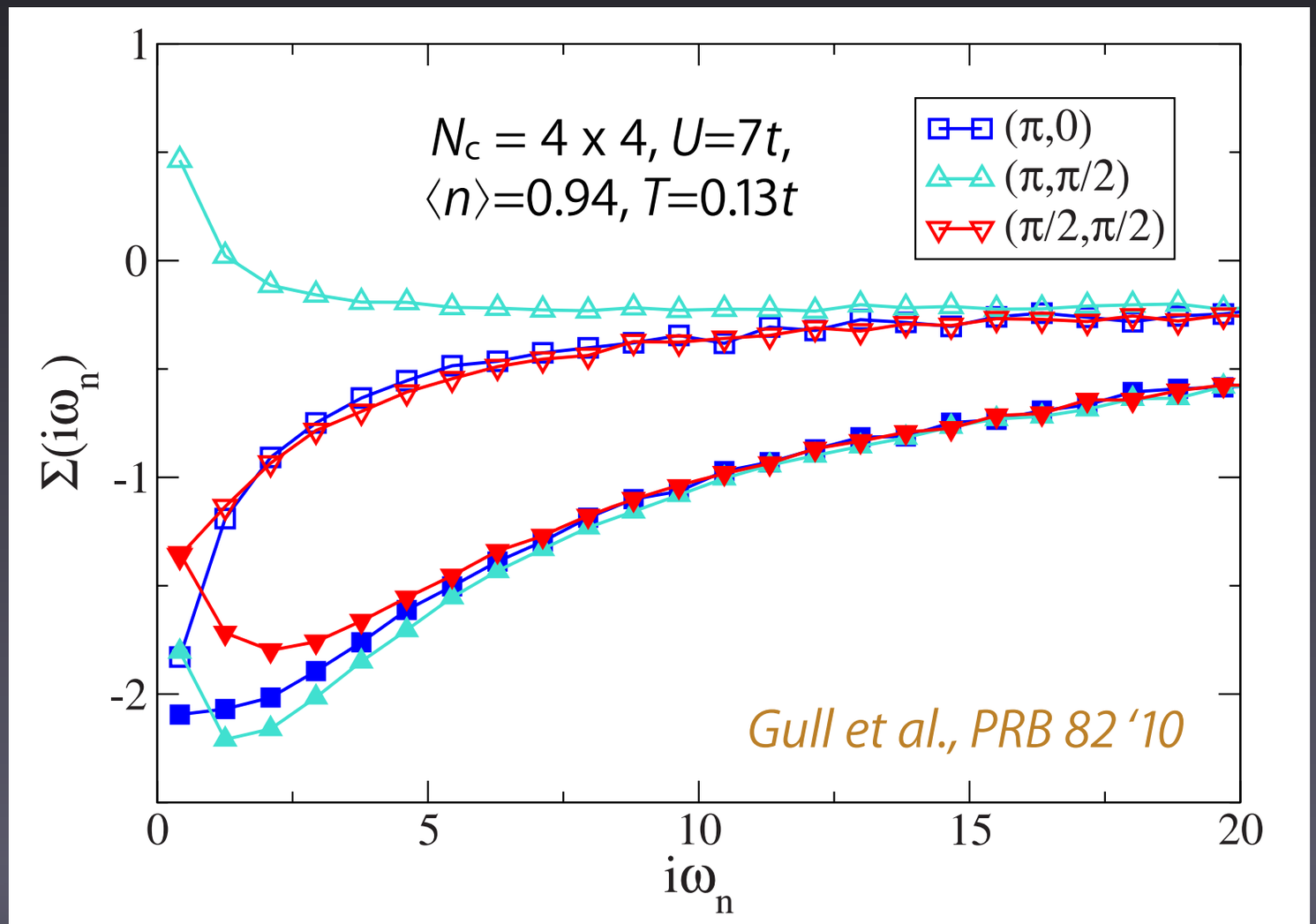
- Average sign decreases exponentially with system size, inverse temperature and U and leads to exponential statistical errors.

Fermion sign problem



DCA/QMC has much weaker sign problem

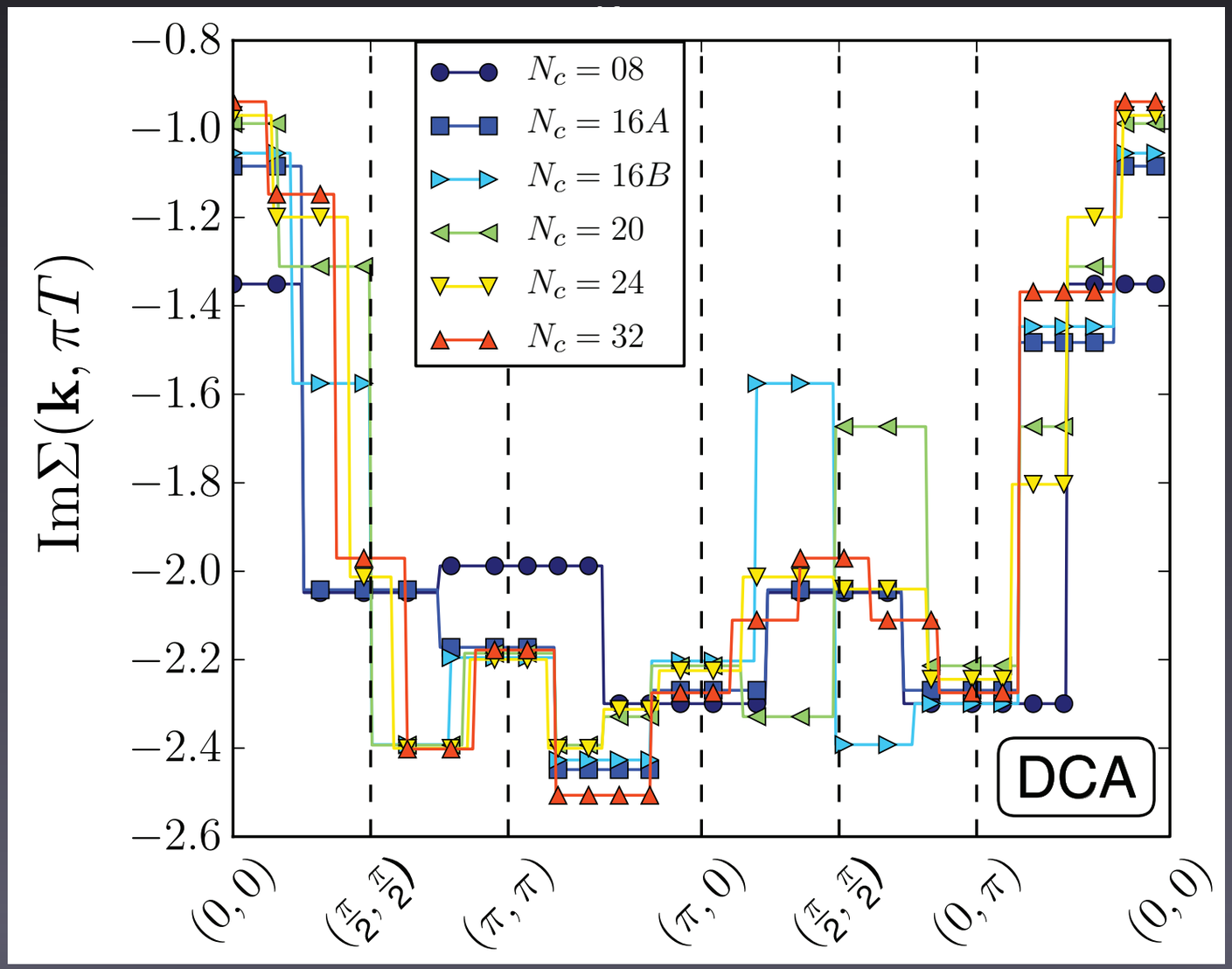
Typical DCA result for self-energy



Strong momentum dependence in "pseudogap" region

DCA self-energy

$$\Sigma^{DCA}(\mathbf{k}, i\omega_n) = \sum_{\mathbf{K}} \phi_{\mathbf{K}}(\mathbf{k}) \Sigma_c(\mathbf{K}, i\omega_n)$$



Jump discontinuities and cluster shape/size dependence

Calculation of response functions (susceptibilities)

- Two approaches

  1. Apply symmetry breaking field and calculate "anomalous" Green's function. E.g. for s-wave superconductivity

$$F_{ij}(\tau) = -\langle T_\tau c_{i\uparrow}(\tau) c_{j\downarrow}(0)\rangle \; ; \quad P_s = \left.\frac{\partial \Delta_s}{\partial \Psi}\right|_{\Psi=0} \; ; \quad \Delta_s = T/N \sum_{\mathbf{k},\omega_n} F(\mathbf{k}, i\omega_n)$$

  2. Calculate susceptibility from two-particle correlation function

$$P_s = \int_0^\beta d\tau \langle \Delta_s(\tau) \Delta_s^\dagger(0)\rangle$$

DCA is "thermodynamically consistent" $\longrightarrow$ two approaches give same result.

Calculation of 2-particle response functions

- Pair-field susceptibility

$$P_\varphi(T) = \int_0^\beta d\tau \langle \Delta_\varphi(\tau)\Delta_\varphi^\dagger(0)\rangle\,; \quad \Delta_\varphi^\dagger = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} g_\varphi(\mathbf{k}) c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger\,;$$

$$g_{d_{x^2-y^2}}(\mathbf{k}) = \cos k_x - \cos k_y$$

- Two-particle Green's functon

$$G_{2,\sigma_1\ldots\sigma_4}(x_1, x_2; x_3, x_4) = -\langle T_\tau c_{\sigma_1}(x_1) c_{\sigma_2}(x_2) c_{\sigma_3}^\dagger(x_3) c_{\sigma_4}^\dagger(x_4)\rangle$$

- Bethe-Salpeter equation $k = (\mathbf{k}, i\omega_n)\,; q = (\mathbf{q}, i\omega_m)$

$$G_2(k, -k+q, -k'+q, k') = G_\uparrow(k) G_\downarrow(-k+q)\delta_{k,k'} - \frac{T}{N}\sum_{k''} G_\uparrow(k) G_\downarrow(-k+q)$$

$$\times\, \Gamma_{pp}(k, -k+q, -k''+q, k'') G_2(k'', -k''+q, -k'+q, k')$$

Irreducible vertex function

DCA approximation of irreducible vertex

- Cluster approximation

$$\Gamma_\alpha(k,k') = \sum_{\mathbf{K},\mathbf{K}'} \phi_{\mathbf{K}}(\mathbf{k}) \Gamma_{c,\alpha}(K,K') \phi_{\mathbf{K}'}(\mathbf{k}')$$

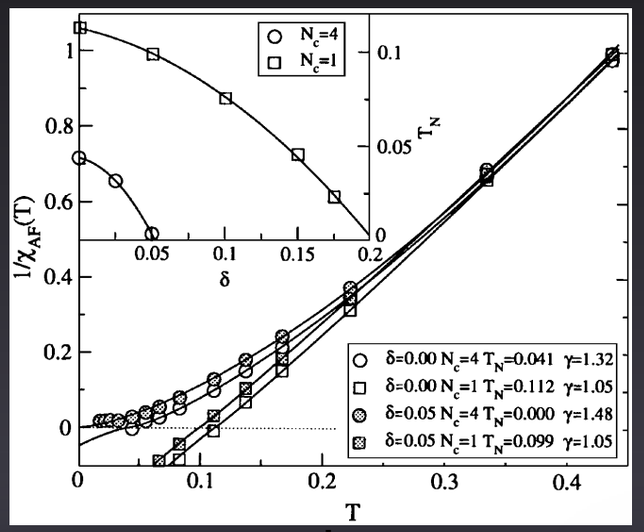
- Bethe-Salpeter equation on cluster

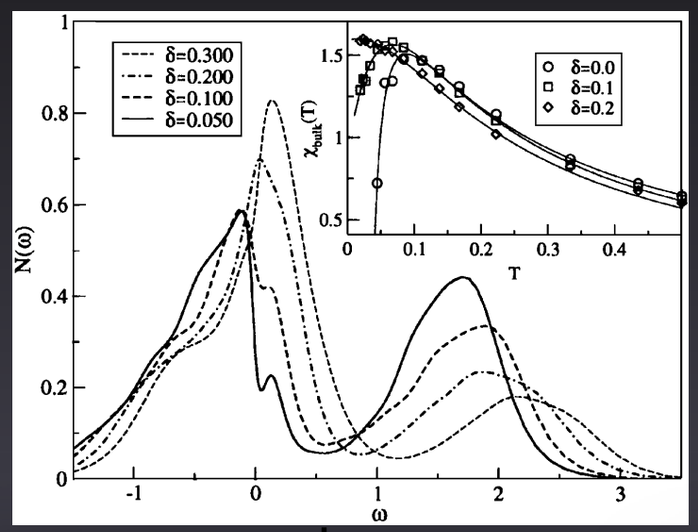
$$G_{2,c}(K,K') = G_{c,\uparrow}(K) G_{c,\downarrow}(-K) \delta_{K,K'} - \frac{T}{N} \sum_{K''} G_{c,\uparrow}(K) G_{c,\downarrow}(-K)$$
$$\times \Gamma_{c,pp}(K,K'') G_{2,c}(K'',K')$$

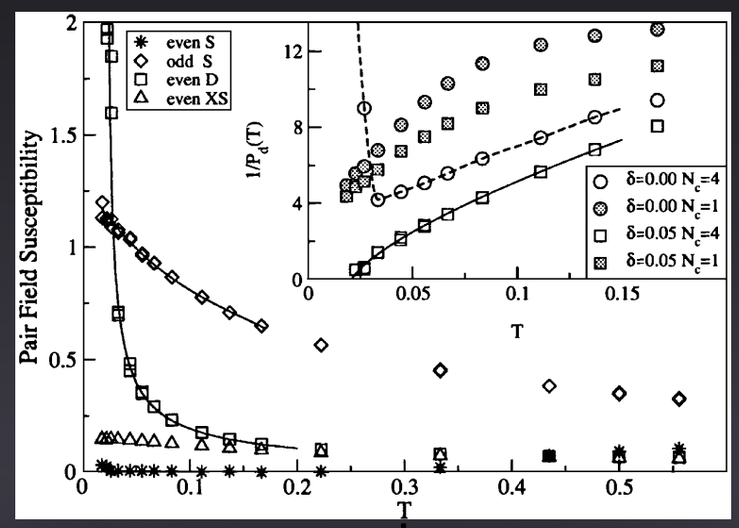
- Determine cluster irreducible vertex

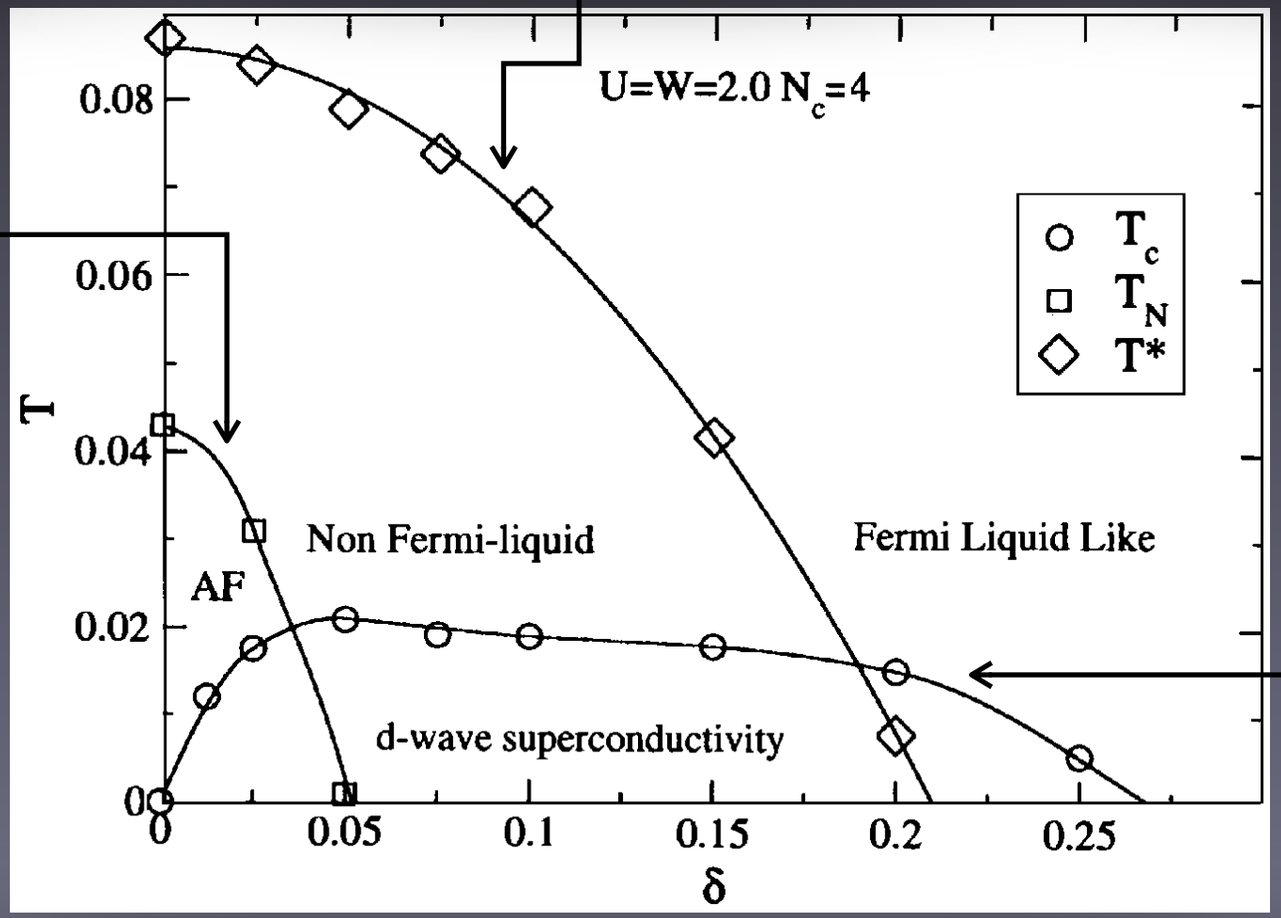
$$\mathbf{\Gamma}_{c,pp} = -\frac{N}{T} \left[[\mathbf{G}^0_{2,c}]^{-1} - [\mathbf{G}_{2,c}]^{-1} \right]$$

Example: Phase diagram of 2 x 2 cluster









Jarrell, TAM et al., EPL '01

Bethe-Salpeter eigenvalues and eigenfunctions

- Eigenvalue equation in particle-particle channel

$$-\frac{T}{N}\sum_{k'}\Gamma_{pp}(k,k')G_{\uparrow}(k')G_{\downarrow}(-k')g_{\alpha}(k') = \lambda_{\alpha}g_{\alpha}(k)$$

- Relation to 2-particle Green's function

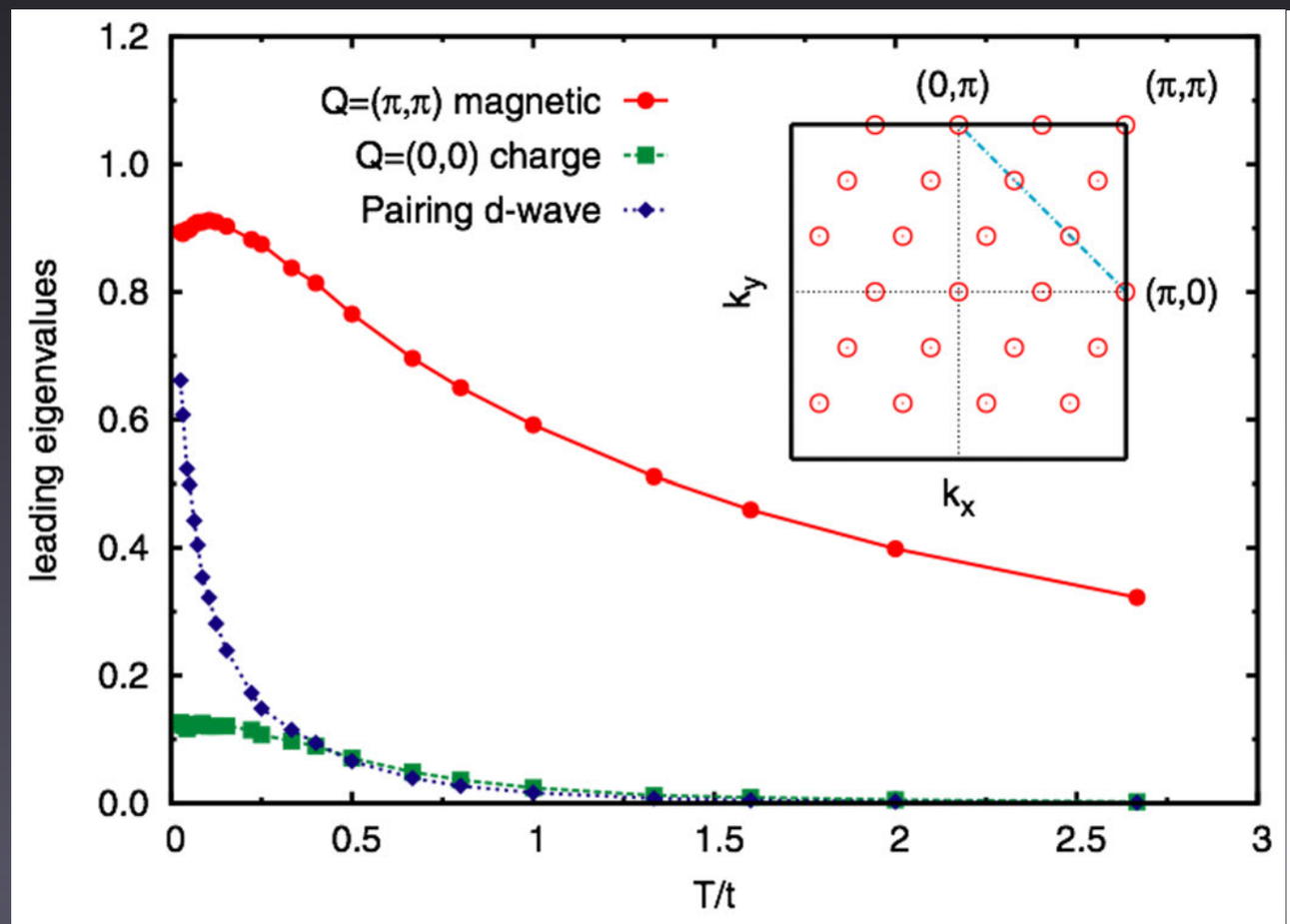
$$G_{2,pp}(k,k') = \sum_{\alpha} G_{\uparrow}(k)G_{\downarrow}(-k)\frac{g_{\alpha}(k)g^{*}_{\alpha}(k')}{1-\lambda_{\alpha}}$$

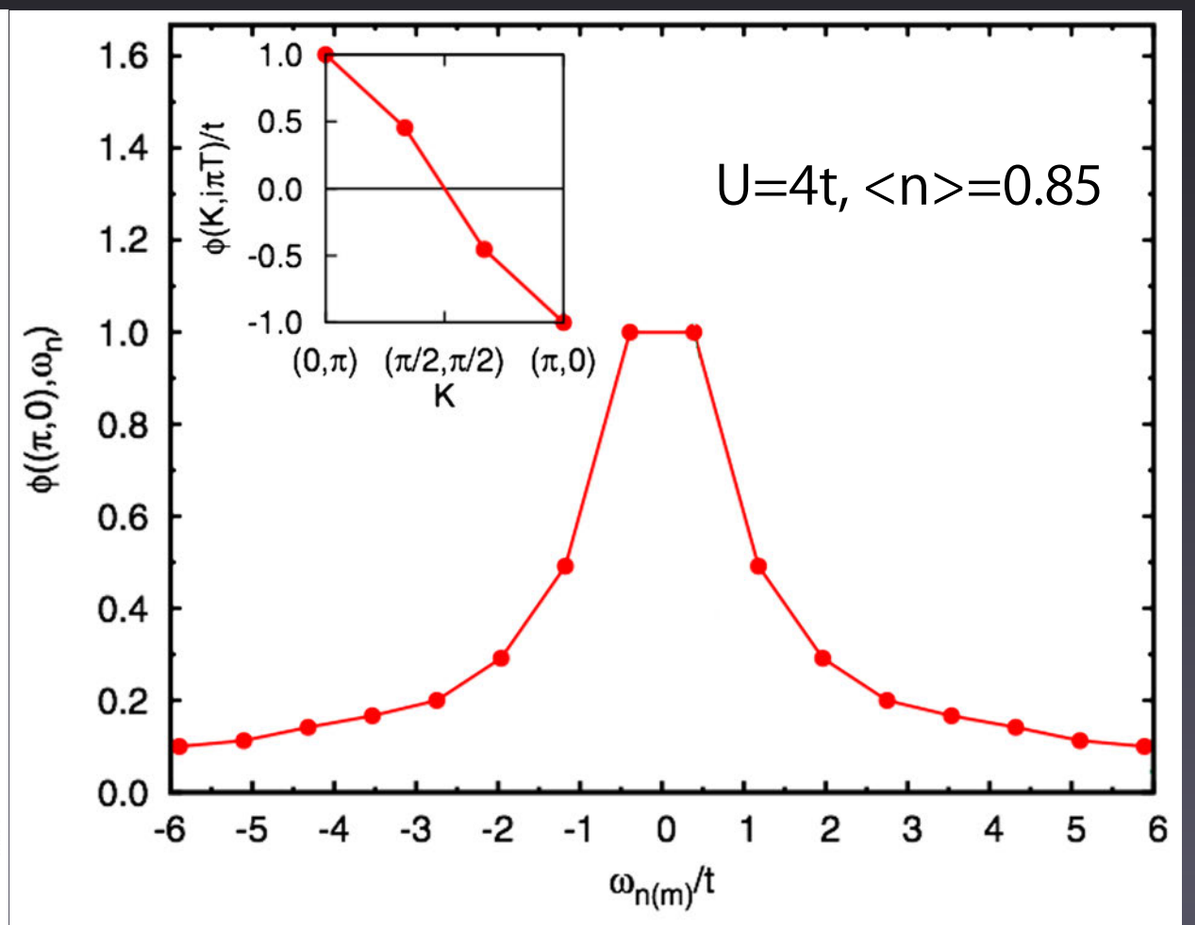
- Coarse-grained eigenvalue equation

$$-\frac{T}{N_c}\sum_{K'}\Gamma_{c,pp}(K,K')\chi_{0,pp}(K')g_{\alpha}(K') = \lambda_{\alpha}g_{\alpha}(K)$$

$$\chi_{0,pp}(K) = N_c/N\sum_{\mathbf{k}}\phi_{\mathbf{K}}(\mathbf{k})G_{\uparrow}(k)G_{\downarrow}(-k)$$

BSE eigenvalues and eigenfunctions: 2D Hubbard model





The Q=(π,π), *S*=1 particle-hole channel dominates but saturates at low *T*. The leading eigenvalue in the singlet Q=0 particle-particle channel has *d*-wave symmetry and increases towards 1 at low *T*.

The DCA+ method

The DCA$^+$ method

General idea:

Introduce lattice self-energy with continuous *k*-dependence and thus reduce its cluster shape and size dependence.

DCA$^+$ self-energy

- DCA self-energy

$$\Sigma(\mathbf{k}) = \sum_{\mathbf{K}} \phi_{\mathbf{K}}(\mathbf{k}) \Sigma_c(\mathbf{K})$$

- Identity

$$\frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) \phi_{\mathbf{K}'}(\mathbf{k}) = \delta_{\mathbf{K}\mathbf{K}'}$$

- DCA$^+$ relation for lattice self-energy

$$\Sigma_c(\mathbf{K}) = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) \Sigma(\mathbf{k})$$

DCA$^+$ algorithm

(2) Coarse-graining

$$\bar{G}(\mathbf{K}, i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) \frac{1}{i\omega_n - \varepsilon_{\mathbf{k}} + \mu - \Sigma(\mathbf{k}, i\omega_n)}$$

$$\Sigma_c(\mathbf{k}, i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) \Sigma(\mathbf{k}, i\omega_n)$$

(3) Bare cluster propagator

$$\mathcal{G}_0(\mathbf{K}, i\omega_n) = \left[\bar{G}^{-1}(\mathbf{K}, i\omega_n) + \Sigma_c(\mathbf{K}, i\omega_n)\right]^{-1}$$

(4) Cluster solver

$$\{\mathcal{G}_0, U\} \rightarrow \Sigma_c(\mathbf{K}, i\omega_n)$$

(5) Interpolation/Deconvolution

$$\Sigma_c(\mathbf{K}, i\omega_n) \rightarrow \Sigma_c(\mathbf{k}, i\omega_n)$$

$$\Sigma_c(\mathbf{k}, i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k}'} \phi_0(\mathbf{k}' - \mathbf{k}) \Sigma(\mathbf{k}', i\omega_n)$$

(1) DCA$^+$ self-energy

$$\Sigma(\mathbf{k}, i\omega_n)$$

Iterate to self-consistency:

$$\Sigma_c^{\text{new}} = \Sigma_c^{\text{old}}$$

From cluster to lattice

$$\Sigma_c(\mathbf{K}) = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) \Sigma(\mathbf{k})$$

- Interpolation $\Sigma_c(\mathbf{K}) \to \Sigma_c(\mathbf{k})$
- Generalized coarse-graining

$$\Sigma_c(\mathbf{k}) = \frac{N_c}{N} \sum_{\mathbf{k}'} \phi_0(\mathbf{k}' - \mathbf{k}) \Sigma(\mathbf{k}') \qquad \phi_{\mathbf{K}}(\mathbf{k}') = \phi_{\mathbf{K}=0}(\mathbf{k}' - \mathbf{K})$$

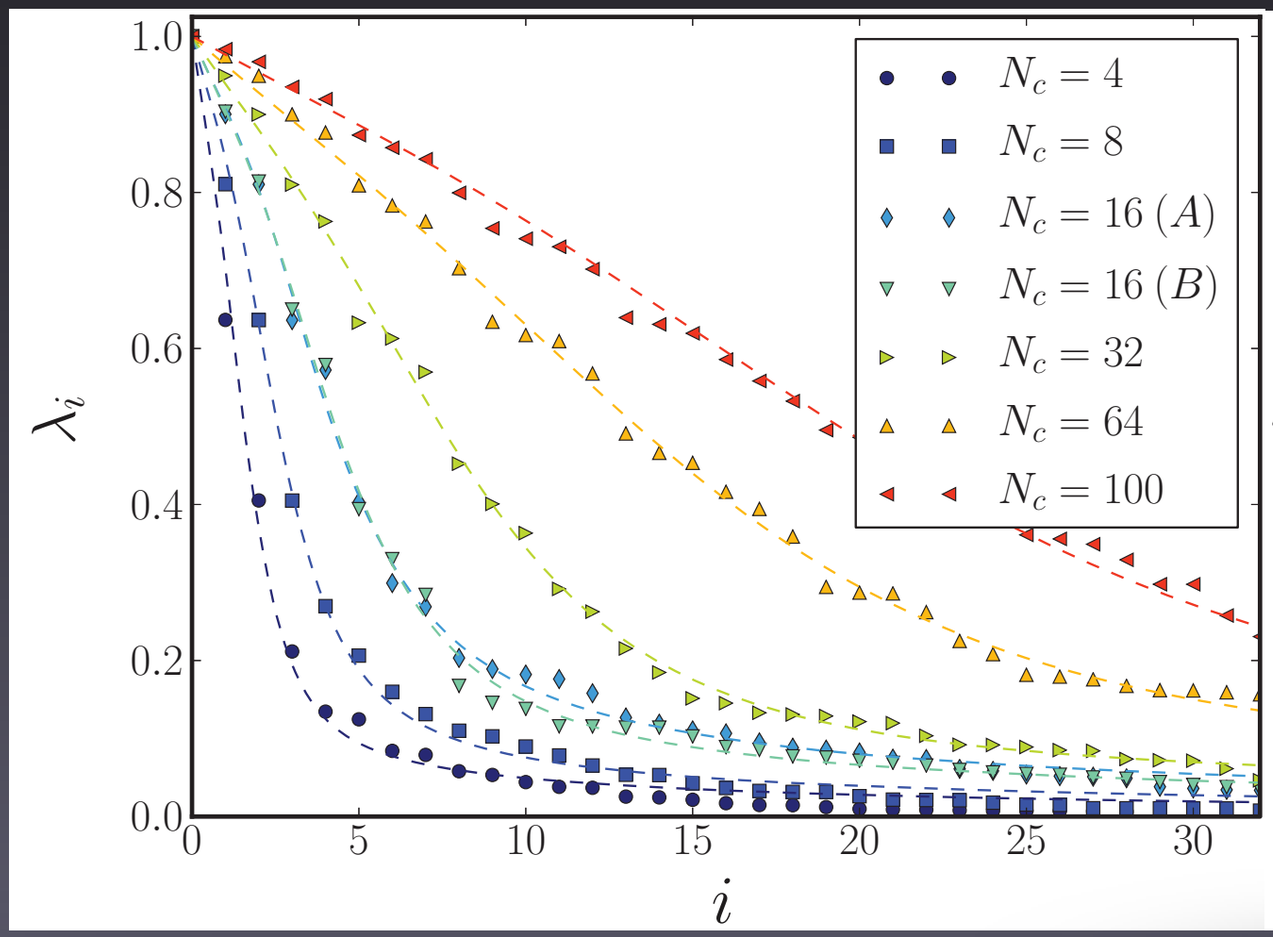
- Expansion of lattice self-energy

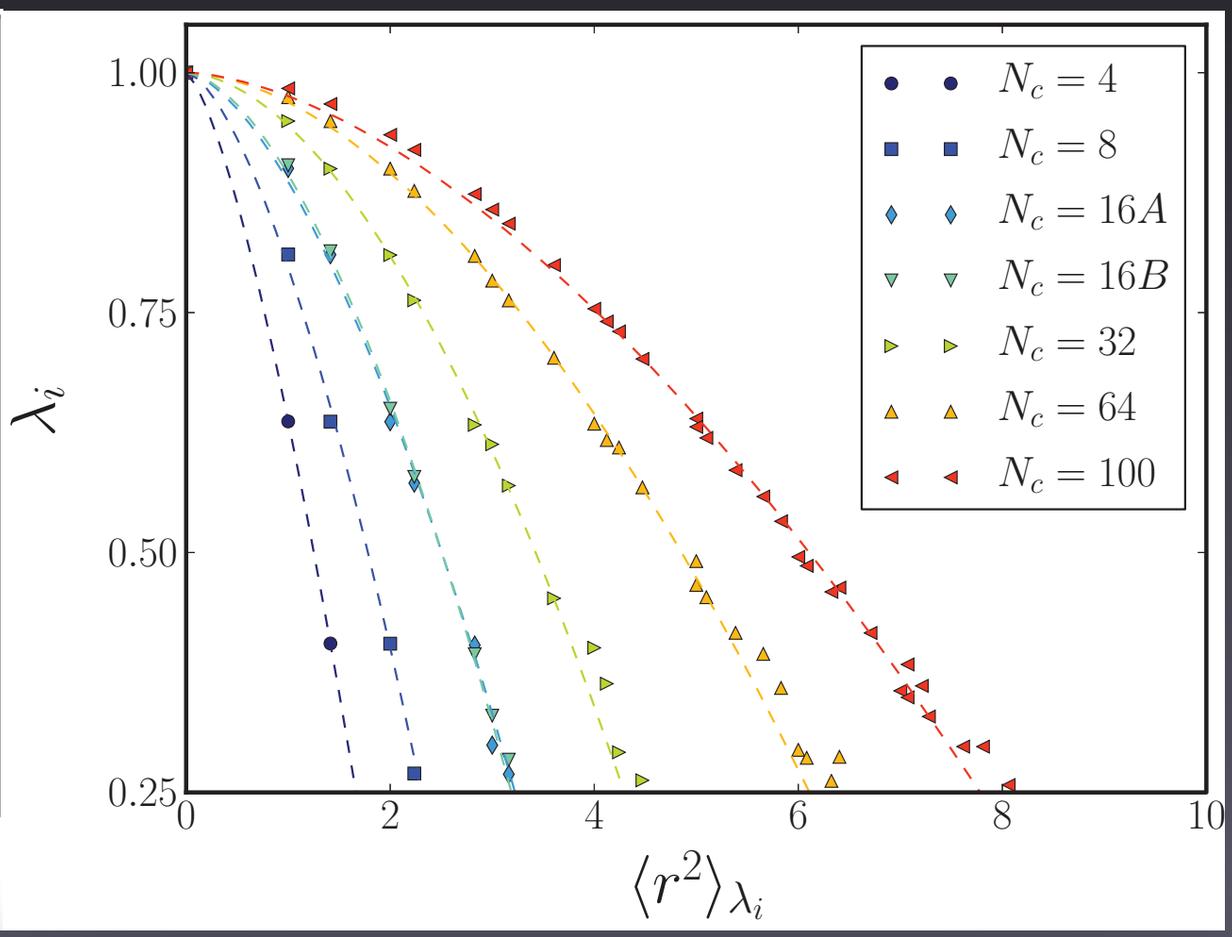
$$\Sigma(\mathbf{k}) = \sum_i \mathcal{B}_{i\omega_n}(\mathbf{k} - \mathbf{k}_i) \sigma(\mathbf{k}_i)$$

- Projection

$$\Sigma_c(\mathbf{k}_i) = \sum_j P_{ij} \sigma(\mathbf{k}_j)\,; \;\; P_{ij} = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_0(\mathbf{k} - \mathbf{k}_i) \mathcal{B}_{i\omega_n}(\mathbf{k} - \mathbf{k}_j)$$

Eigenvalues of projection operator

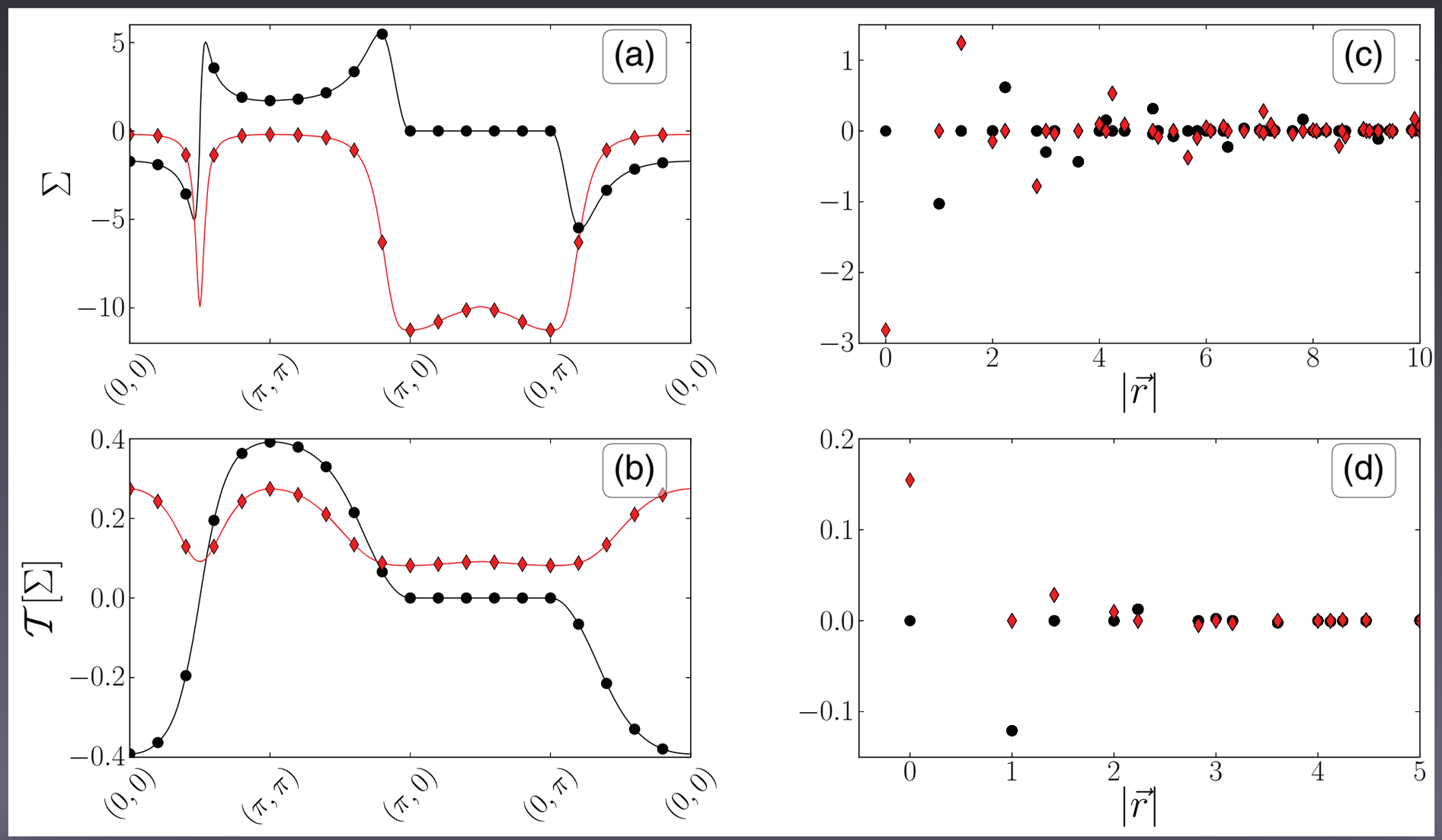




Inversion only possible if self-energy contained within the cluster

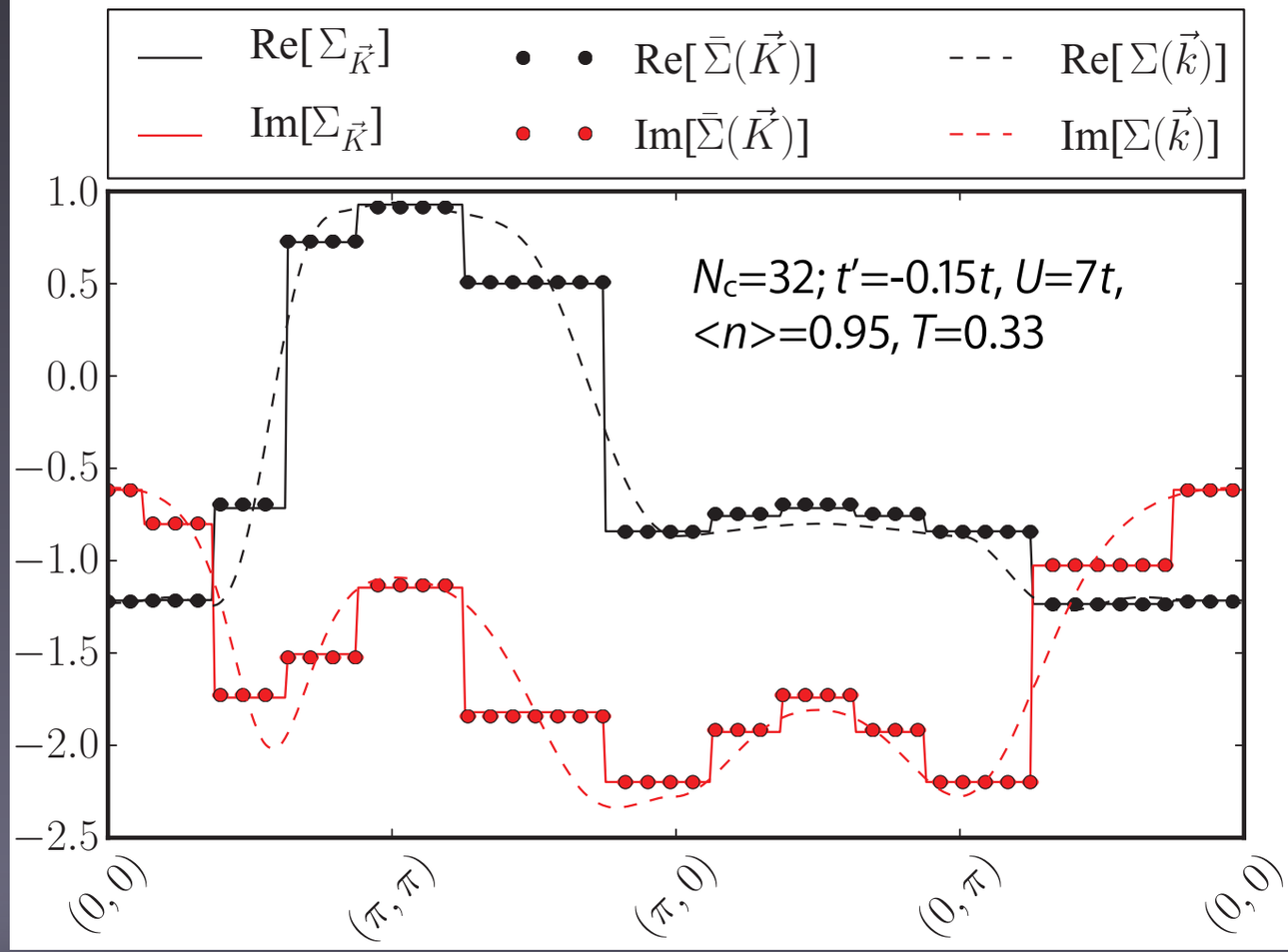
Interpolation of cluster self-energy

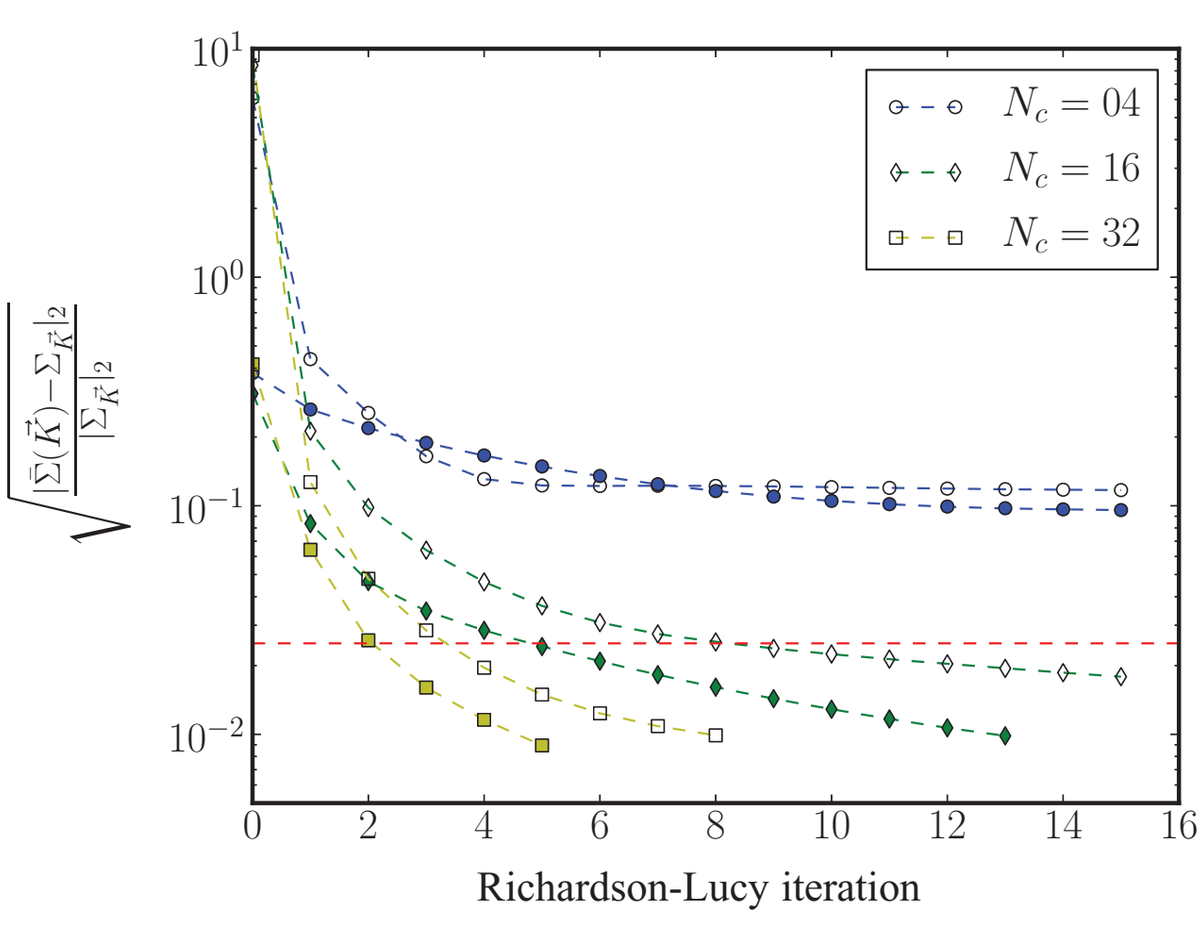
$$\Sigma_c(\mathbf{k}) = \mathcal{T}^{-1}\Big[\sum_{\mathbf{R}} e^{-i\mathbf{k}\mathbf{R}} \underbrace{\Big(\sum_{\mathbf{K}} e^{i\mathbf{K}\mathbf{R}}\mathcal{T}(\Sigma_c(\mathbf{K}))\Big)}_{(\mathcal{T}\Sigma)_{\mathbf{R}}}\Big];\ \mathcal{T}(z) = (z-i)^{-1}$$



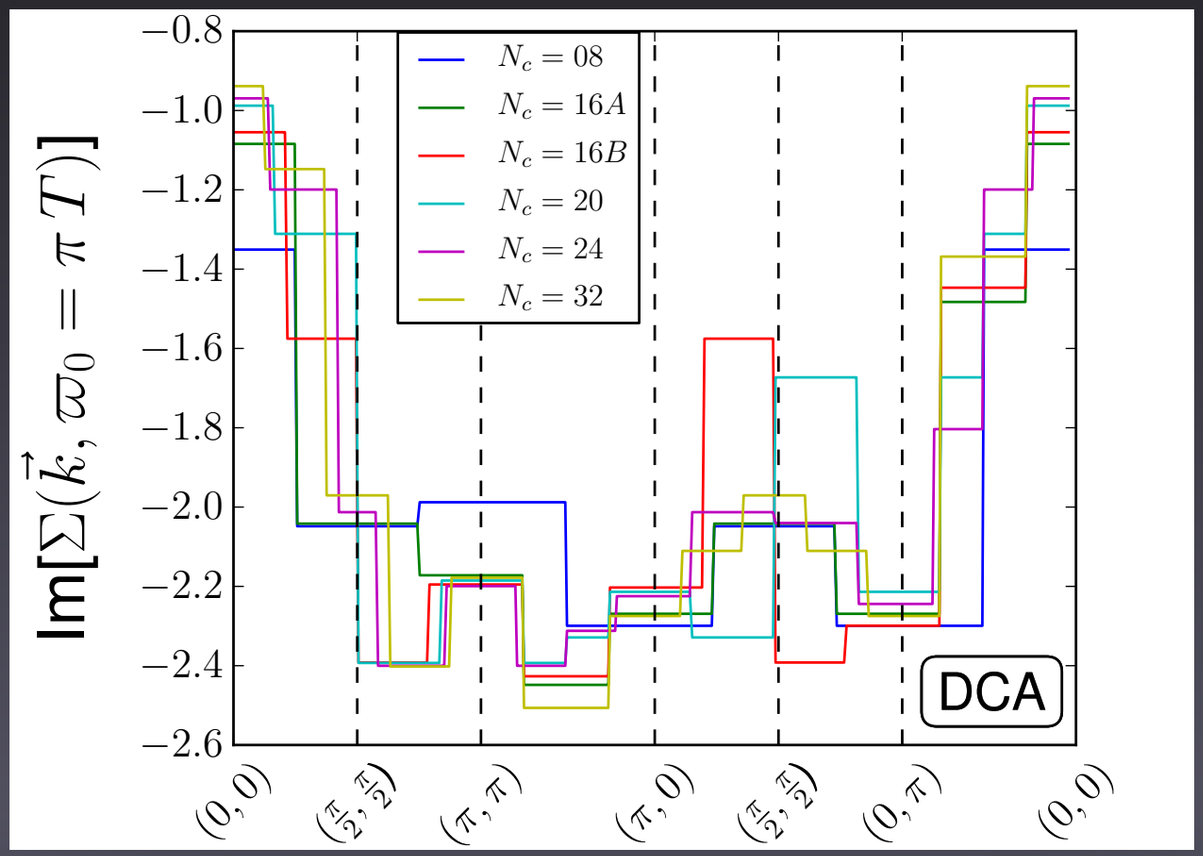
Deconvolution of interpolated cluster self-energy

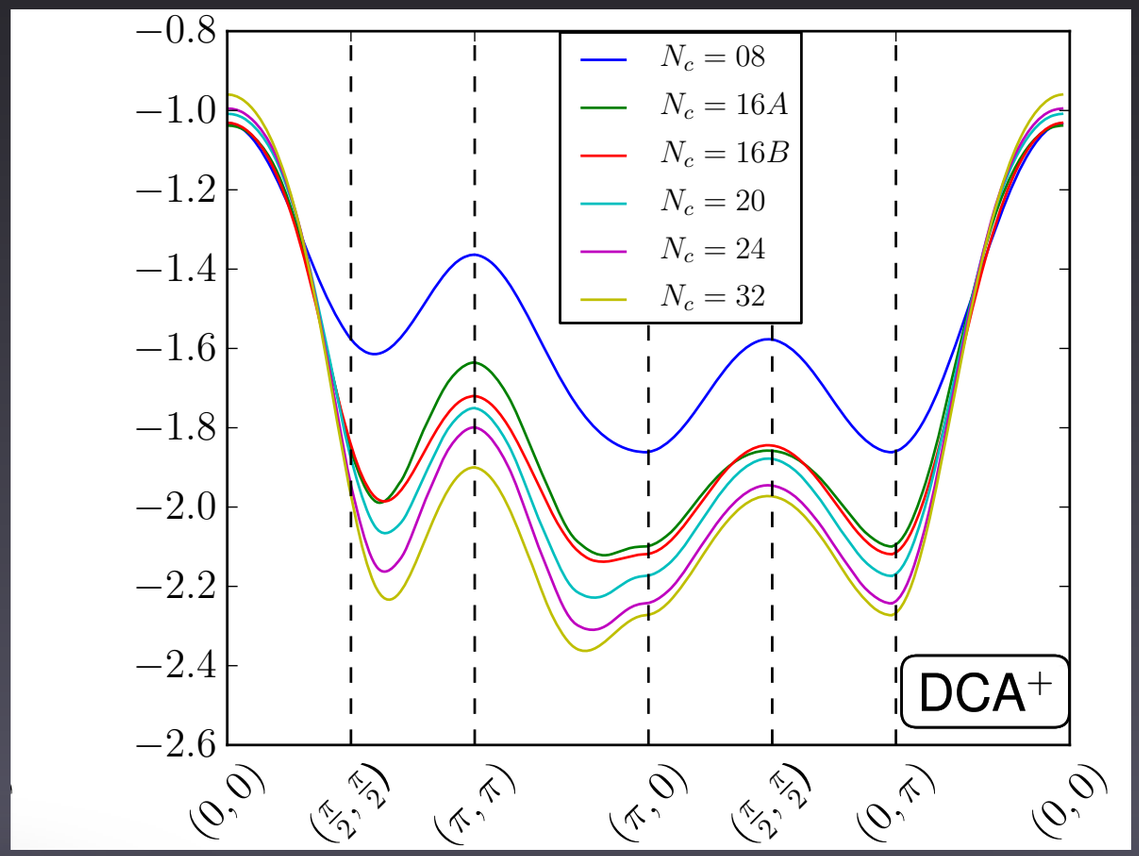
- Richardson-Lucy fixed-point iteration (converges to maximum likelihood solution): $\Sigma^{(i+1)}(\mathbf{k}) \leftarrow \Sigma^{(i)}(\mathbf{k}) \int d\mathbf{k}' \frac{\phi_0(\mathbf{k}-\mathbf{k}')\Sigma_c(\mathbf{k}')}{\int d\mathbf{k}\, \phi_0(\mathbf{k}-\mathbf{k}')\Sigma^{(i)}(\mathbf{k})}$





DCA vs. DCA$^+$ self-energy





DCA$^+$ gives smooth momentum dependence
and mitigates cluster shape/size dependence

Lattice irreducible vertex function

- DCA vertex

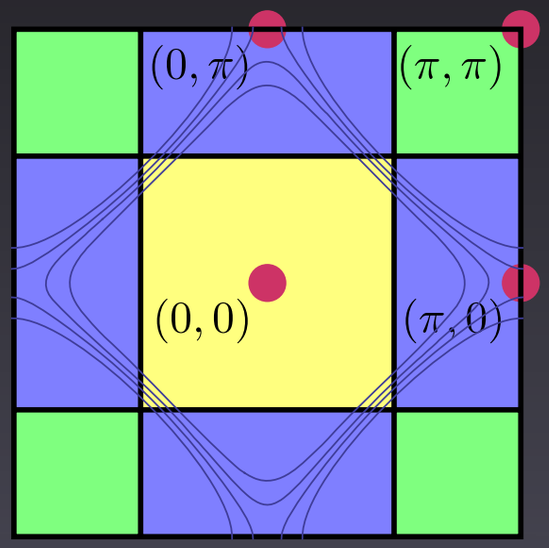
$$\Gamma_\alpha(k, k') = \sum_{\mathbf{K},\mathbf{K}'} \phi_{\mathbf{K}}(\mathbf{k}) \Gamma_{c,\alpha}(K, K') \phi_{\mathbf{K}'}(\mathbf{k}')$$

- DCA$^+$ relation for lattice vertex

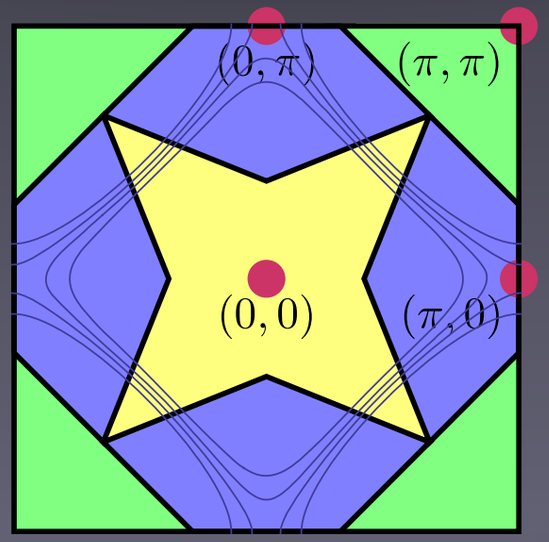
$$\Gamma_{c,\alpha}(K, K') = \frac{N_c^2}{N^2} \sum_{\mathbf{k},\mathbf{k}'} \phi_{\mathbf{K}}(\mathbf{k}) \Gamma_\alpha(k, k') \phi_{\mathbf{K}'}(\mathbf{k}')$$

- Use interpolation, then inversion to determine lattice vertex $\Gamma_\alpha(k,k')$

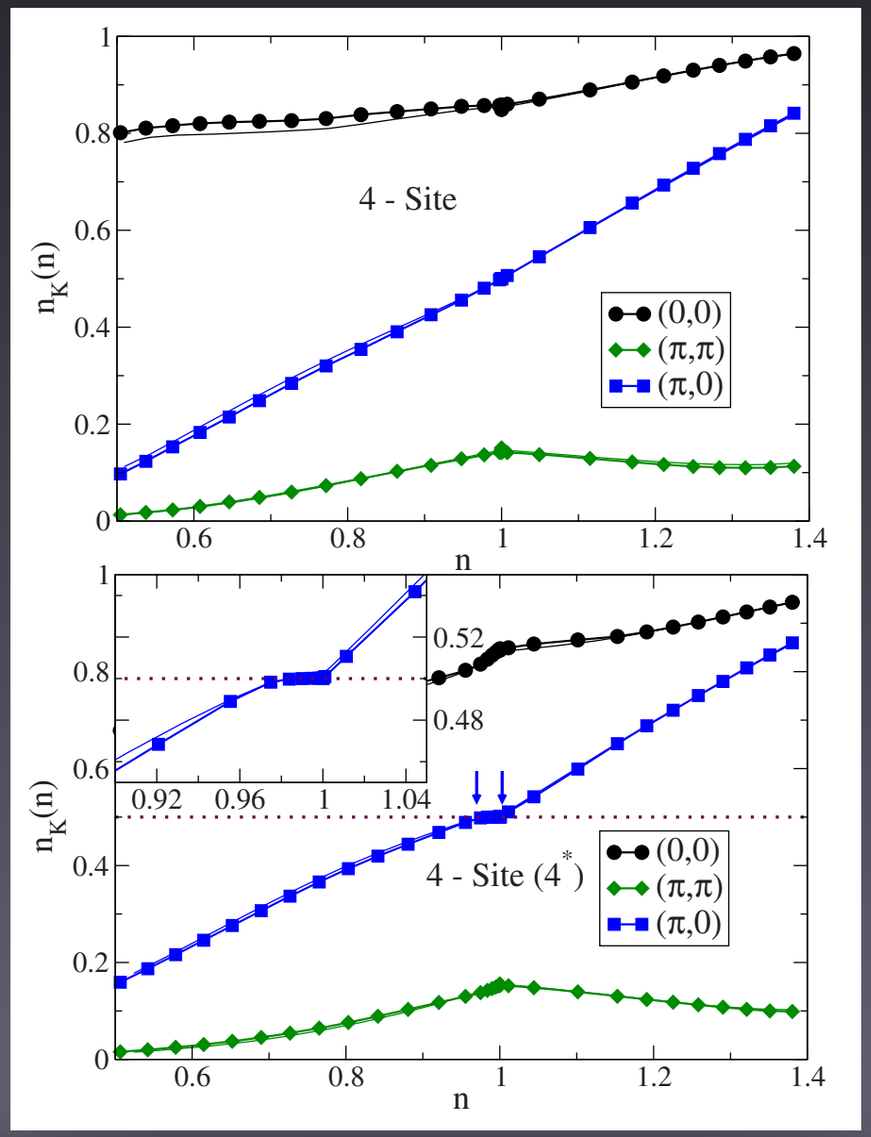
Choice of coarse-graining patch function



Star-like patching



Partial occupancies



Gull et al., PRB '10

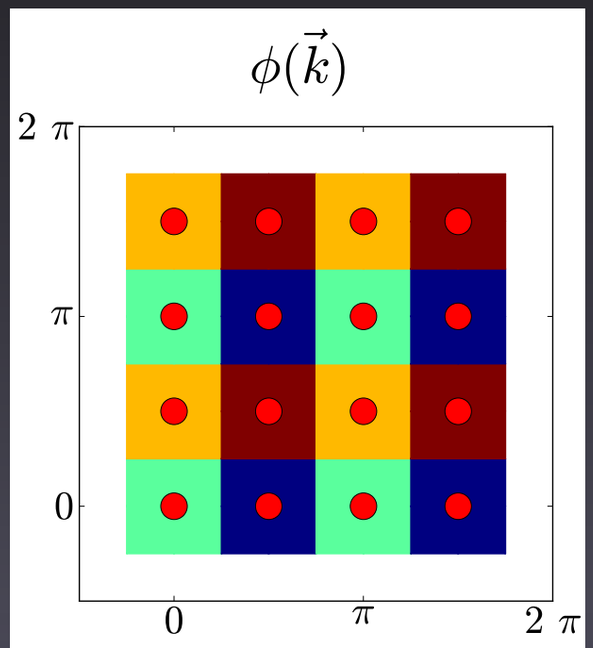
"Interleaved" coarse-gra

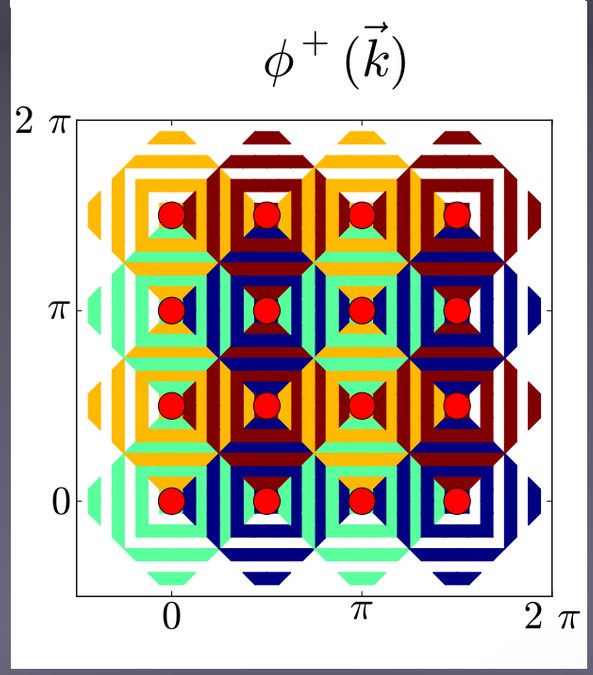
for L=6:

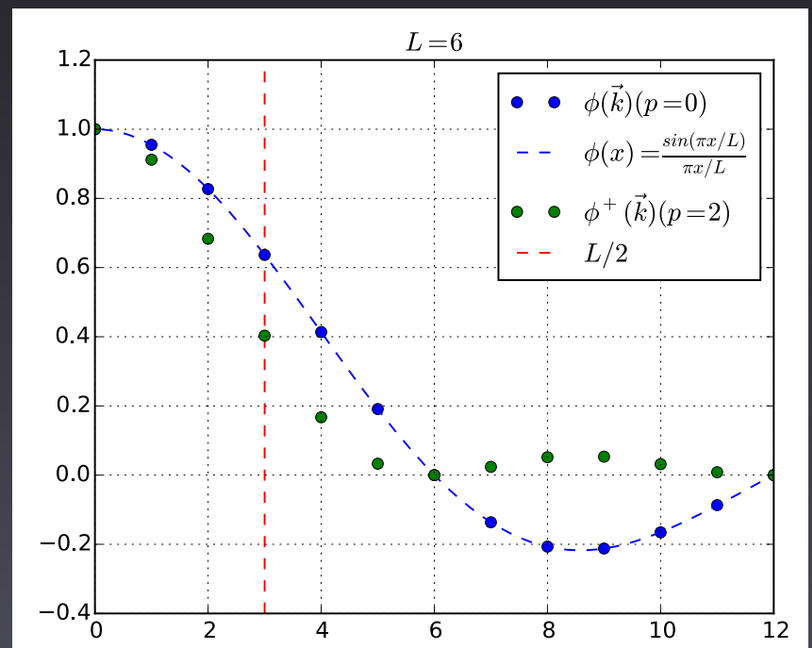
Gbar(1) = Phi(1)G(1) + Phi(-5)G(-5)
Gbar(5) = Phi(5)G(5) + Phi(-1)G(-1)

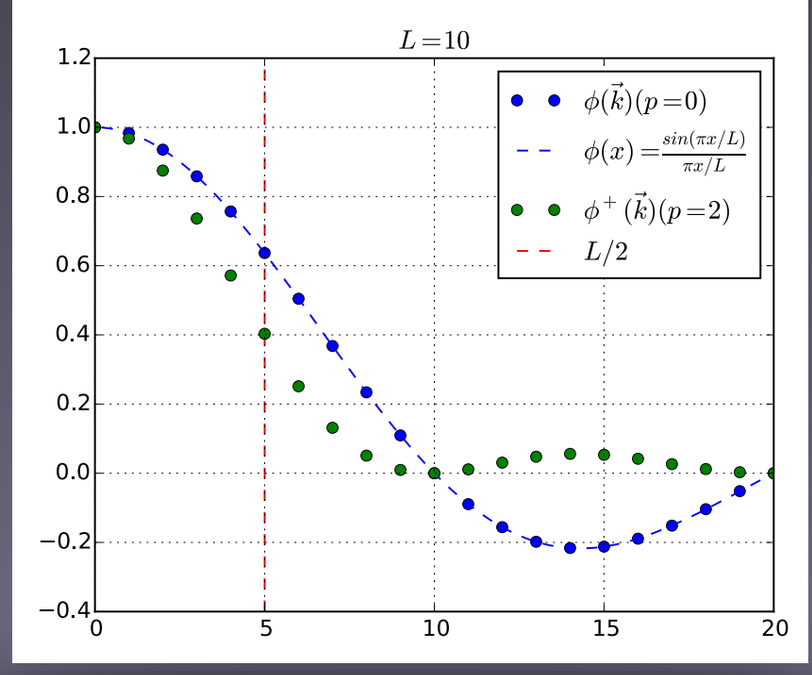
-> Gbar(1) = Gbar(5) (with inv. symmetry)

$$\bar{G}(\mathbf{K}) = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) G(\mathbf{k}) \qquad \bar{G}(\mathbf{R}) = \sum_{\mathbf{r}} \phi(\mathbf{R}+\mathbf{r}) G(\mathbf{R}+\mathbf{r})$$



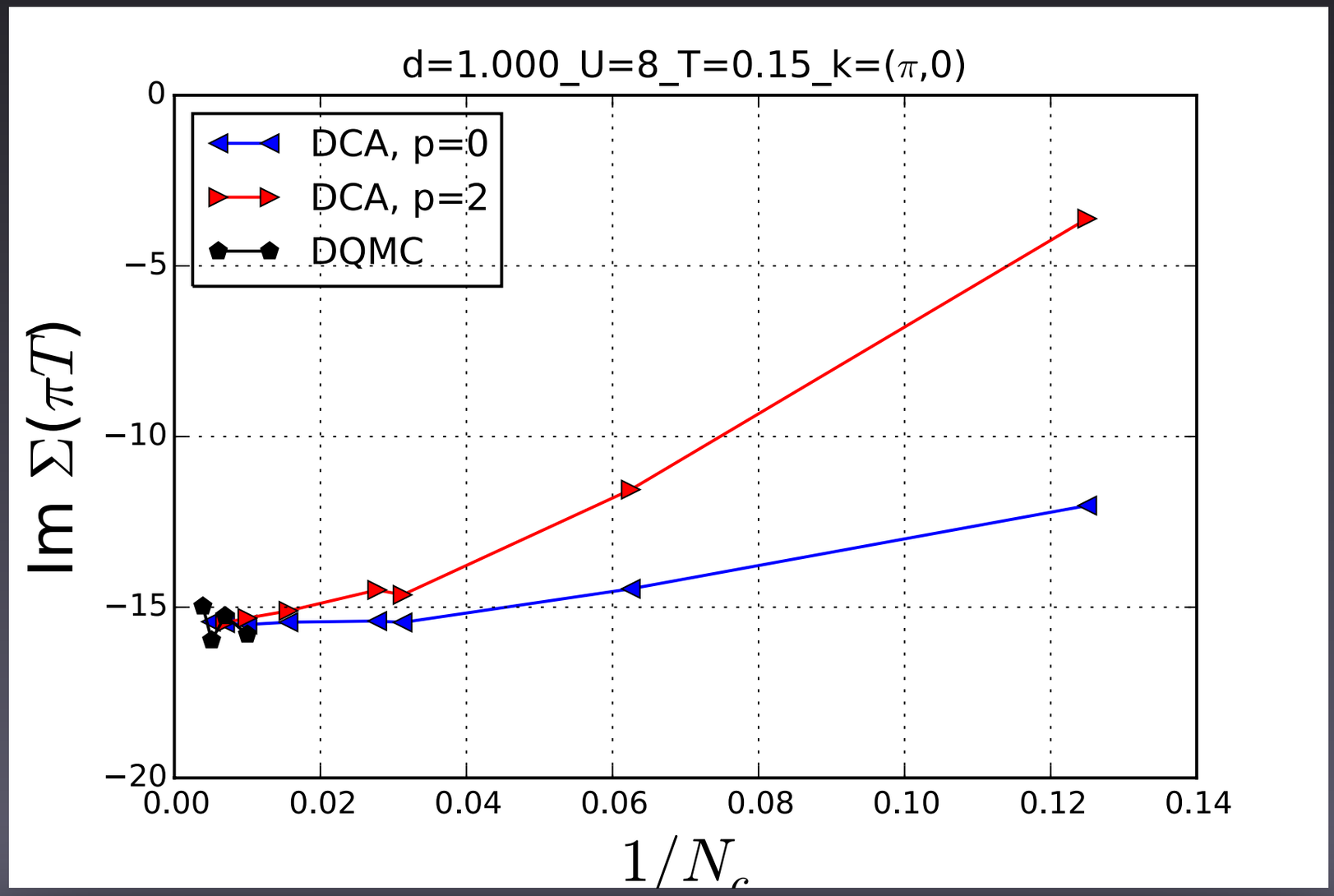






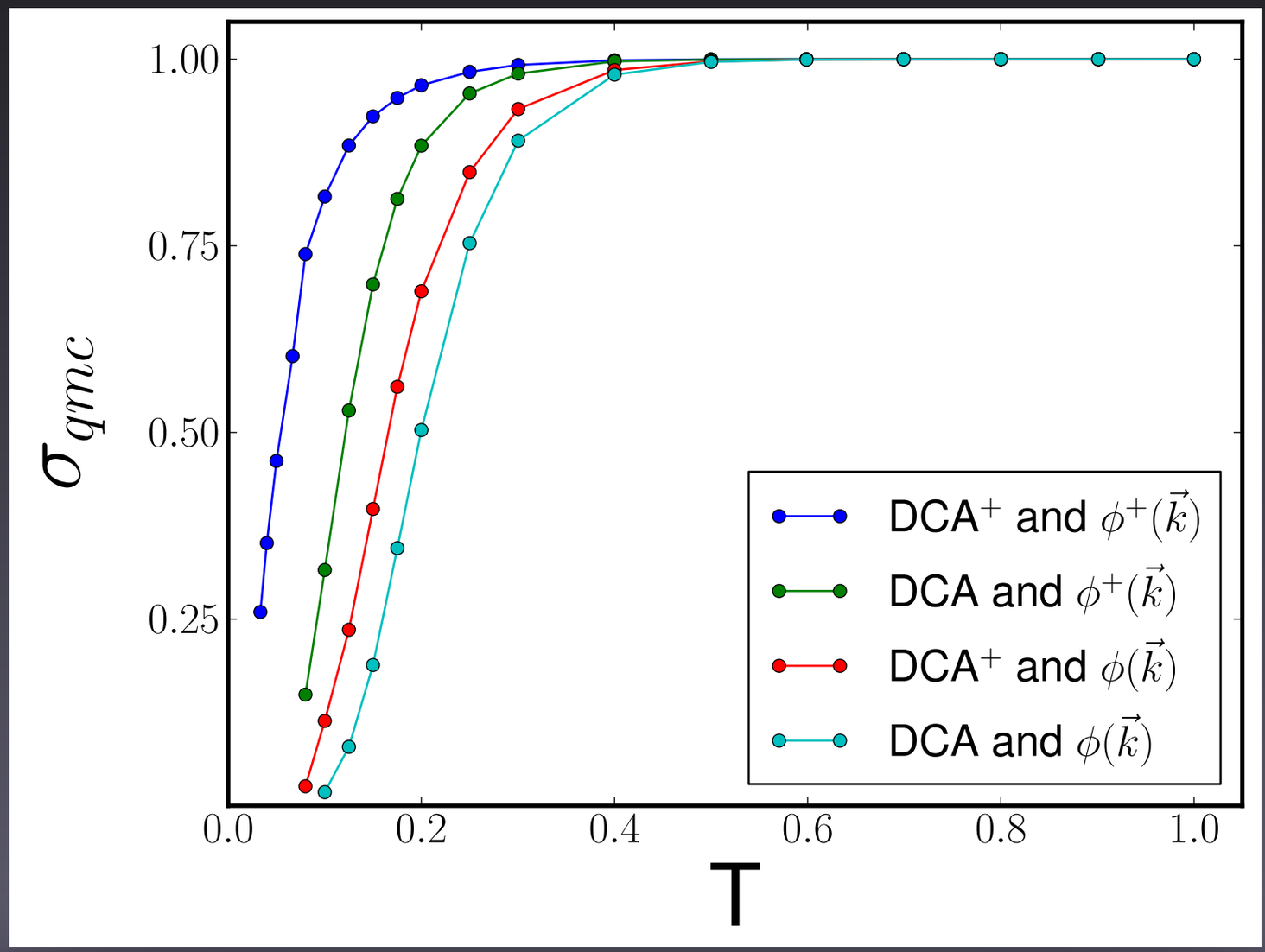
Staar, Jiang, Hähner, TAM, Schulthess, in preparation

Coarse-graining and cluster size



Effects of coarse-graining gradually diminish with increasing cluster size

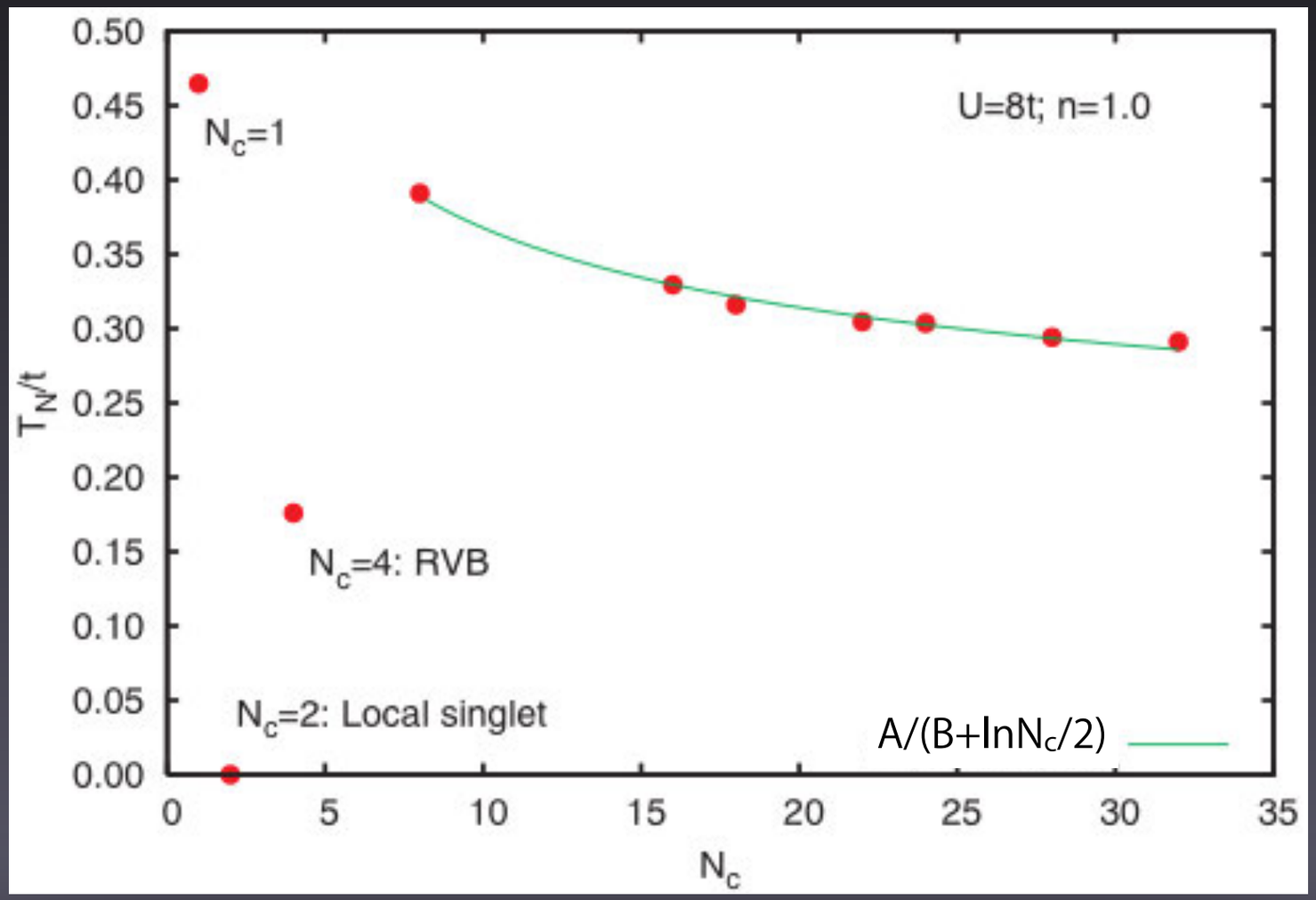
Reduction of QMC sign problem



DCA$^+$ with interleaved coarse-graining significantly reduces sign problem

Applications to 2D Hubbard model

Antiferromagnetism



$$\chi_s(\mathbf{q}) = \int_0^\beta d\tau \langle T_\tau S^z(\mathbf{q},\tau) S^z(-\mathbf{q},0)\rangle$$

$$S^z(\mathbf{q}) = 1/N \sum_{\mathbf{k}} (c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} c_{\mathbf{k}\uparrow} - c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\downarrow})$$

$$\xi(T_N) = \sqrt{N_c}$$

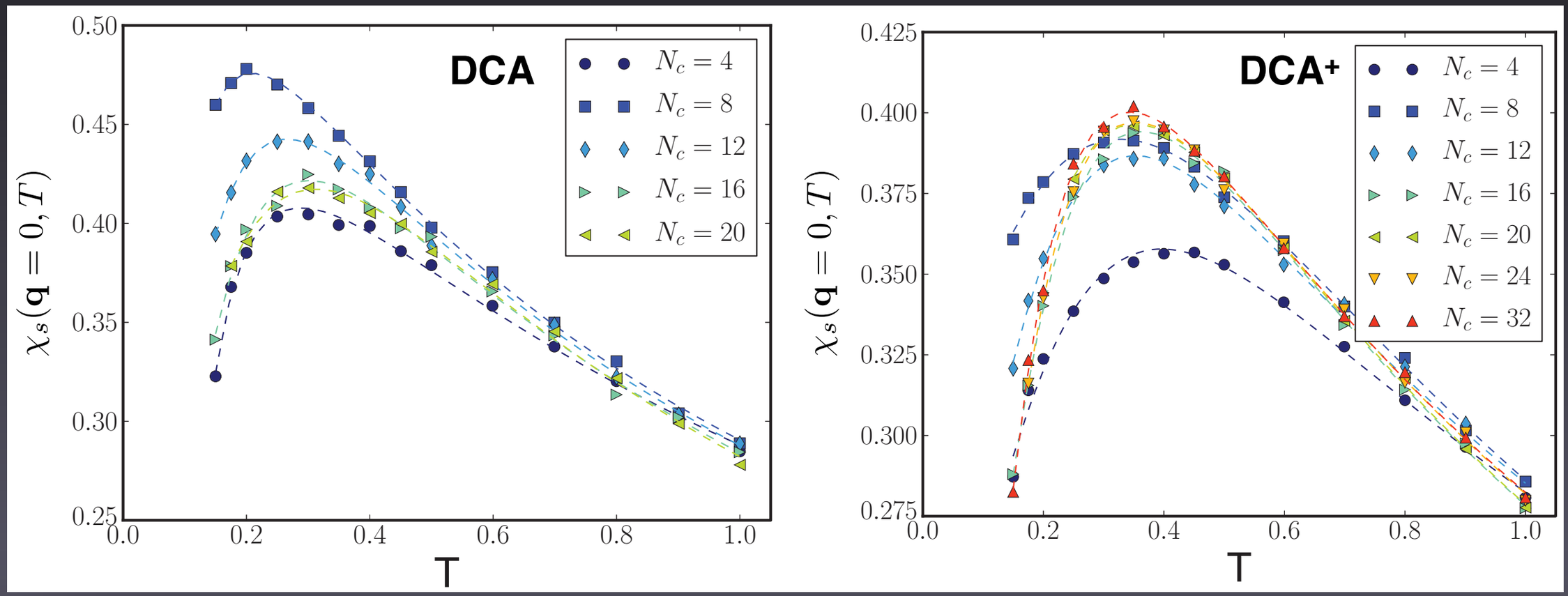
$$\xi(T) \sim e^{A/T}$$

$$\rightarrow T_N(N_c) \sim \frac{A}{B + \ln(N_c)/2}$$

From scaling analysis: Logarithmic decrease of T_N with N_c

Pseudogap at $T=T^*$

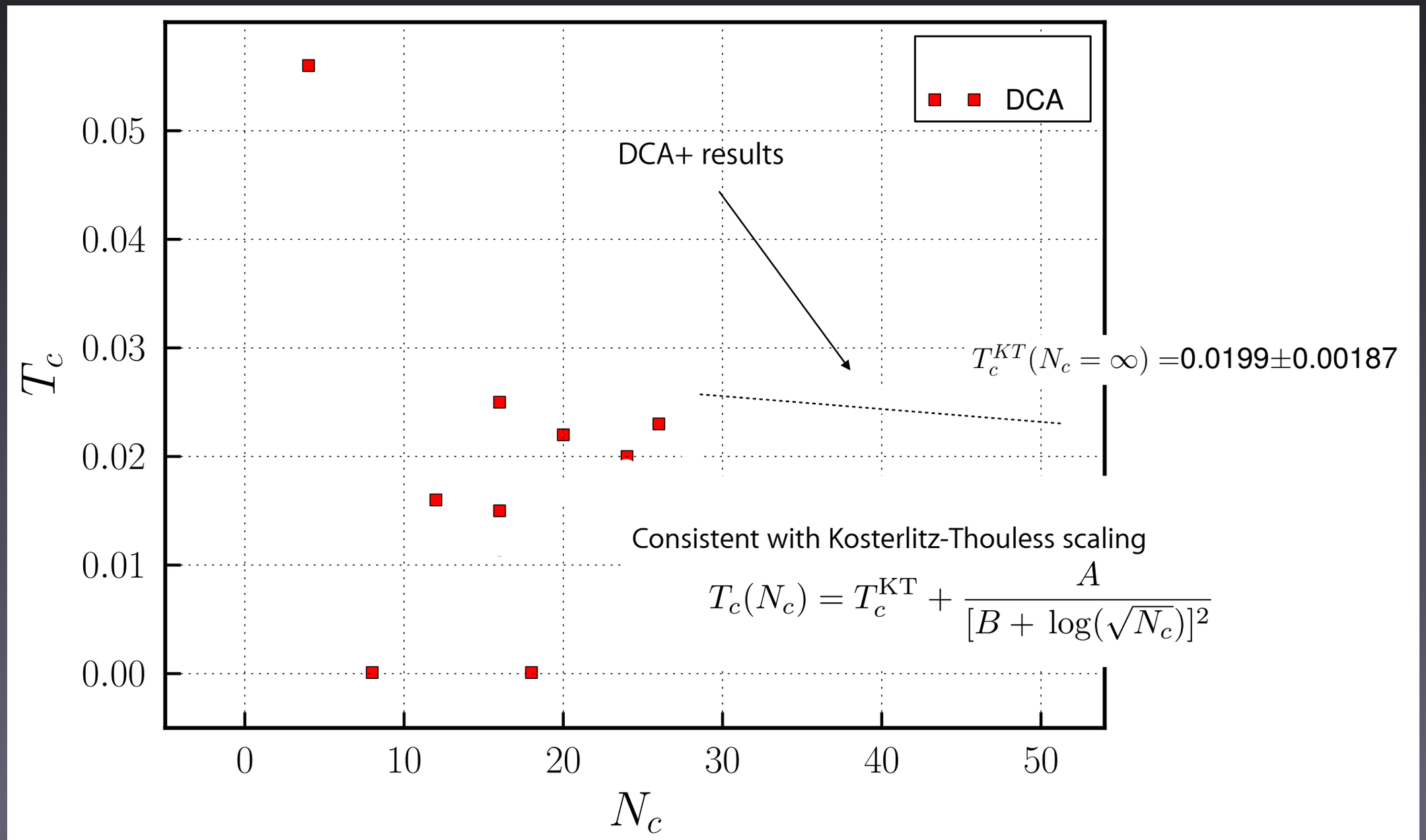
$U=7t$, $t'=-0.15t$, $\langle n\rangle=0.95$



DCA$^+$ converges $T^*(N_c)$ faster

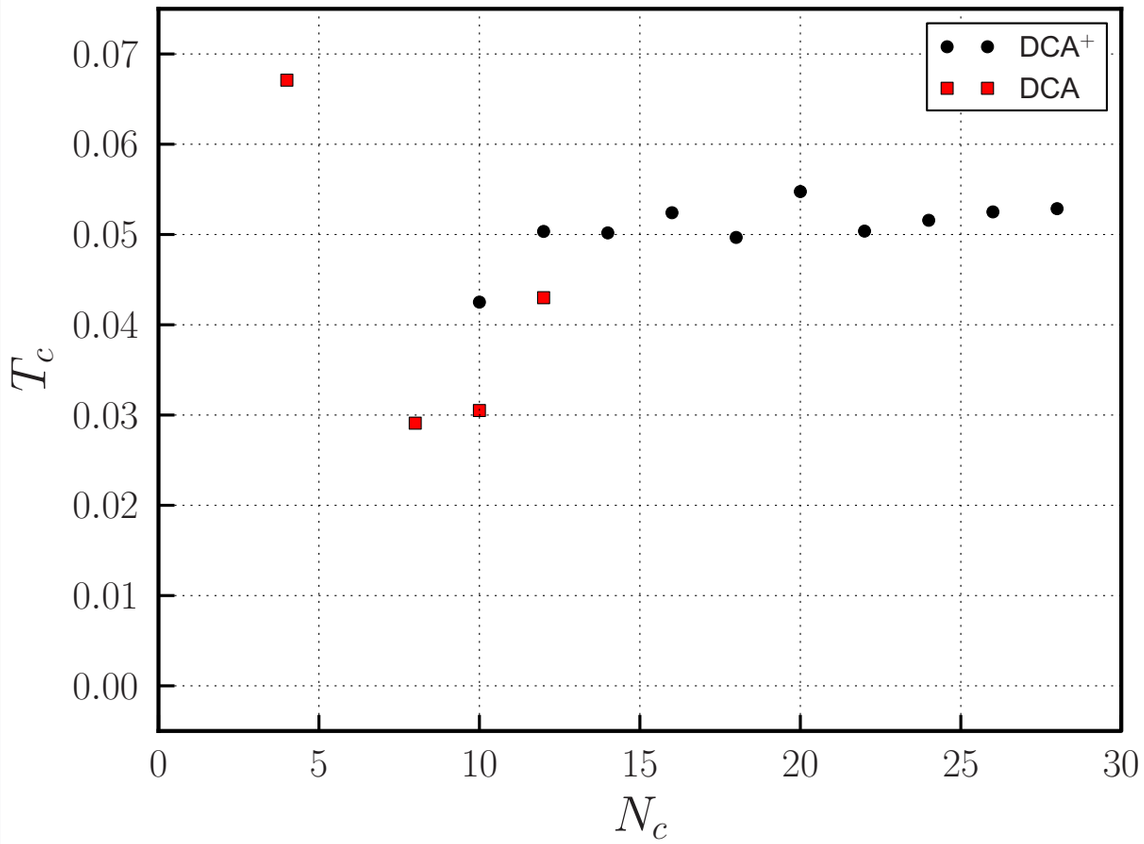
$d_{x^2-y^2}$ superconductivity

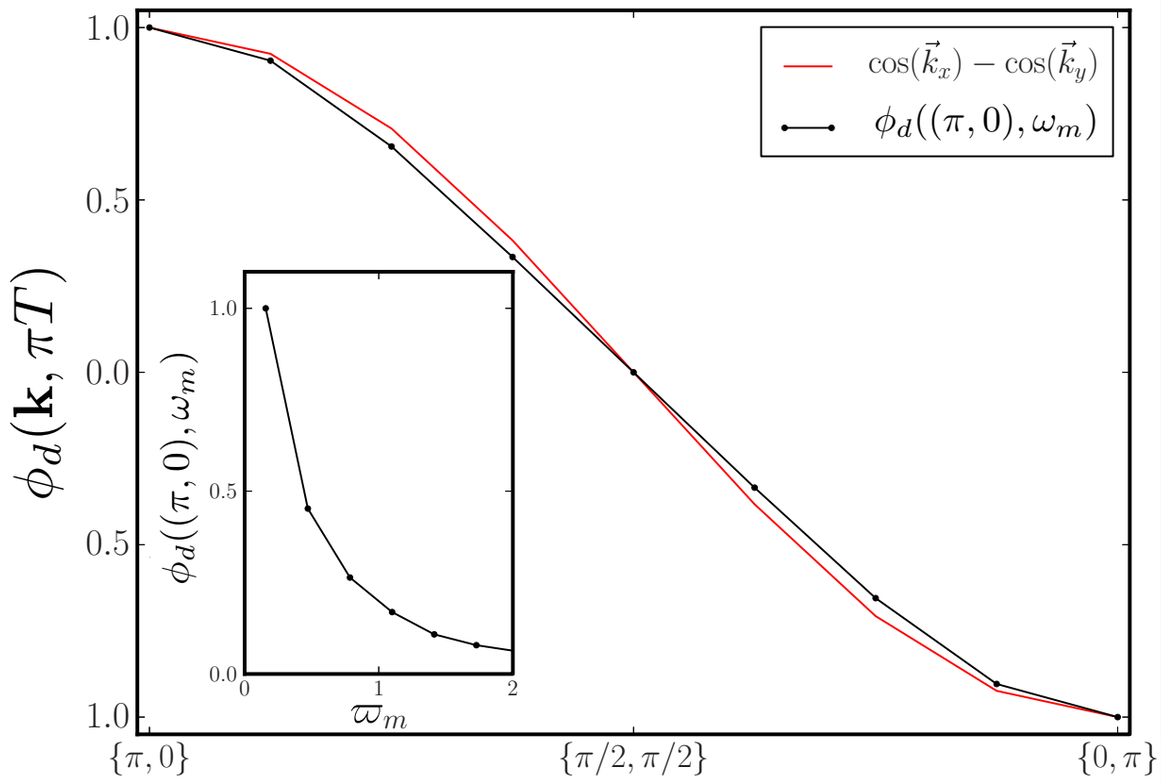
$U=4t$, $\langle n \rangle = 0.9$



$d_{x^2-y^2}$ superconductivity

U=7*t*, <*n*>=0.9





General remarks

Nature of approximation

- DCA and DCA+ are cluster dynamical mean-field theories that map the bulk lattice problem onto a finite size, periodic cluster embedded in a self-consistent dynamic mean-field

- Correlations on the cluster are treated accurately, those beyond the cluster at a mean-field level

- Approximation assumes short-ranged correlations that do not extend beyond $L_c/2$

- Breaks down near classical or quantum phase transition, where mean-field behavior is generated, but finite size scaling can give exact results

Causality

- Causality requires that $\mathrm{Im}\,\Sigma(\mathbf{k}, \omega + i0^+) < 0$
- Causality was a particular challenge in the early attempts to develop of cluster extensions of DMFT
- The DCA can be proven to be causal
- Simple interpolations of the cluster self-energy in the coarse-graining are likely to lead to acausal results
- The DCA+ cannot be proven to be causal, but causality violations have not been observed

Thermodynamic consistency

- Thermodynamic consistency implies that a quantity calculated from the single-particle Green's function is identical to the respective quantity calculated from the two-particle Green's function

$$P_s = \left.\frac{\partial \Delta_s}{\partial \psi}\right|_{\psi=0} \quad \text{or} \quad P_s = \int_0^\beta d\tau \langle \Delta_s(\tau) \Delta_s^\dagger(0) \rangle$$

- An algorithm is thermodynamically consistent if it is self-consistent and if

$$\Gamma = \delta \Sigma[G] / \delta G$$

- Both the DCA and DCA$^+$ are thermodynamically consistent

DCA and DCA$^+$ as self-energy functional approximations

Grand potential

$$\Omega[\mathbf{G}] = \mathrm{Tr}\,\ln[-\mathbf{G}] - \mathrm{Tr}\left[(\mathbf{G}_0^{-1} - \mathbf{G}^{-1})\mathbf{G}\right] + \Phi[\mathbf{G}, \mathbf{U}]$$

Self-energy from Baym-Kadanoff functional

$$\mathbf{\Sigma} = \frac{\delta\Phi[\mathbf{G}]}{\delta\mathbf{G}}$$

and Dyson equation

$$\mathbf{G}^{-1} = \mathbf{G}_0^{-1} - \mathbf{\Sigma}$$

imply stationarity

$$\frac{\delta\Omega[\mathbf{G}]}{\delta\mathbf{G}} = 0$$

Self-energy functional

Grand potential

$$\Omega[\mathbf{\Sigma}] = \mathrm{Tr}\,\ln\left[-(\mathbf{G}_0^{-1} - \mathbf{\Sigma})\right] - (\mathcal{L}\Phi)[\mathbf{\Sigma}]$$

Legendre transform

$$(\mathcal{L}\Phi)[\mathbf{\Sigma}] = \Phi - \mathrm{Tr}[\mathbf{\Sigma}\mathbf{G}]$$

Green's function

$$\mathbf{G} = -\delta(\mathcal{L}\Phi)[\mathbf{\Sigma}]/\delta\mathbf{\Sigma}$$

Dyson equation

$$\mathbf{G} = \left[\mathbf{G}_0^{-1} - \mathbf{\Sigma}\right]^{-1}$$

imply stationarity

$$\delta\Omega[\mathbf{\Sigma}]/\delta\mathbf{\Sigma} = 0$$

DCA approximation

DCA self-energy

$$\Sigma(\mathbf{k}) \simeq \Sigma^{DCA}(\mathbf{k}) = \sum_{\mathbf{K}} \phi_{\mathbf{K}}(\mathbf{k}) \Sigma_c(\mathbf{K})$$

reduces degrees of freedom in functional

$$(\mathcal{L}\Phi)[\mathbf{\Sigma}_c] = \Phi - \frac{N}{N_c} \sum_{\mathbf{K}} \mathrm{Tr}[\Sigma_c(\mathbf{K}) G_c(\mathbf{K})]$$

with cluster Green's function

$$G_c(\mathbf{K}) = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) G(\mathbf{k}) = \frac{N_c}{N} \sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k}) \frac{1}{G_0^{-1}(\mathbf{k}) - \Sigma^{DCA}(\mathbf{k})}$$

DCA grand potential

$$\Omega^{DCA}[\mathbf{\Sigma}_c] = \mathrm{Tr}\,\ln\left[-(\mathbf{G}_0^{-1} - \mathbf{\Sigma}^{DCA})\right] + \Phi - \frac{N}{N_c} \sum_{\mathbf{K}} \mathrm{Tr}[\Sigma_c(\mathbf{K}) G_c(\mathbf{K})]$$

is stationary

$$\delta\Omega[\mathbf{\Sigma}_c]/\delta\Sigma_c(\mathbf{K}) = 0$$

DCA$^+$

DCA$^+$ grand potential

$$\Omega^{DCA^+}[\mathbf{\Sigma}] = \mathrm{Tr}\,\mathrm{ln}\left[-(\mathbf{G}_0^{-1} - \mathbf{\Sigma})\right] + \Phi - \frac{N}{N_c}\sum_{\mathbf{K}} \mathrm{Tr}[\Sigma_c(\mathbf{K})G_c(\mathbf{K})]$$

Self-energy relation between cluster and lattice

$$\Sigma_c(\mathbf{K}) = \frac{N_c}{N}\sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k})\Sigma(\mathbf{k})$$

At stationarity

$$\delta\Omega^{DCA^+}[\Sigma(\mathbf{k})]/\delta\Sigma(\mathbf{k}) = 0$$

one obtains

$$\left[G_0^{-1}(\mathbf{k}) - \Sigma(\mathbf{k})\right]^{-1} = \sum_{\mathbf{K}} \phi_{\mathbf{K}}(\mathbf{k})G_c(\mathbf{K})$$

Multiplying both sides with $N_c/N\sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k})$ gives

$$G_c(\mathbf{K}) = \frac{N_c}{N}\sum_{\mathbf{k}} \phi_{\mathbf{K}}(\mathbf{k})\frac{1}{G_0^{-1}(\mathbf{k}) - \Sigma(\mathbf{k})}$$

Summary & Outlook

- DCA and DCA+ enable insightful and often controlled studies of correlated systems
- They allow for the calculation of various single-particle and two-particle observables to make contact with experiments
- Studies have been mainly based on single-band models. Multi-orbital models are challenging but possible in the near future.