Does the 2D Hubbard model describe high-temperature superconductors?

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Outline

- Motivation
- The Dynamical Cluster Approximation
- Results for Small Clusters
- Large Cluster Scaling: Betts Clusters
- Superconductivity in 2D Hubbard Model
- Conclusion

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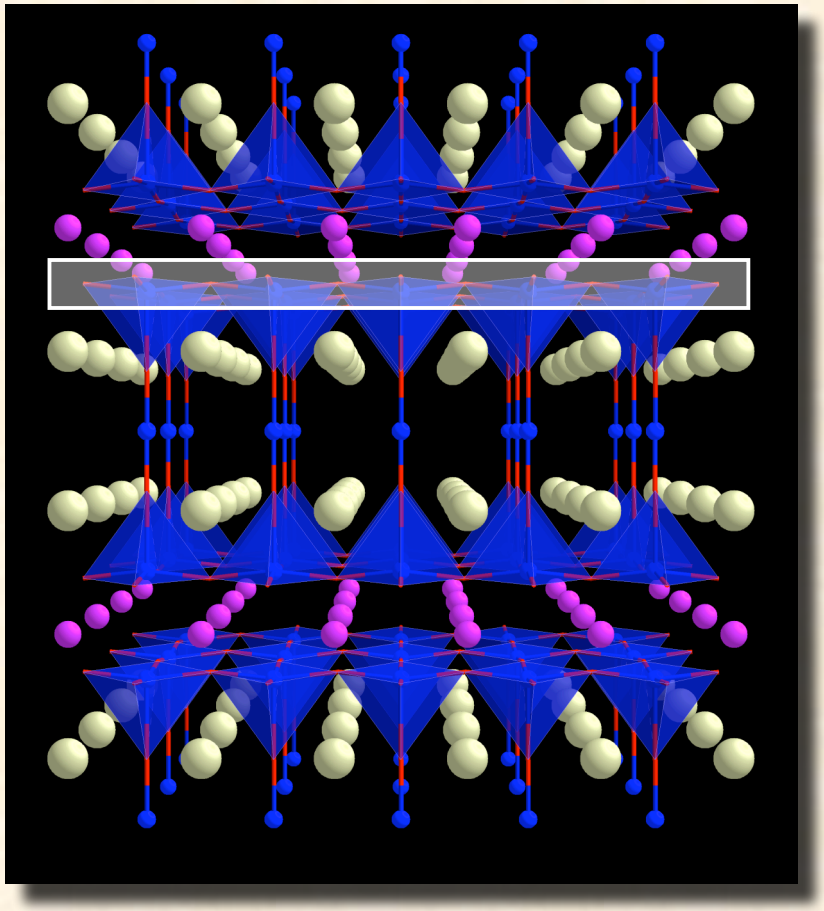
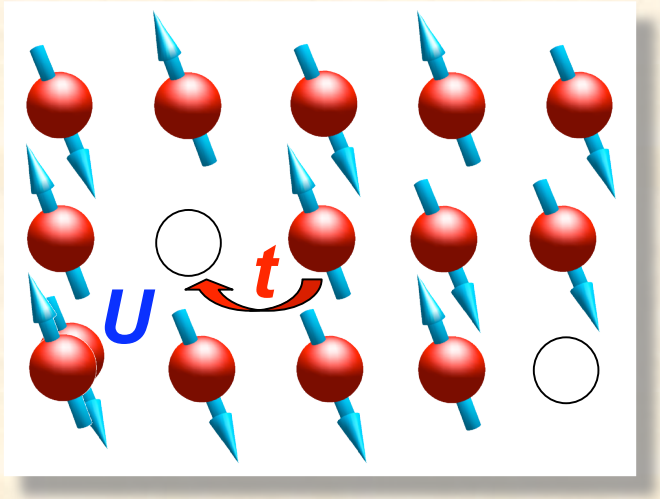
2D Hubbard model of HTSC





(Zhang and Rice, PRB 1988, P.W. Anderson)

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

More than 1000 publications yearly!

Search for superconductivity in 2D Hubbard model

- **Weak coupling (U << W)**
  - **AF spin fluctuations mediate pairing with d-wave symmetry**
    (Bickers, PRL 1989; Monthoux, PRL 1991; Scalapino, JLTP 1999)
  - **RG → Groundstate d-wave superconducting**
    (Halboth, PRB 2000; Zanchi, PRB 2000)
- **Strong coupling (U >> W)**
  - **Finite size simulations of t-J model → Groundstate superconducting**
    (Sorella, PRL 2002; Poilblanc, cond-mat 2002)
- **Intermediate coupling (U ≈ W)**
  - **Inconclusive! QMC sign problem!**

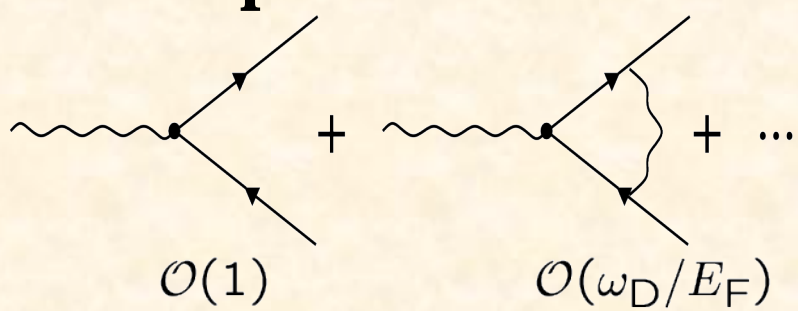
Small Parameter?

BCS (conventional) SC:

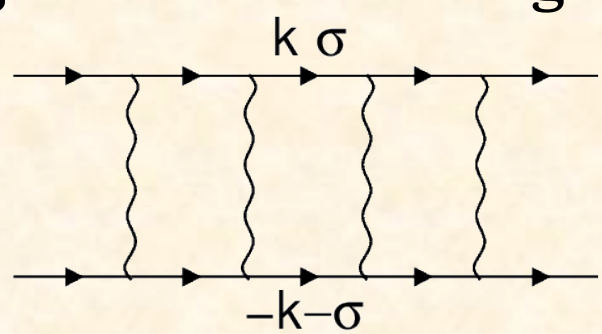
Small parameter:

$$\omega_D/E_F \propto \sqrt{m/M} \ll 1$$

Electron-phonon vertex:



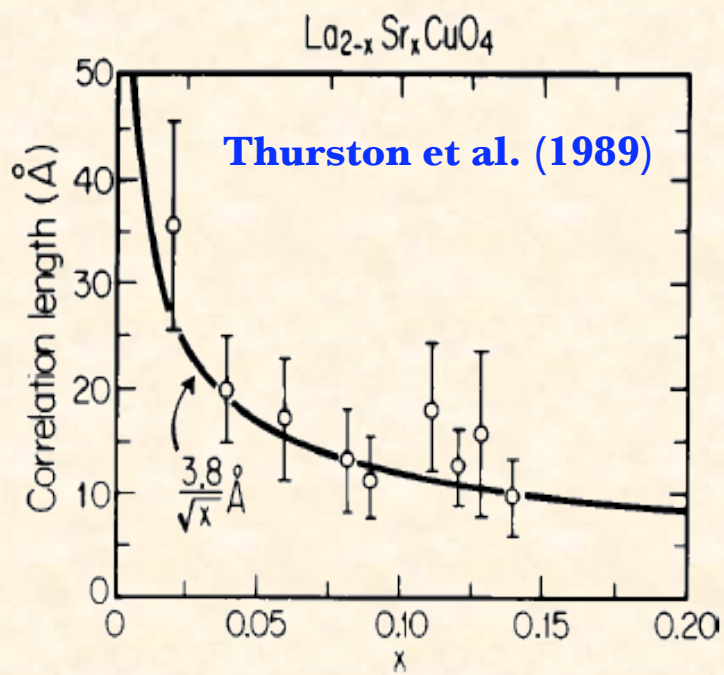
Neglect classes of diagrams:



Cuprate (unconventional) SC:

No small energy scale: $U/W \approx 1$

But in Cuprates:



Short-ranged AF correlations

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- Large Cluster Scaling: Betts Clusters
- Case Study: 3D Phase Diagram
- Superconductivity in 2D Hubbard Model
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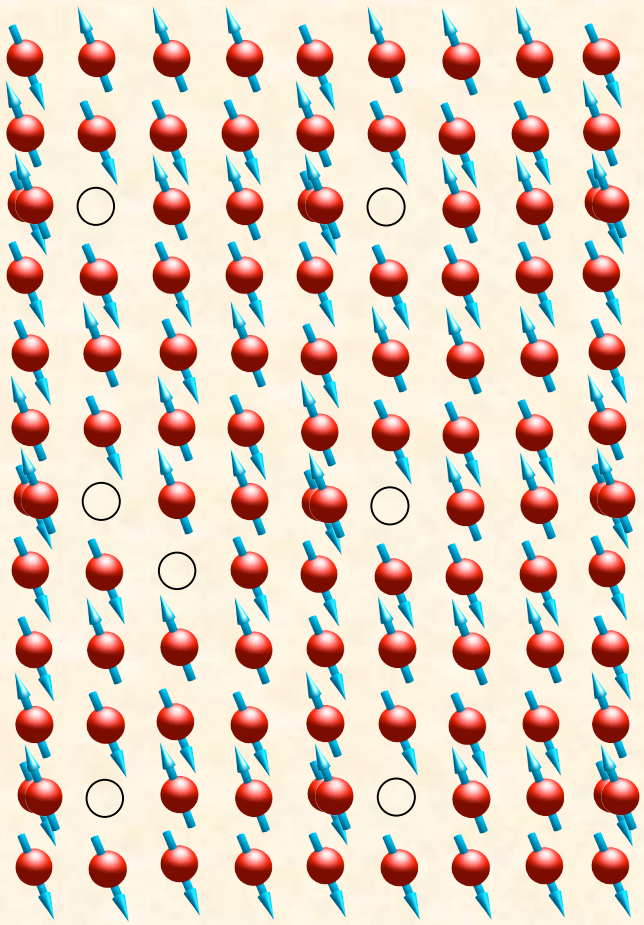
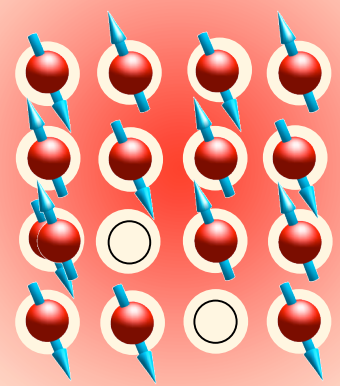
Dynamical Cluster Approximation: Schematic

Infinite lattice



DCA

Cluster coupled to mean-field

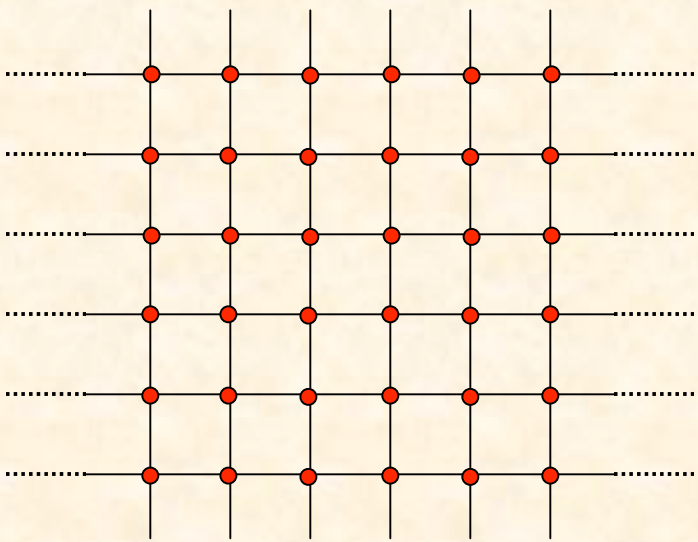


- **Short-ranged correlations within cluster treated explicitely**
- **Longer length scales treated on mean-field level**

DCA: Kinetic vs. interaction energy

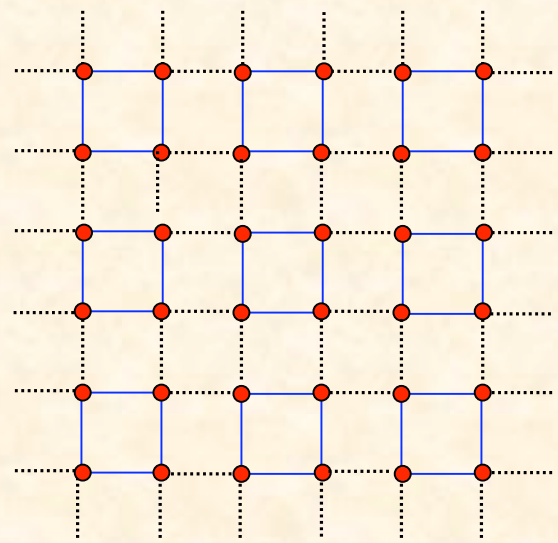
$$H = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Kinetic energy: $\mathrm{Tr}(\mathbf{tG})$



Treat exactly in infinite system

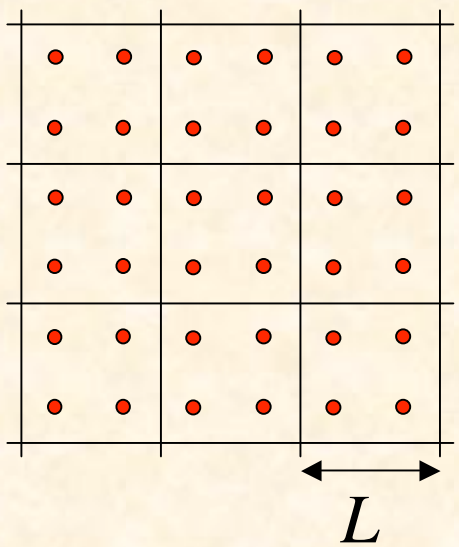
Interaction energy: $\mathrm{Tr}(\mathbf{\Sigma G})$



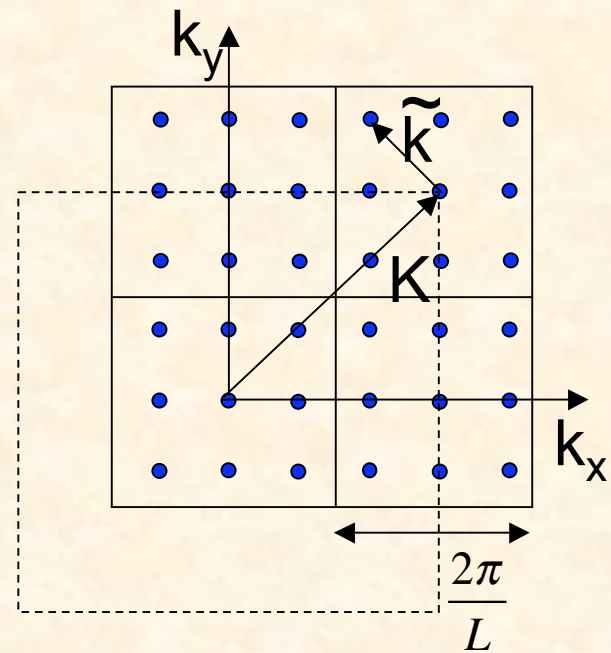
Cut off correlations beyond cluster

Dynamical Cluster Approximation: Formalism

- **Divide lattice into clusters of size $N_c = L \times L$**



- **1st Brillouin zone**

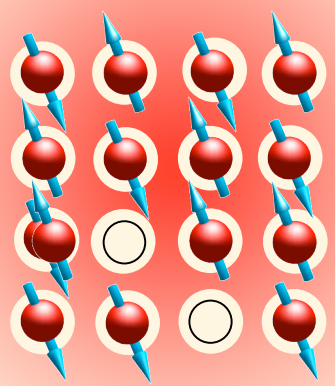


- **Dispersion** $t(\mathbf{k}) = \bar{\epsilon}_{\mathbf{K}} + \delta t(\mathbf{K}, \tilde{\mathbf{k}}); \quad \bar{\epsilon}_{\mathbf{K}} = \frac{N_c}{N} \sum_{\tilde{\mathbf{k}}} t(\mathbf{K} + \tilde{\mathbf{k}})$

- **Self-energy** $\Sigma(\mathbf{k}, z) = \Sigma_c(\mathbf{K}, z) + \delta\Sigma(\mathbf{K}, \tilde{\mathbf{k}}, \omega)$

Dynamical Cluster Approximation

$$G_0(K,\omega) = \left[\left(\frac{N_c}{N} \sum_{\tilde{k}} \frac{1}{\omega + \mu - \varepsilon_{K+\tilde{k}} - \Sigma_c(K,\omega)} \right)^{-1} + \Sigma_c(K,\omega) \right]^{-1}$$



QMC $\rightarrow \Sigma_c[G_0(K,\omega),U]$

- ✓ **Thermodynamic limit**
- ✓ **Non-local correlations**

Cluster in reciprocal space

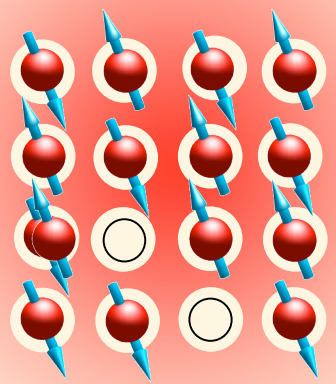
↓

- ✓ **Translational symmetry**

Other quantum cluster approaches: CDMFT (Kotliar *et al.*, PRL 2001); CPT (Gros *et al.*, Ann. Phys. 1996, Sènèchal *et al.*, PRL 2000); For a review see TM *et al.*, cond-mat/0404055

DCA/QMC: Numerically expensive

$$G_0(K,\omega) = \left[\left(\frac{N_c}{N} \sum_{\tilde{k}} \frac{1}{\omega + \mu - \varepsilon_{K+\tilde{k}} - \Sigma_c(K,\omega)} \right)^{-1} + \Sigma_c(K,\omega) \right]^{-1}$$



QMC $\rightarrow \Sigma_c[G_0(K,\omega),U]$

Numerical expense ~$(N_c N_l)^3$

Cray X1 @ CCS ORNL

- **Powerful processors**
- **Large memory bandwidth**
- **Runs at ~50% efficiency**

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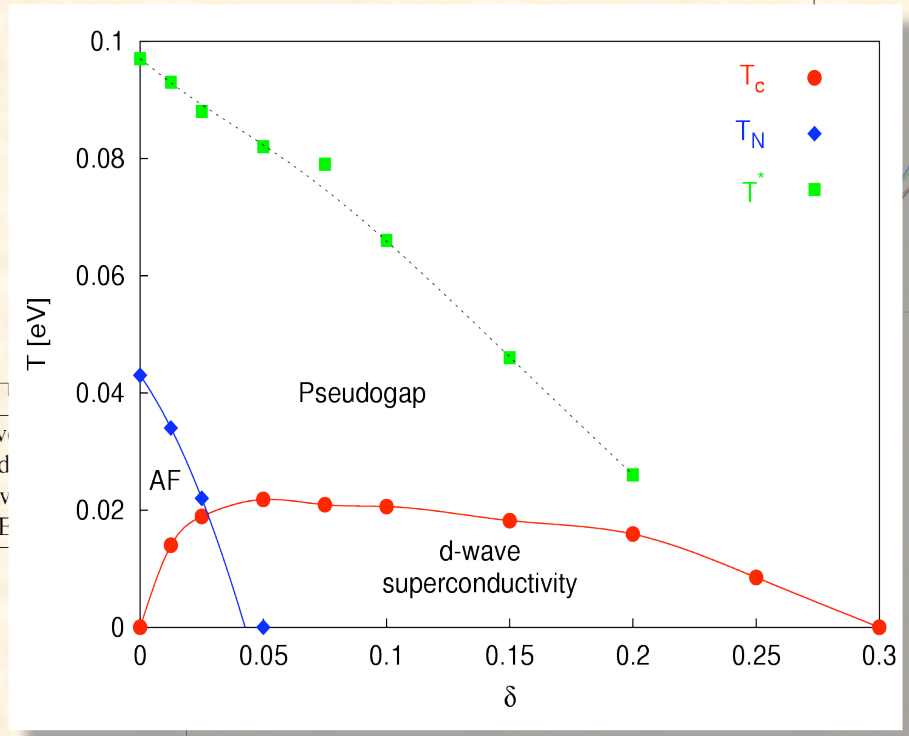
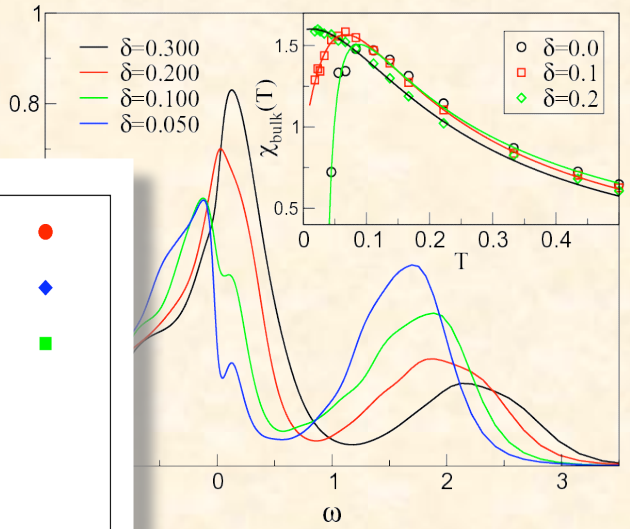
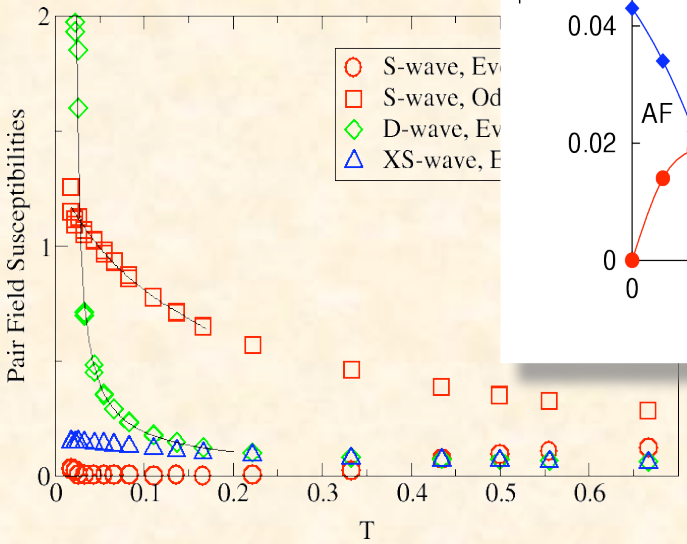
4-site cluster DCA - 2D Hubbard model

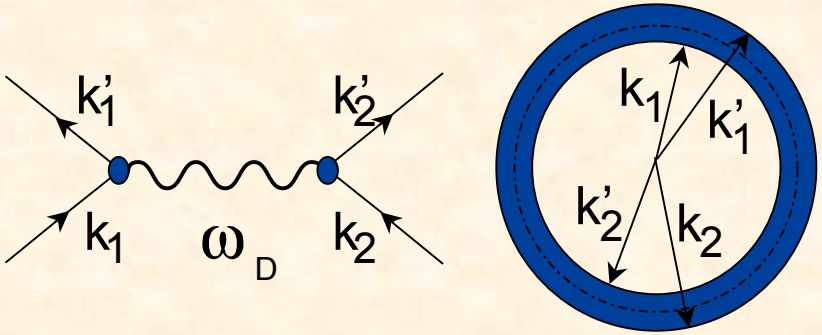


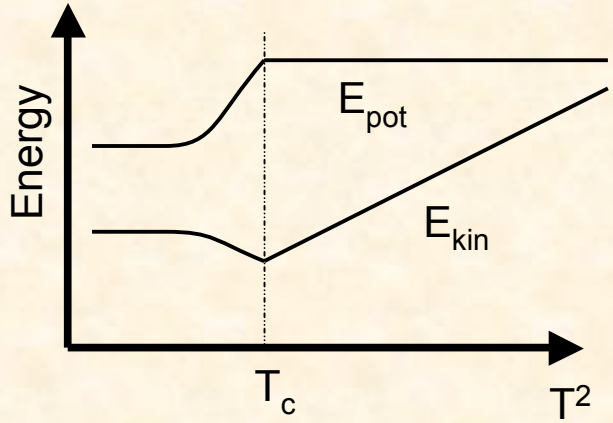




Superconducting transition: Energies

BCS (conventional) SC:

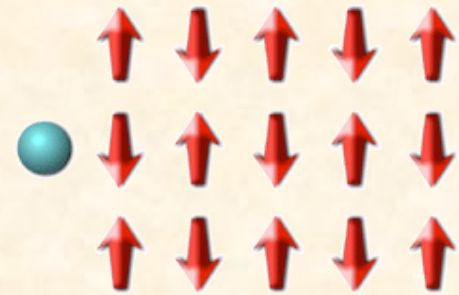




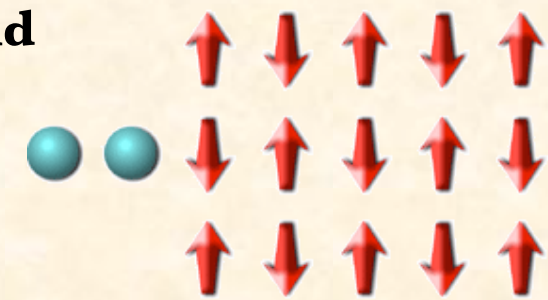
Pairing due to pot. energy gain

Cuprate (unconventional) SC:

Single hole in AF background

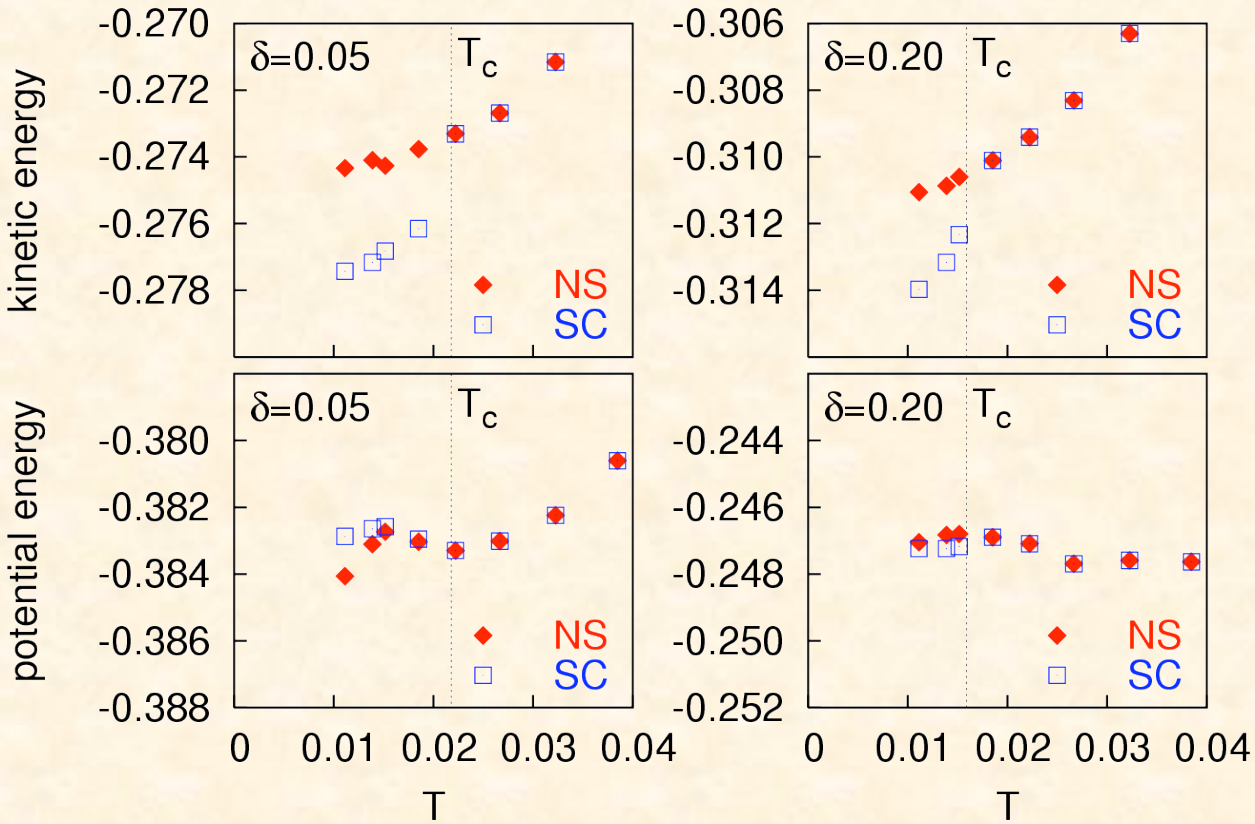


Two holes in AF background



Pairing due to kinetic energy gain

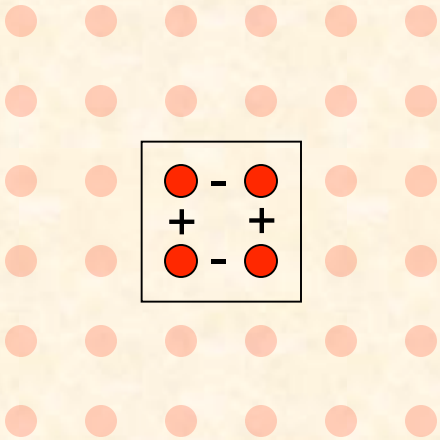
Superconductivity with kinetic energy gain



- **Kinetic energy is lower in superconducting state**
- **Consistent with experiments** (Molegraf et al., Science 2002)

But …

- **Antiferromagnetism**
  - **Finite T order in contradiction to Mermin-Wagner theorem**
- **Superconductivity**
  - **N_c=4 results represent mean-field result for d-wave order**
  - **No fluctuations of d-wave order parameter included**



- **Questions:**
  - **KT transition to d-wave super-conductivity in larger clusters ?**
  - **Exact limit $N_c \rightarrow \infty$?**

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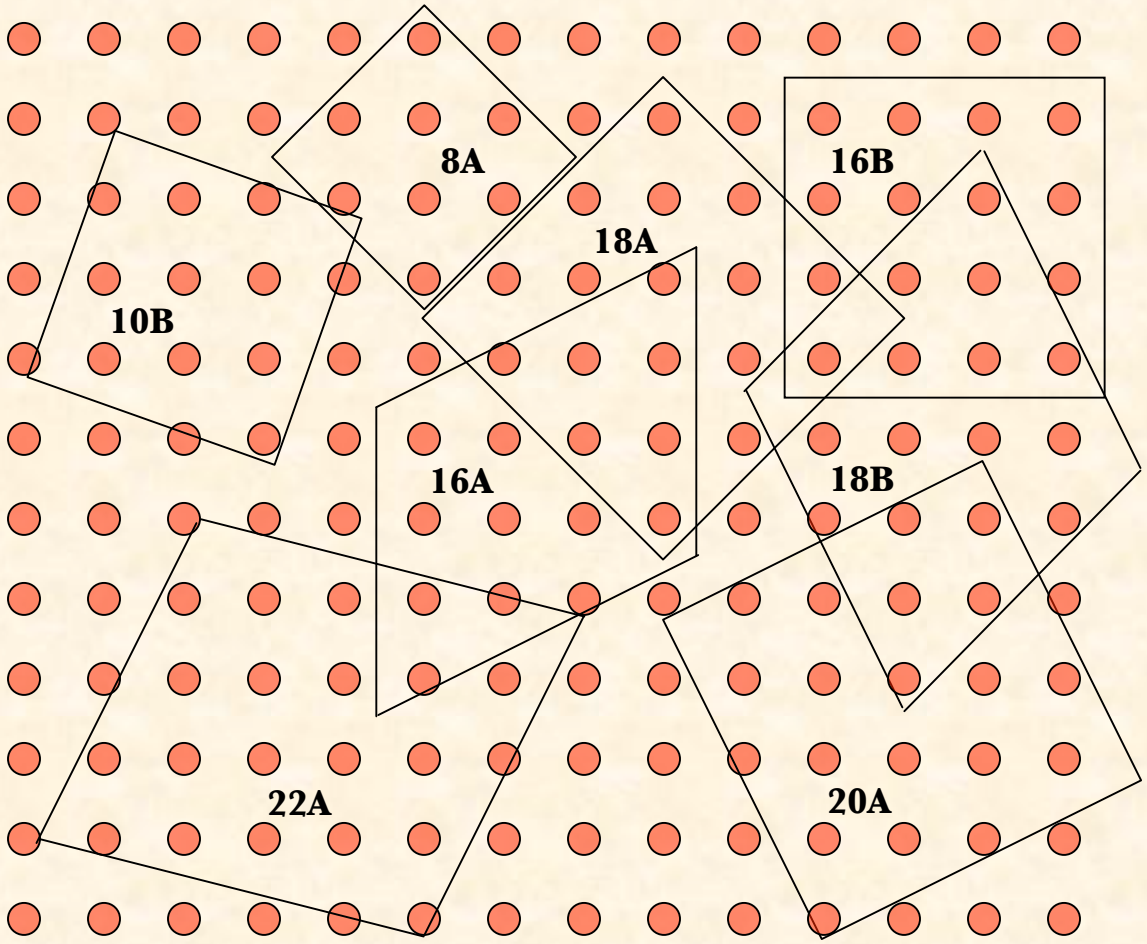
Larger (Betts) clusters

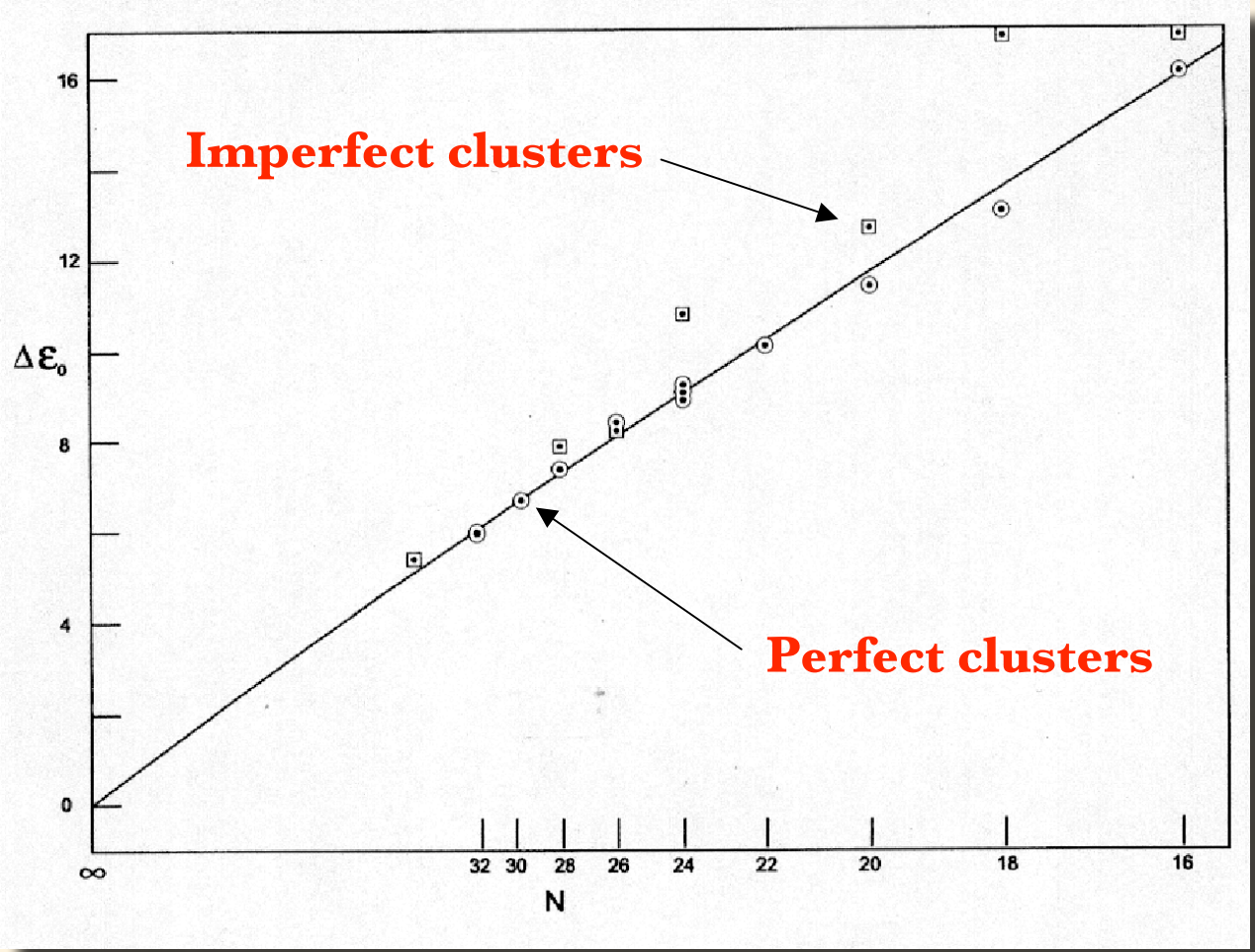


Selection criteria:

(Betts, Can. J. Phys. 1999)

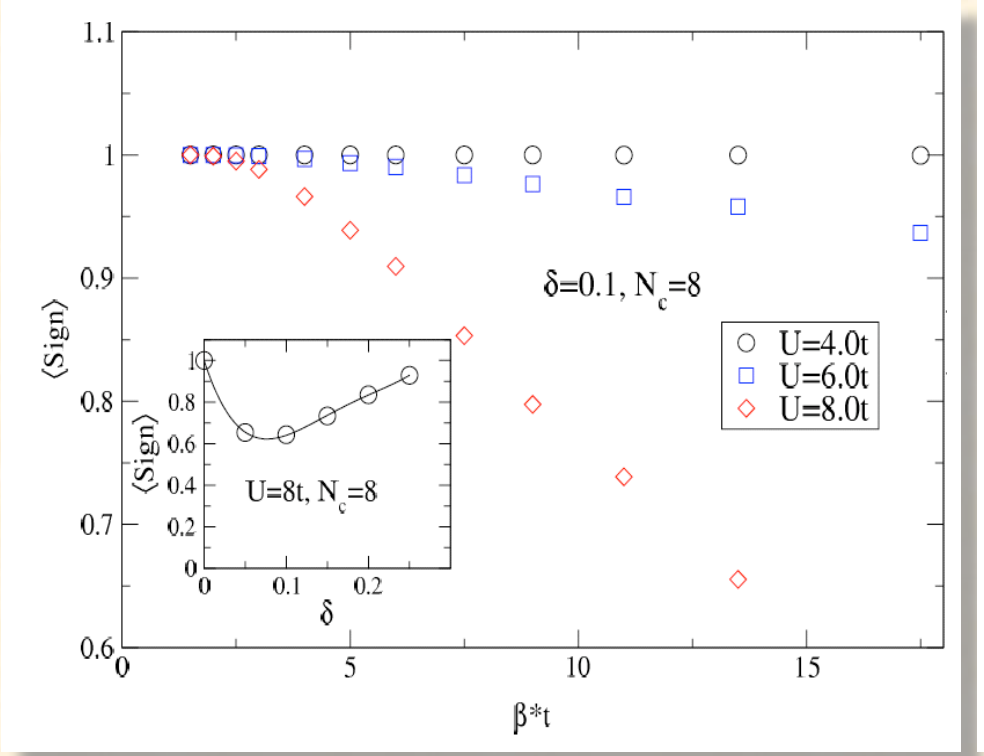
- Symmetry
- Squareness
- Neighbors in a given shell

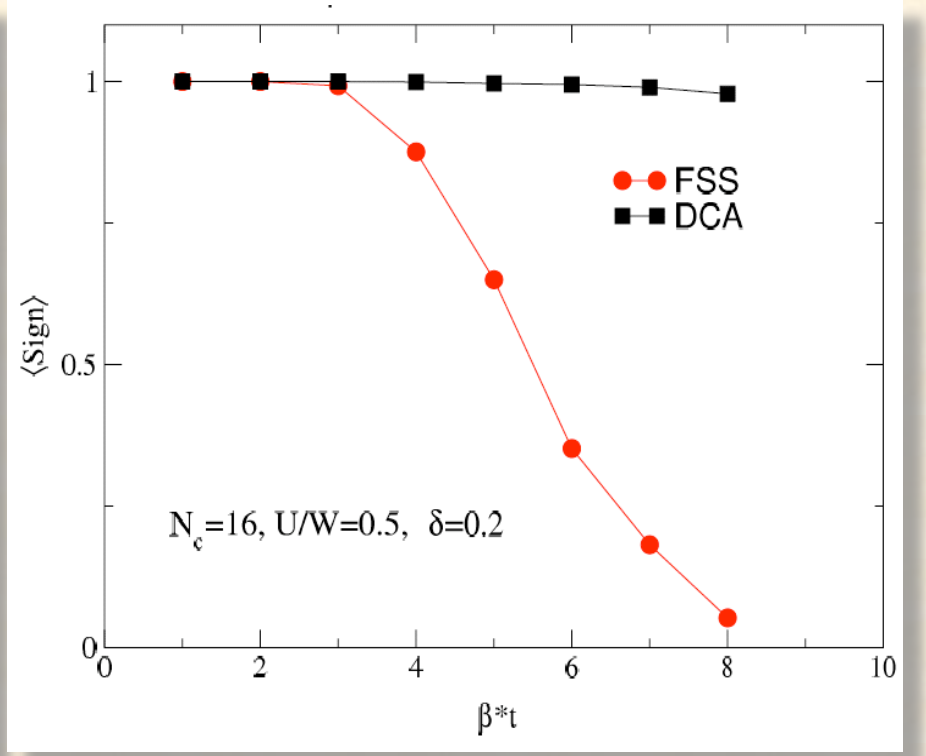
Groundstate energy of 2D S=1/2 Heisenberg AF



(Betts, Can. J. Phys. 77, 353)

QMC sign problem: DCA vs. FSS





- **Sign problem in DCA/QMC**
- **Much weaker than in finite size simulations**

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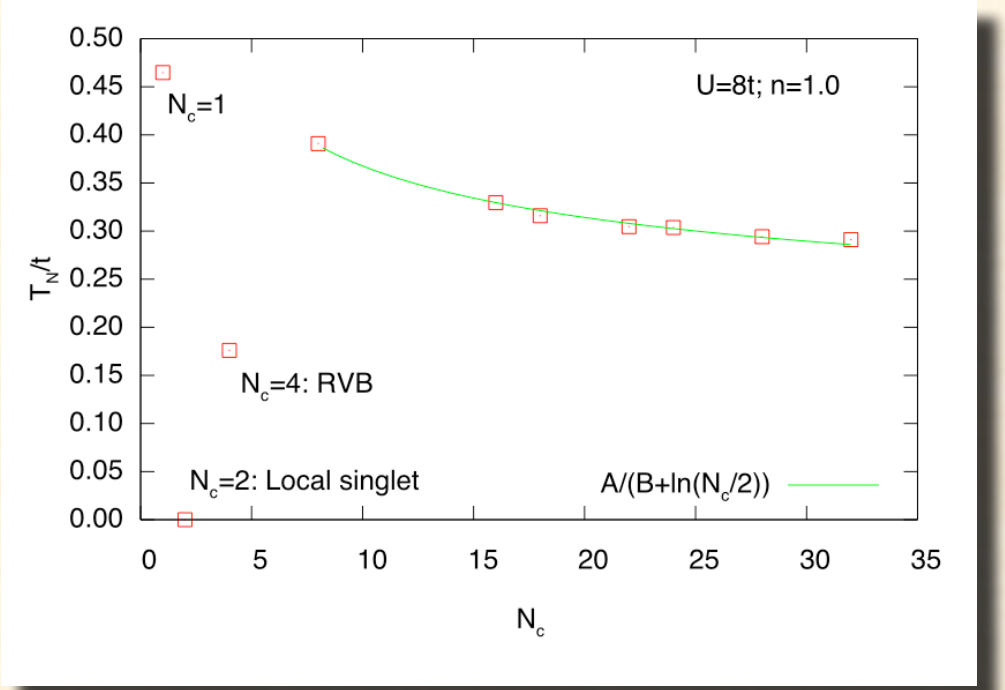
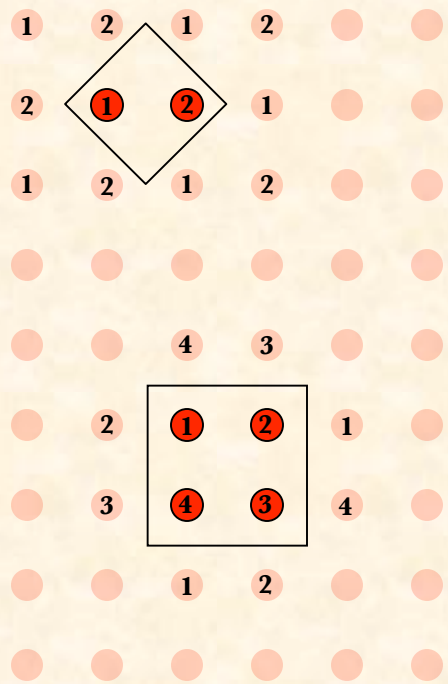
Antiferromagnetism: Cluster size dependence





Nc=2:

1 neighbor

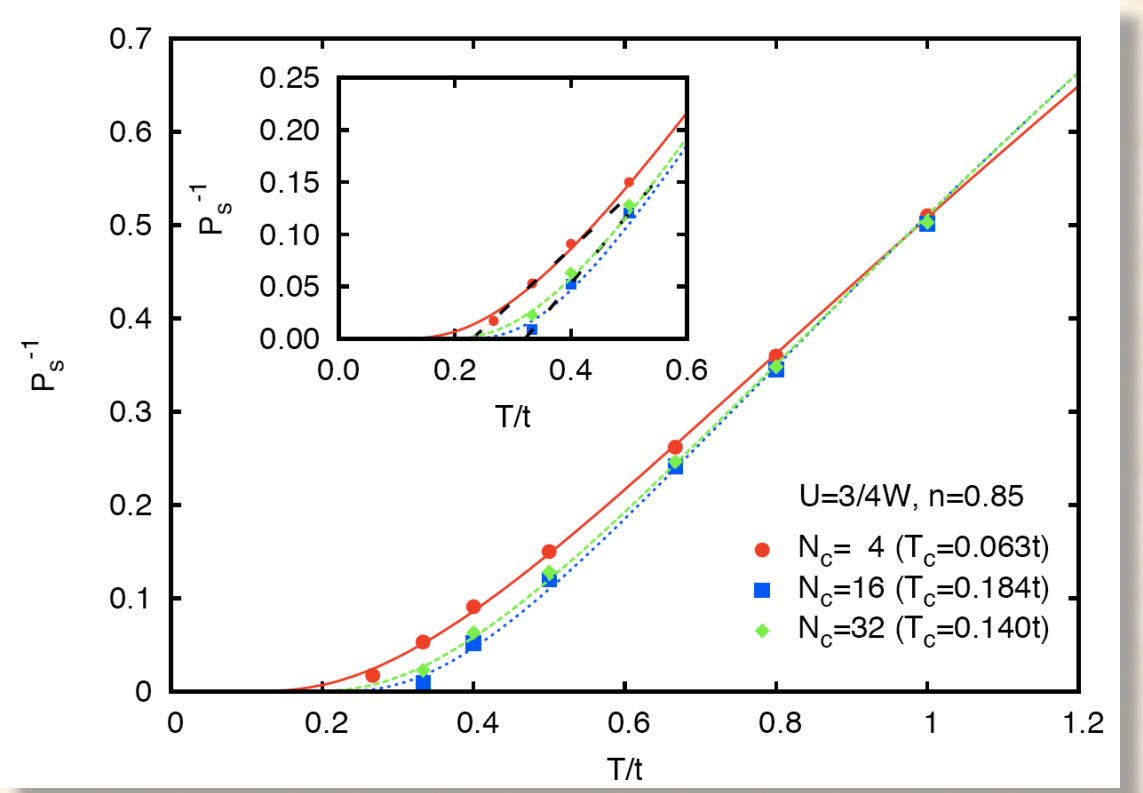
Nc=4:

2 neighbors

- $T_N \rightarrow 0$ logarithmically with $N_c \rightarrow \infty$ (since AF correlations build exponentially with decreasing T)

KT superconducting transition with DCA?

- **Test DCA on 2D attractive Hubbard model** (*U*=-6*t*; *n*=0.85)



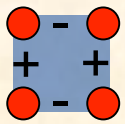
- **DCA reproduces KT transition to s-wave superconducting state**

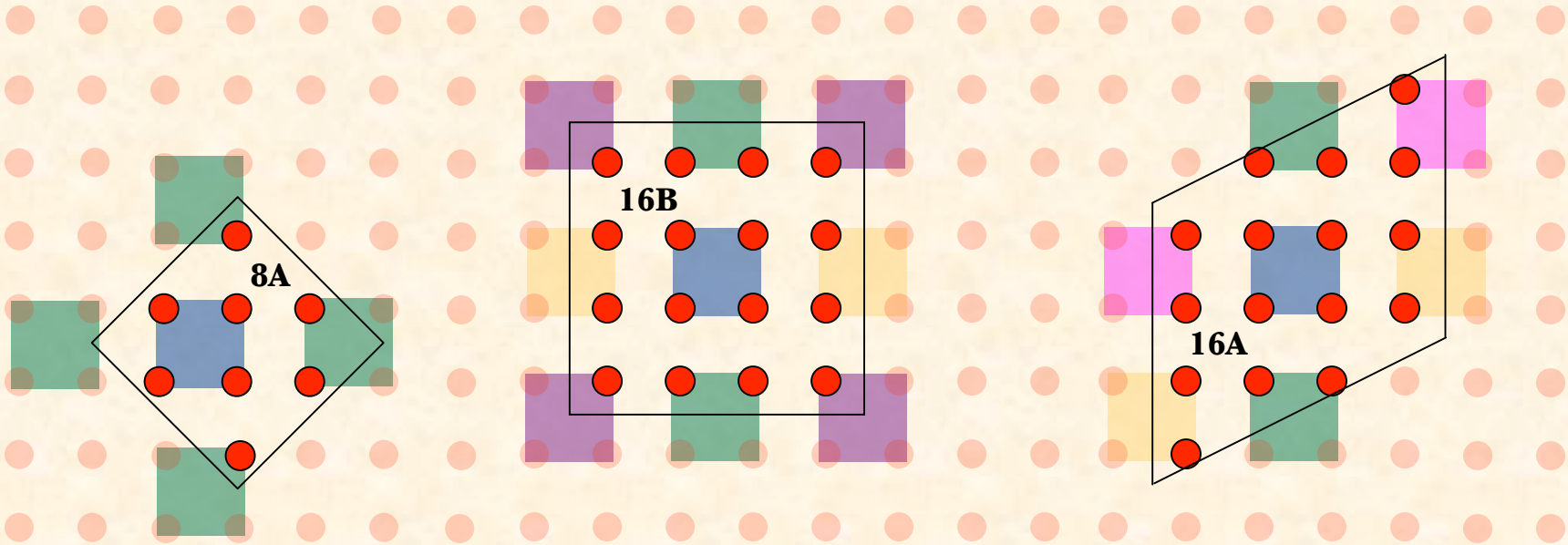
$$P_s = A\exp(2B/(T-T_c)^{0.5})$$

- **Mean-field divergence**
- **Results converge fast with N_c**

d-wave order in repulsive 2D Hubbard model

- **Dilemma:**
  - **d-wave order parameter non-local (4 sites)**
  - **Expect large size and geometry effects in small clusters**

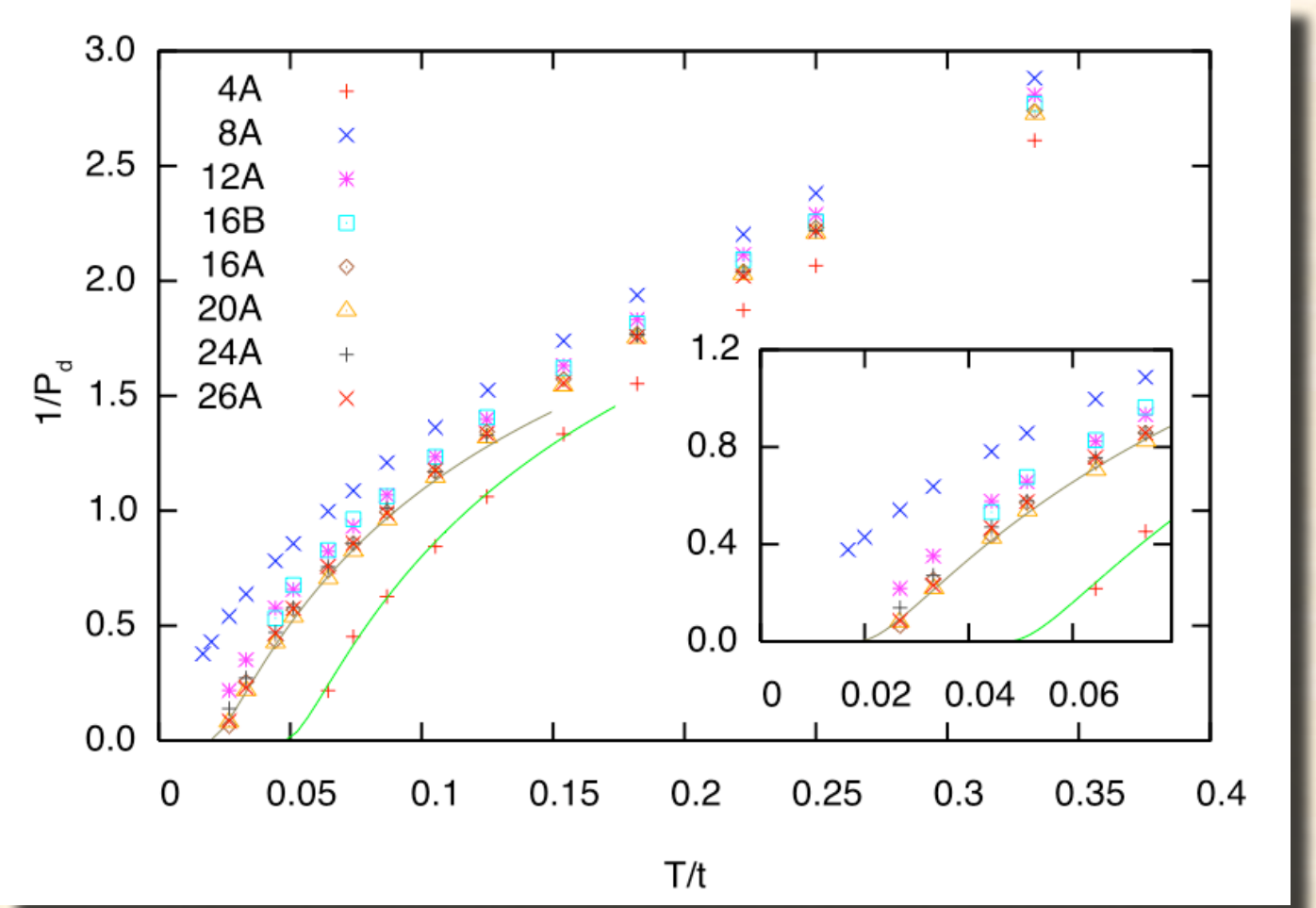




Number of independent neighboring d-wave plaquettes:

$Z_d=1$ $Z_d=2$ $Z_d=3$

d-wave pairing susceptibility (U=4t; n=0.90)



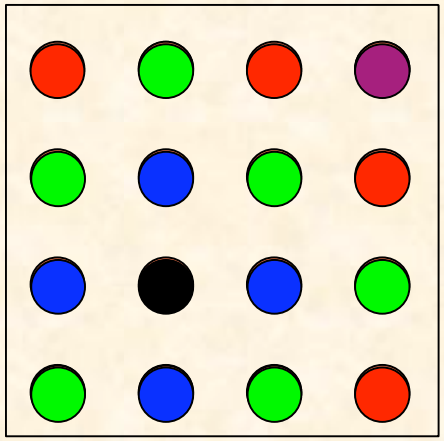
Cluster	Z_d
4A	0(MF)
8A	1
12A	2
16B	2
16A	3
20A	4
24A	4
26A	4

$T_c \approx 0.025t$

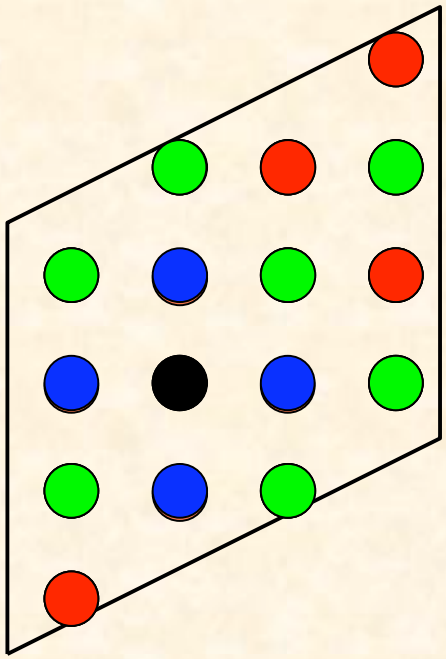
Conclusions - DCA/QMC for 2D Hubbard model

- N_c=4 mean field result = excellent description of cuprates
- AF vanishes logarithmically with increasing N_c
- Large size and geometry effects for d-wave SC in small clusters
- Finite T_c's in large enough clusters
- $T_c(N_c) \approx$ const. within error bars
- Cannot exclude $T_c = T_c^* + a/\ln(N_c)$ (even with $T_c^*=0$)
- Future: Phonons, frustration, disorder

Betts clusters: Neighbor shells

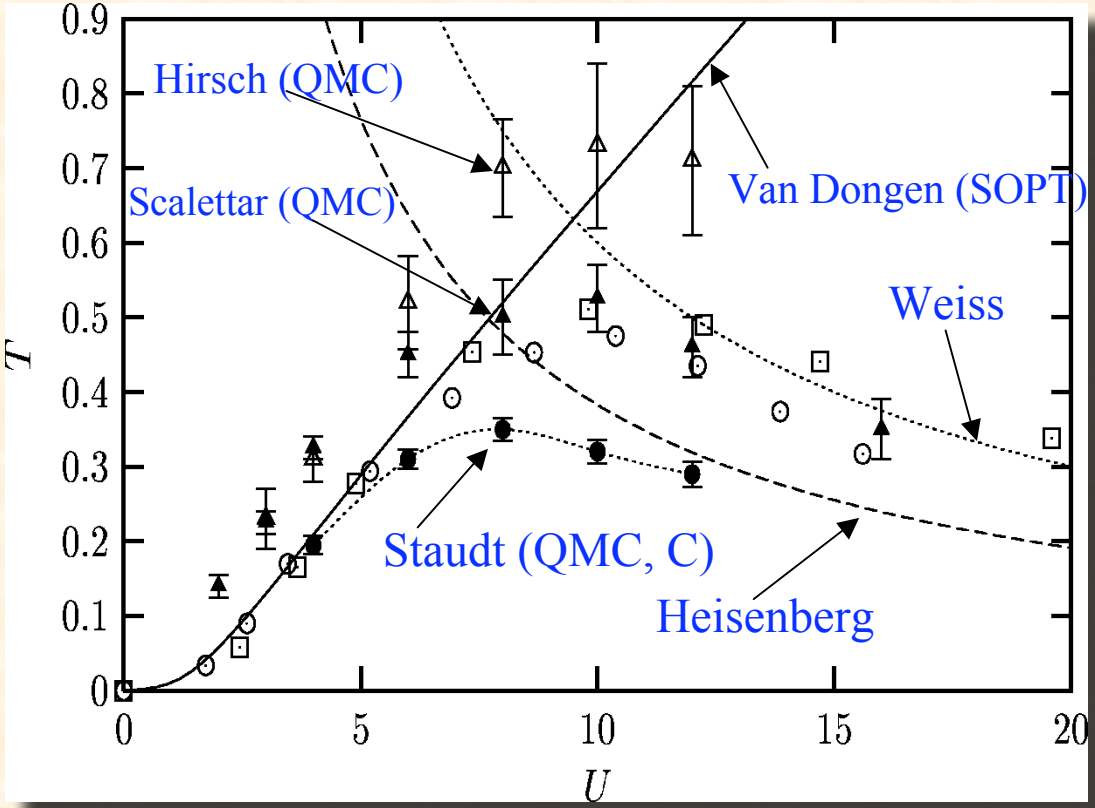


16B	
n	#
0	1
1	4
2	6
3	4
4	1



16A	
n	#
0	1
1	4
2	7
3	4

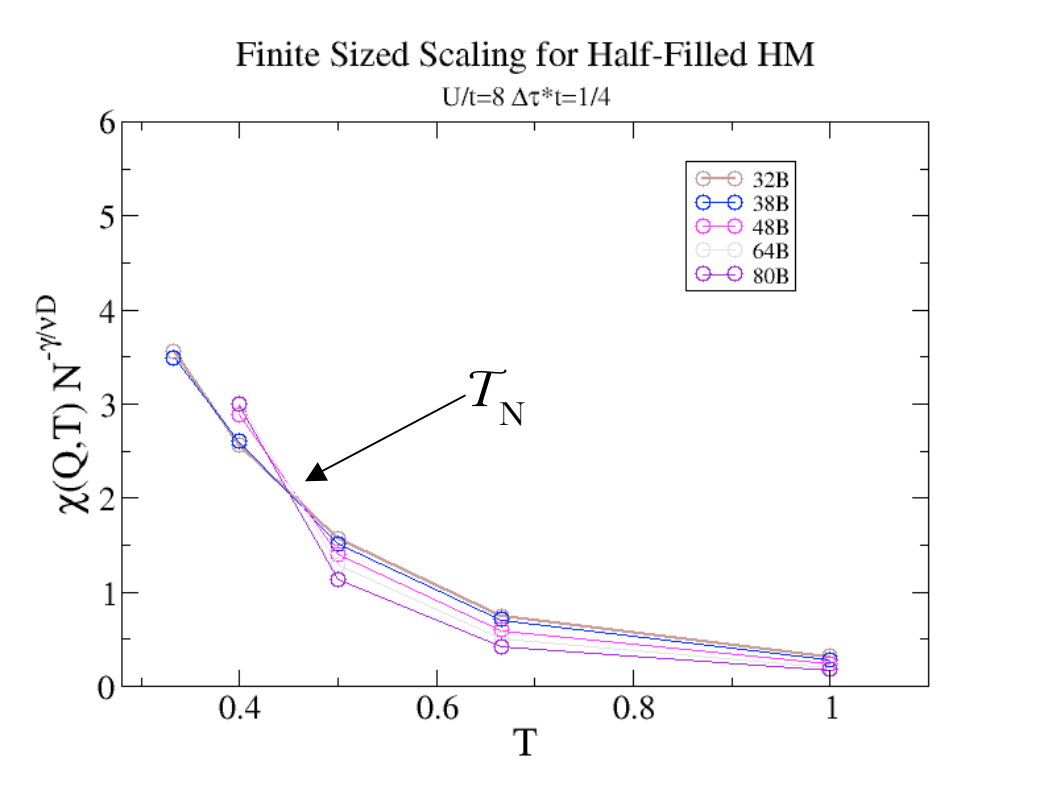
3D Hubbard model: Phase diagram



- **Different results do not agree**
- **Staudt: specific heat**
- **Hirsch and Scalettar: spin susceptibility**

(Staudt, EPJ 2000)

Betts clusters: Finite size scaling



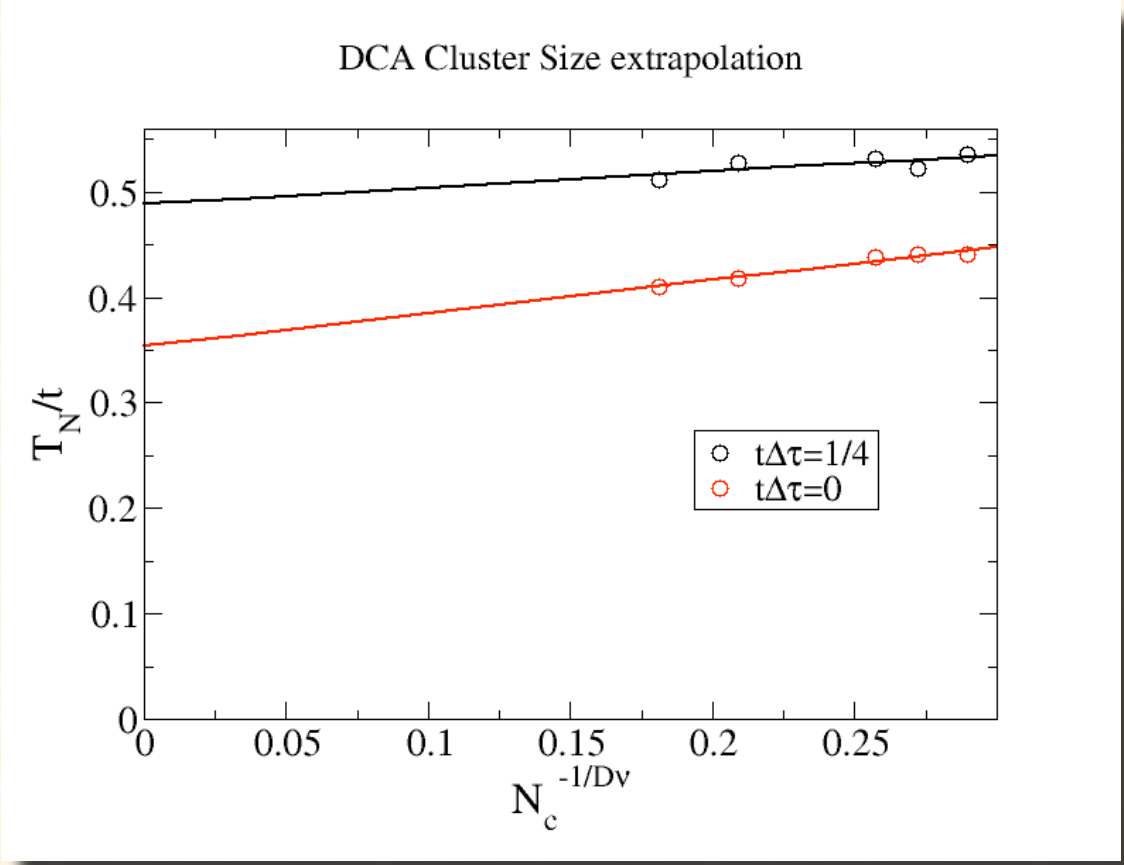
- **Scaling ansatz**

$$\chi \propto L^{\gamma/\nu} g(L^{1/\nu} t)$$

- **$\gamma \approx 1.38$** (Amit)
- **$\nu \approx 0.71$** (Sandvik, PRL 1998)
- **$T_N \approx 0.46 \pm 0.04$**

Preliminary (unpublished)

DCA: Cluster size scaling



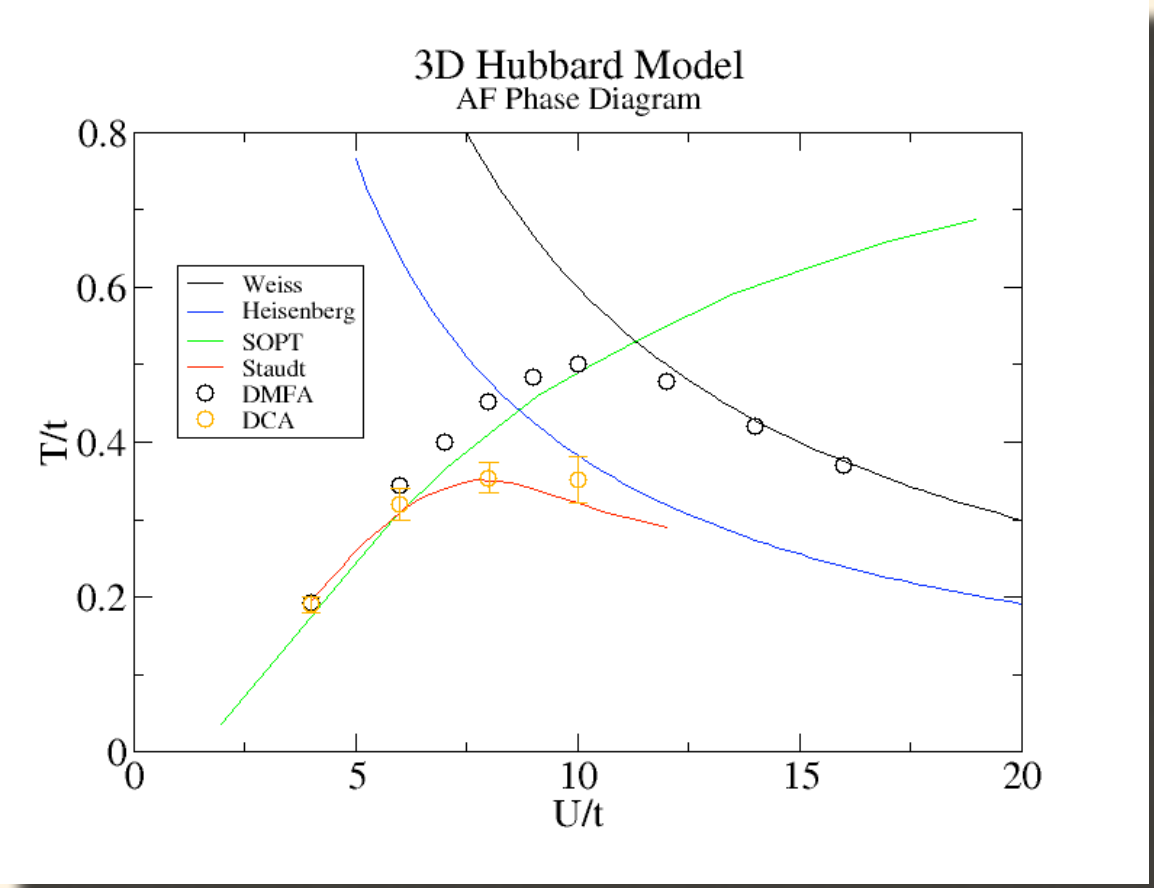
- **Scaling**

$$\xi(T_{\mathrm{N}}) = L$$
$$T_{\mathrm{N}}(L_c) = T_{\mathrm{N}}(\infty) + aL_c^{-1/\nu}$$

- **$T_N(\Delta\tau=1/4) \approx 0.48 \pm 0.04$**

Preliminary (unpublished)

3D Hubbard model: Phase diagram



- **Results agree with Staudt's**
- **Previous QMC used clusters with N=1000**
- **Our results:**
  - **$N \leq 80$ (FSS) and**
  - **$N_c \leq 48$ (DCA)**

Preliminary (unpublished)

Dynamical Cluster Approximation: Locator approach

$$G(\mathbf{k}) = g(\mathbf{K}) + g(\mathbf{K})[\delta t(\mathbf{K}, \tilde{\mathbf{k}}) + \delta\Sigma(\mathbf{K}, \tilde{\mathbf{k}})]G(\mathbf{k})$$

$$g(\mathbf{K}) = [z - \bar{\epsilon}_{\mathbf{K}} - \Sigma_c(\mathbf{K}, z)]^{-1}$$

Neglect inter-cluster correlations

$$G(\mathbf{k}) = [g(\mathbf{K})^{-1} - \delta t(\mathbf{K}, \tilde{\mathbf{k}})]^{-1}$$

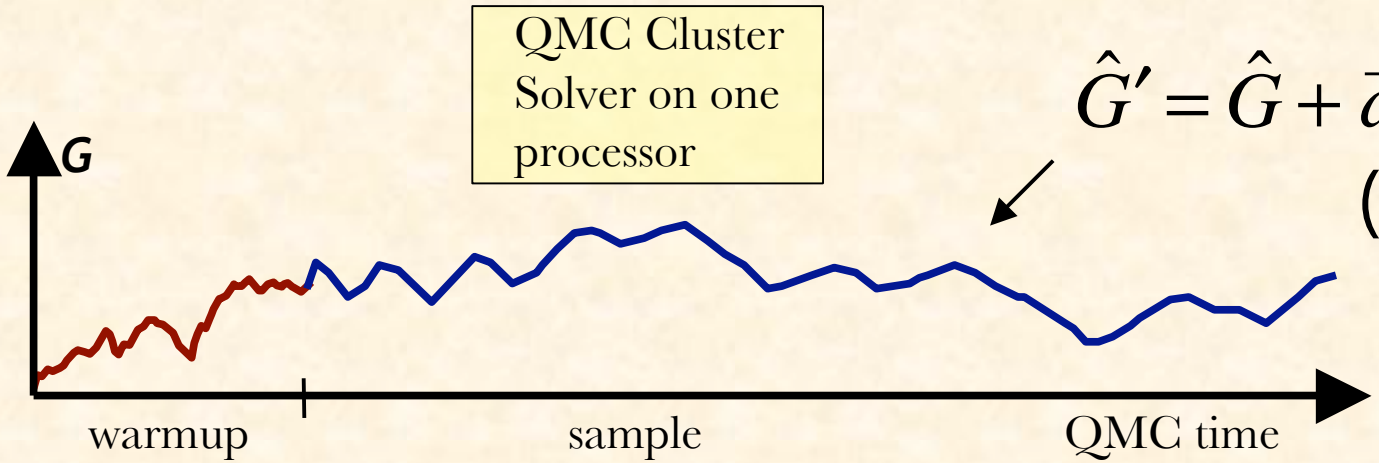
Self-energy may be calculated in effective cluster problem:

$$\Sigma_c(\mathbf{K}, z) = \mathcal{F}[\bar{G}(\mathbf{K}, z)]; \quad \bar{G}(\mathbf{K}) = \frac{N_c}{N} \sum_{\tilde{\mathbf{k}}} G(\mathbf{K} + \tilde{\mathbf{k}})$$

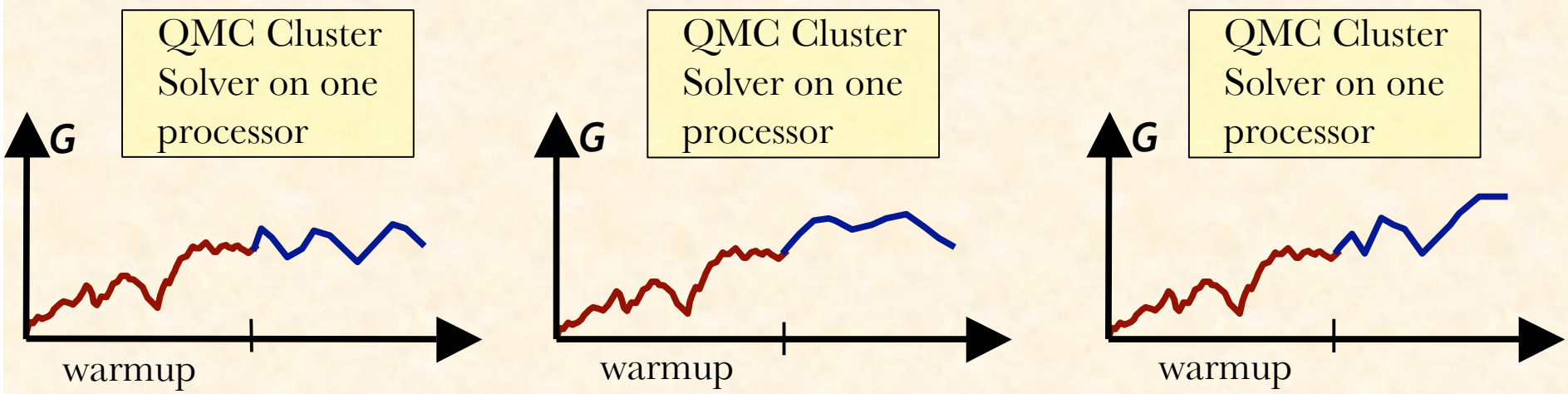
Green function localized on cluster

DCA/QMC Cluster solver

Serial:



$$\hat{G}' = \hat{G} + \vec{a} \otimes \vec{b}$$

(dger)

Perfectly parallel: