On the nature of pairing in the cuprates

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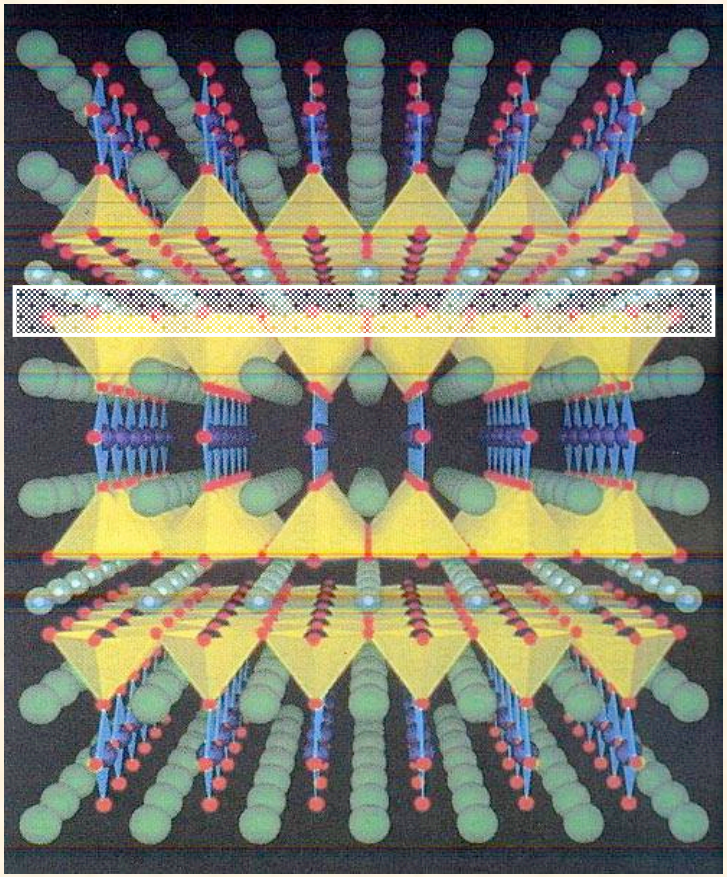
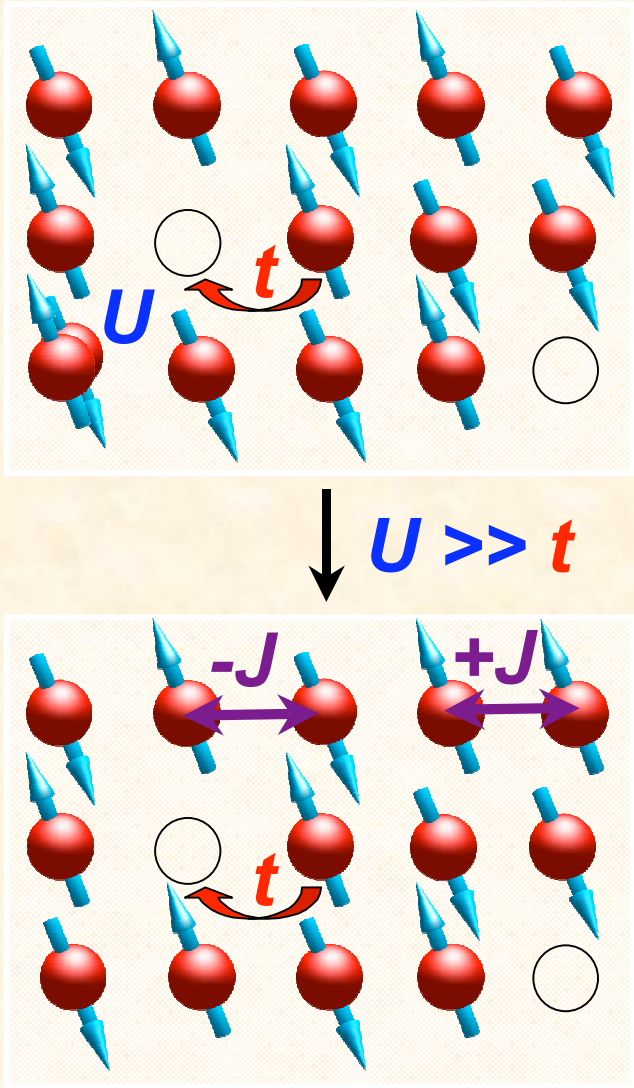
- *Models of HTSC*
- *4-site DCA results*
- *Nature of Pairing*
- *Larger clusters*

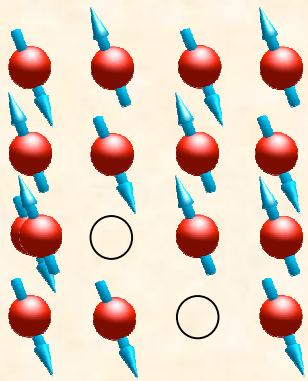
Hubbard and t-J models of HTSC





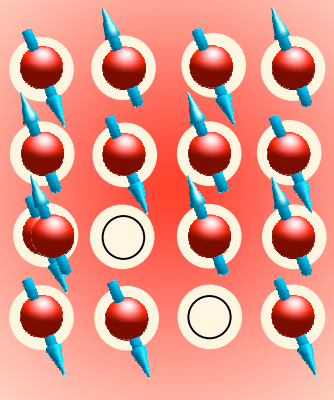
Quantum Cluster Approach

Finite size simulations



Dynamical mean field theory

✓ Non-local correlations

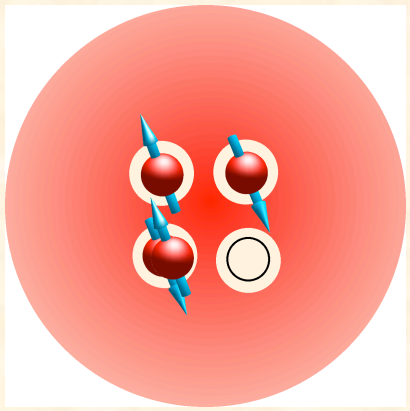


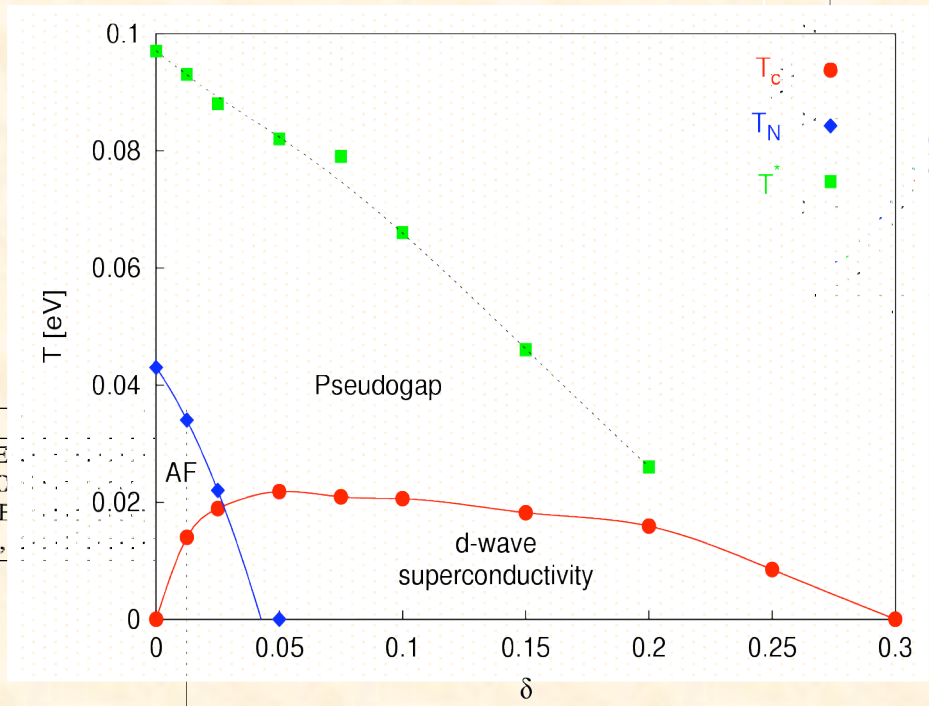
✓ Thermodynamic limit

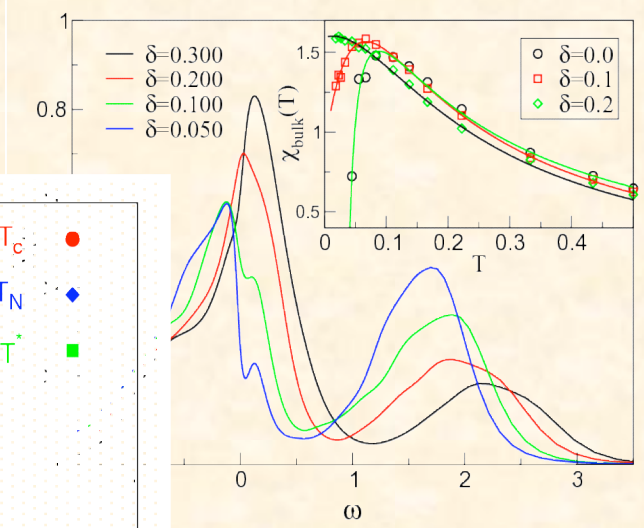
DCA: Coarse-grain momentum space

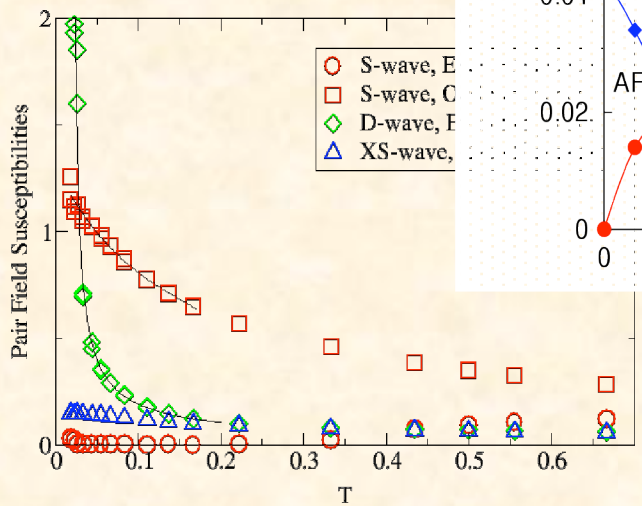
Cluster with periodic Boundary conditions

4-site cluster









Condensation energy

BCS superconductors:

Chester: condensation energy $\propto$ change in ion kinetic energy
(Chester, Phys. Rev., (1956))

Link: Pairing $\longleftrightarrow$ Electron - ion interaction

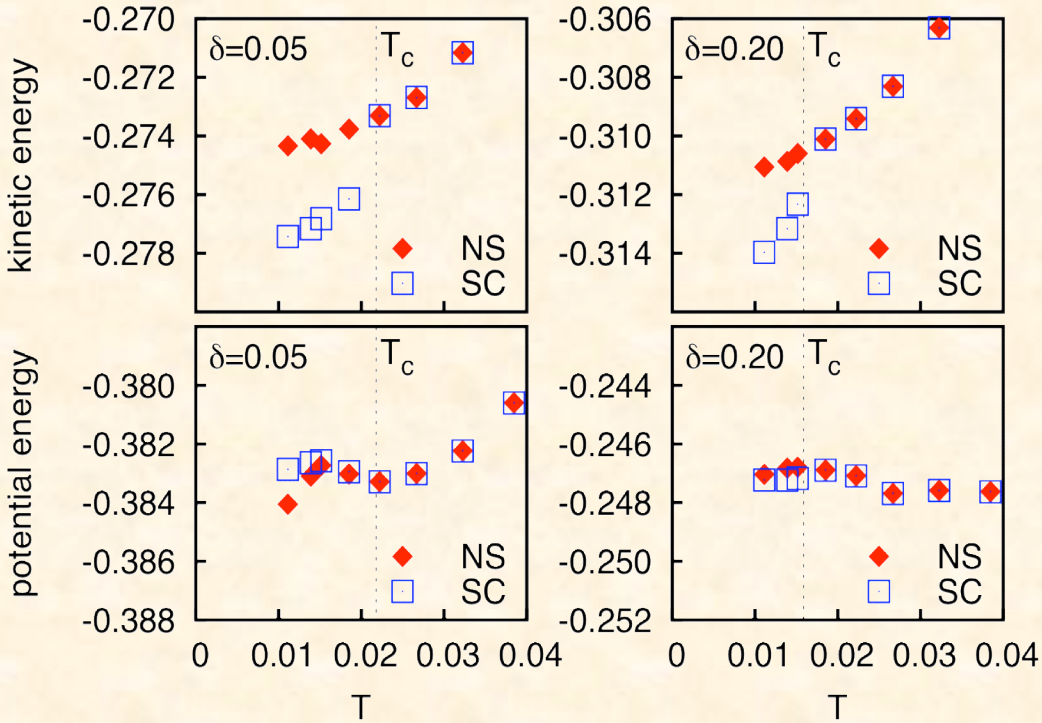
Cuprate superconductors:

Scalapino & White: AF spin-correlations important
(Scalapino & White, PRB, 1998)

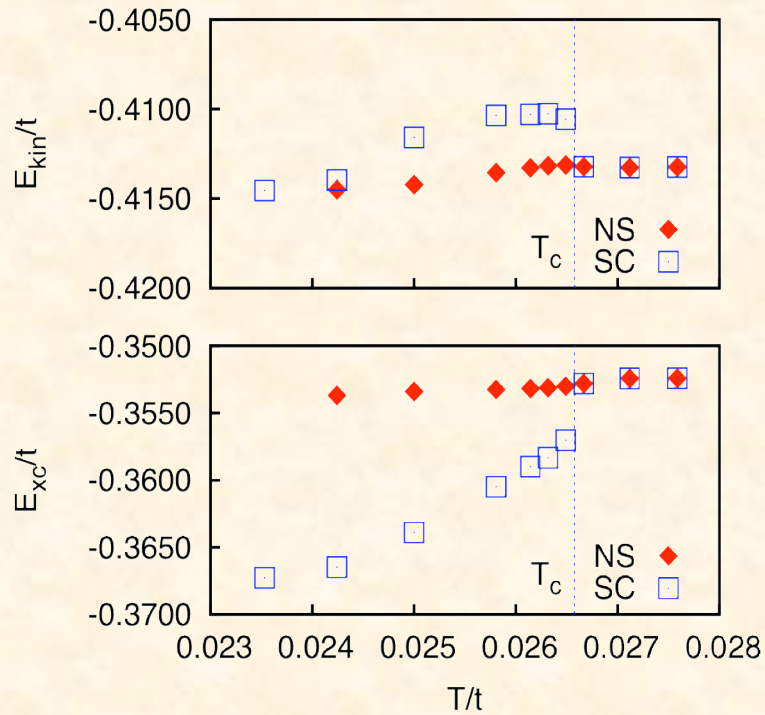
Condensation energy $\propto$ Change in exchange energy

Condensation energy in Hubbard and t-J models

Hubbard model



t-J model



Compare optical experiments:

H. Molegraaf et al., Science 2002

Compare neutron scattering:

Dai et al., Science, 1999

… Larger Cluster Sizes

Mermin-Wagner:

No antiferromagnetism at finite *T* in 2D

? Cluster size too small

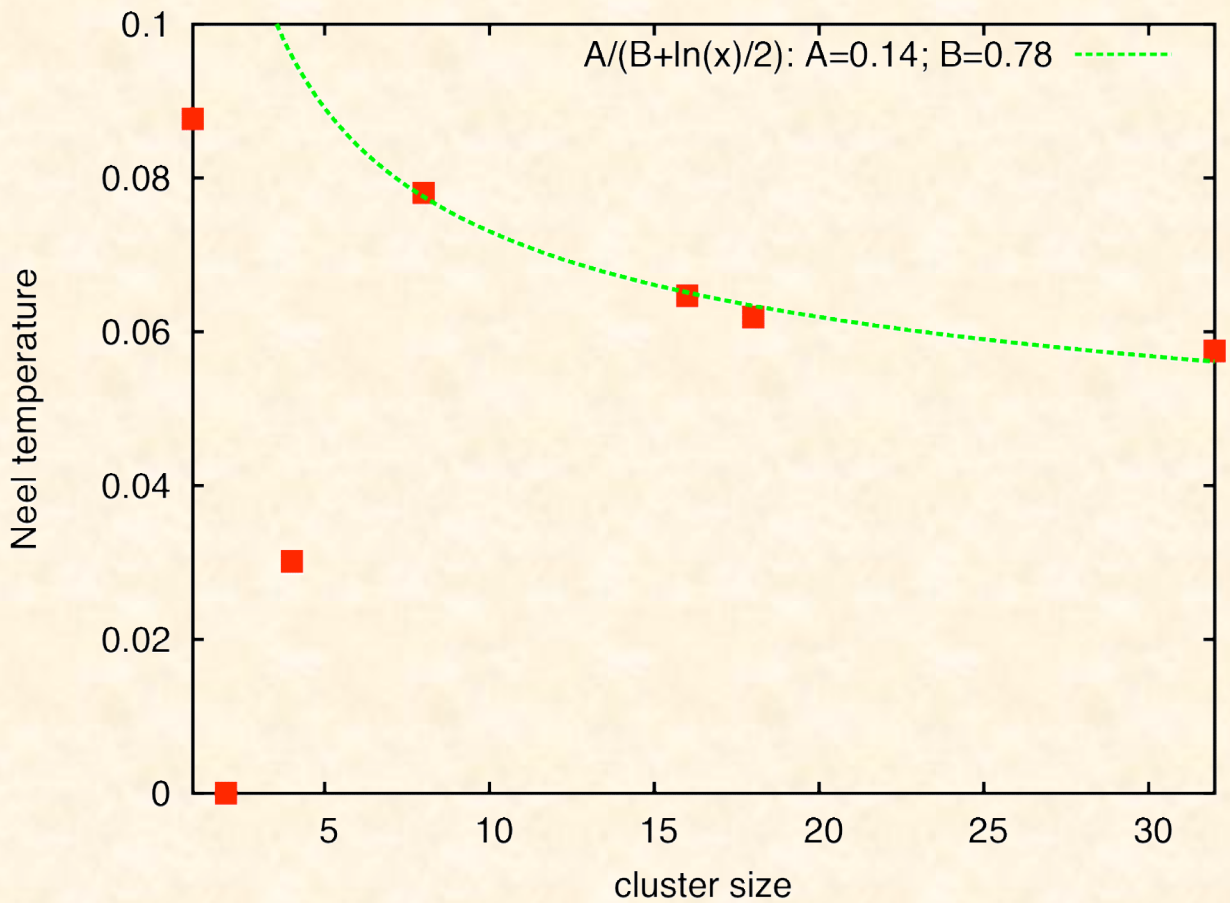
Systematic study with larger clusters important

Problem: Computational cost ~ (cluster size)^3

Solution: Cray X1 (Phoenix)

Antiferromagnetism

U=6t, n=0.95

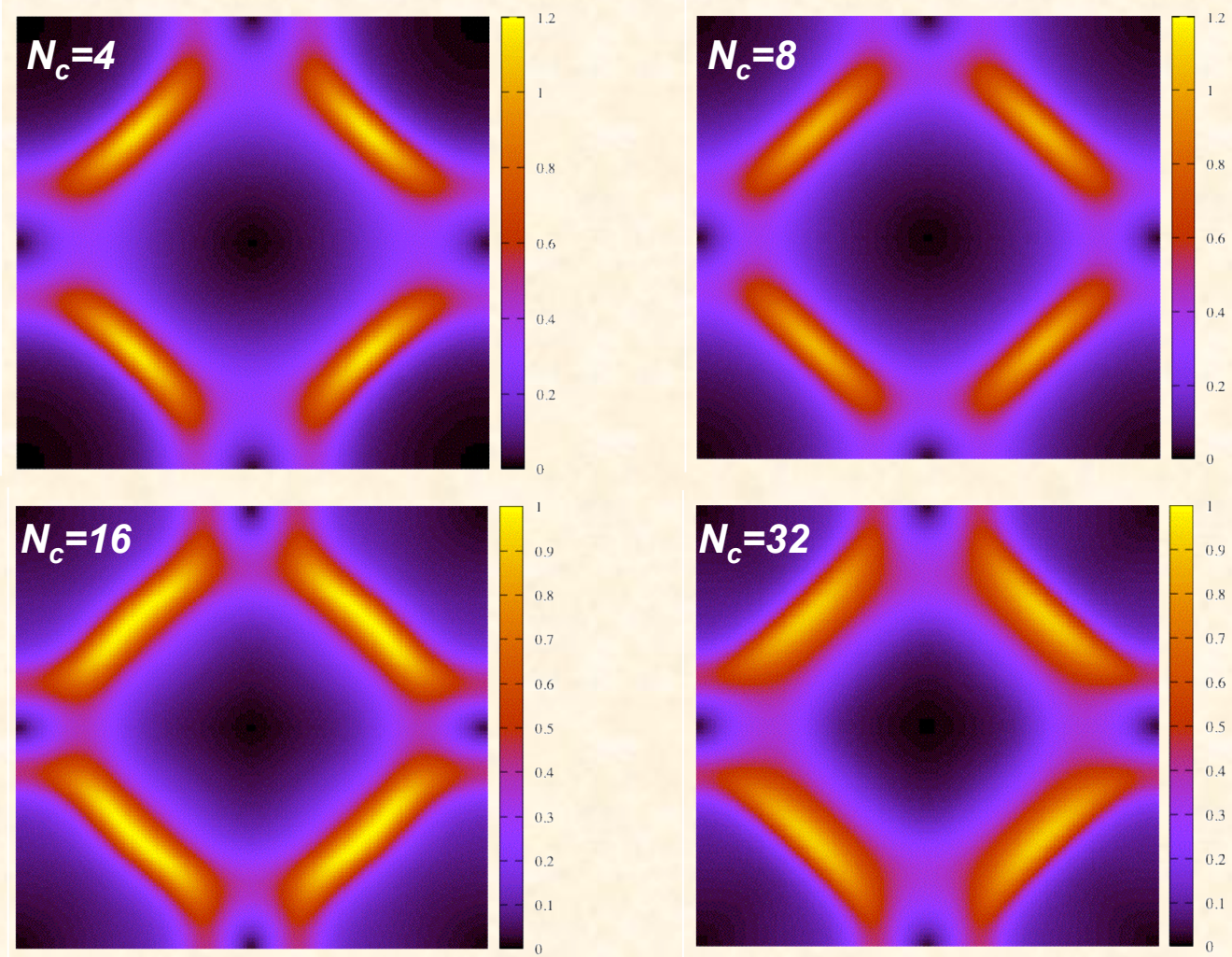


Correlation length:

$\xi \propto \exp(A/T)$

Fermi surface

U=6t
n=0.95



Summary & Conclusions

DCA = Tool with predictive capability:

- ✓ *Phase diagram of Hubbard model consistent with HTSC*
- ✓ *Kinetic energy driven pairing in Hubbard model*
- ✓ *Exchange energy driven pairing in t-J model*
- ✓ *Larger clusters recover fundamental physics of 2D systems*

LDA+DCA ⟶ *Material specific properties*