Does the 2D Hubbard describe high-temperature superconductors?

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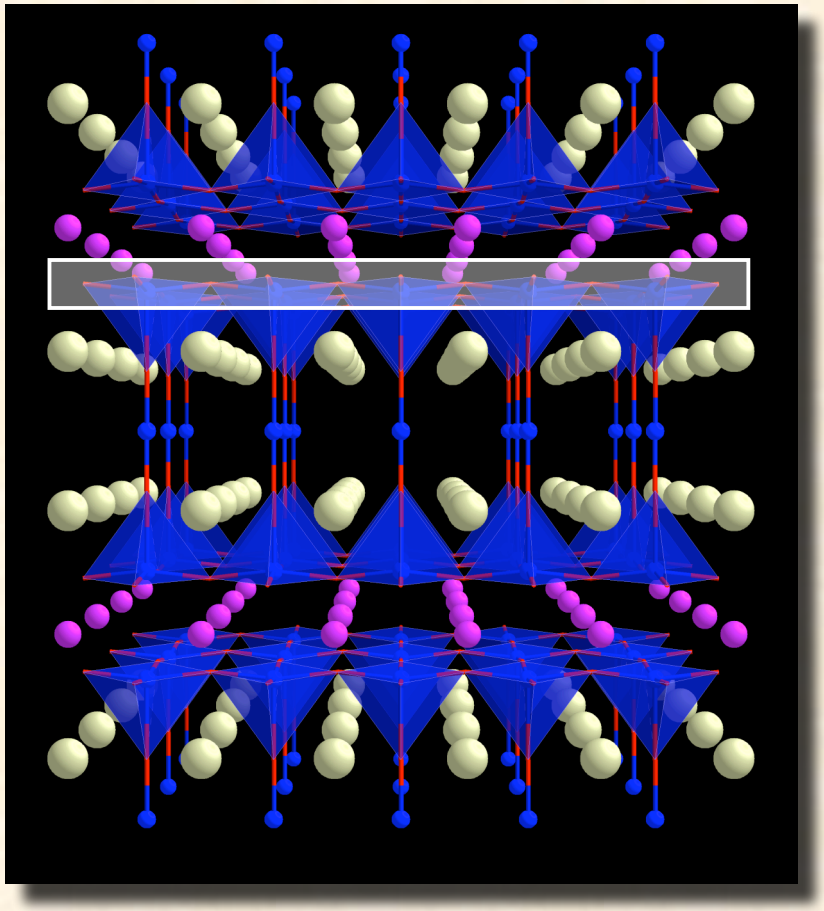
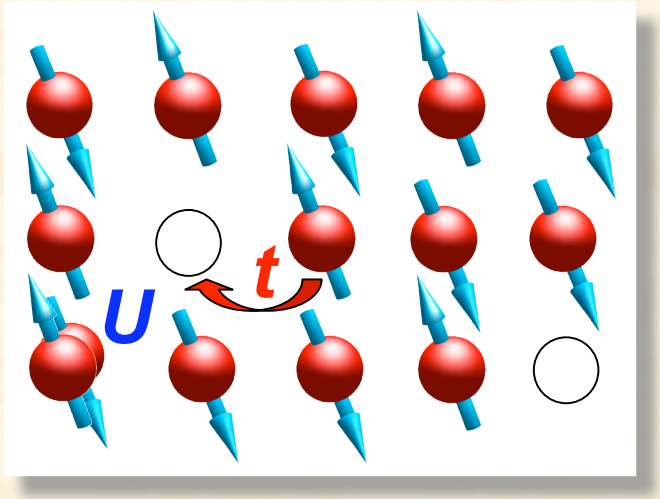
2D Hubbard model of HTSC





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

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

Search for superconductivity in 2D Hubbard model

- **Weak coupling (U/W << 1)**
  - **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 (W/U << 1)**
  - **Finite size simulations of t-J model → Groundstate superconducting**
    (Sorella, PRL 2002; Poilblanc, cond-mat 2002)
- **Intermediate coupling (W ≈U)**
  - **Inconclusive!**

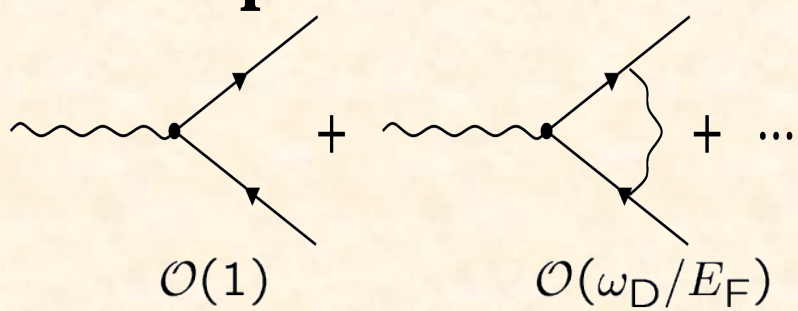
Small Parameter?

BCS (conventional) SC:

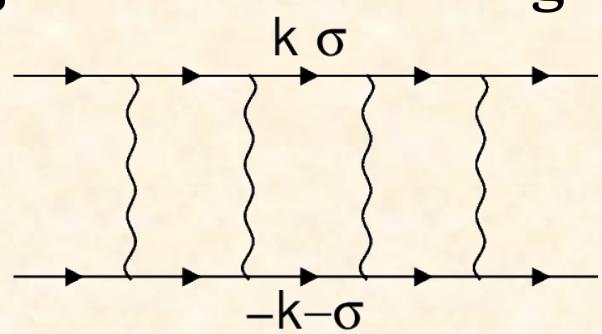
Small parameter:

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

Electron-phonon vertex:



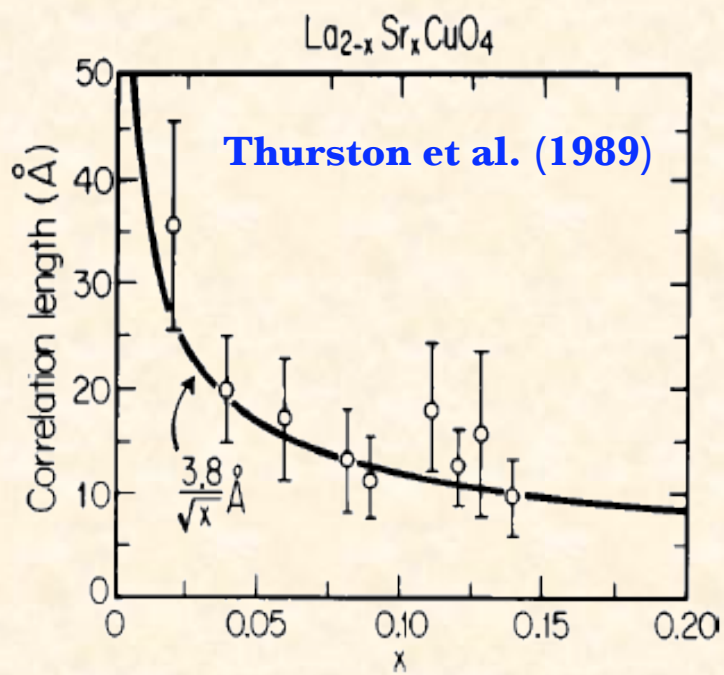
Neglect classes of diagrams:



Cuprate (unconventional) SC:

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

But in Cuprates:

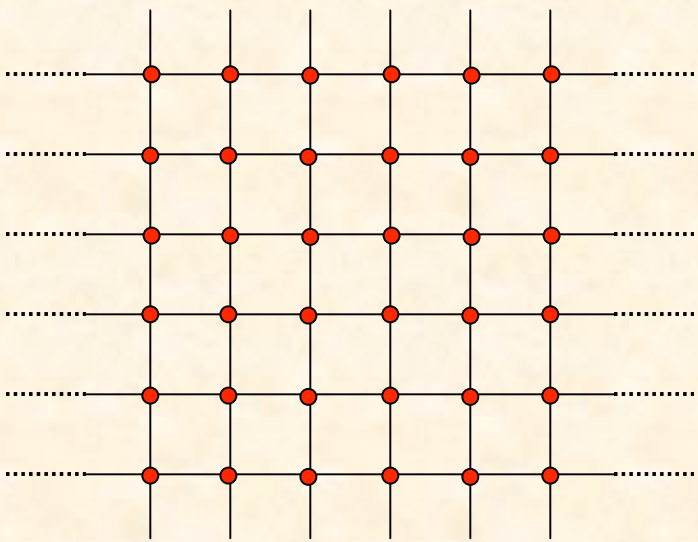


Short-ranged AF correlations

Quantum cluster approach for Hubbard model

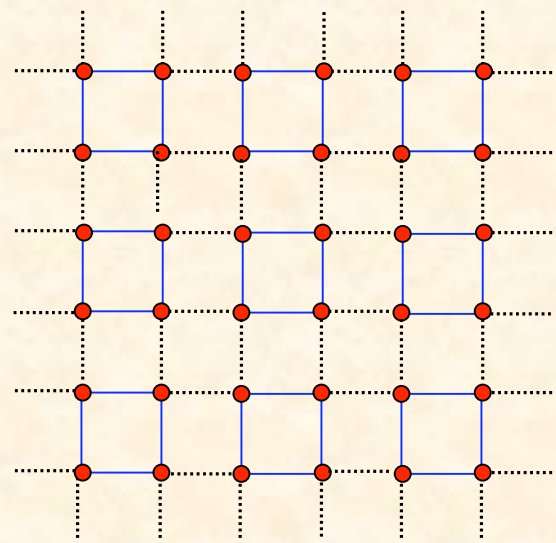
$$H = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

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



Treat exactly in infinite system

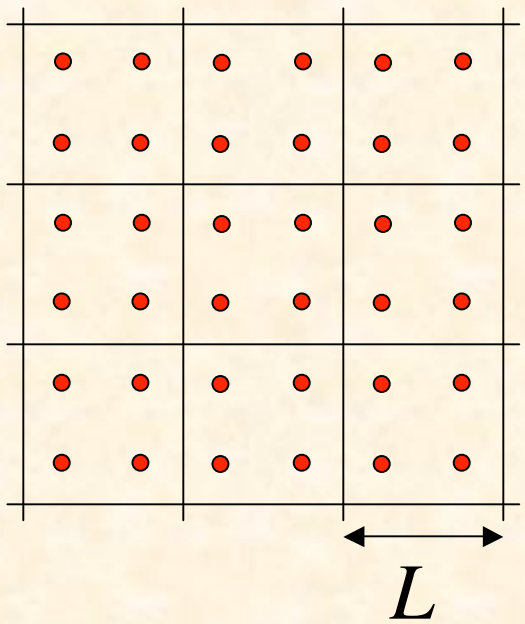
Potential energy: $\mathrm{Tr}(\mathbf{\Sigma G})$



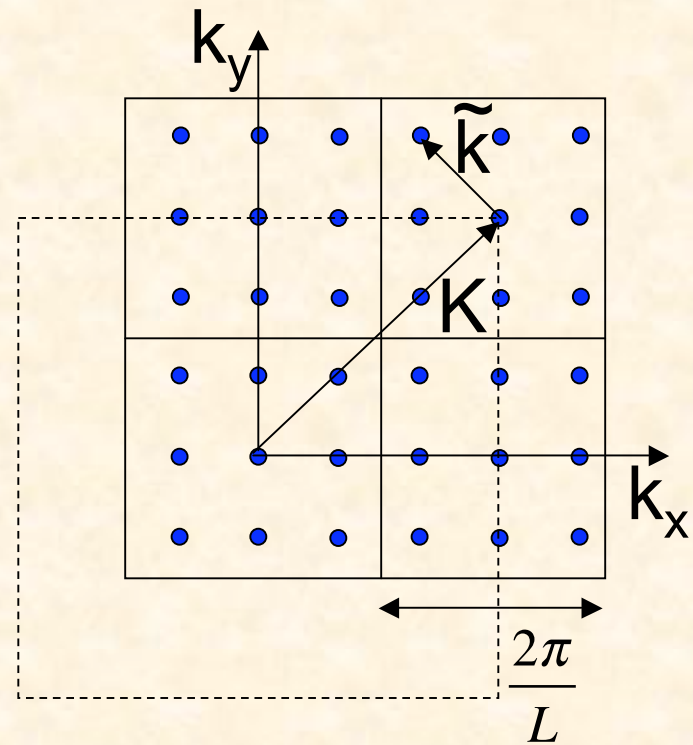
Cut off correlations beyond cluster

DCA: Coarse-graining

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



- **1st Brillouin zone**

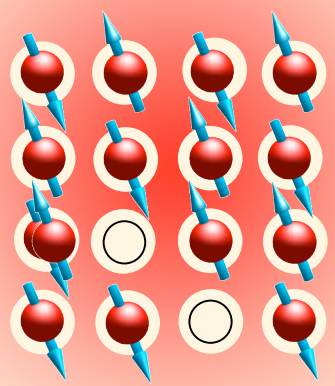


- **Neglect correlations between clusters →**

  Self-energy: $\Sigma\left(K+\tilde{k},\omega\right) \approx \Sigma\left(K,\omega\right)$

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**

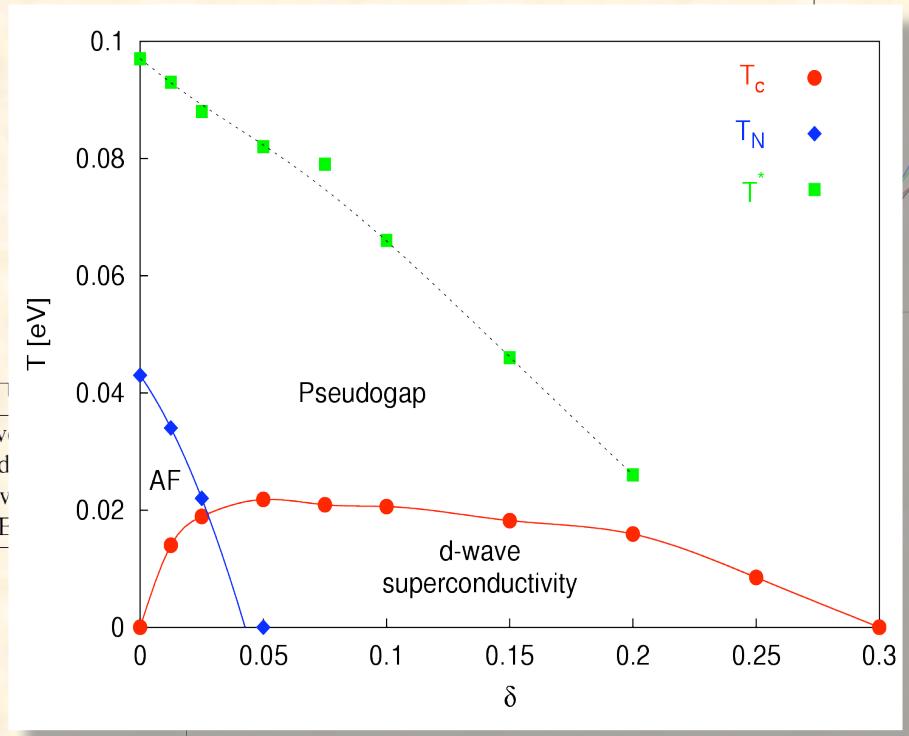
Cluster in reciprocal space

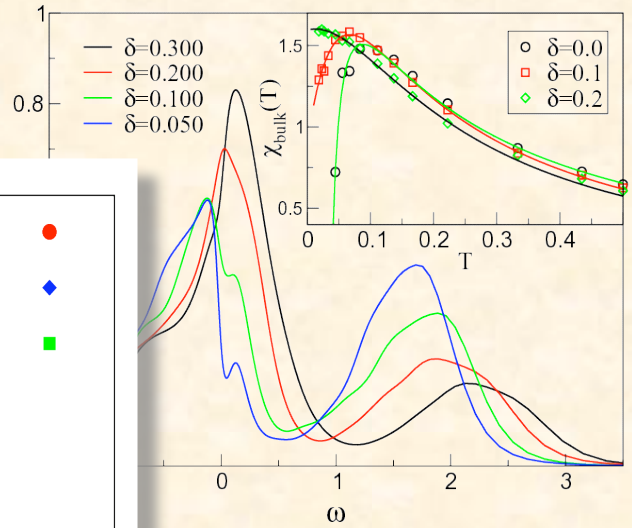
↓

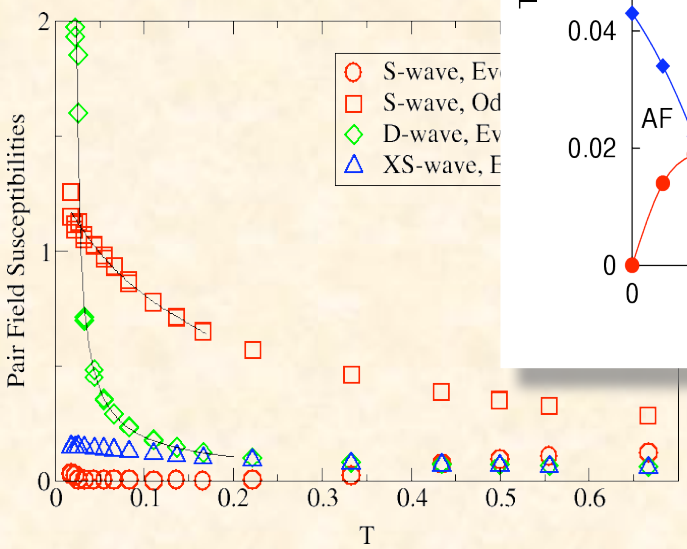
- ✓ **Translational symmetry**

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

4-site cluster DCA - 2D Hubbard model

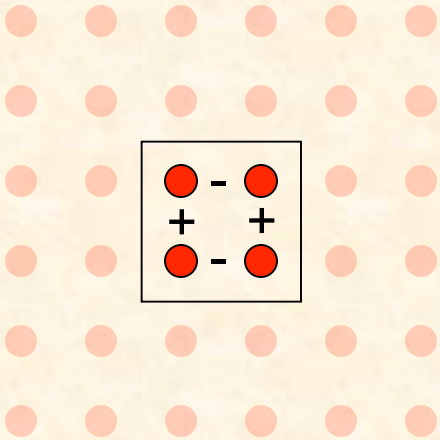






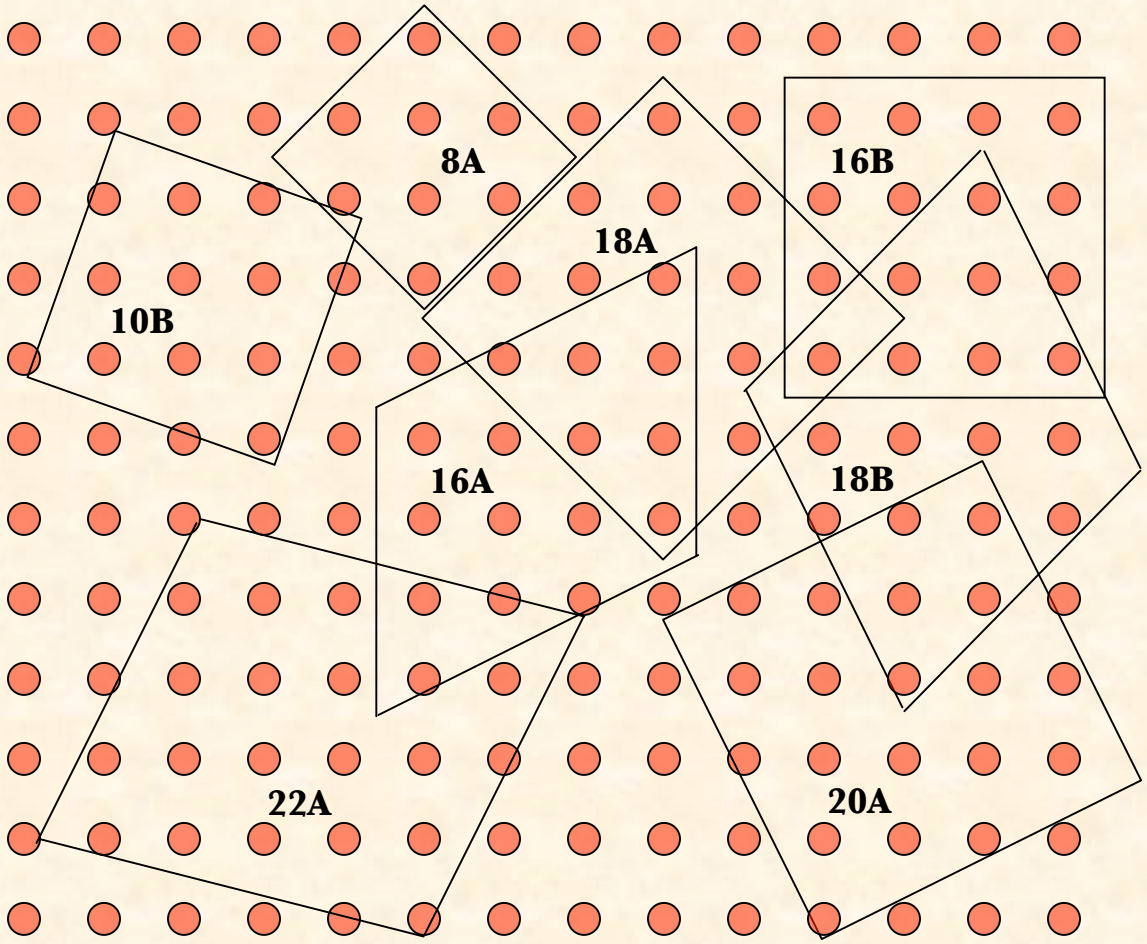
But …

- **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:**
  - **d-wave superconductivity in larger clusters ?**
  - **Exact limit $N_c \rightarrow \infty$?**

Larger (Betts) clusters

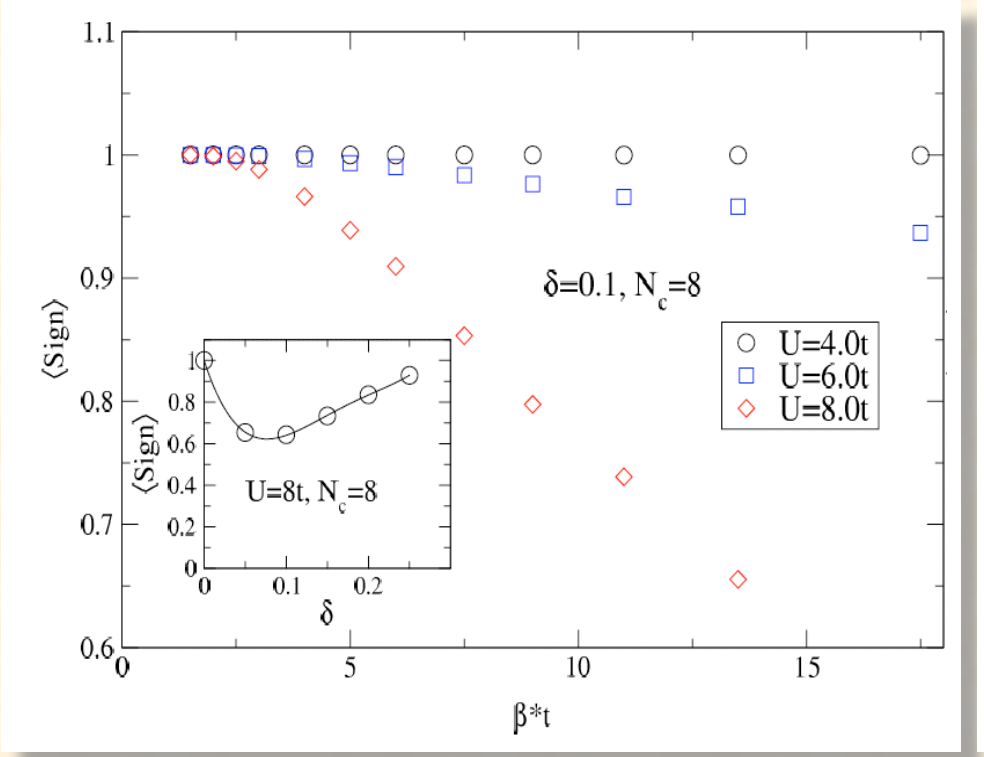


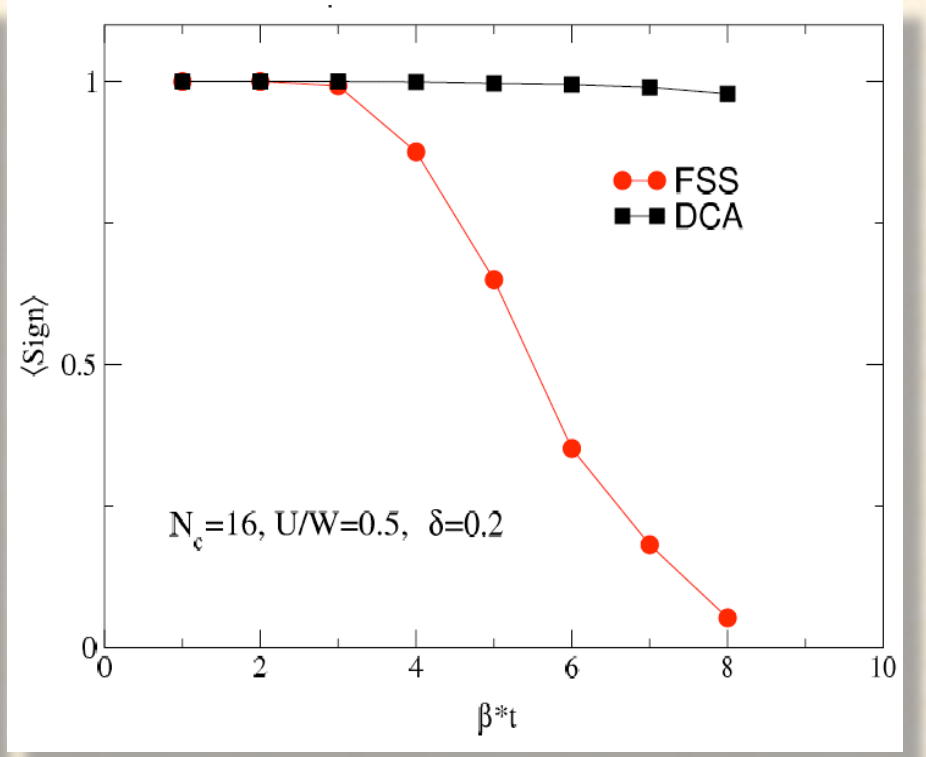
Selection criteria:

(Betts, Can. J. Phys. 1999)

- Symmetry
- Squareness
- Neighbors in a given shell

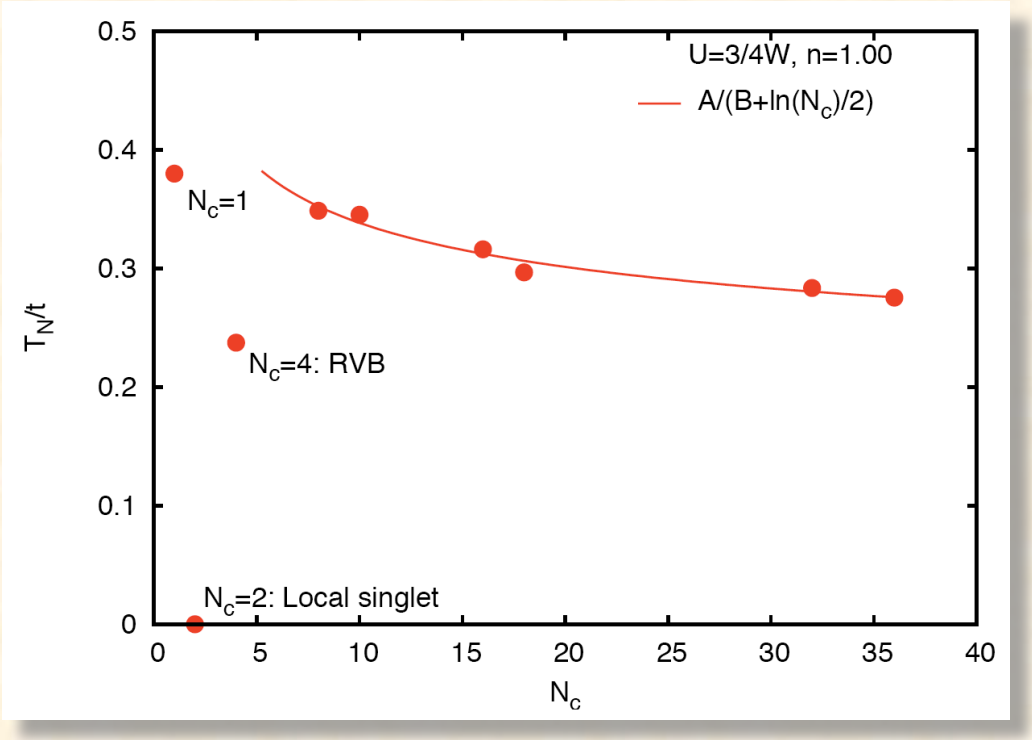
QMC sign problem: DCA vs. FSS

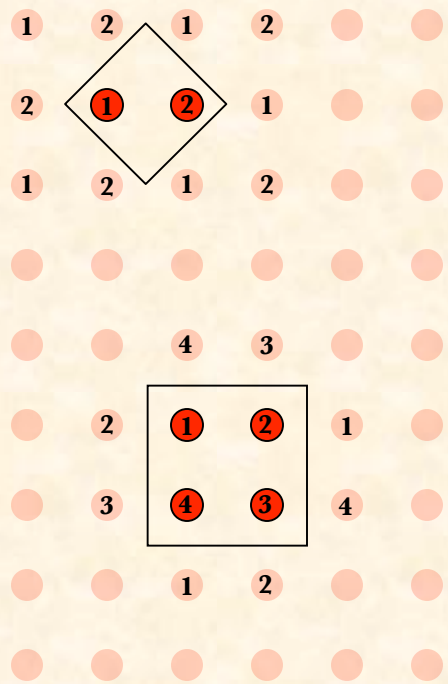




- **Sign problem in DCA/QMC**
- **Much weaker than in finite size simulations**

Antiferromagnetism: Cluster size dependence





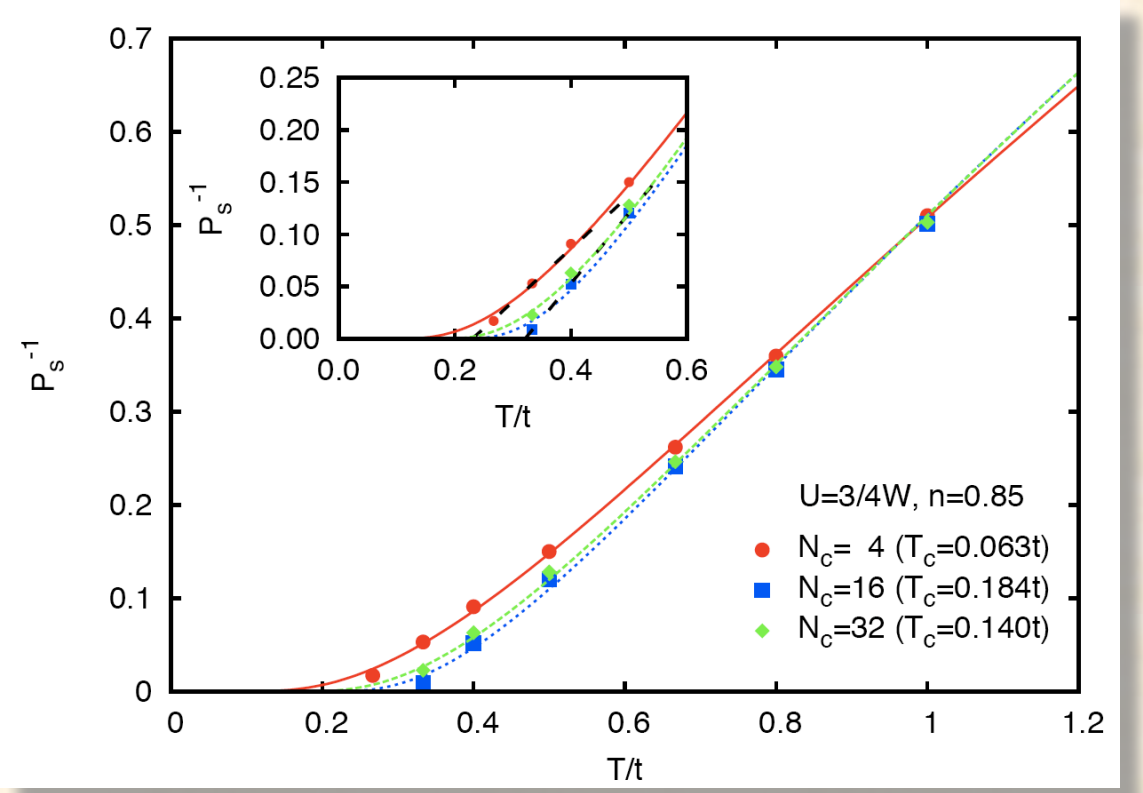
Nc=2:
1 neighbor

Nc=4:
2 neighbors

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

Kosterlitz-Thouless superconducting transition

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



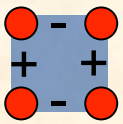
- **DCA reproduces KT transition to s-wave superconducting state**

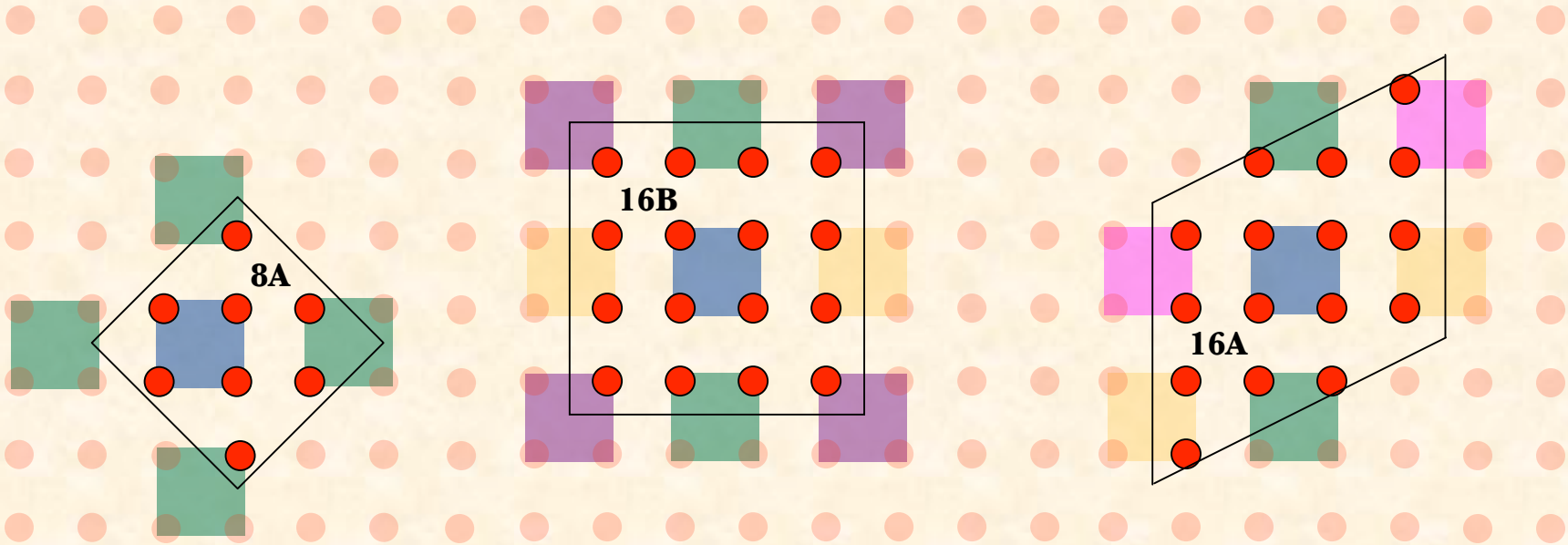
$$P_s = A\exp(2B/(T-T_c)^{0.5})$$

- **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**

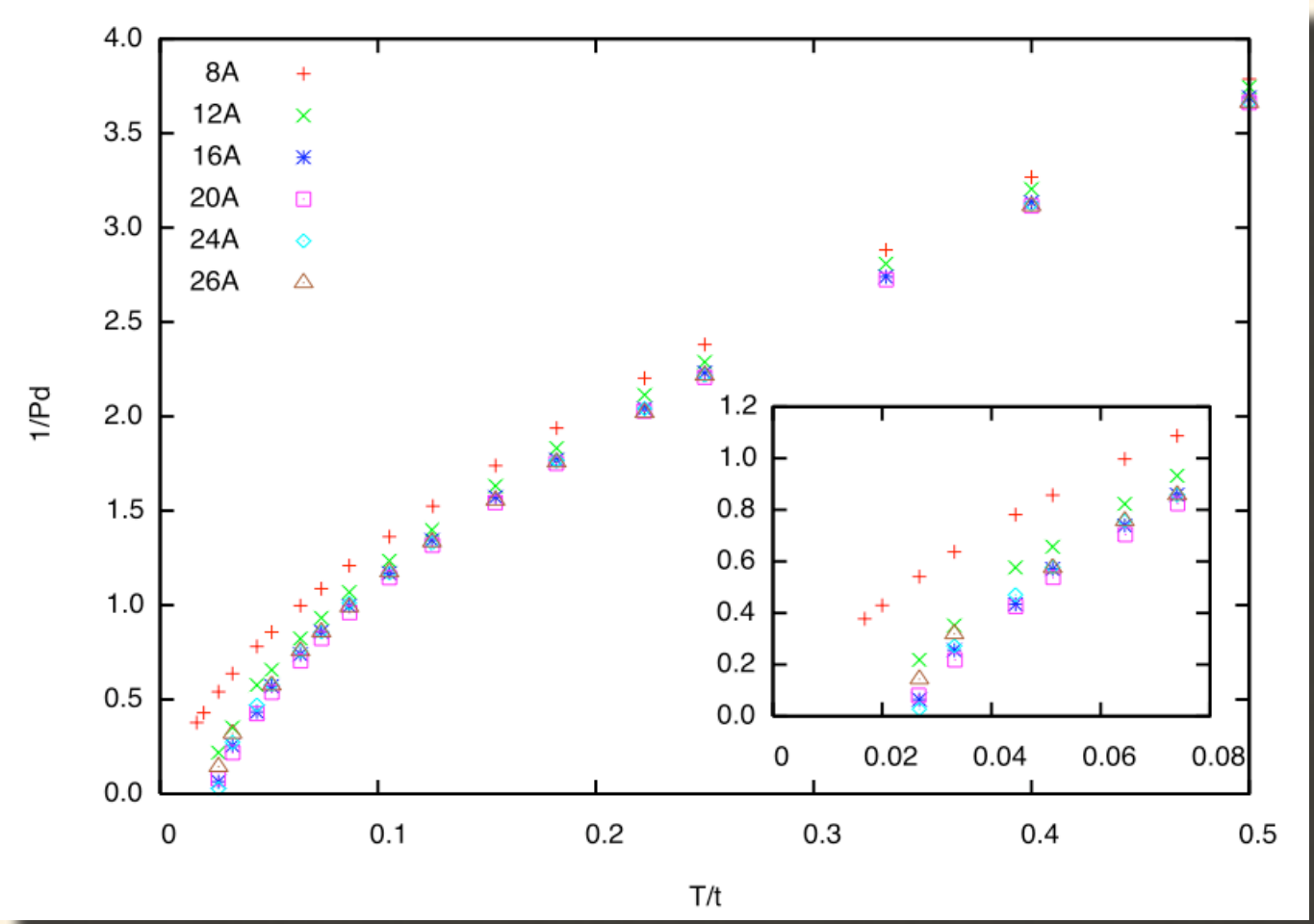




Number of independent neighboring d-wave plaquettes:

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

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



Cluster	Z_d
8A	1
12A	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 slowly 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 $T_c = T_c^* + \ln(f(N_c))$ (even with $T_c^* = 0$).
- Future: Phonons, frustration, disorder