On the origin of pairing in cuprate superconductors

Th. A. Maier

Oak Ridge National Laboratory

Research performed as Eugene P. Wigner Fellow and staff member at the Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy under Contract DE-AC05-00OR22725.

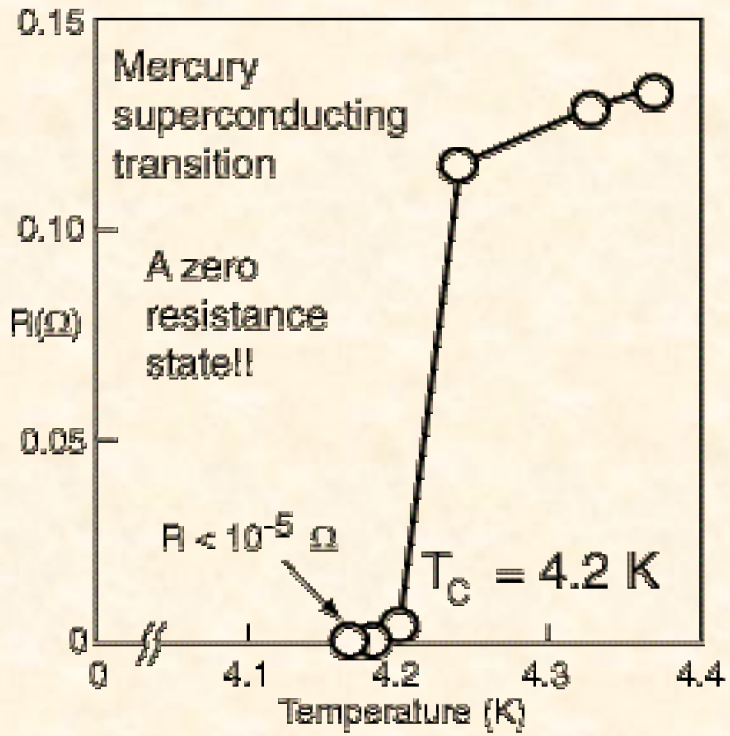
Collaborators: M. Jarrell, Th. Pruscke, T.C. Schulthess, M. Hettler,

A. Macridin, A.N. Thavildarzadeh, C. Huscroft, F.C. Zhang, Cyrill Slezak

- *BCS (conventional) superconductors*
- *Cuprate (unconventional) superconductors*
- *Dynamical cluster approximation*
- *Pairing phenomenologies*

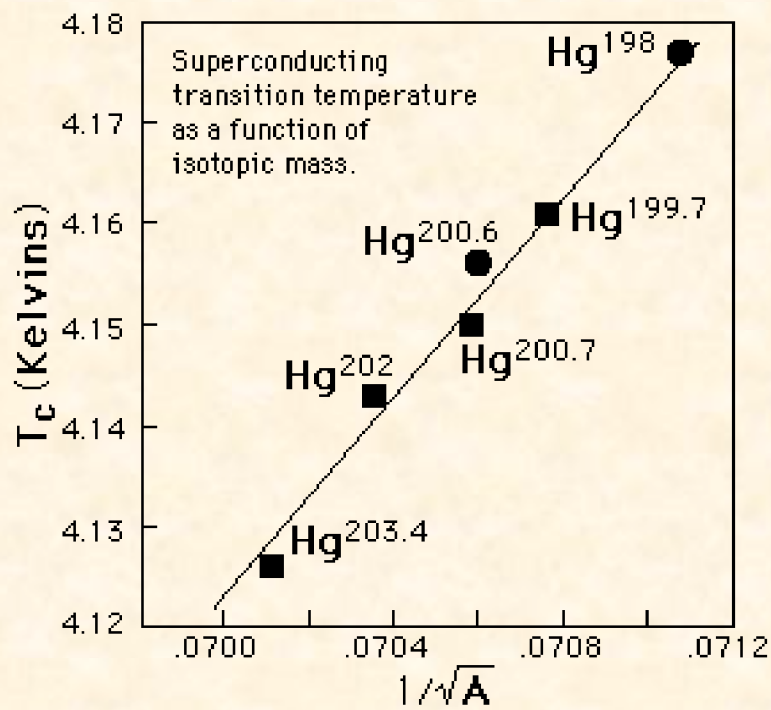
BCS superconductors

Conventional superconductivity:



K. Omnes, Commun. Phys. Lab. (1911).

Smoking gun: Isotope effect



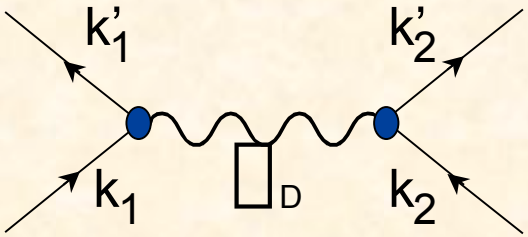
E. Maxwell, Phys. Rev. (1950)
C.A. Reynolds et al., Phys. Rev. 78 (1950).

Phonon mediated pairing

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

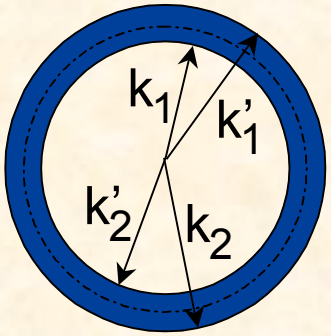
Link: Pairing $\longleftrightarrow$ *Electron - ion interaction*

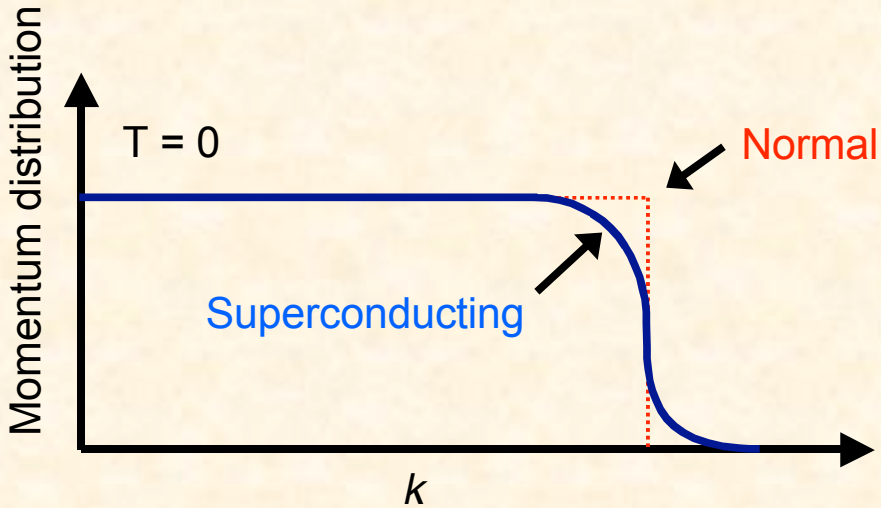
Scattering of quasiparticles by phonons:

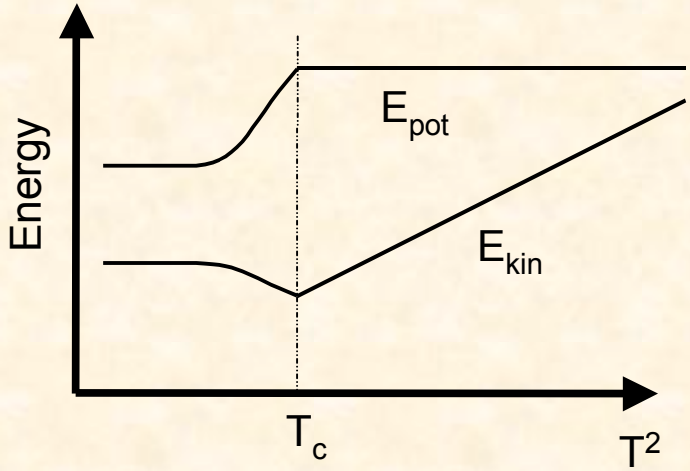


Attractive potential

Electronic sub-system





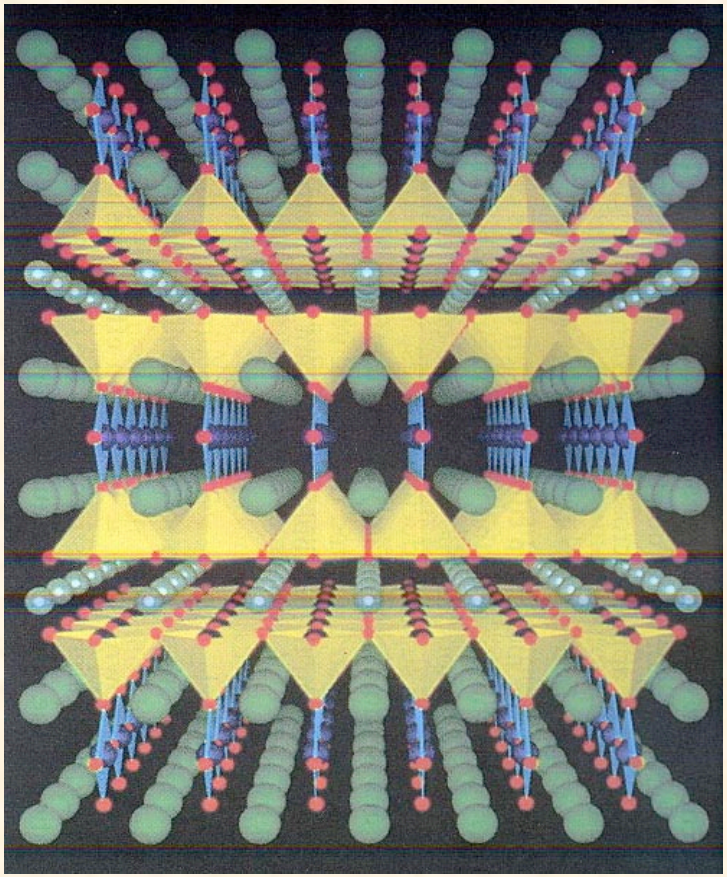


Pairing due to potential energy

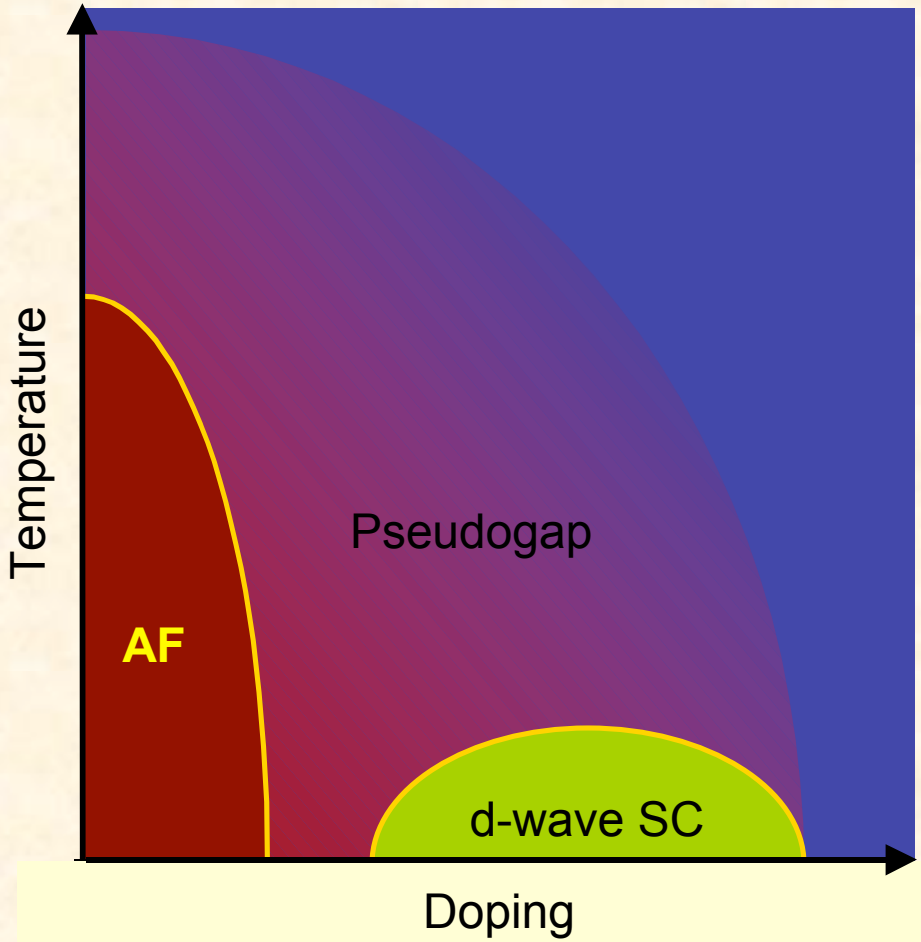
Kinetic energy increases upon pairing

Cuprate superconductors

$Yba_2Cu_3O_7$



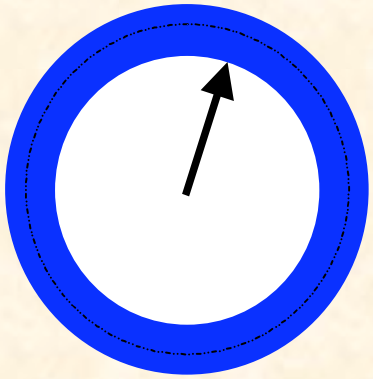
Schematic phase-diagram



Pairing Symmetry

BCS (conventional) superconductors:

Local pairing induced by phonons

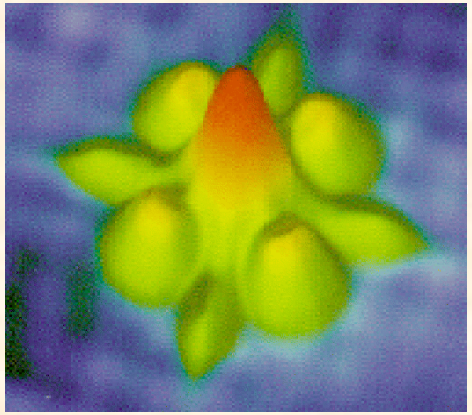


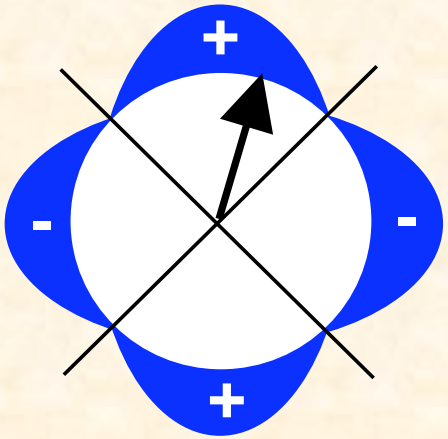
Pairing state has *s-wave* symmetry

Cuprate(unconventional) superconductors:

STM near Zn impurity:

(S. Pan, Physics Today)





Pairing state has *d-wave* symmetry

Exchange-based Pairing?

Scalapino & White: AF spin-correlations important

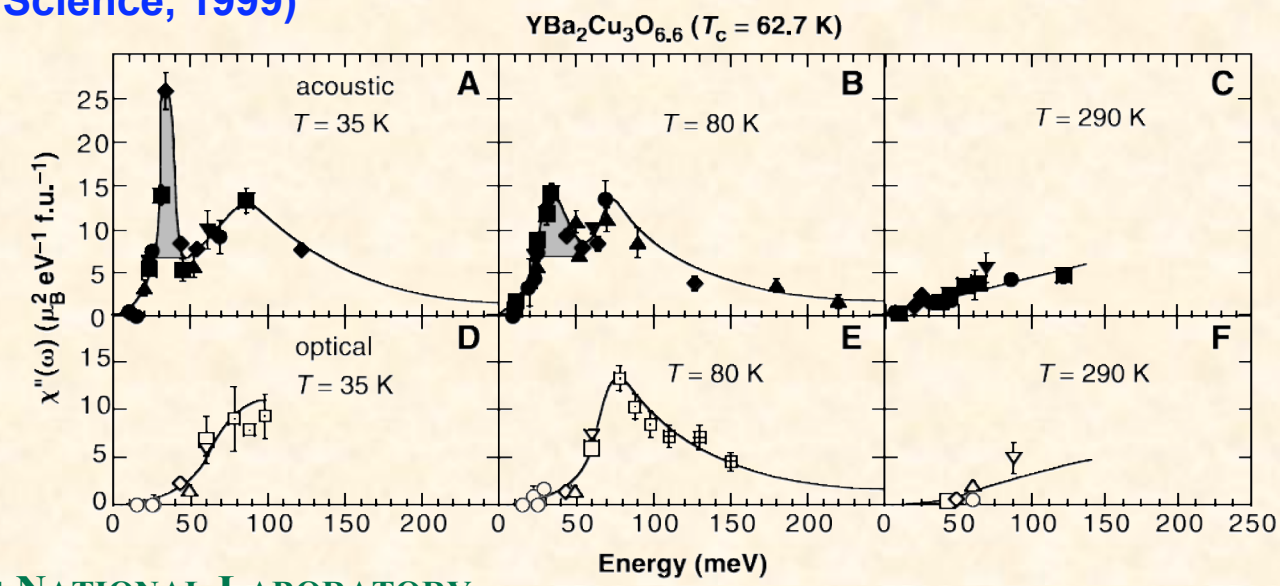
(Scalapino & White, PRB, 1998)

Condensation energy $\propto$ *Change in exchange energy*

$$J\langle \vec{S}_i \cdot \vec{S}_j \rangle = 3 \int \frac{d^2q}{2\pi^2} \int \frac{d\omega}{\pi} S(\vec{q},\omega) \cos[\vec{q}\cdot(\vec{x}_i - \vec{x}_j)]$$

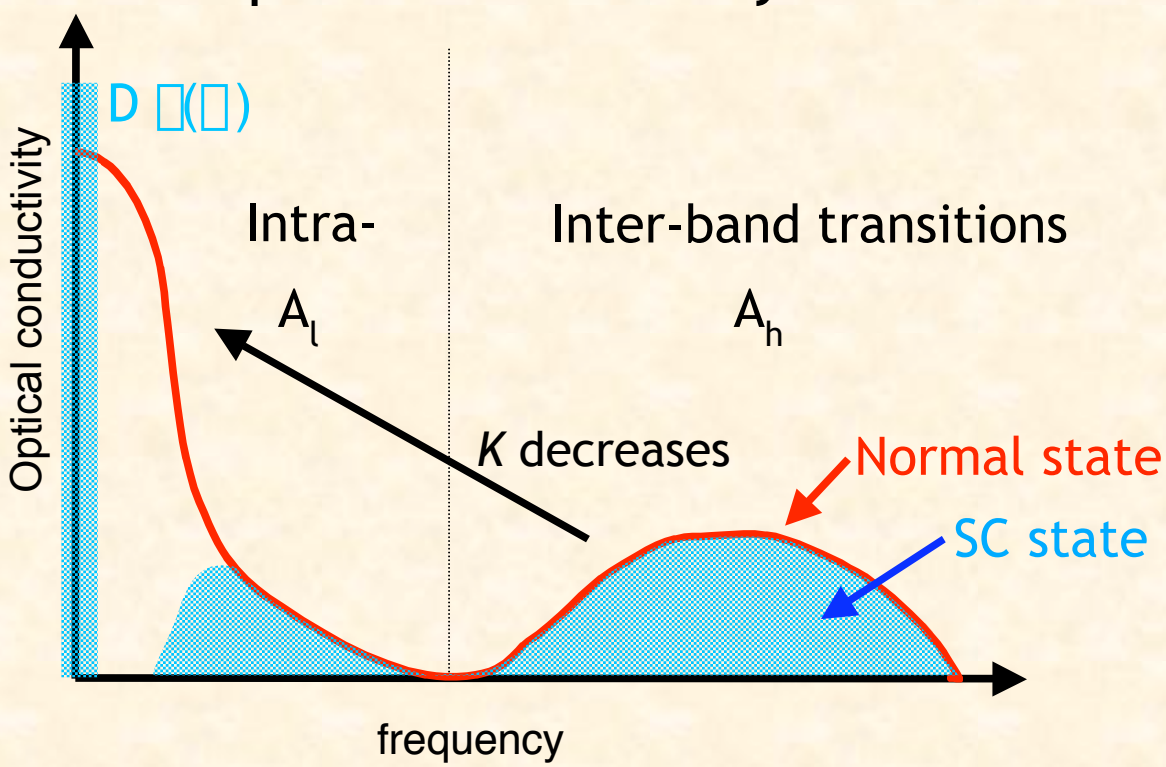
Neutron scattering: Resonance peak accounts for E_{cond}

(Dai et al., Science, 1999)



Optical conductivity - Kinetic energy

Optical conductivity:



f-sum rule:

$$\int_0^\infty \sigma(\omega)d\omega = \frac{\pi n e^2}{2m} = const.$$

Ferrell-Glover-Tinkham sum rule:

$$D = A_l^N - A_l^S + A_h^n - A_N^S$$

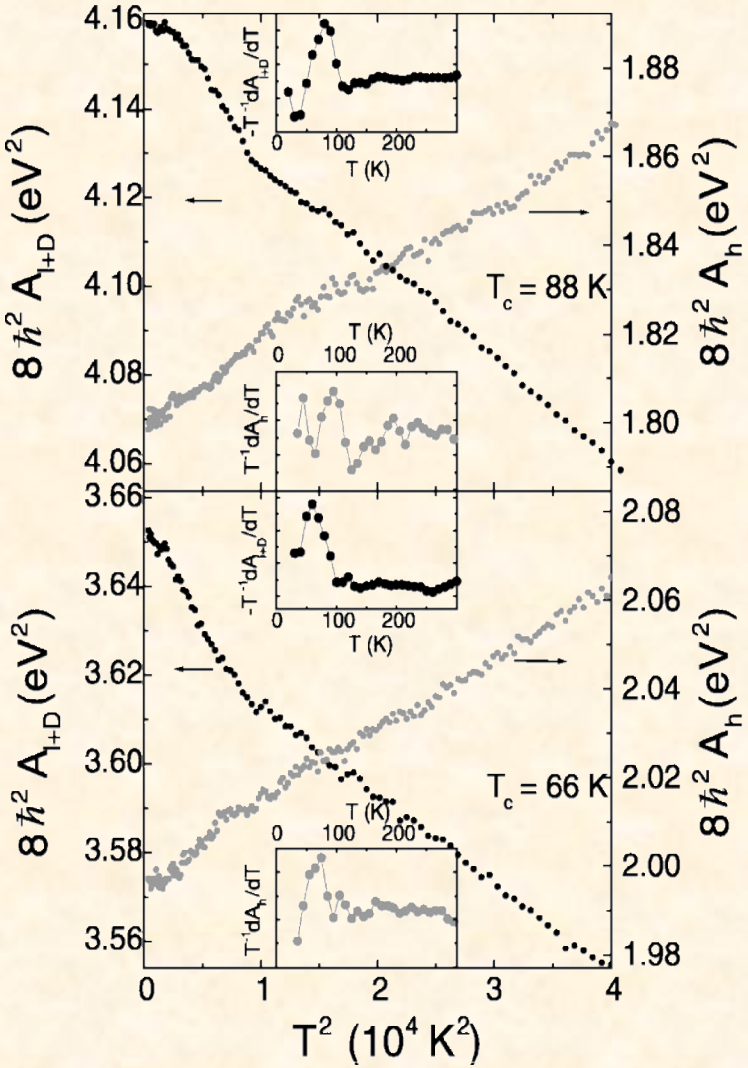
Kinetic energy:

$$K = -\frac{h^2 V_{Cu}}{\pi^2 e^2}(A_l + D)$$

Kinetic energy ∝ negative low frequency spectral weight

Transfer of Spectral Weight in BSCCO

(H. Molegraaf, D. van der Marel, Science 2002)



$$A_I + D = -\frac{\pi^2 e^2}{h^2 V_{Cu}} K$$

$$A_h = \frac{\pi n e^2}{2m} + \frac{\pi^2 e^2}{h^2 V_{Cu}} K$$

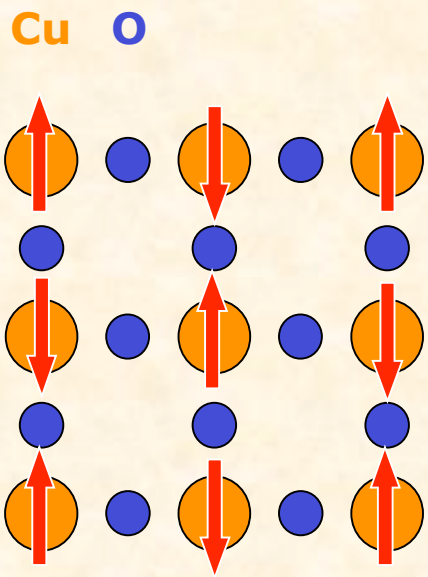
Pairing driven by lowering of kinetic energy

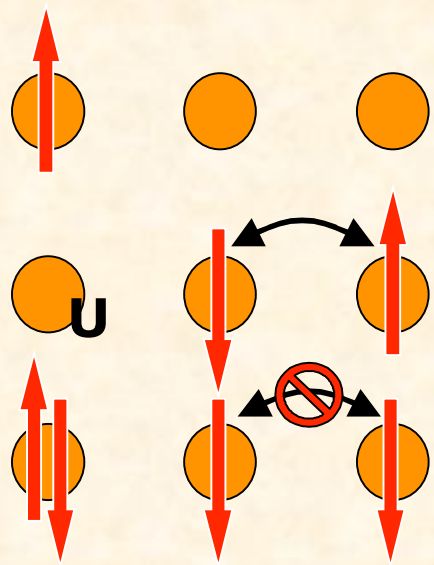
Cuprates - Strong Correlations

CuO_2-plane

2D Hubbard model: $H = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$

(Anderson, Zhang)





$$\left.\begin{aligned} E_1 &= \frac{-2t^2}{U} \\ E_2 &= 0 \end{aligned}\right\} \quad J = -\frac{2t^2}{U}$$

U>>*t* : tJ-model: $H_{tJ} = -t \sum_{\langle ij \rangle, \sigma} \tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} + J \sum_{\langle ij \rangle} [\vec{S}_i \cdot \vec{S}_j - \frac{n_i n_j}{4}]$

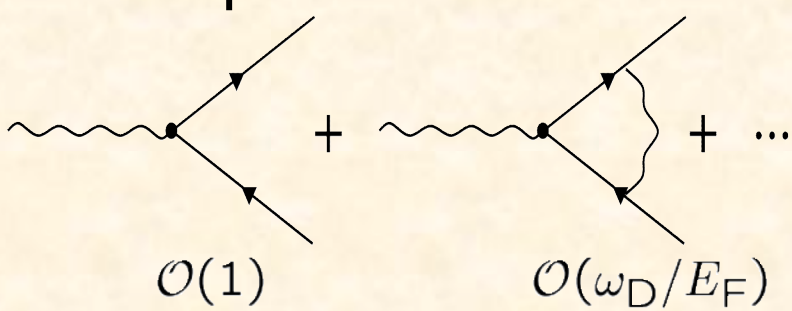
Small Parameter?

BCS (conventional) SC:

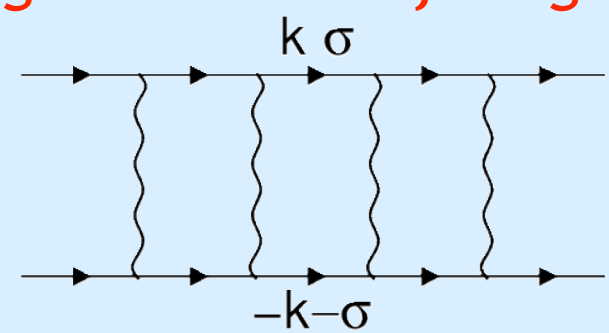
Small parameter:

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

Electron-phonon vertex:



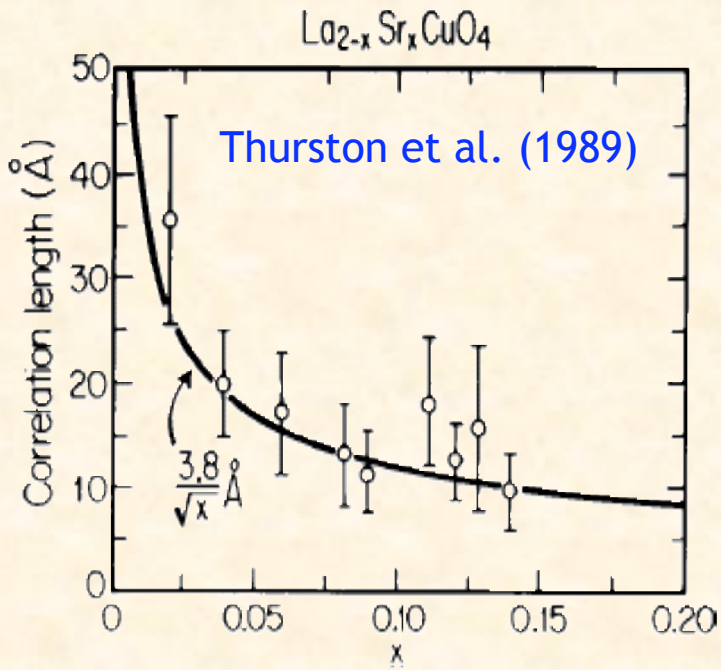
Neglect classes of diagrams:



Cuprate (unconventional) sc:

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

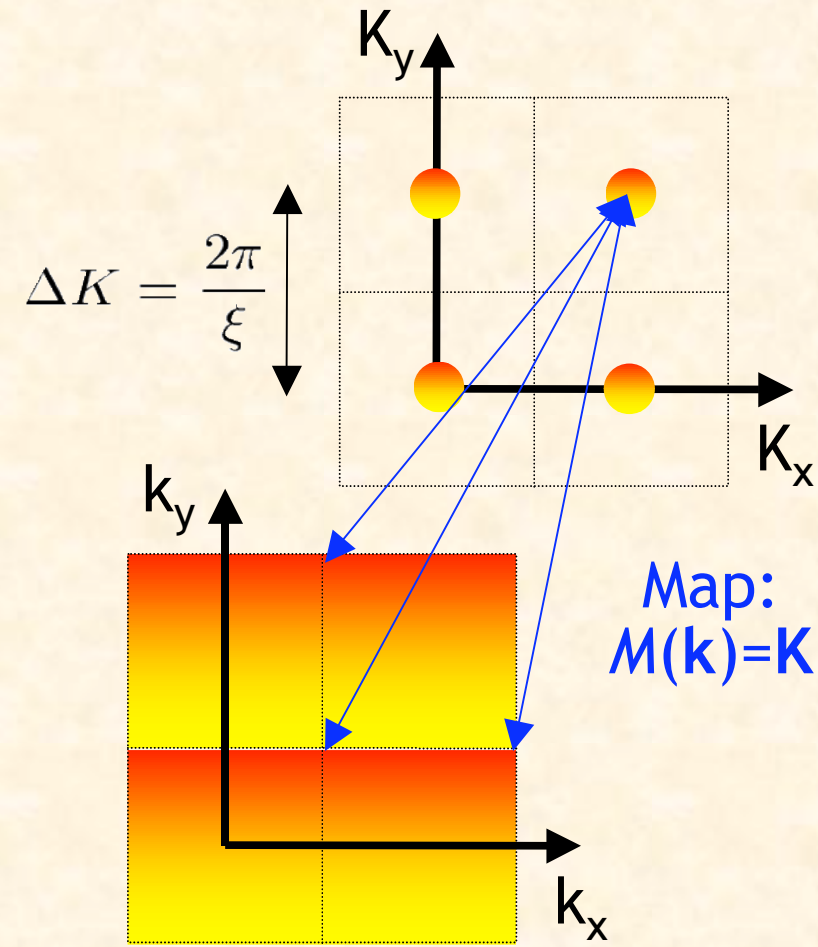
But in Cuprates:



Short-ranged AF correlations

Dynamical Cluster Approximation

Cluster (N_c degees of freedom)

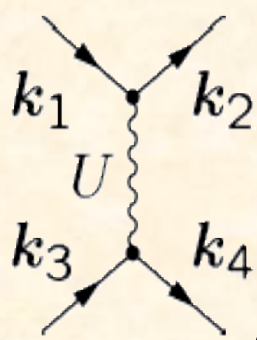


Lattice (N degrees of freedom)

Short-ranged correlations within the cluster treated exactly

Longer-ranged dynamics described on mean-field level

Microscopic definition:



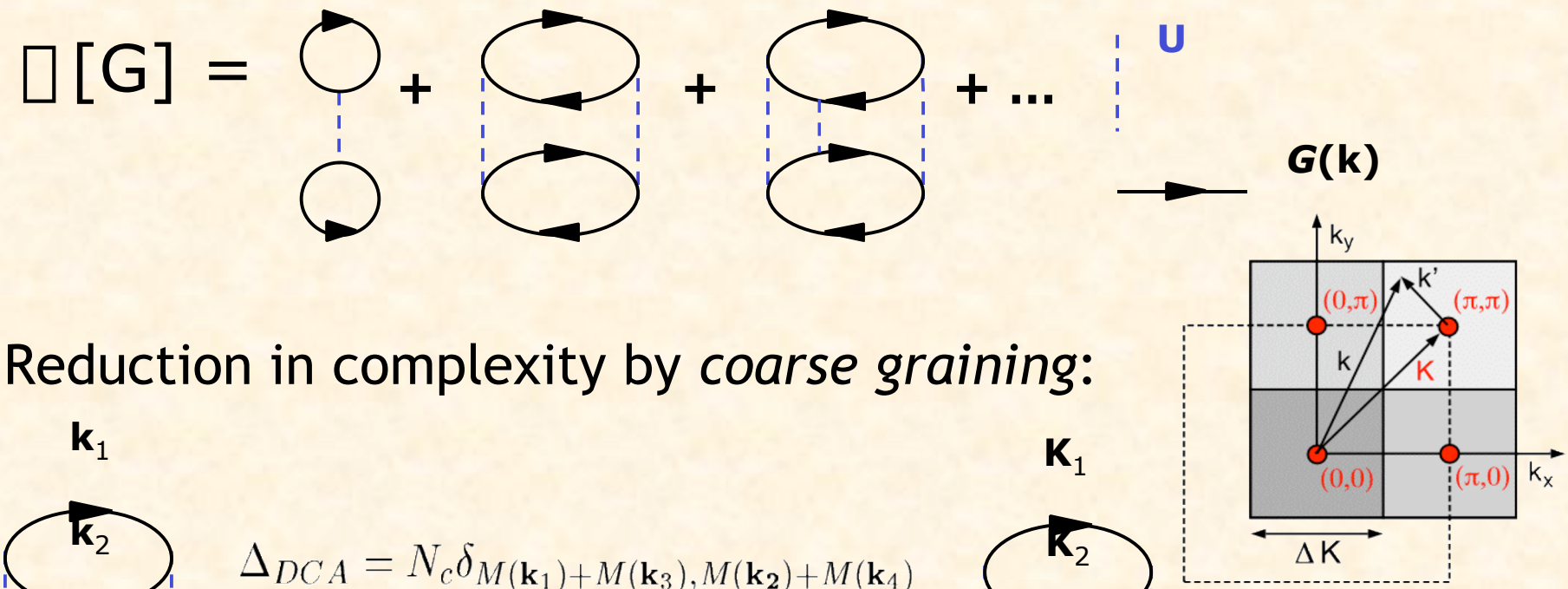
$$N\delta_{\mathbf{k}_1+\mathbf{k}_3,\mathbf{k}_2+\mathbf{k}_4}$$

DCA

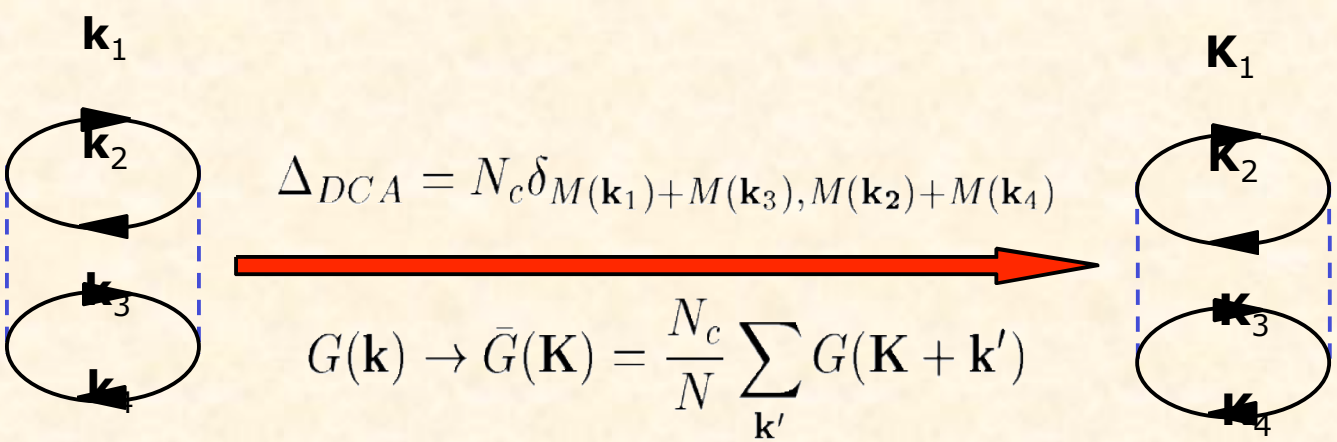
$$N_c\delta_{M(\mathbf{k}_1)+M(\mathbf{k}_3),M(\mathbf{k}_2)+M(\mathbf{k}_4)}$$

DCA - Free Energy

Free energy: $\mathcal{F} = -k_B T \left\{ \Phi\left[\mathbf{G}\right] + \mathrm{Tr}\left[\mathbf{\Sigma G}\right] - \mathrm{Tr}\left[\ln\left(-\mathbf{G}\right)\right] \right\}$



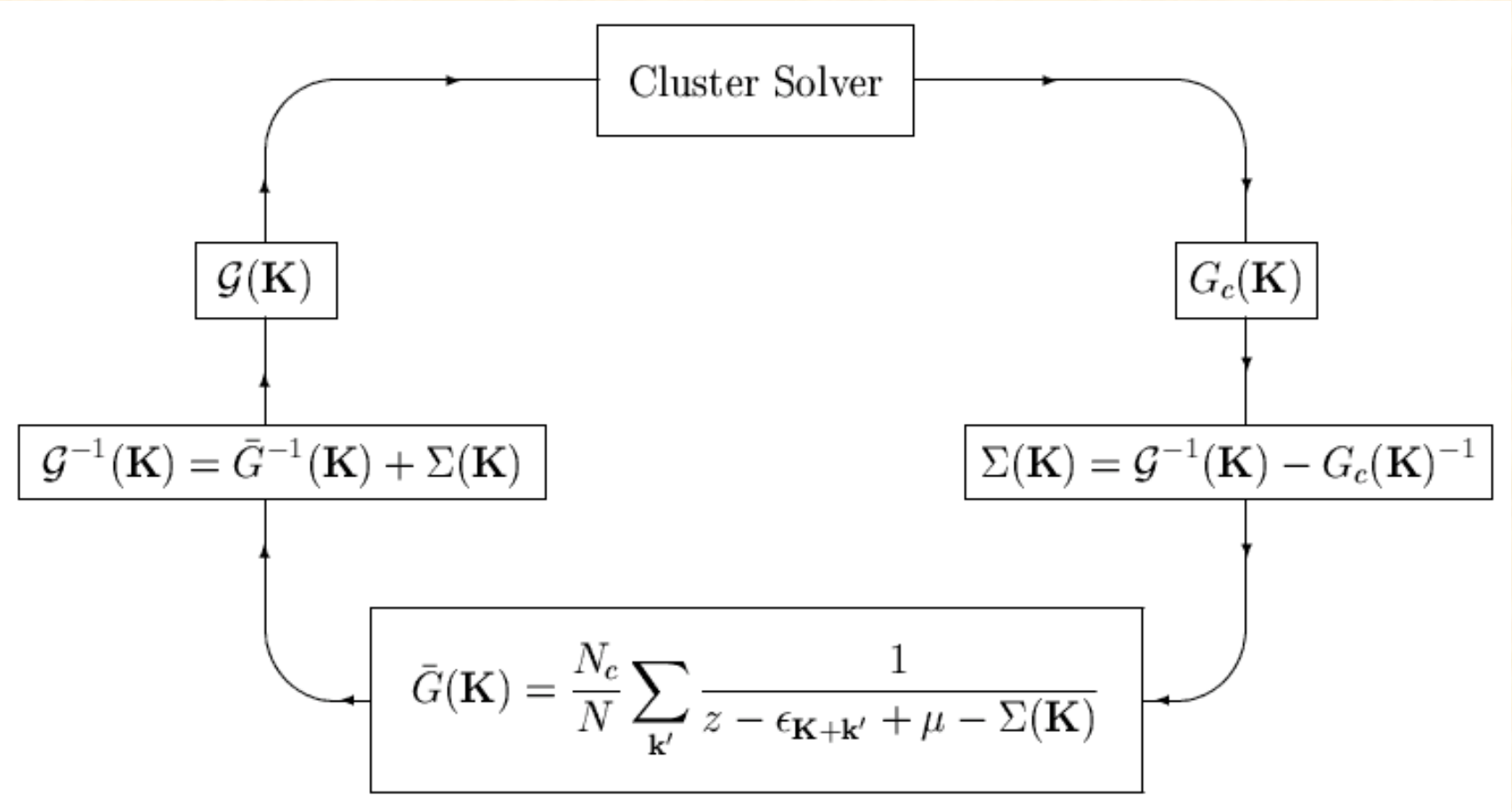
Reduction in complexity by *coarse graining*:



$$\Delta_{DCA} = N_c \delta_{M(\mathbf{k}_1)+M(\mathbf{k}_3),M(\mathbf{k}_2)+M(\mathbf{k}_4)}$$

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

DCA - Algorithm



DCA - t-J model

Non-local interaction: $J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$

Coarse-graining: $\bar{J}(Q) = \frac{N_c}{N} \sum_{\tilde{q}} J(Q + \tilde{q})$

Bosonic field □(Q,□) via spin-susceptibility:

$$\bar{\chi}_s(Q) = \frac{N_c}{N} \sum_{\tilde{q}} \frac{M(Q,z)}{1 + (J(Q+\tilde{q}) - \bar{J}(Q)))M(Q,z)}$$

$$= \frac{M(Q,z)}{1 + \Theta(Q,z)M(Q,z)}$$

Self-consistency also on two-particle level

Calculation of Energy densities

- Kinetic energy:

$$\langle T \rangle = \frac{2}{N} \sum_k \varepsilon_k \langle c^\dagger_{k\sigma} c_{k\sigma} \rangle = -\frac{2}{N\pi} \sum_k \varepsilon_k \int d\omega f(\omega) \Im m G(k,\omega)$$

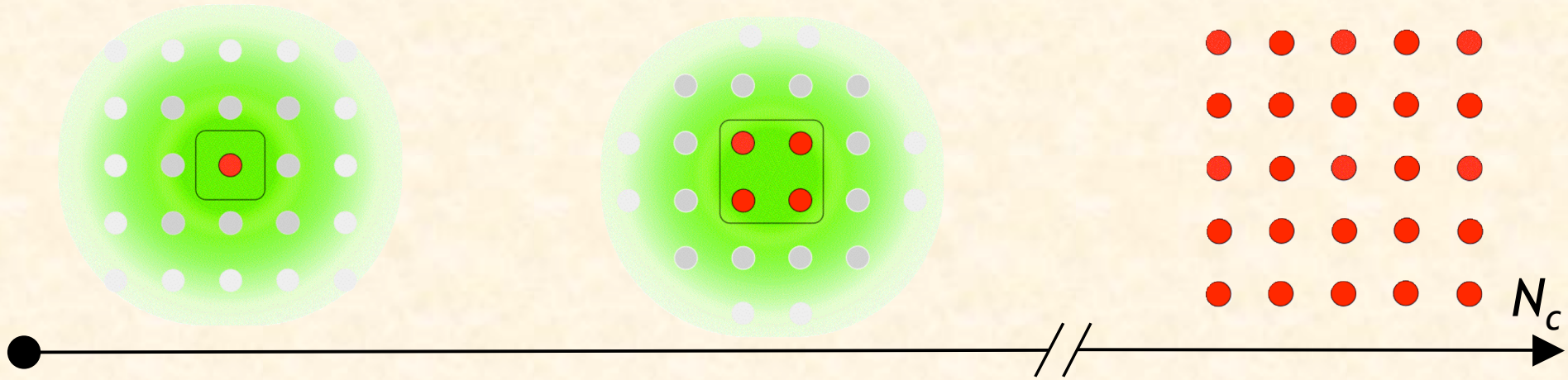
- Potential energy:

$$\langle V \rangle = \frac{U}{N} \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle = \frac{U}{2} [\langle n \rangle - \langle m^2 \rangle]$$

- Exchange energy:

$$\langle W \rangle = \frac{1}{N} \sum_q J(q) \langle \vec{S}(q) \vec{S}(-q) \rangle = -\frac{3}{N\pi} \sum_q J(q) \int d\omega \frac{\Im m \chi(q,\omega)}{1 - e^{-\beta\omega}}$$

DCA - Systematic in $1/N_c$



N_c=1: DMFT

Local approximation:

$$\Sigma(k,\omega) = \Sigma(\omega)$$

Local dynamical correlations included!

No nonlocal correlations!

N_c=4: DCA

Cluster approximation:

$$\Sigma(k,\omega) = \Sigma(K,\omega)$$

$$\frac{\pi}{\Delta K} = 1$$

Correlations between nearest and n.n neighbors

Neglect of correlations on length-scales > 1!

N_c=N: exact result

All length scales:

$$\Sigma(k,\omega)$$

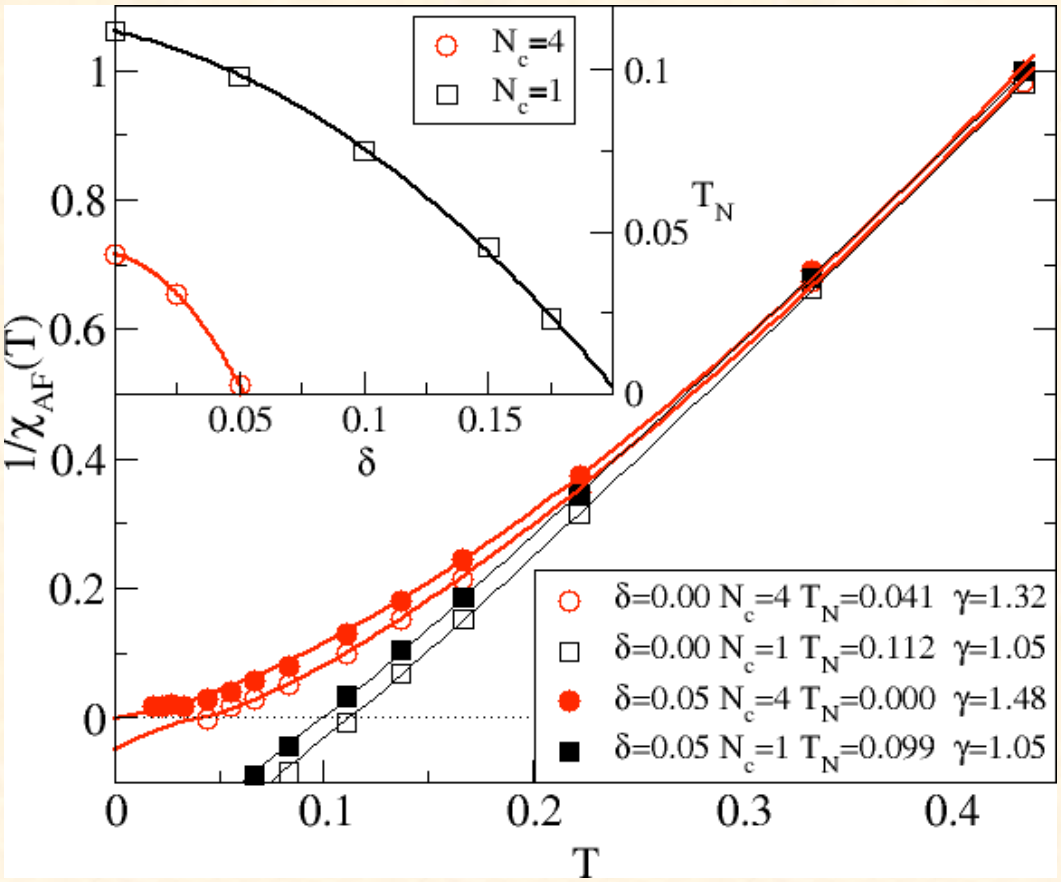
$$\frac{\pi}{\Delta K} = \infty$$

Possible correlations on all length-scales

Antiferromagnetism - Hubbard model

Parameters: $U=W=8t=2$

Inverse antiferromagnetic susceptibility



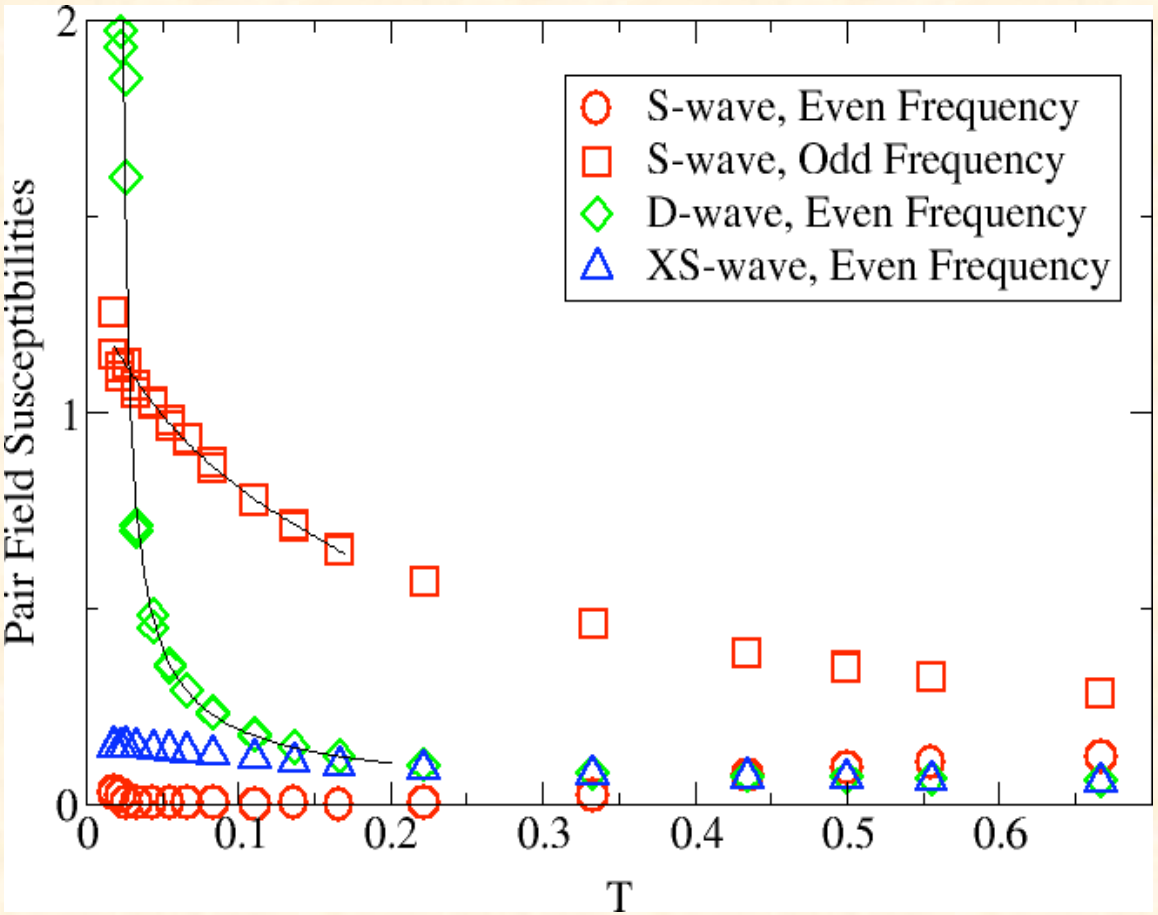
$T_N(N_c=4) < T_N(N_c=1)$

Nonlocal fluctuations suppress ordering

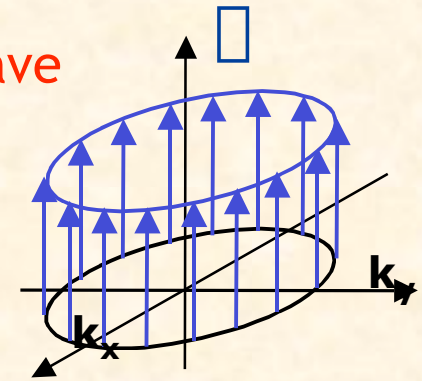
Pairing - Hubbard model

Parameters: $U=W=8t=2$, $\square=0.05$

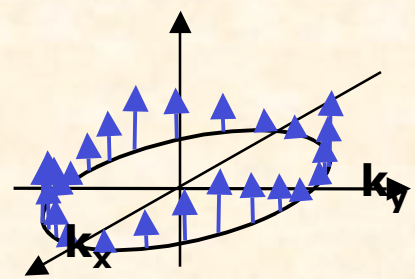
Pairfield susceptibility



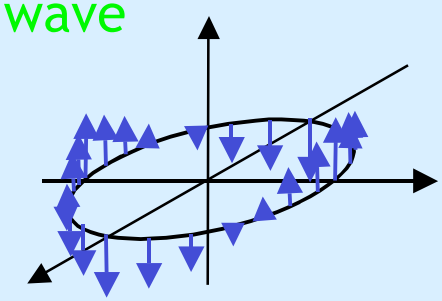
- s-wave



- Extended s-wave



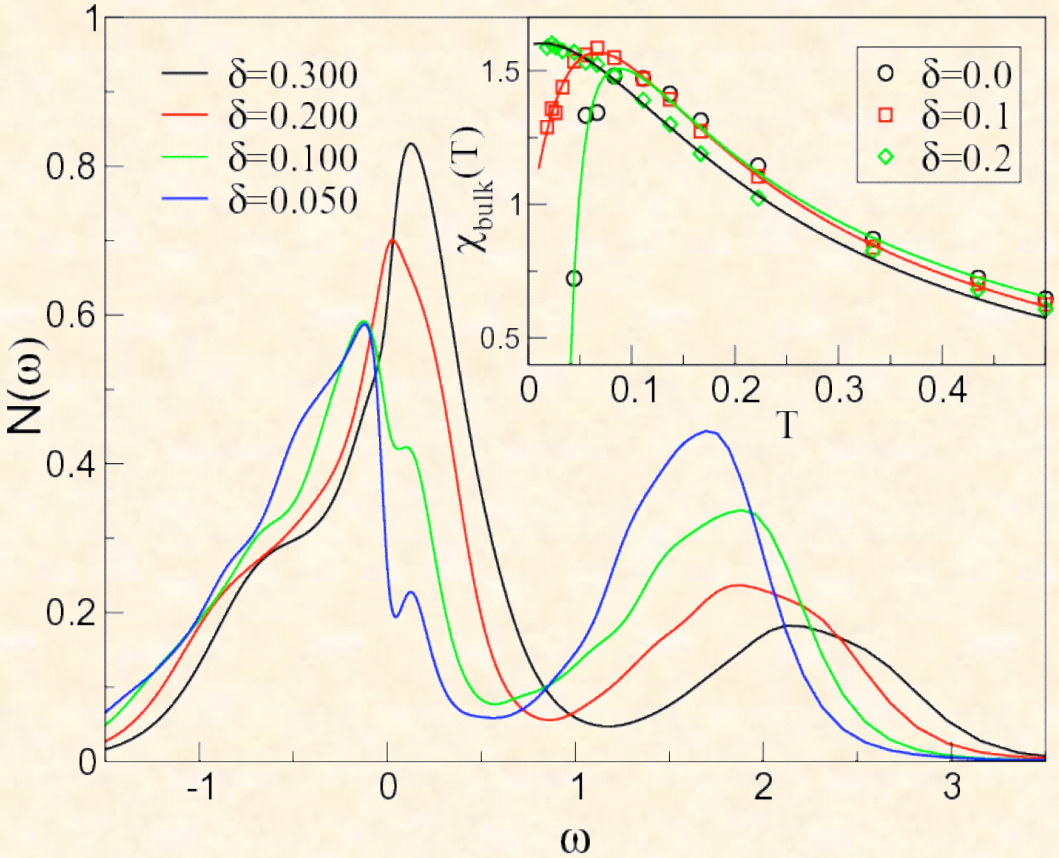
- d-wave



Pseudogap - Hubbard model

Parameters: $U=W=8t=2$

Density of states, spin susceptibility



Pseudogap in DOS and spin excitations at low T and doping.

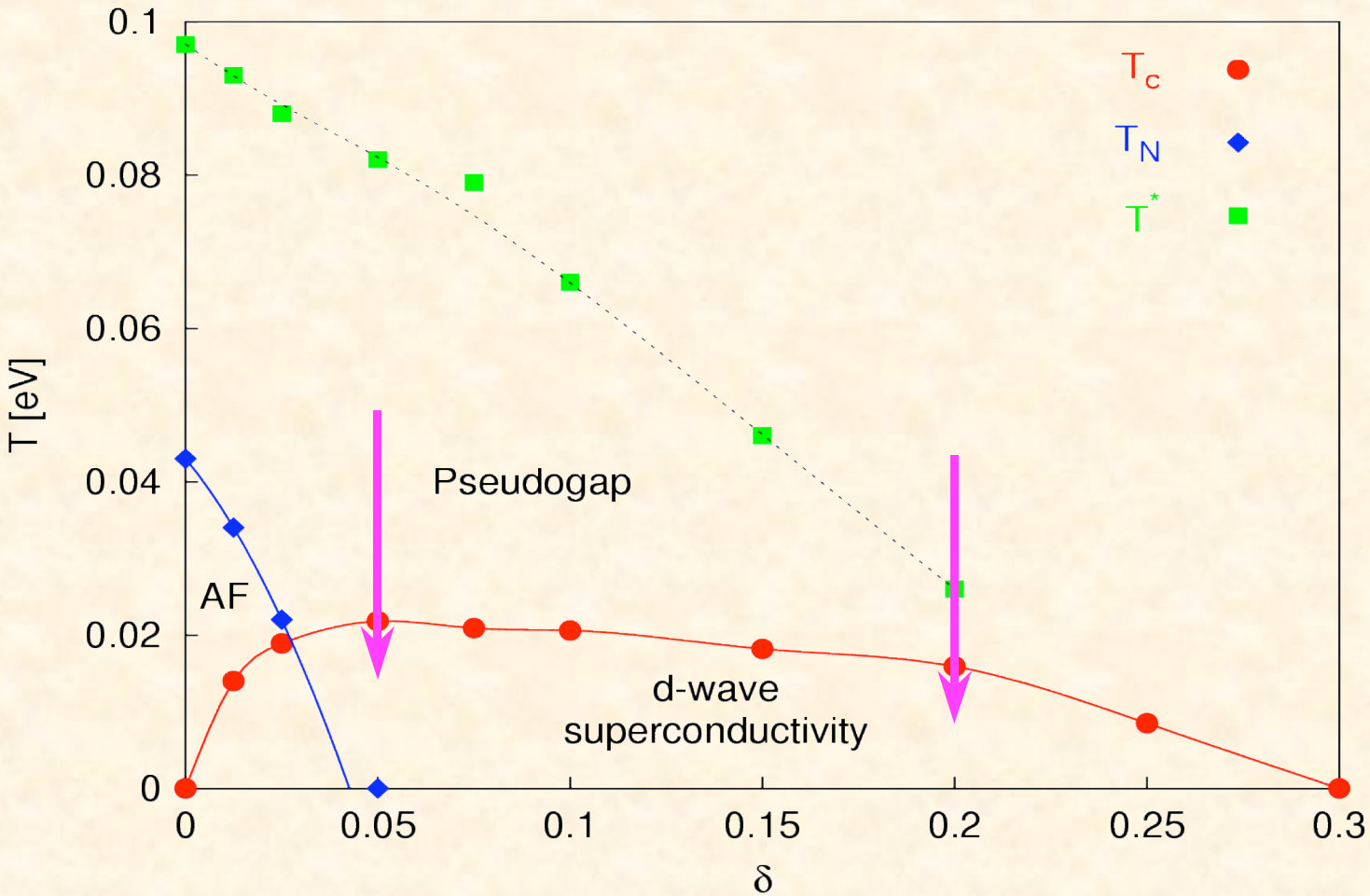
Characteristic temperature:

$$T^*(\delta = 0) \approx J$$

FL-behavior at high doping recovered.

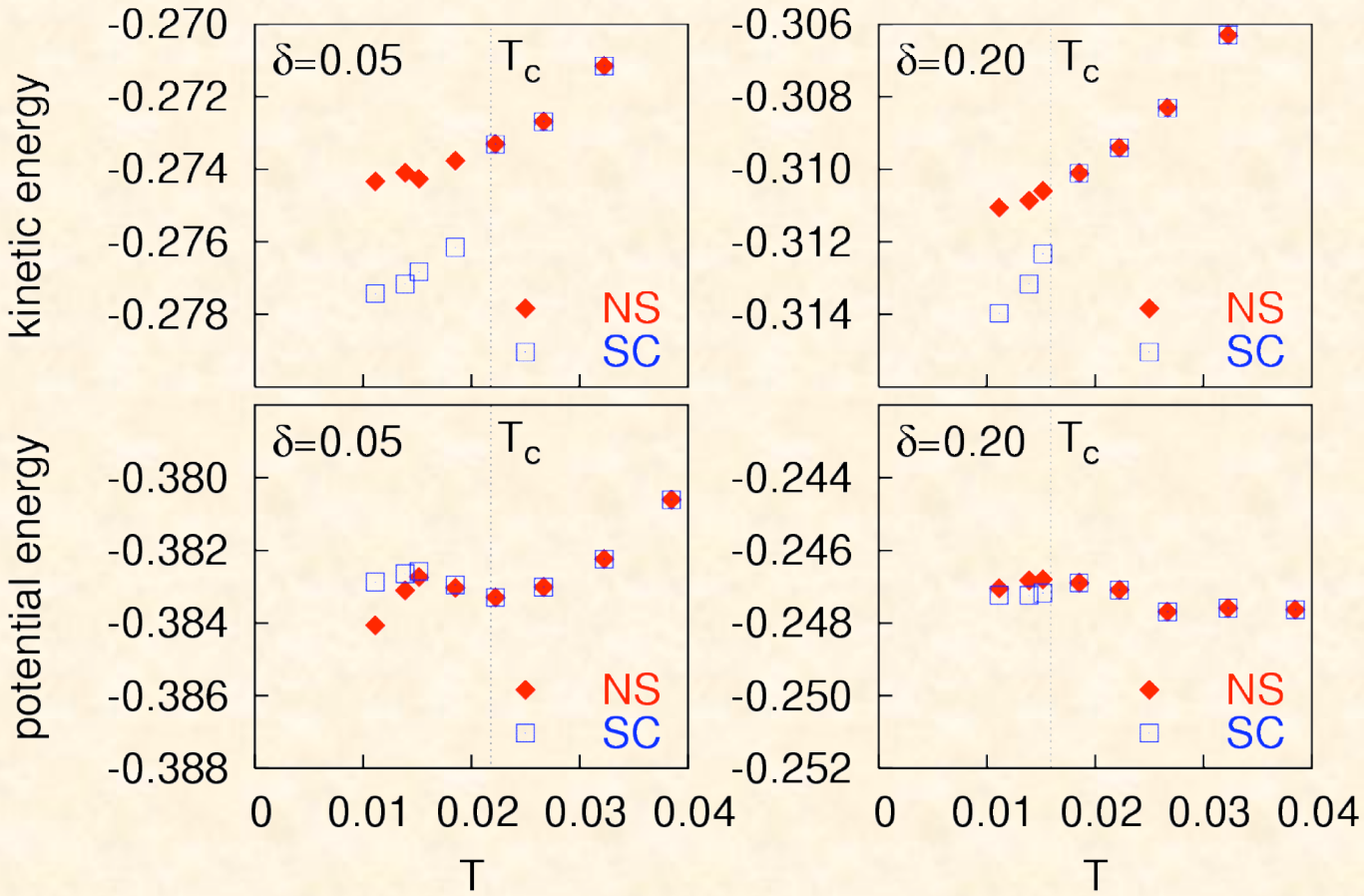
Phase Diagram - Hubbard model

Parameters: $U=W=8t=2$



Energetics - Hubbard model

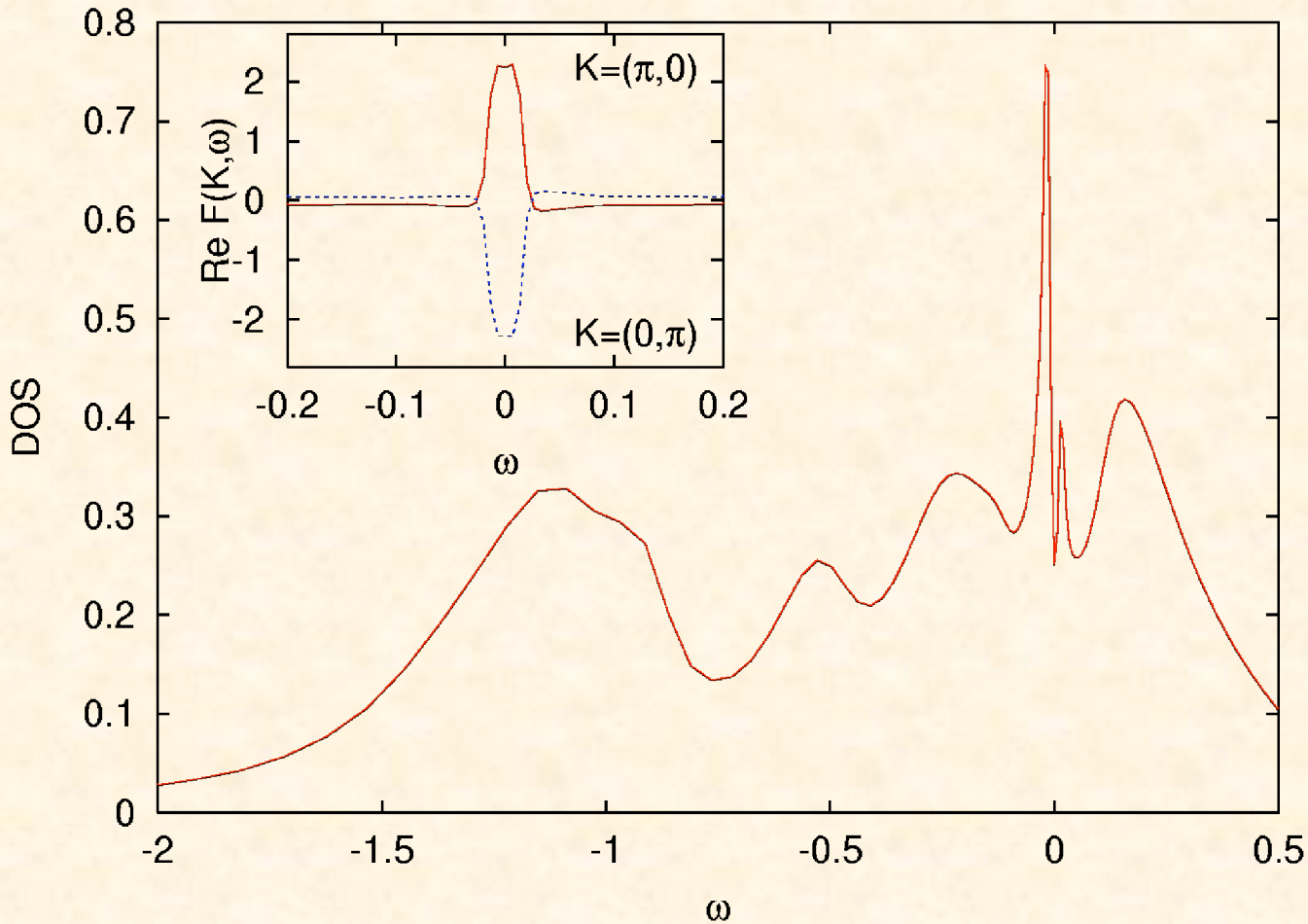
Parameters: $U=W=8t=2$



Pairing driven by lowering of kinetic energy

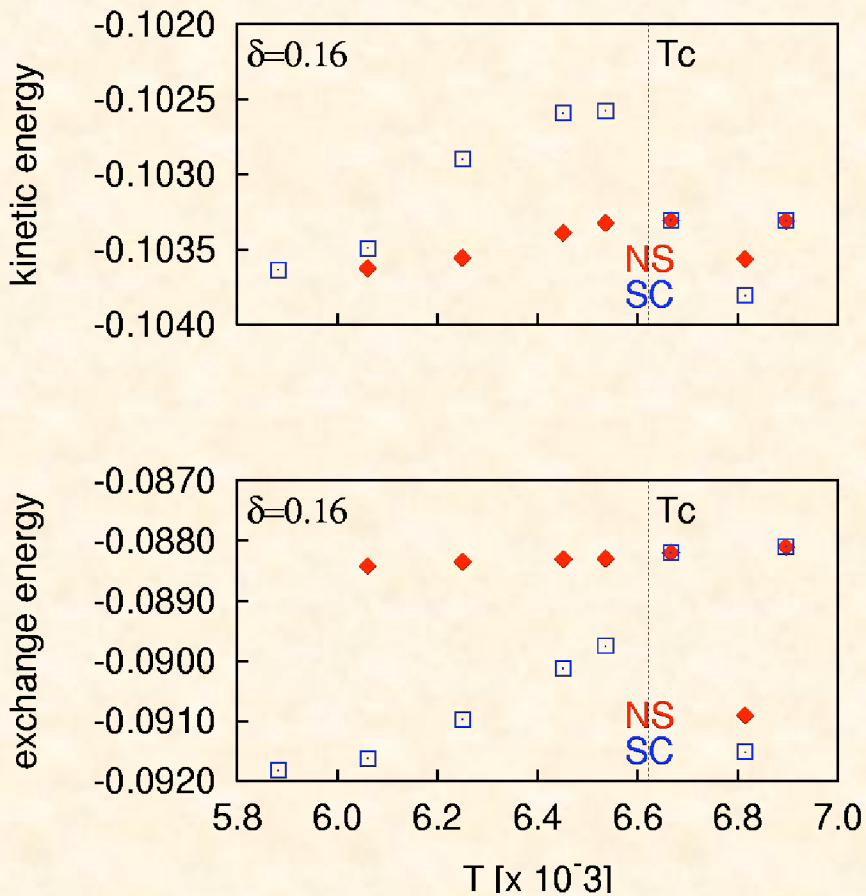
Pairing - t-J model

Parameters: *J=0.5t=0.125* , *δ=0.16*



Energetics - t-J model

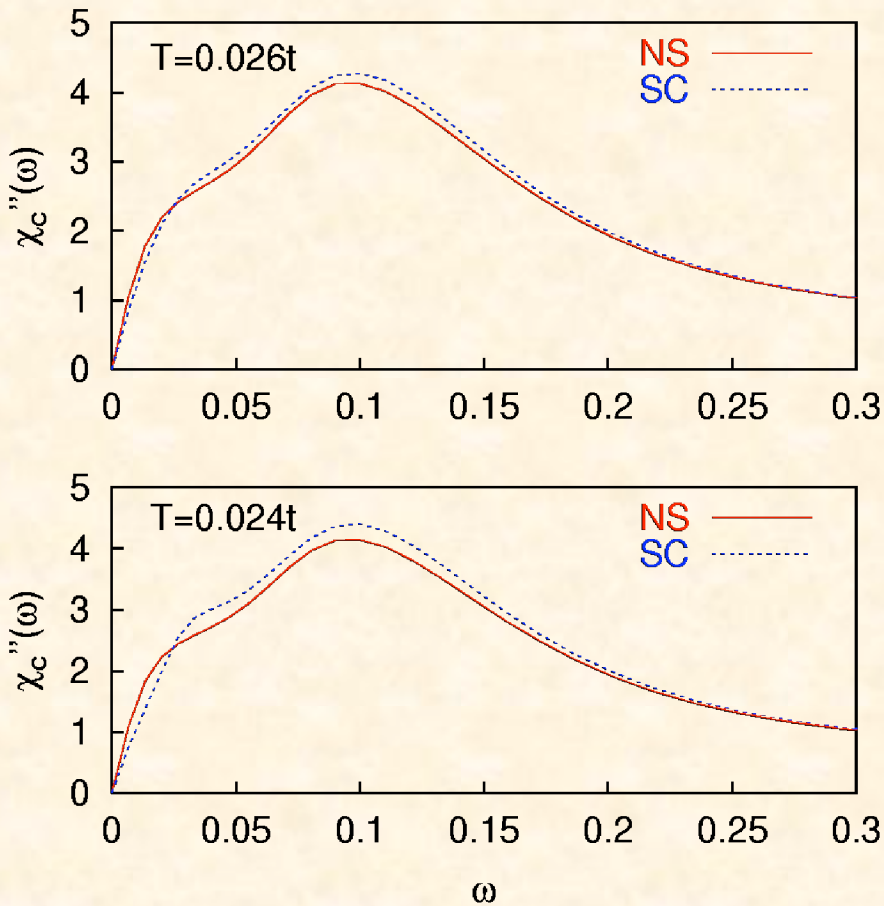
Parameters: *J=0.5t=0.125, δ=0.16*



Pairing driven by lowering of exchange energy

Magnetic susceptibility - t-J model

Parameters: *J=0.5t=0.125*, *δ=0.16*



Origin of kinetically driven pairing

Strong short-ranged
AF spin correlations

Quasiparticle-picture:

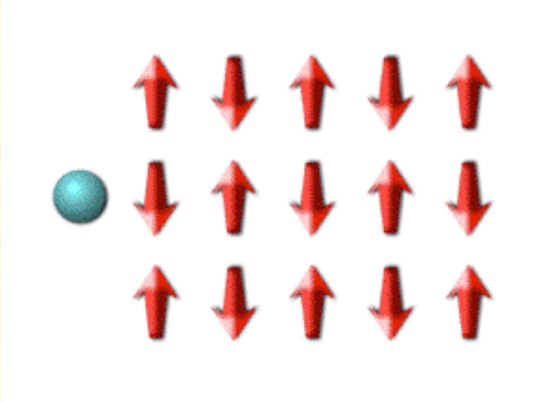
Quasiparticles in
antiferromagnetic background
(Brinkman '70, Hirsch '02)

Spin-charge separation:

Resonating valence bonds
(Anderson '87)

Quasiparticles in AF background

Motion of single hole:

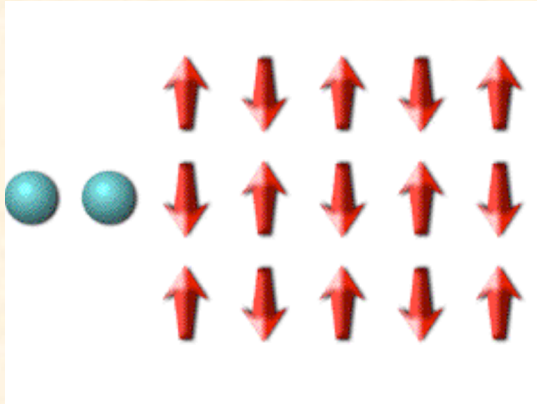


Moving hole breaks AF bonds

Motion of single hole suppressed

Hole's kinetic energy increased

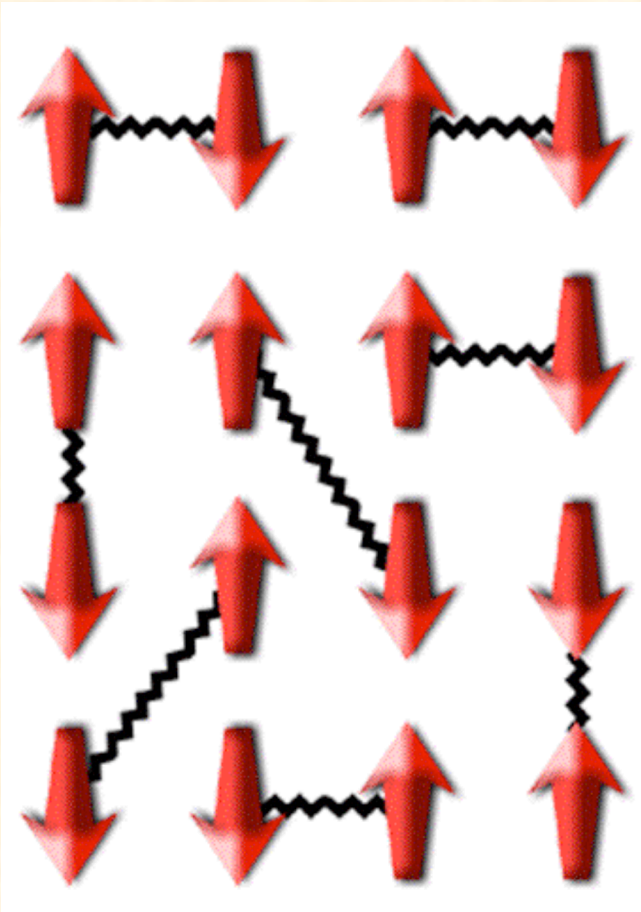
Motion of paired holes:



Second hole restores AF bonds

Kinetic energy lowered upon pairing

Resonating Valence Bonds



Elementary excitations:

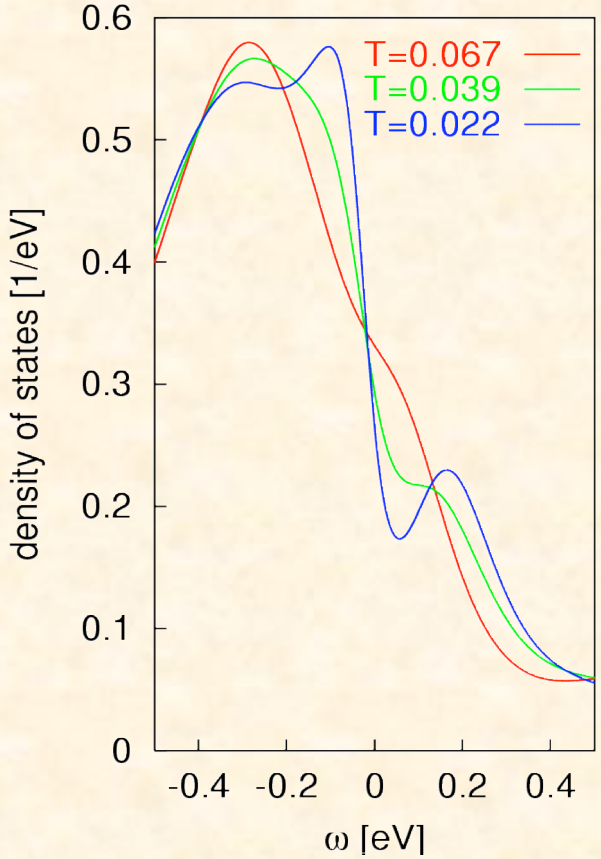
Spinons: Spin 1/2, Charge 0 Fermions
Paired spinons → Pseudogap
increased kinetic energy

Holons: Spin 0, Charge *e* Bosons
quasi-free

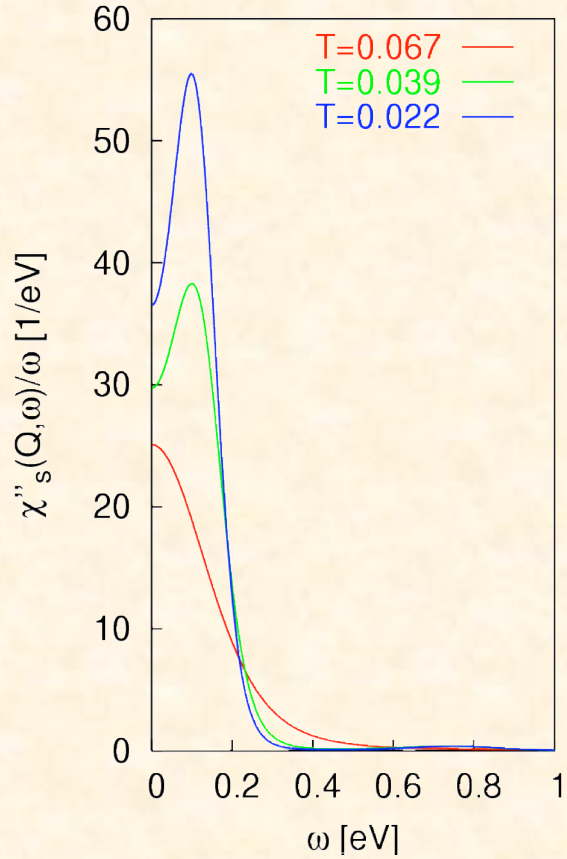
$T<T_c$: Quasiparticles are formed by *recombination of spinons and holons*
Frustrated kinetic energy is recovered

Excitations - Hubbard model

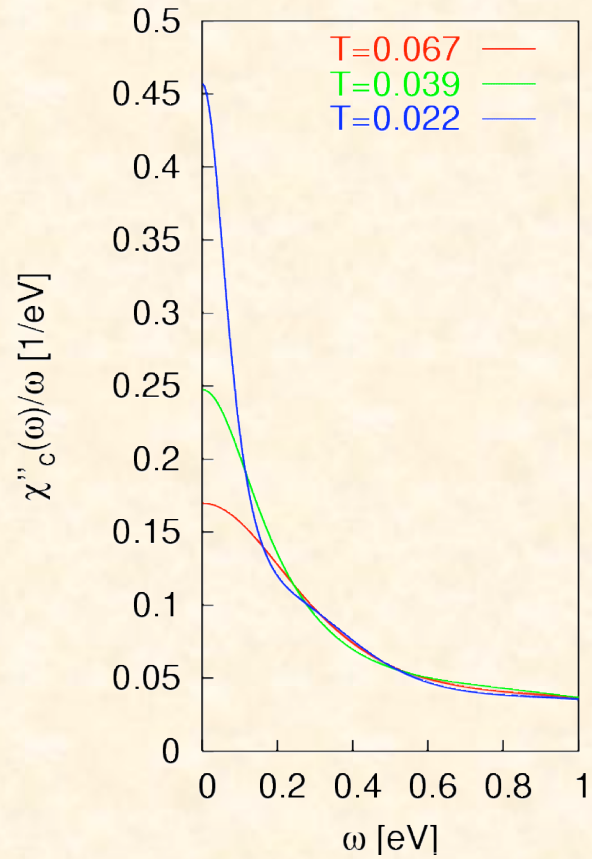
Quasiparticles



Spin



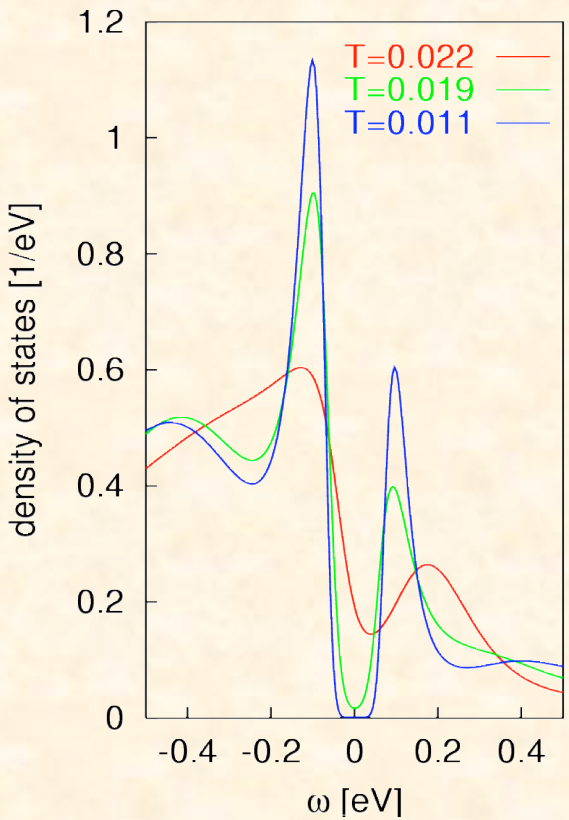
Charge



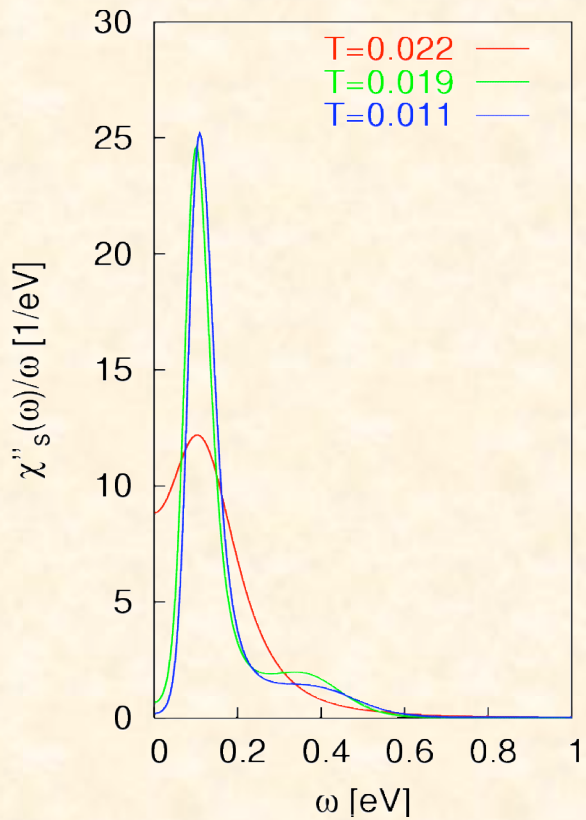
$T_c<T<T^*$: *Spin excitations suppressed, charge more coherent*

Excitations $T<T_c$ - Hubbard model

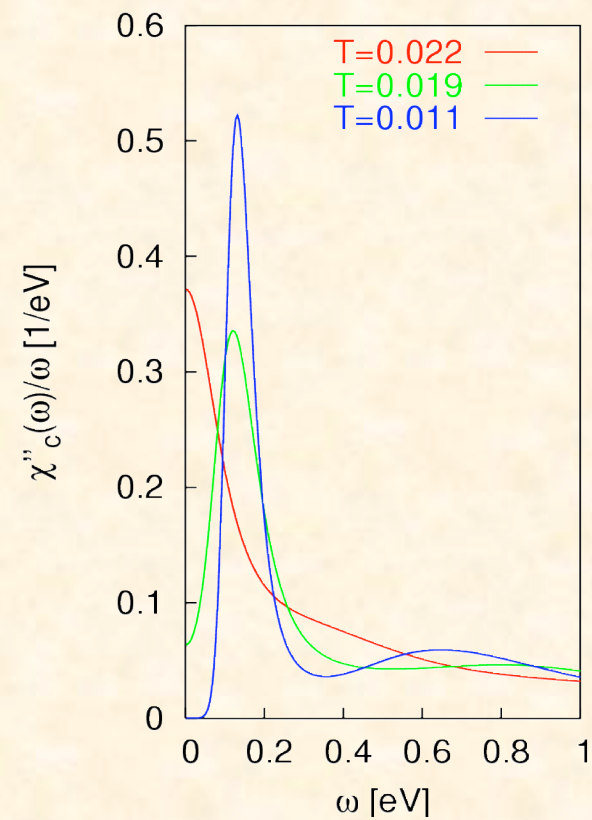
Quasiparticles



Spin



Charge



$T< T_c$: *Spin & Charge qualitatively similar, gapped*

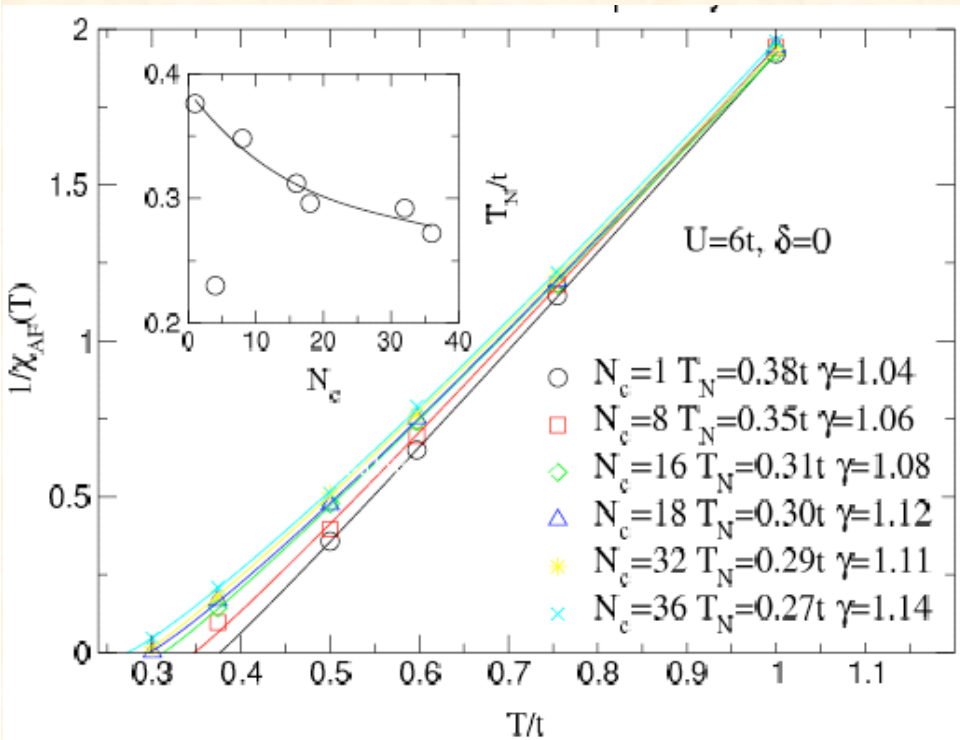
Summary, Conclusions & Outlook

- *Short-ranged AF correlations* ⟶ *DCA*
- *Kinetic energy driven pairing in Hubbard model*
- *Exchange energy driven pairing in t-J model*
- *Exchange energy driven pairing in t-J model*
- *Anomalous normal state and pairing consistent with RVB*

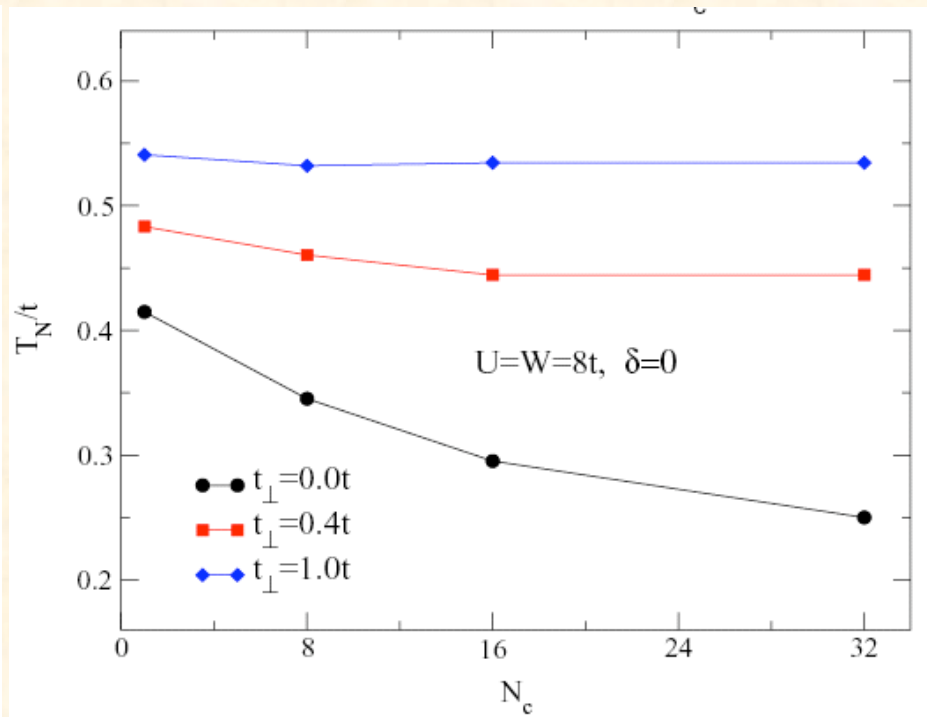
- *Frustration* ⟶ *Gossamer superconductor?*
- *Larger clusters*
  Superconductivity? Spin-charge separation?
- *LDA + DCA* ⟶ *Material specific properties*

Larger N_c & Interplanar coupling

inverse AF susceptibility



Neél temperature vs. N_c



- 2D model
- Periodic array of Hubbard planes

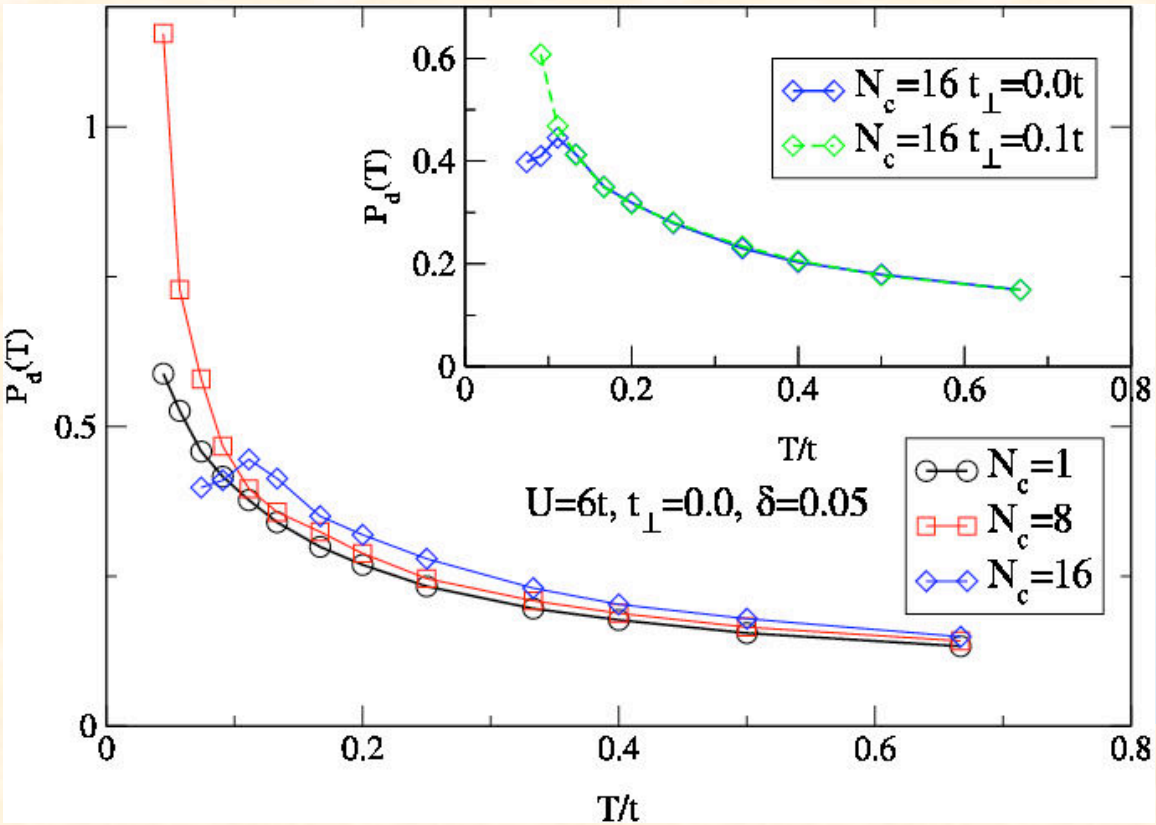
T_N → 0 for N_c →

consistent with Mermin-Wagner

stabilizes Antiferromagnetism

Pairing & Interplanar coupling

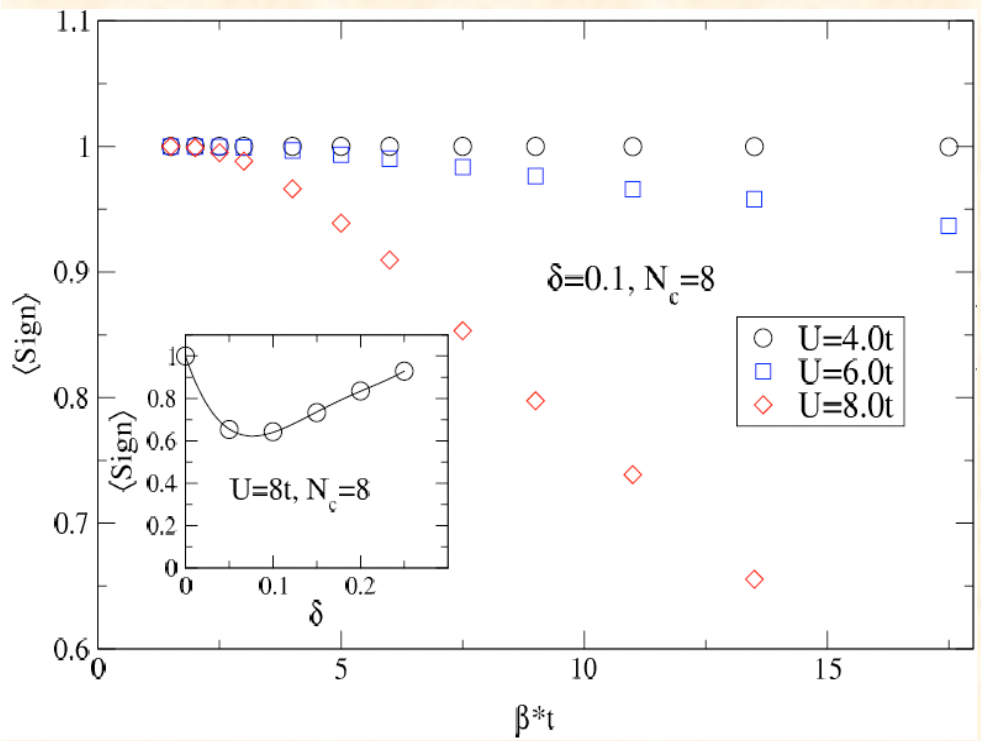
Pairfield susceptibility for different N_c's



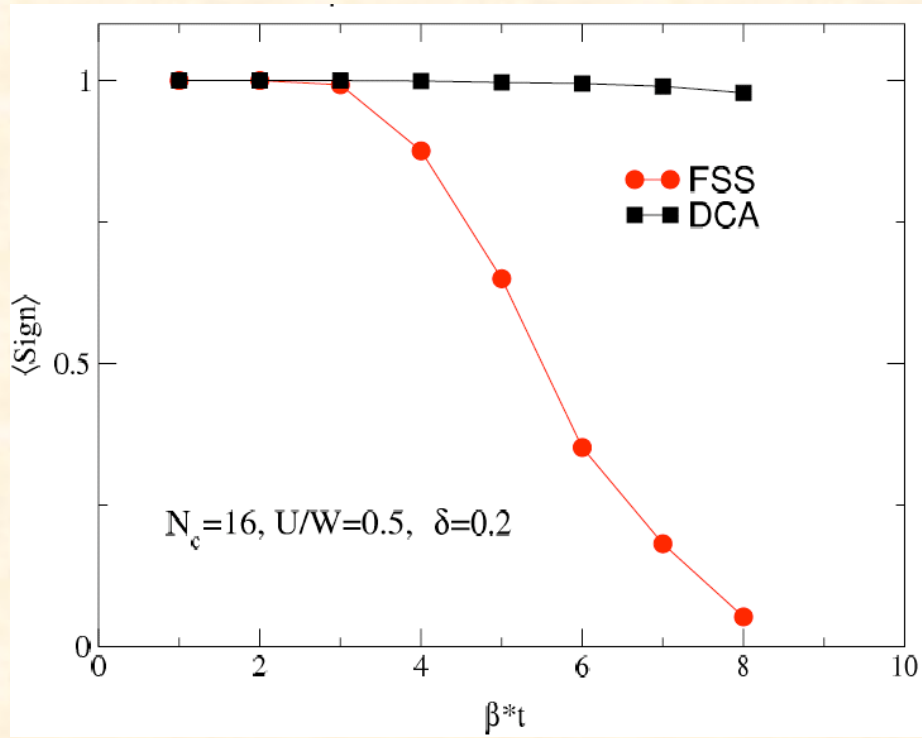
Finite interplanar coupling seems to stabilize transition

QMC Sign Problem

DCA average sign



Comparison DCA-FSS



- Sign problem still present in DCA
- But less severe than in finite size system QMC calculations