The Pairing Mechanism of the Hubbard Model

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CMSN

PIRE DMR

Collaborators: A. Macridin, B. Moritz, Th. Maier, P. Kent, D.J. Scalapino

University of Cincinnati

Kyoto, Japan, Nov. 2007

Outline

- Cuprates + Hubbard Model
- Hubbard Model
  - N_c=4
  - Larger Clusters?
  - The pairing mechanism.
- Hubbard-Phonon Model
  - Phonon-Enhanced spin Polarons
  - Phonons and T_c
- Conclusions and Outlook

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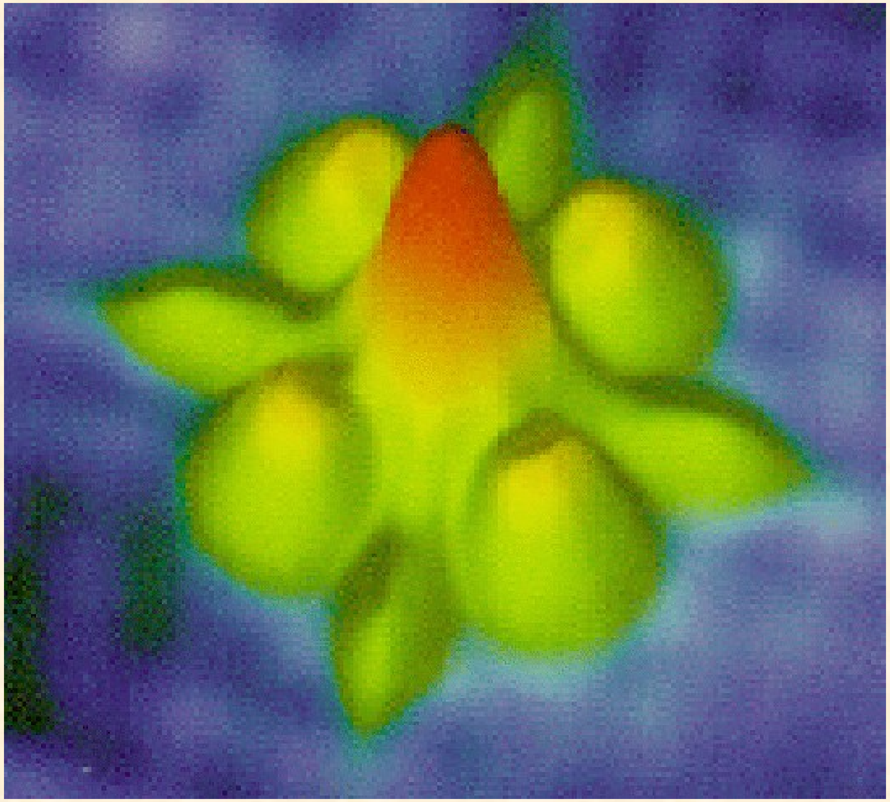
Cuprates: Unusual Superconductors

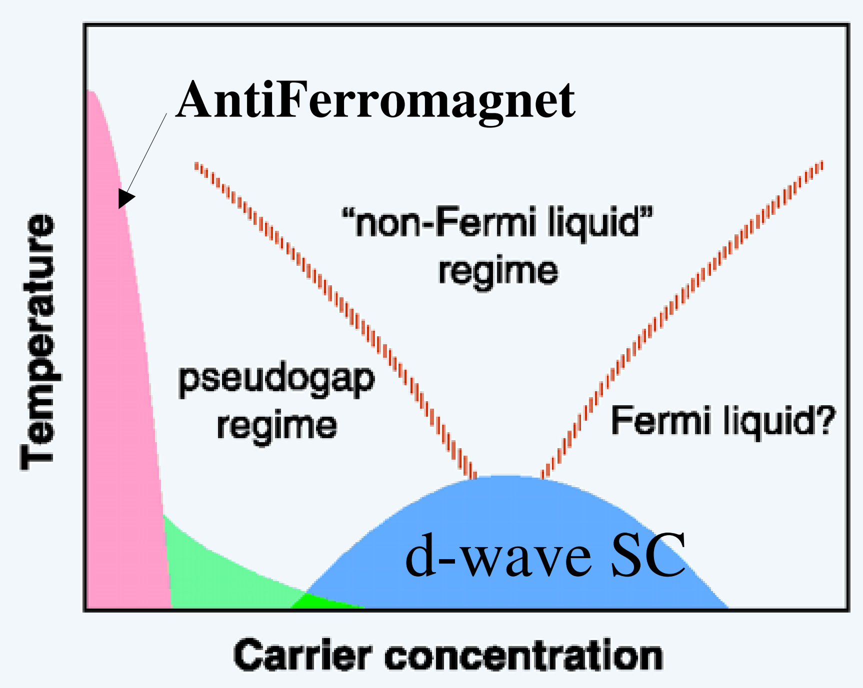


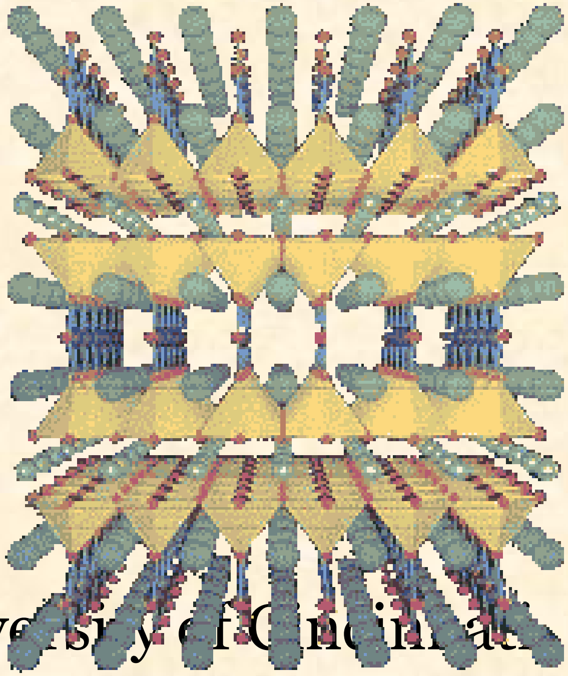
S. Pan, dI/dV at resonance

- **Doped Mott insulator.**
- **d-wave SC order**
- **Non-Fermi liquid underdoped normal state**
- **Pseudogap**
- **Kinetically Driven Pairing?**

Alex Müller
Georg Bednorz

Cuprate structure and phase





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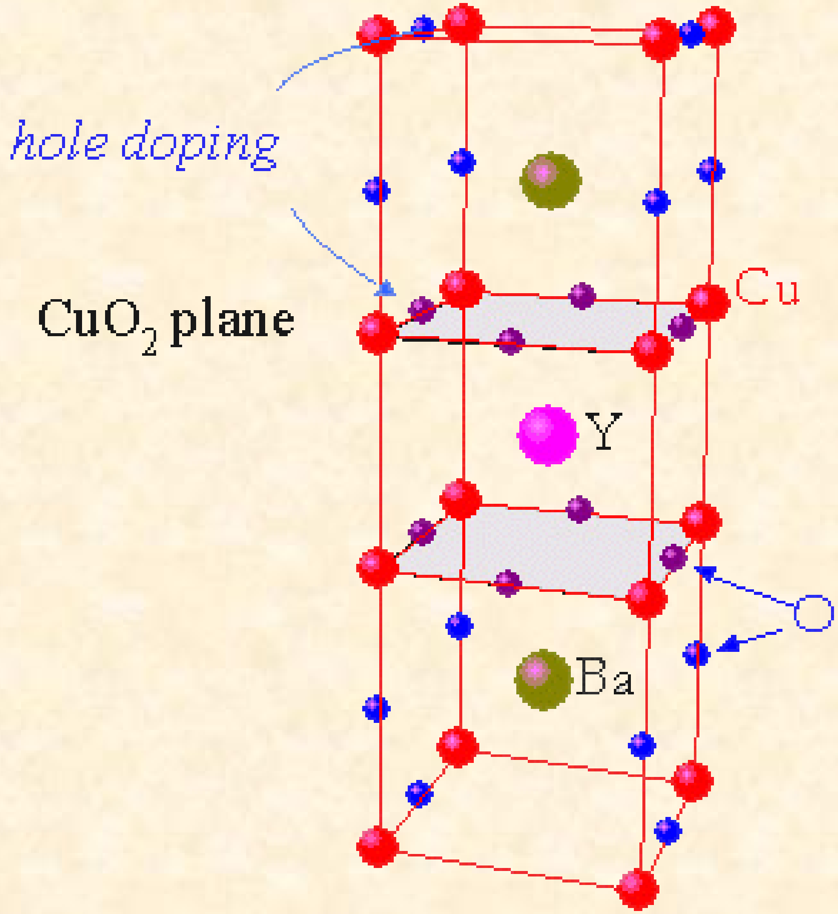
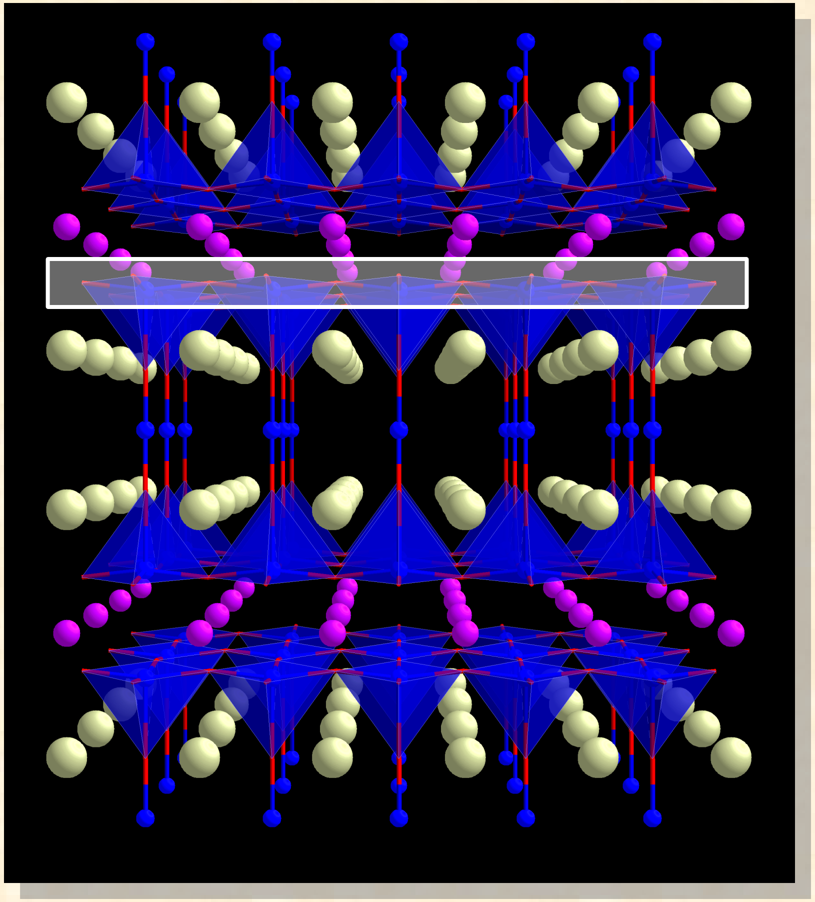
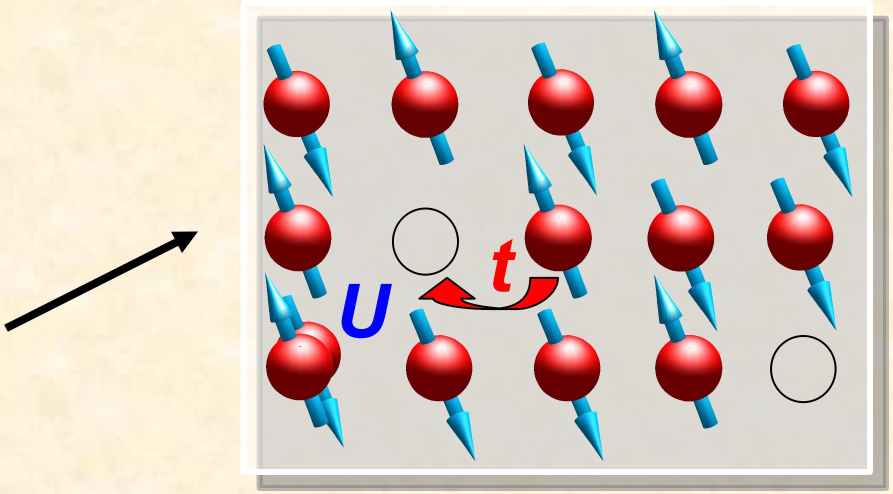


$$YBa_2Cu_3O_{7-\delta}, T_c = 93\,K$$

Modelling The Cuprates





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

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

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 $\rightarrow$ Groundstate d-wave superconducting**
    (Halboth, PRB 2000; Zanchi, PRB 2000)
- **Strong coupling (W/U << 1)**
  - **Finite size simulations of t-J model $\rightarrow$ Groundstate superconducting**
    (Sorella, PRL 2002; Poilblanc, cond-mat 2002)
- **Intermediate coupling (W $\approx$U)**
  - **Inconclusive!**

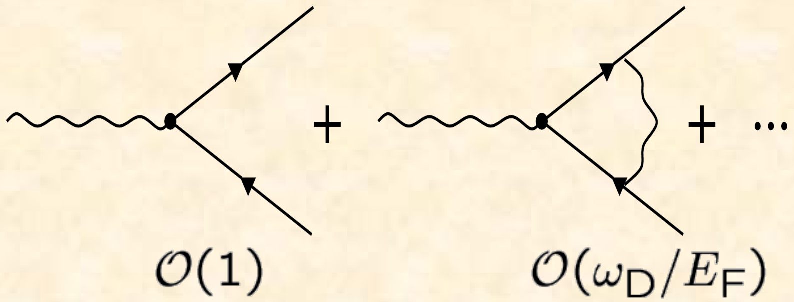
Small Parameter?

BCS (conventional) SC:

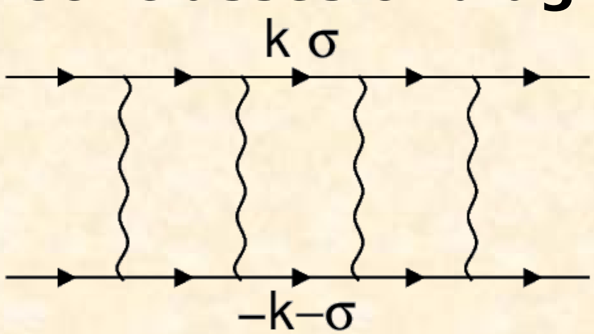
Small parameter:

$$\omega_{\mathrm{D}}/E_{\mathrm{F}} \propto \sqrt{m/M} \ll 1$$

Electron-phonon vertex:



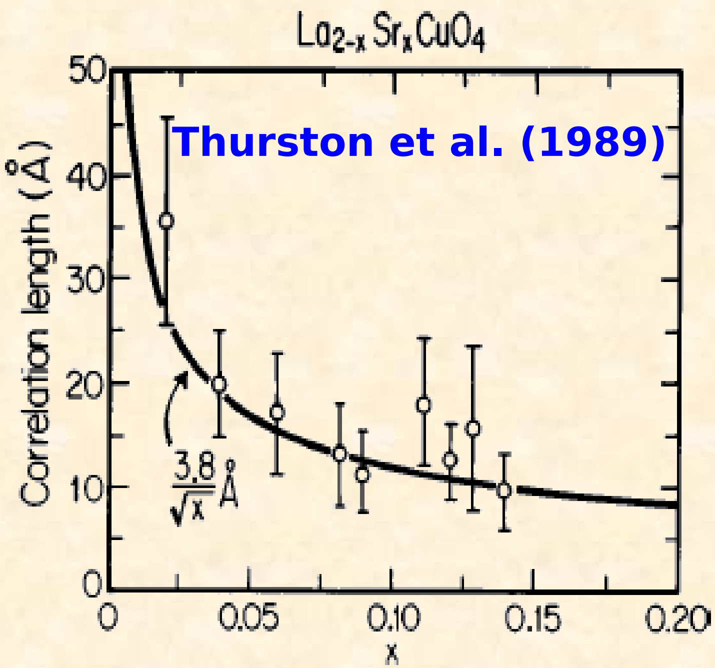
Neglect classes of diagrams:



Cuprate (unconventional) SC:

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

But in Cuprates:



Short-ranged AF correlations

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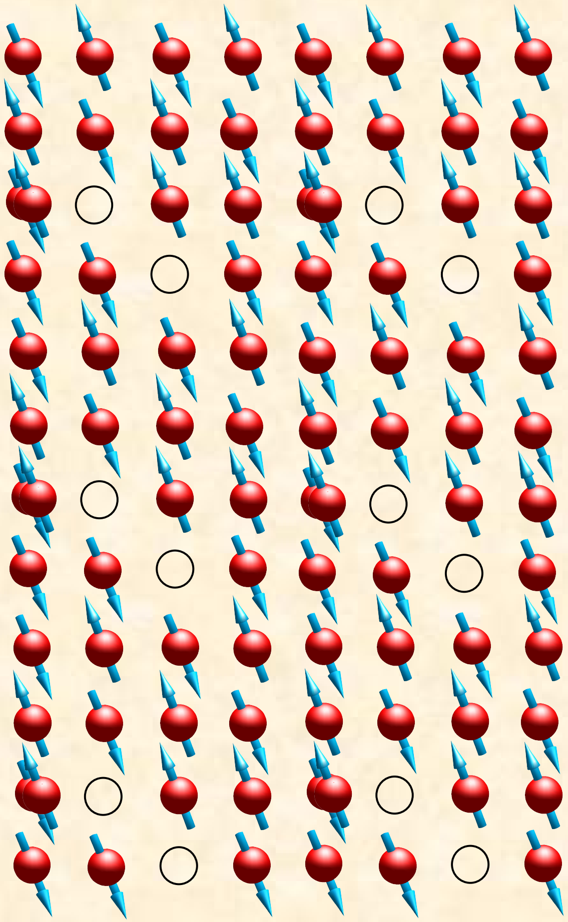
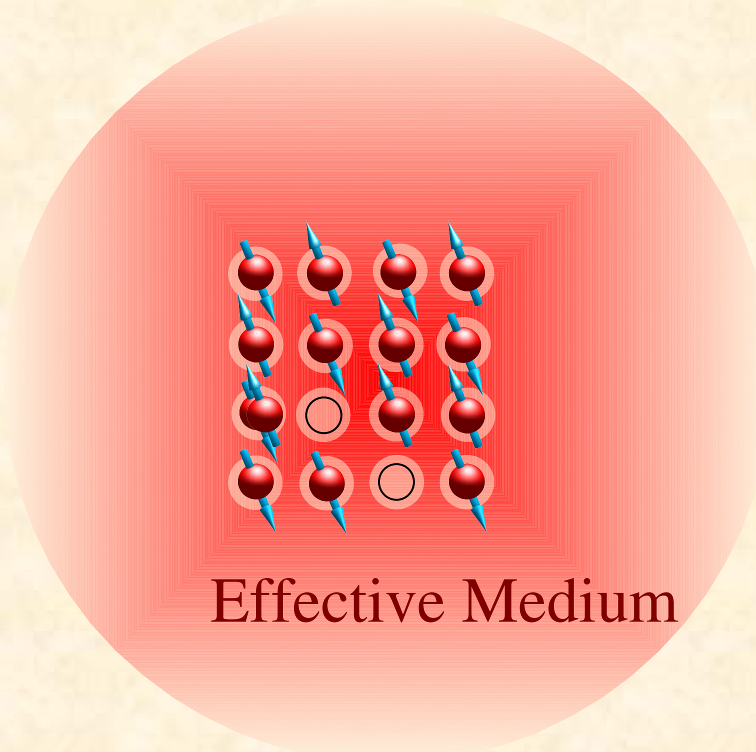
Dynamical Cluster Approximation

Periodic Lattice



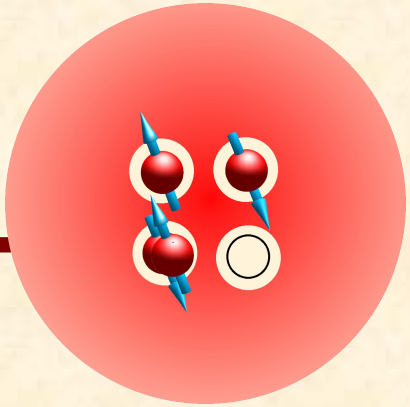
DCA



- **Short length scales, within the cluster, treated explicitly.**
- **Long length scales treated within a mean field.**
- **N_c=1 DMF, N_c=∞, exact**

For a review of quantum cluster approaches: Th. Maier *et al., Rev. Mod. Phys. 77, pp. 1027 (2005).*

Outline



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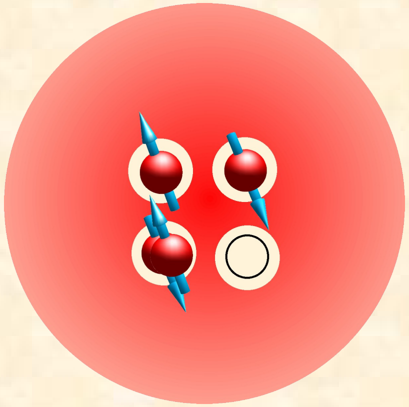
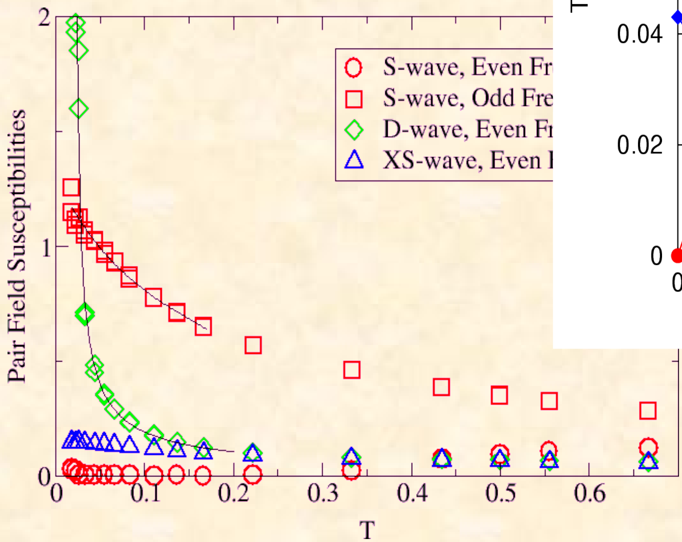
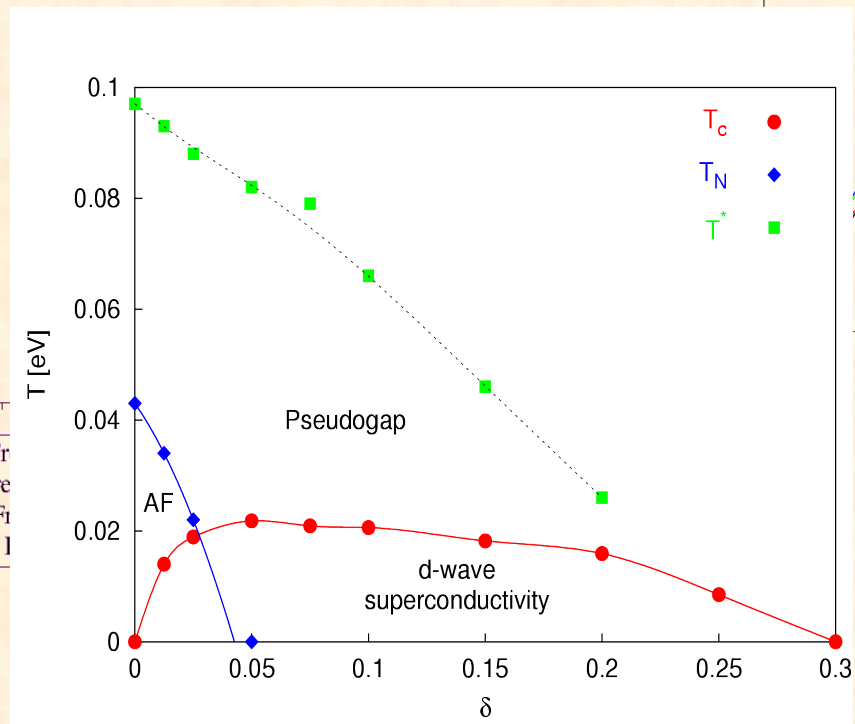
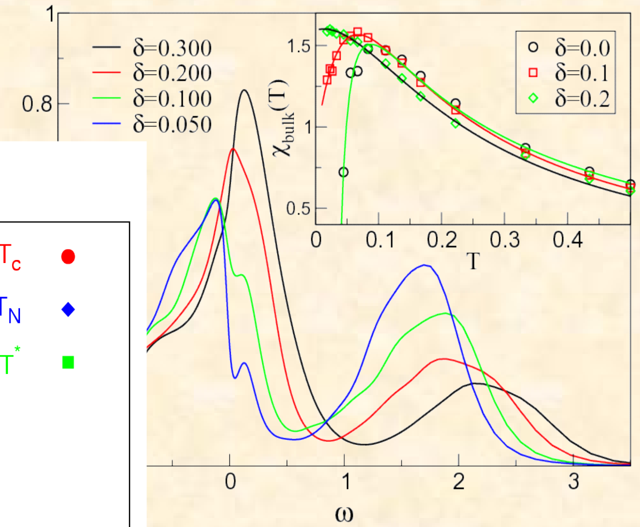
4-site cluster DCA - 2D Hubbard model









$N_c=4$, $U=W=2$, $t'=0$

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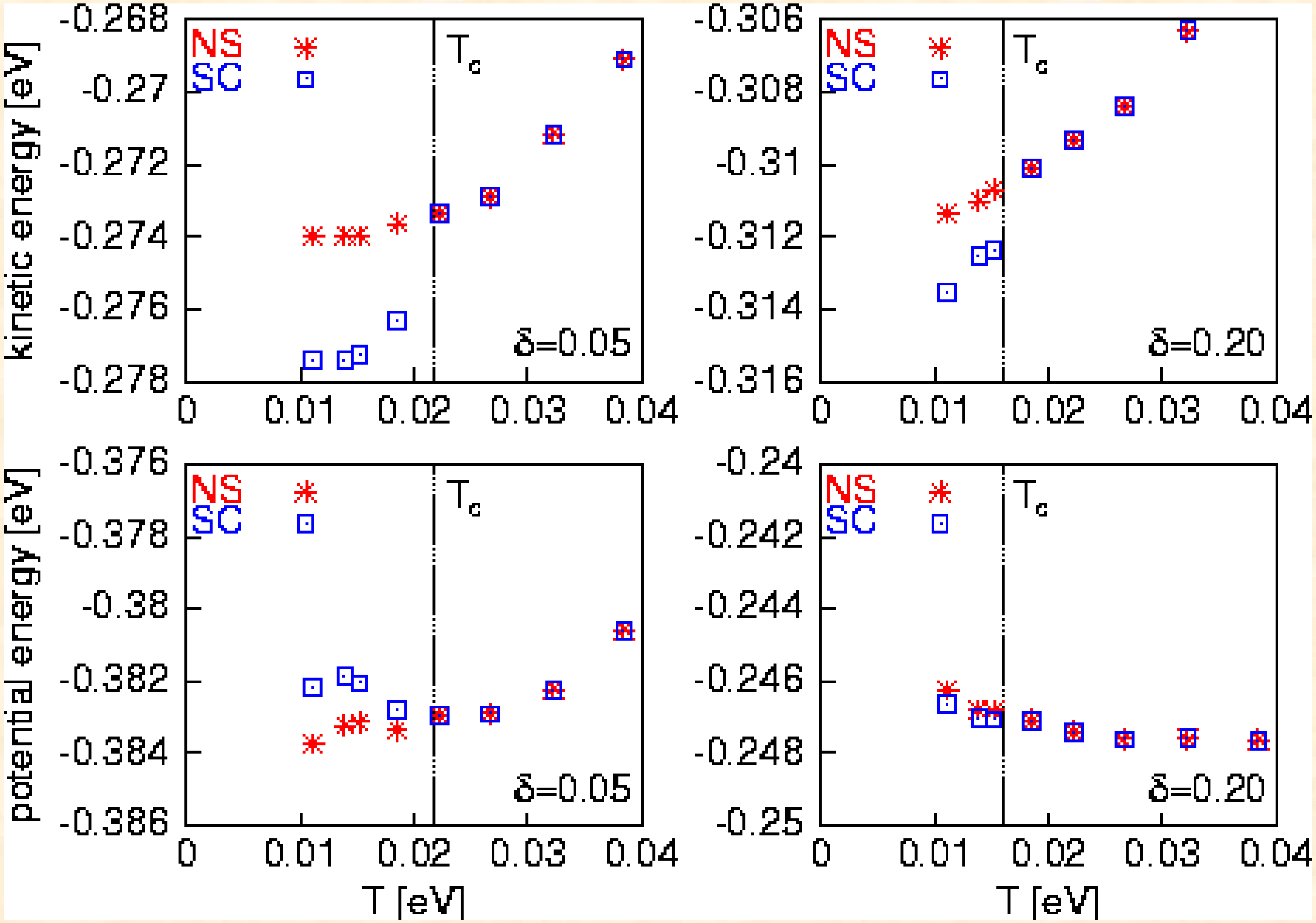
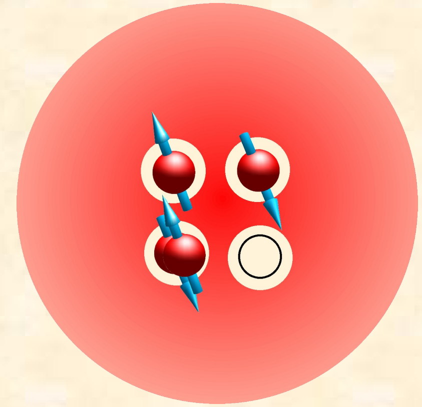
(MJ, Th. Maier several papers)

Kinetic and Potential Energies



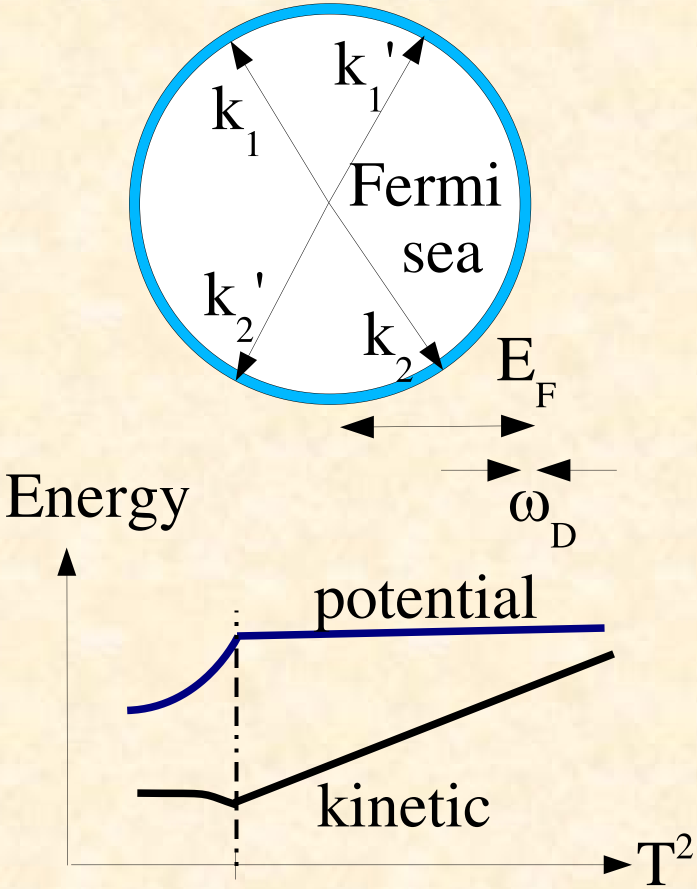


- **SC driven by kinetic energy gain**
- **D. Molegraaf, Science 2002**

University of Cincinnati $N_c=4$, U=W=2, t'=0

Energy of the SC transition

BCS (conventional) SC:



Pairing due to potential energy gain

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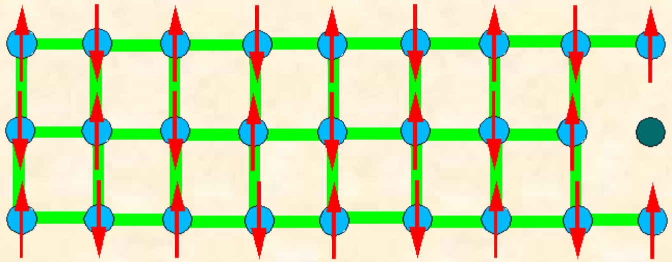
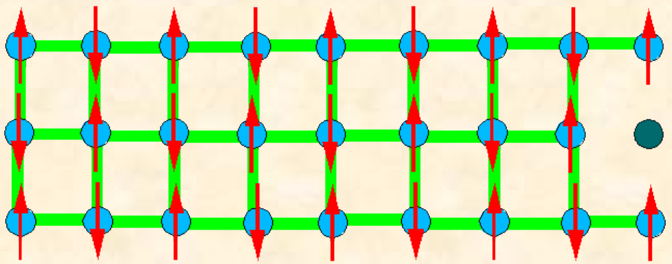
Cuprate (unconventional) SC:

- One hole motion breaks AF bonds



- A bound second hole restores the AF bonds

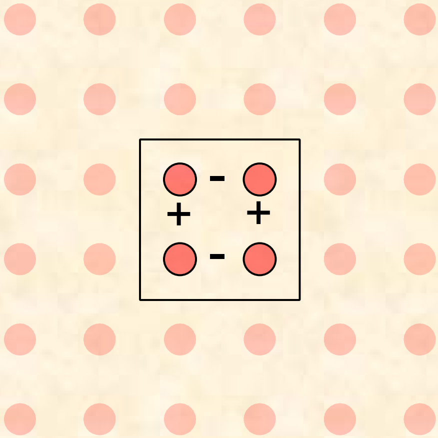


Pairing due to kinetic energy gain

(Brinkman, Hirsch)

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 $N_c \to \infty$?
  - True nature of the pairing mechanism

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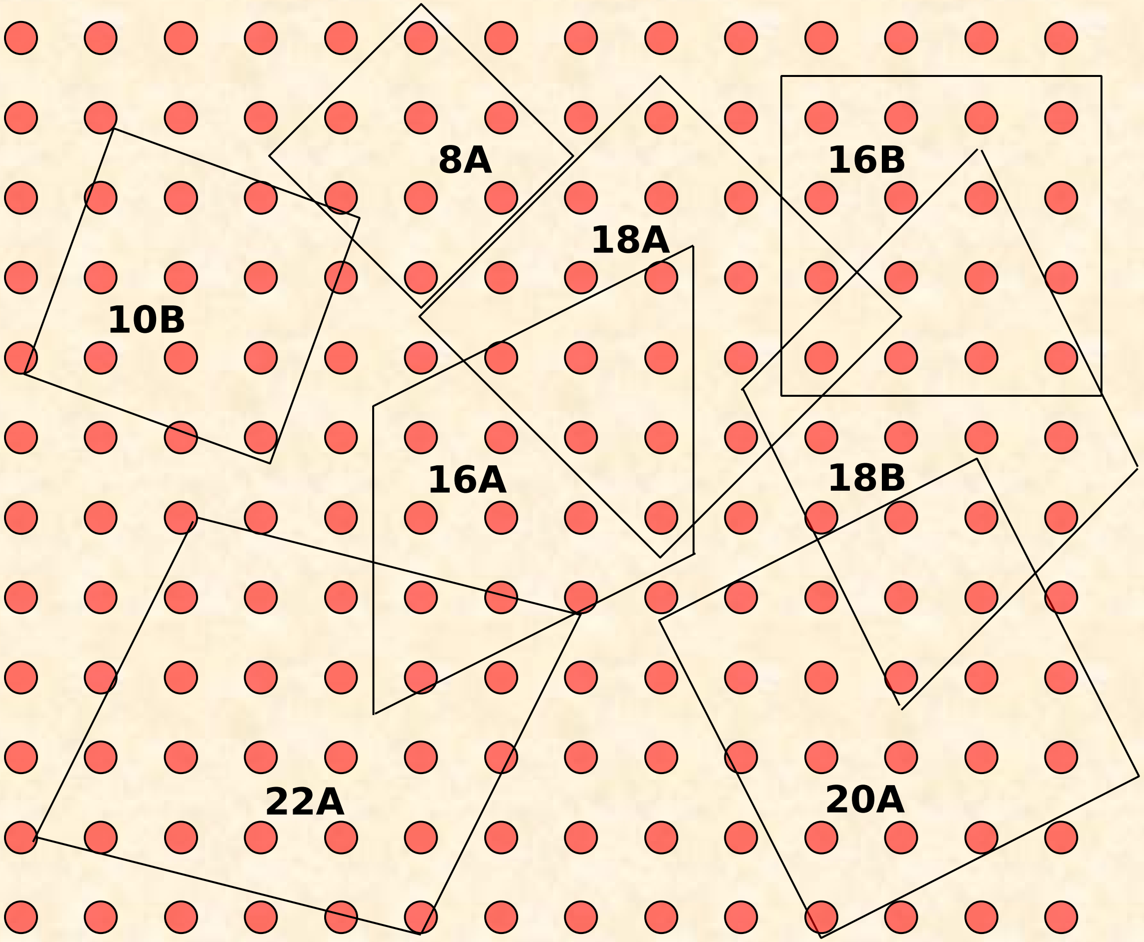
Scaling in Cluster Size (Betts Clusters)

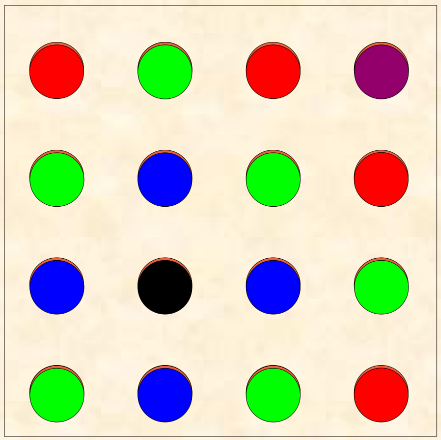


- **Scaling is difficult**
  - **There are few clusters with the same symmetry as the lattice**
- **Solution: Betts clusters, selected for**
  - **Neighbors in a given shell**
  - **Symmetry**
  - **Squareness**

(Betts, Can. J. Phys. 1999)

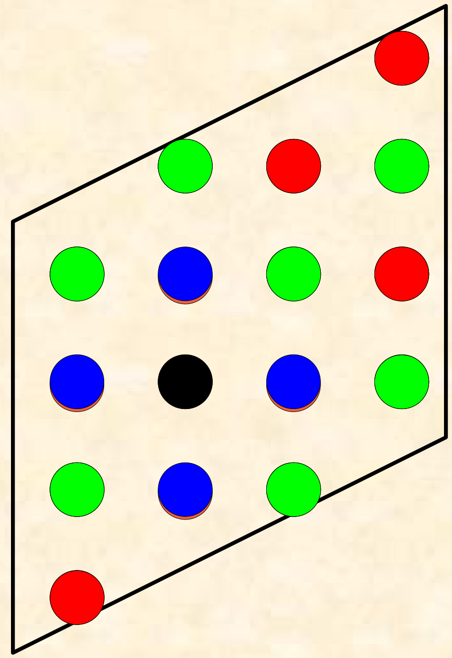
Betts Clusters: Neighbor Shells

Bad N_c=16 cluster



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

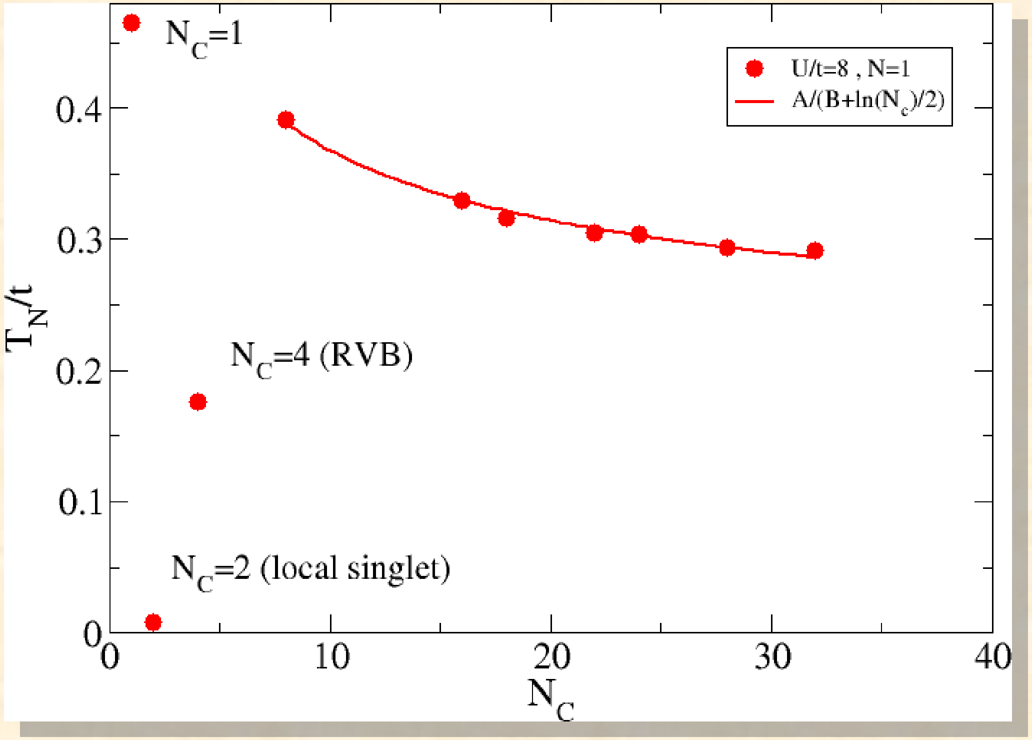
Better N_c=16 cluster

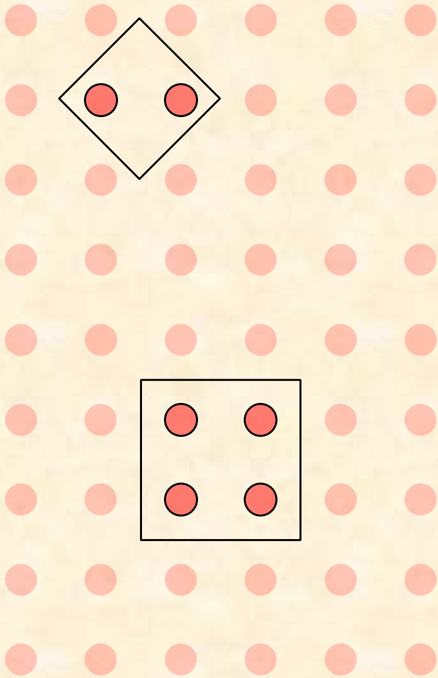


16A	
n	#
0	1
1	4
2	7
3	4

- In the lattice, the shells have 4, 8, 12... neighbors
- Good scaling clusters emulate the lattice
- Betts clusters have the smallest number of imperfections in filling

Antiferromagnetism: Cluster size dependence



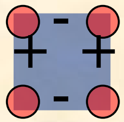


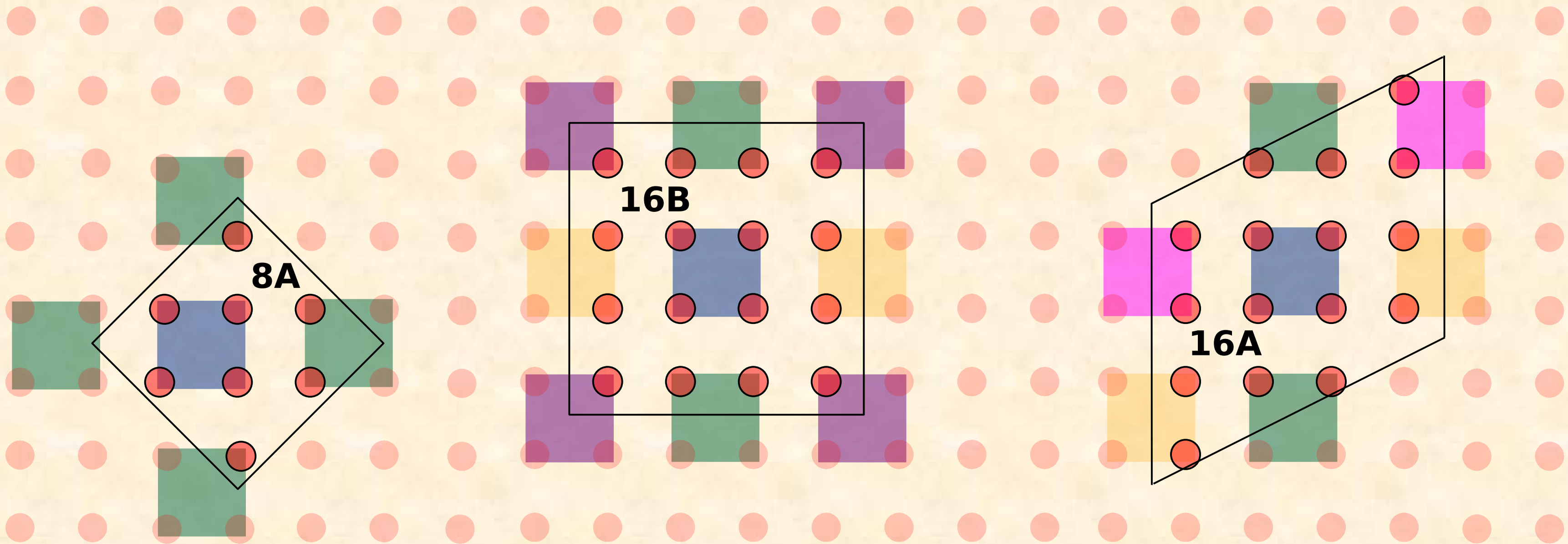
- **Scaling Ansatz $\xi(T_N) = L_c$, or T_N=A/(B+ln(N_c)/2)**
- **$T_N \rightarrow$ 0 logarithmically with $N_c \rightarrow \infty$ (SRW 89, Hirsch 87)**
- **$N_c \geq 8$ lie on line (not true w/o Betts clusters)**

(Th. Maier, PRL)

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

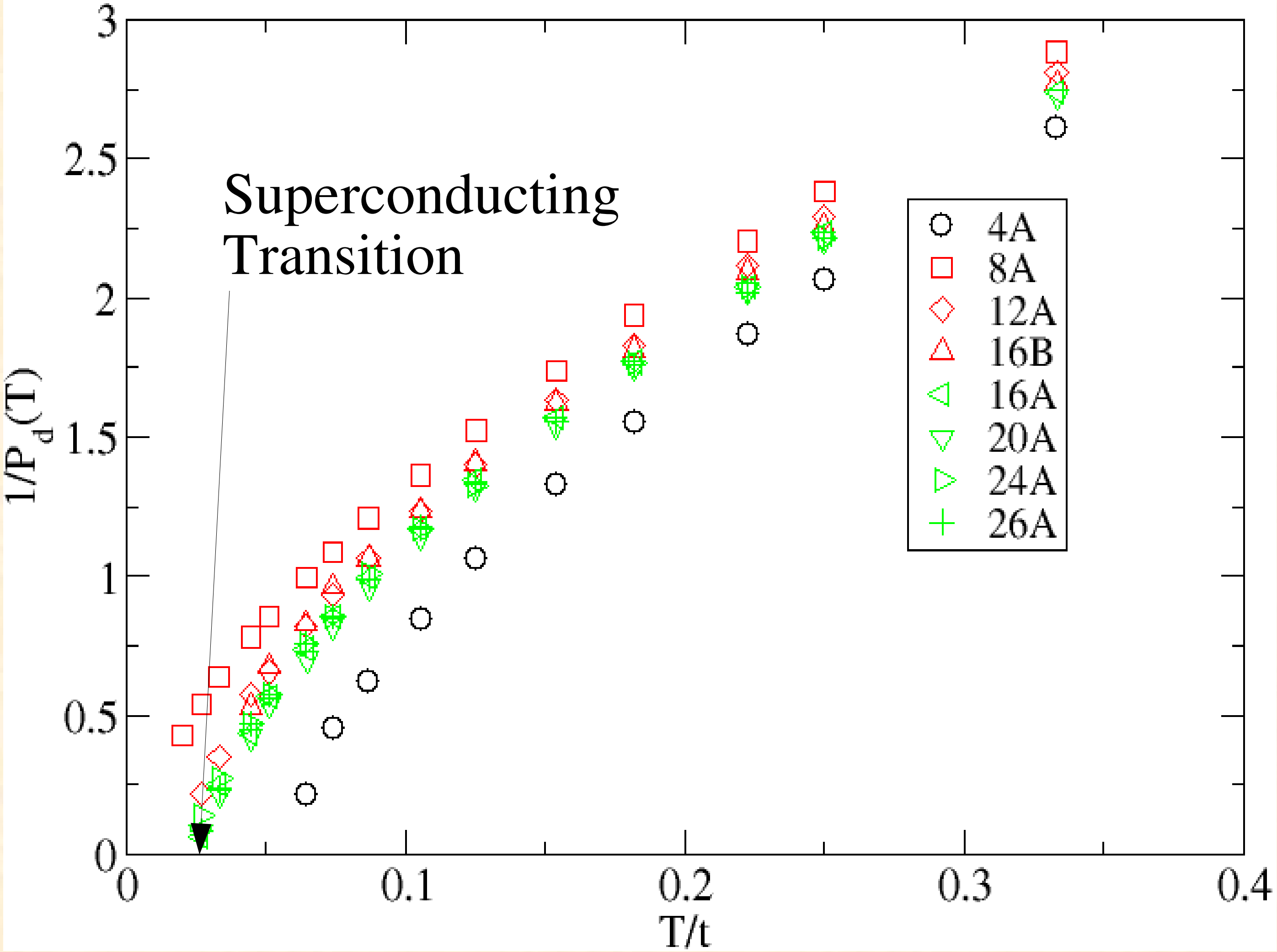




Number of independent neighboring d-wave plaquettes:

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

Inverse 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

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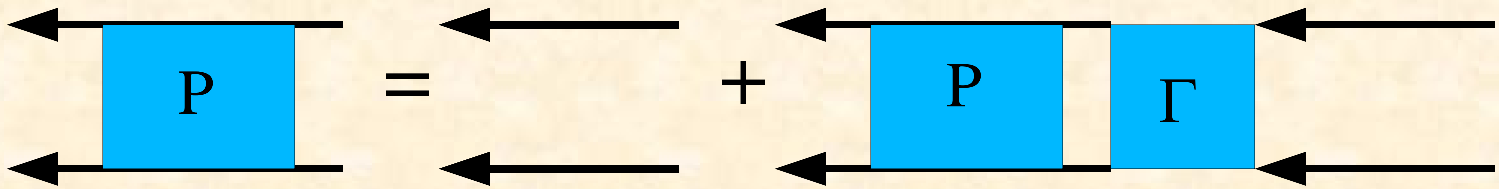
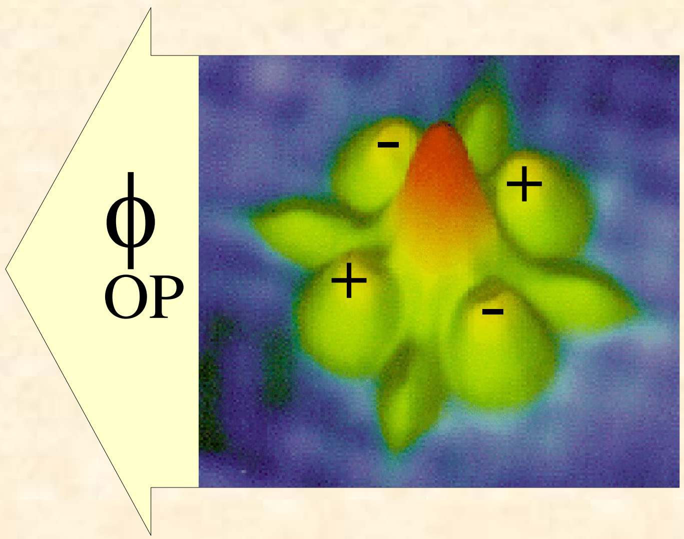
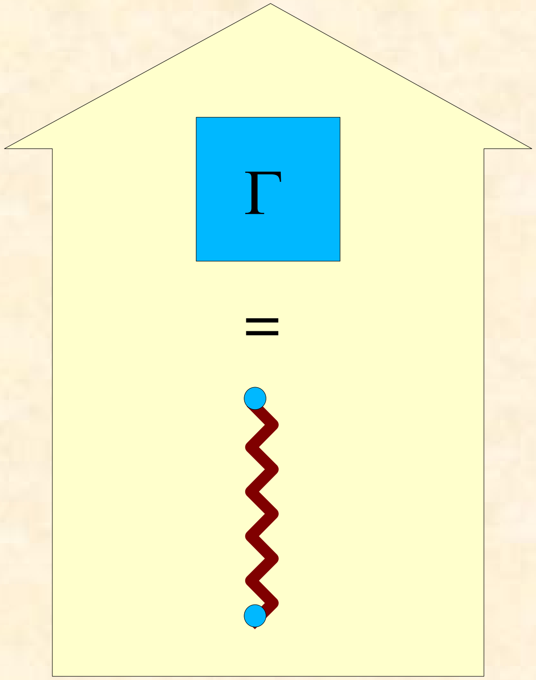
The Mechanism

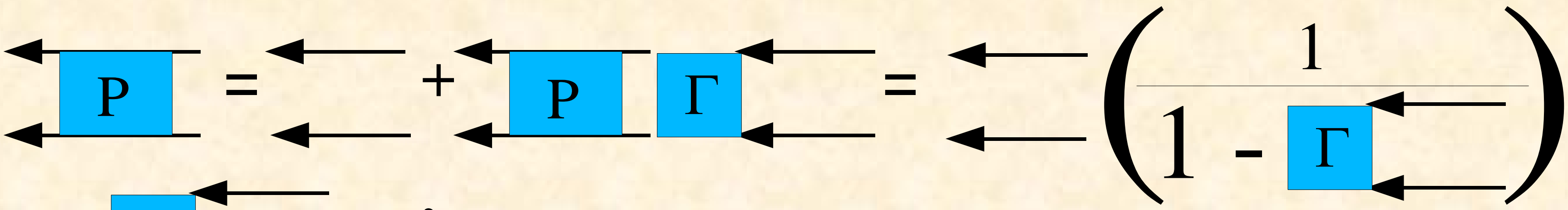


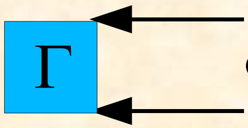




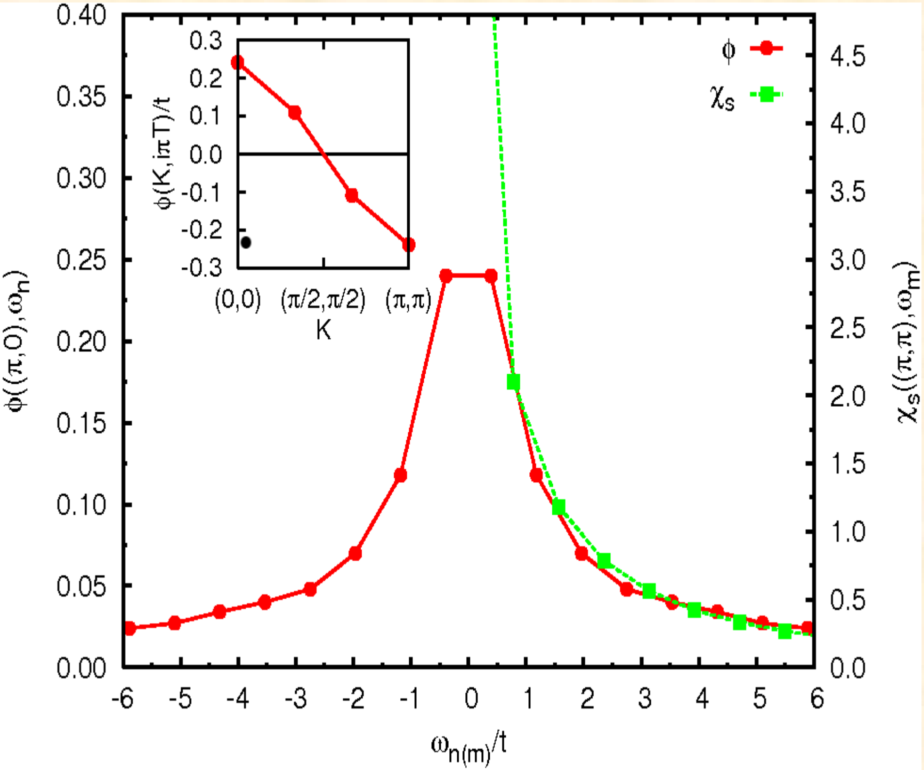
The Mechanism

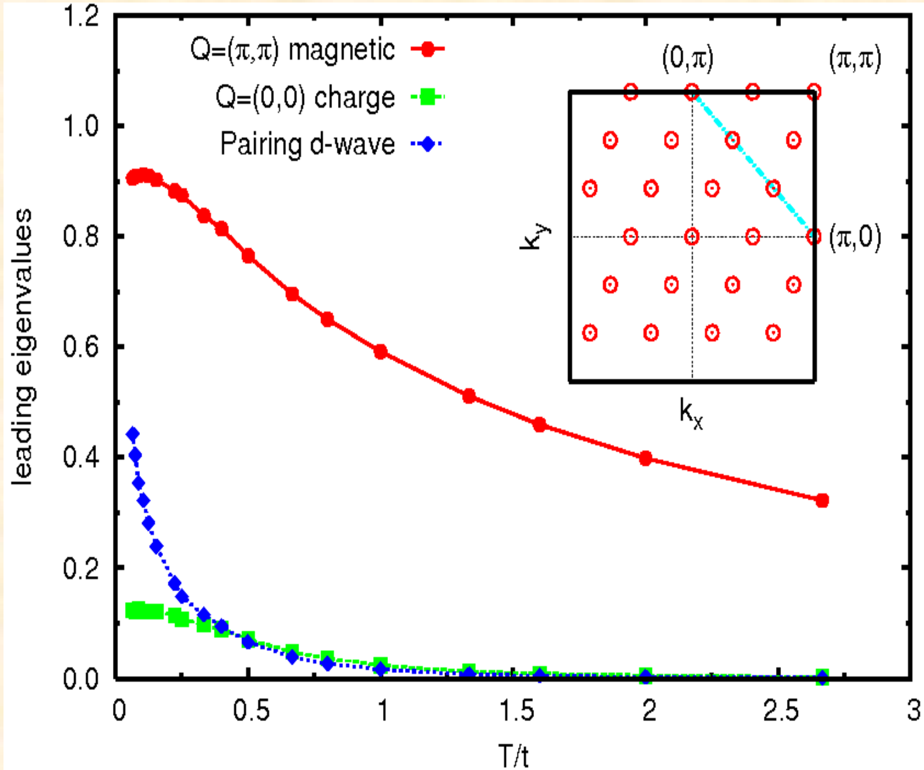
$N_c=24$, $U=4t$, $N=0.9$



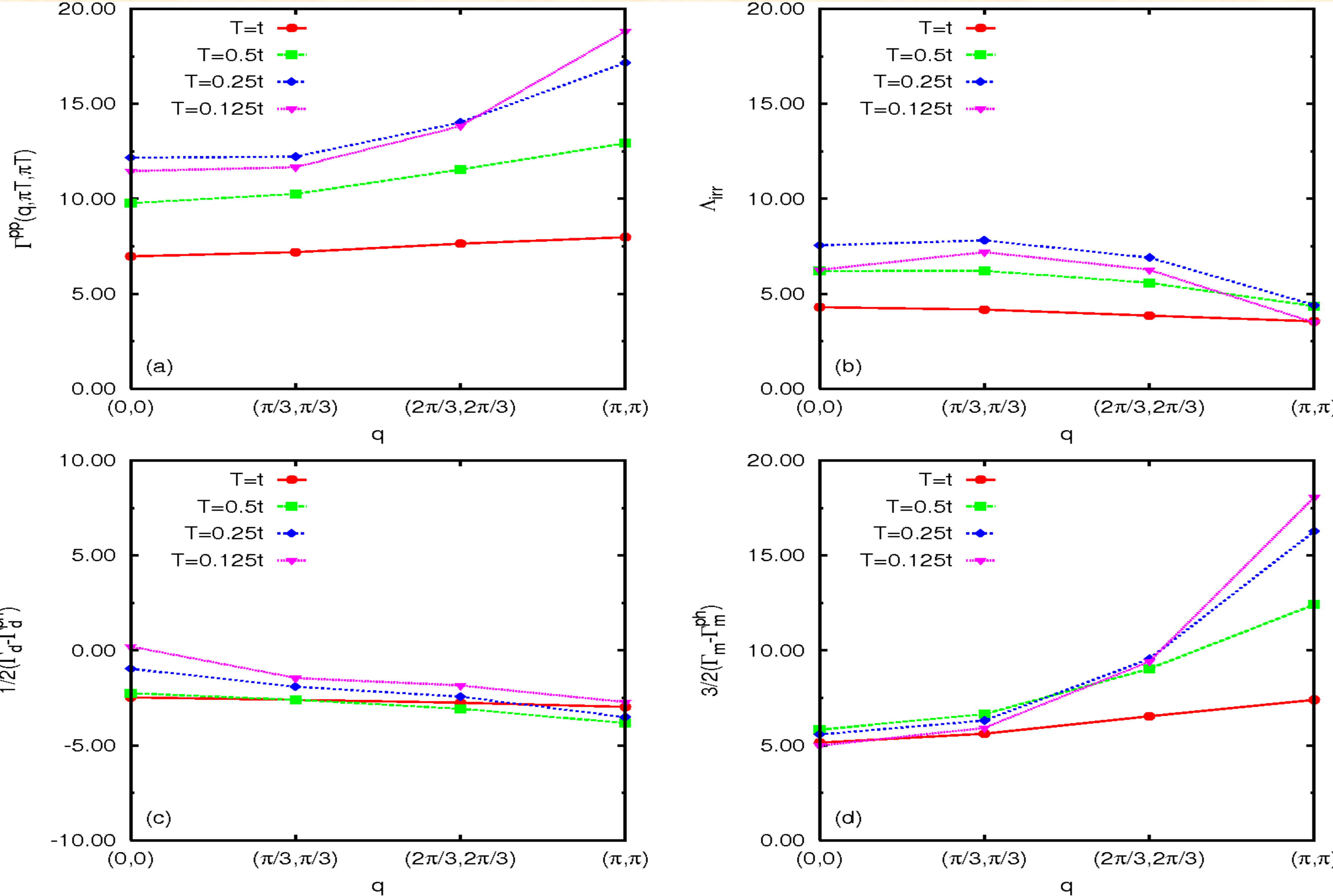


$\Phi=\lambda\Phi$ at T_c $\lambda=1$





Channel Decomposition of Pairing Vertex



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    - Way to fit experimental data?
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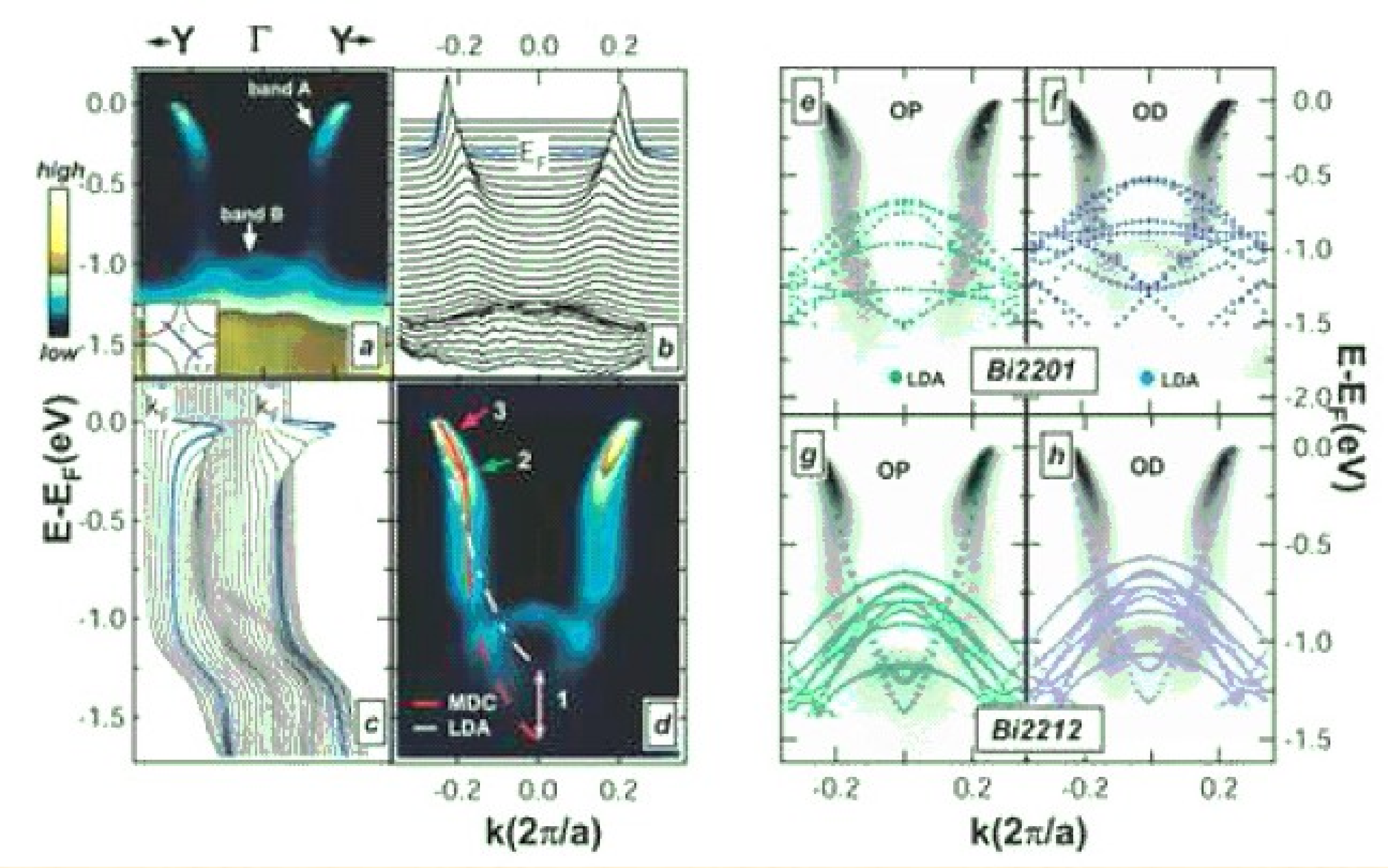
High-Energy Kink (overdoped Bi2201)

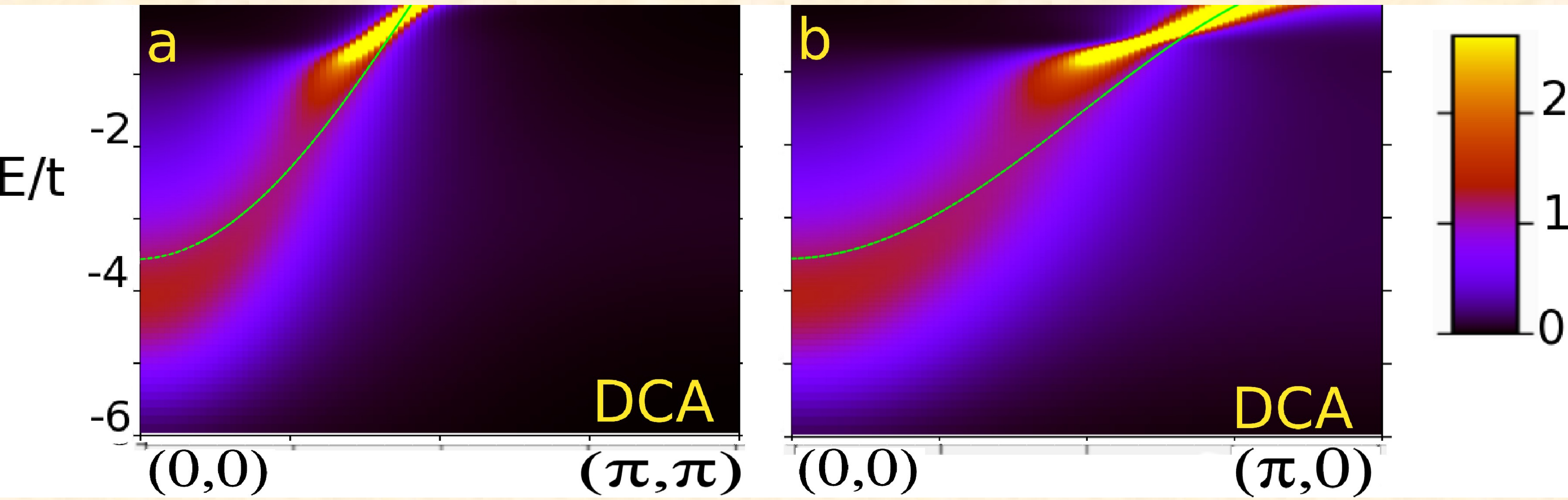


University of Cincinnati Meevasana et al., cond-mat/0612541

High-Energy Kink in the 2D Hubbard Model

n=0.8, U=8t, cluster 16B, E_{kink} = - t

$(0,0) \rightarrow (\pi,\pi)$ $(0,0) \rightarrow (\pi,0)$



A. Macridin
PRL to appear
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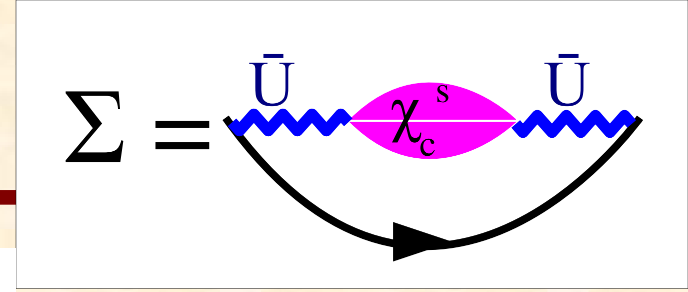
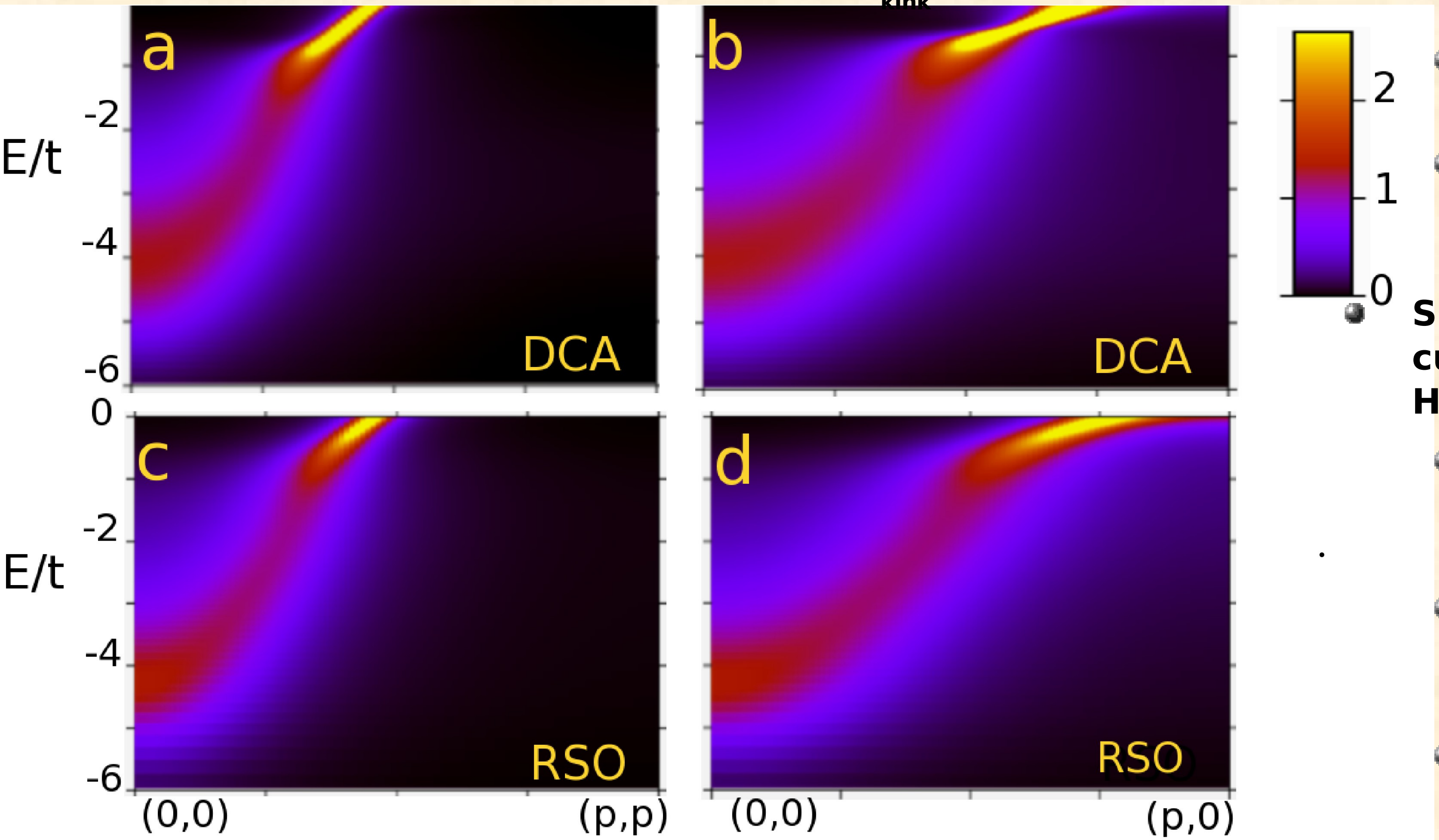
- Kink at $E_{kink} \approx -t$
- (0,0) Dispersion below bare band

Origin of the HE Kink



$$\Sigma^{RSO}(\mathbf{k}, i\omega) = \frac{3}{2}\bar{U}^2 \sum_q \sum_\nu G_c(\mathbf{k}-q, i\omega - i\nu)\chi_c(q, i\nu)$$

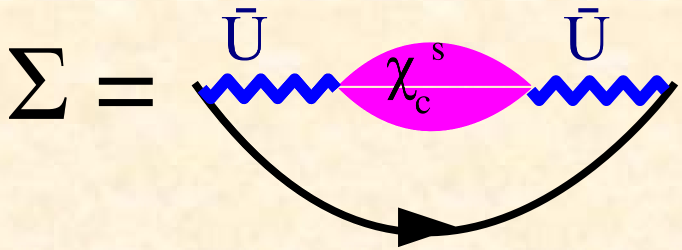
n=0.8, U=8t, cluster 16B, E_{kink} = - t



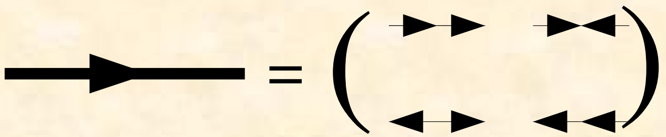
$(0,0) \rightarrow (\pi,\pi)$ $(0,0) \rightarrow (\pi,0)$

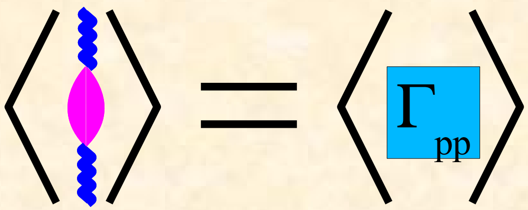
- **Spin, charge, and pair terms (different χ).**
- **Spin dominates**
- **$\bar{U}$<U due to QP renormalization.**
- **Spin RSO used for cuprates and Heavy Fermions**
  - **Kampf & Schrieffer, RPB 42 (1990).**
  - **M. Norman, PRL. 59, 232 (1987).**
  - **Berk & Schrieffer, PRL 17 433 (1966).**
  - **Valla, ibid.**

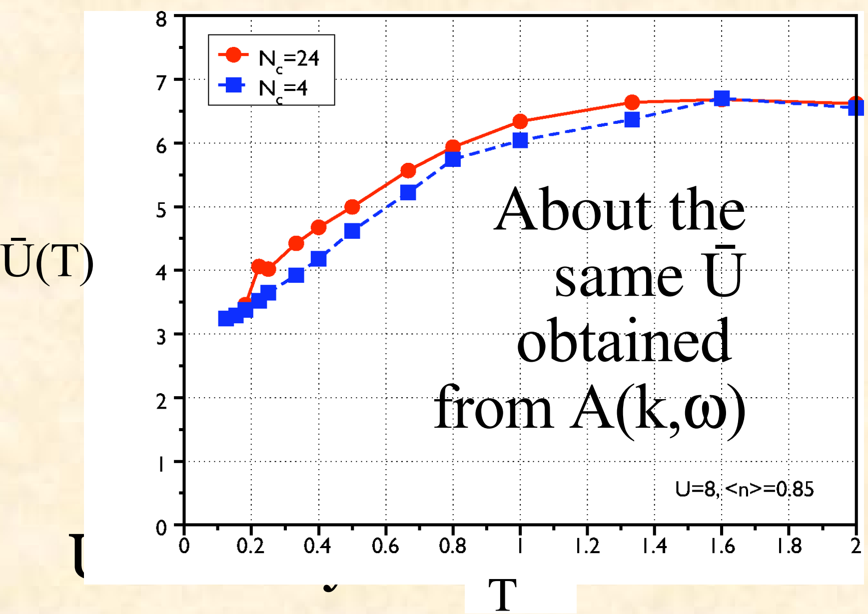
RSO Applied to Superconductivity

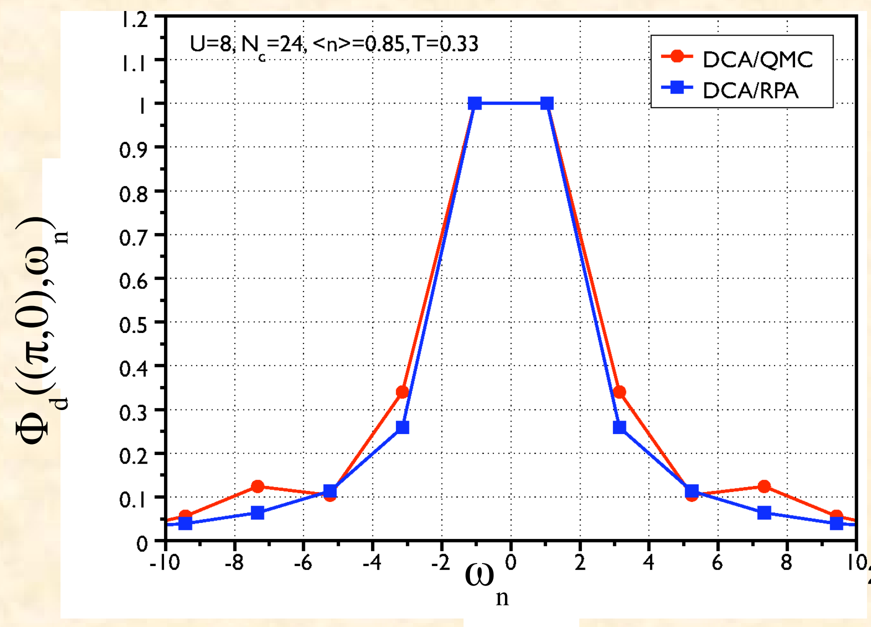


where now

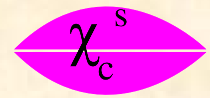


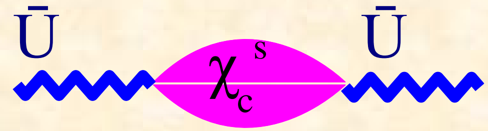


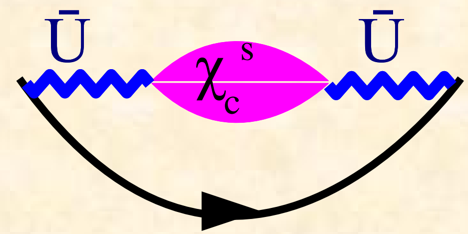




Possible method to analyze experiment

- **Extract spin S(q,ω) from neutron scat.**
  - **use to calculate χ(k,ω)=** 

- **Compare to ARPES to determine Ū**
  - 

- **Use interaction in a DCA extension of Migdal Eliashberg (J. Hague) to calculate superconducting properties**
  - $\Sigma =$ 

  -
  - **Test 1-band model and spin-fluctuation mediated pairing for the cuprates.**

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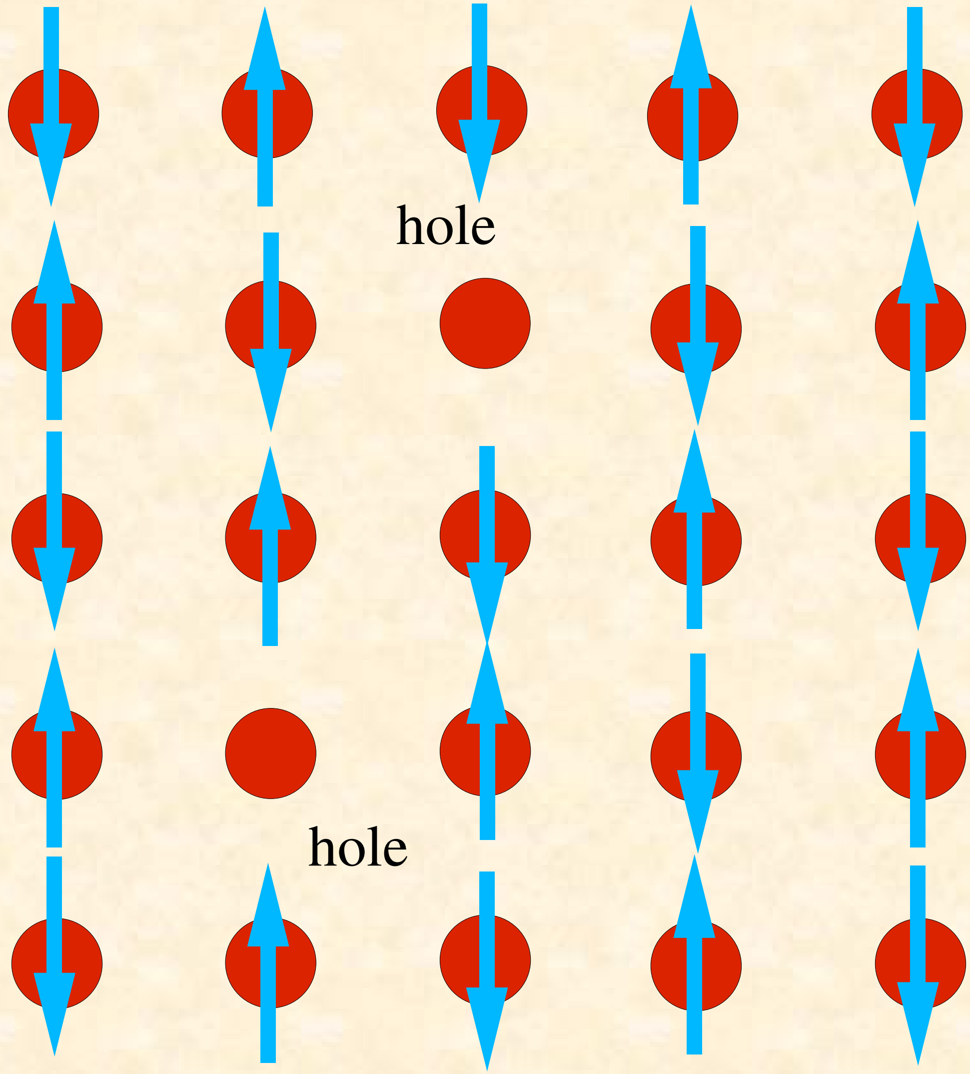
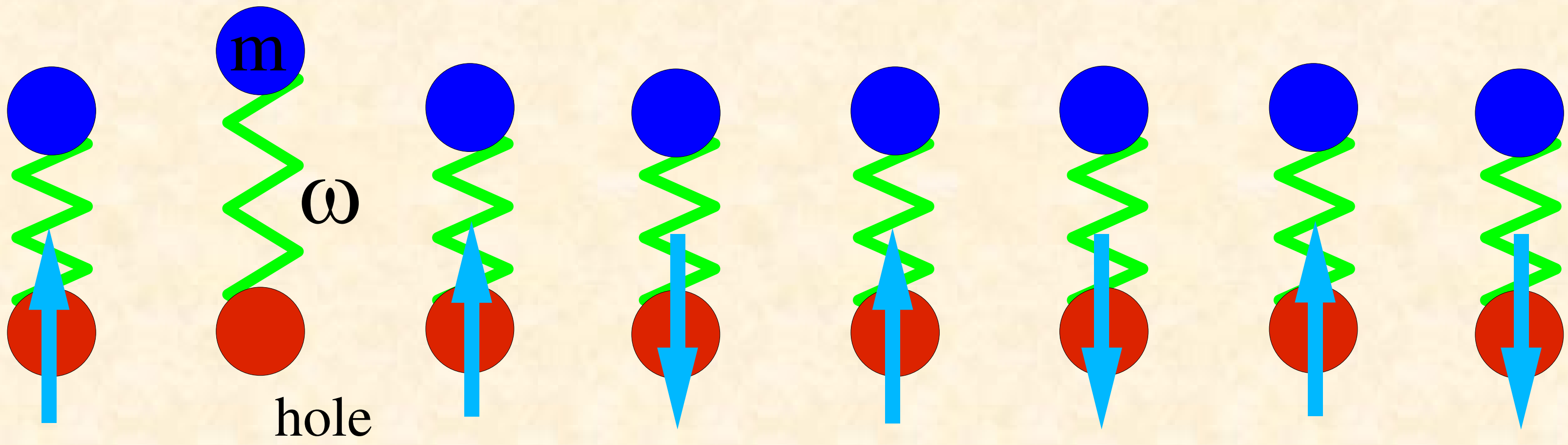
Hubbard Model: Nearly AF Metal



- **Holes in AFM**
  - **many stationary holes are needed to drive T_N to zero**
  - **Itinerant holes do far more damage**
- **Phonons tend to localize holes and increase AFM**

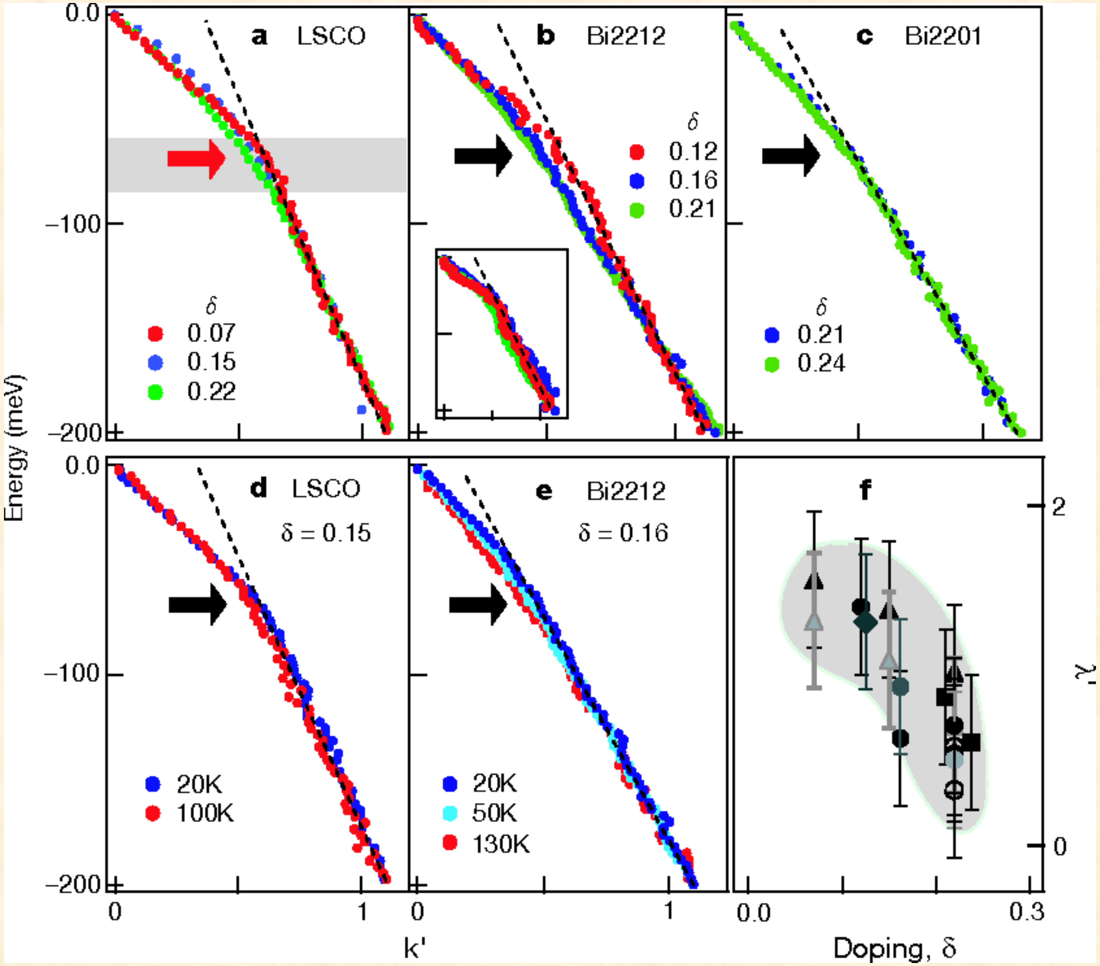
Holstein Phonons



- **Simplest Model, Hubbard+Holstein Phonons**
- **Don't contribute to the d-wave pairing channel**
- $\lambda = g^2 / (8 t m \omega^2)$

Experimental Evidence for Strong EP Coupling

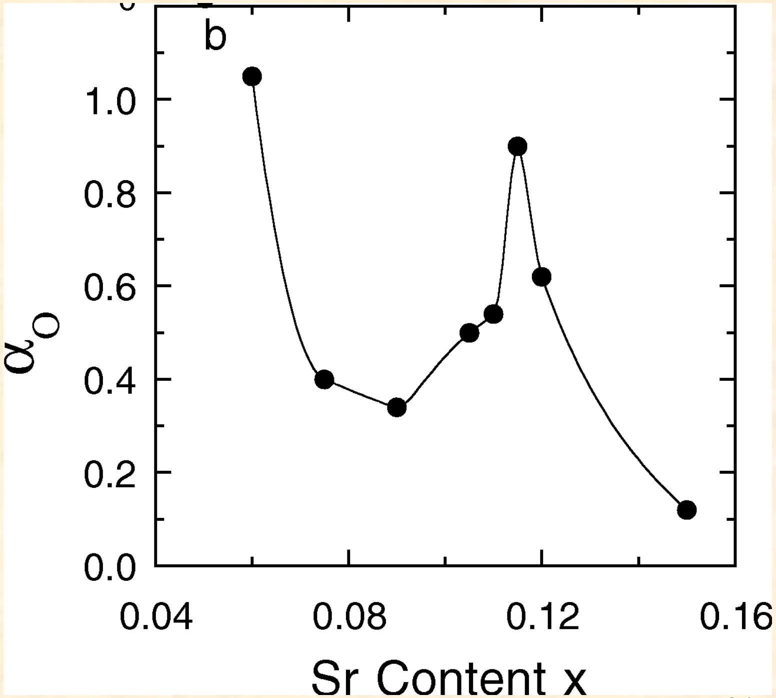
ARPES Kink



A. Lanzara, Nature, 410, 510

O Isotope Effect in 214

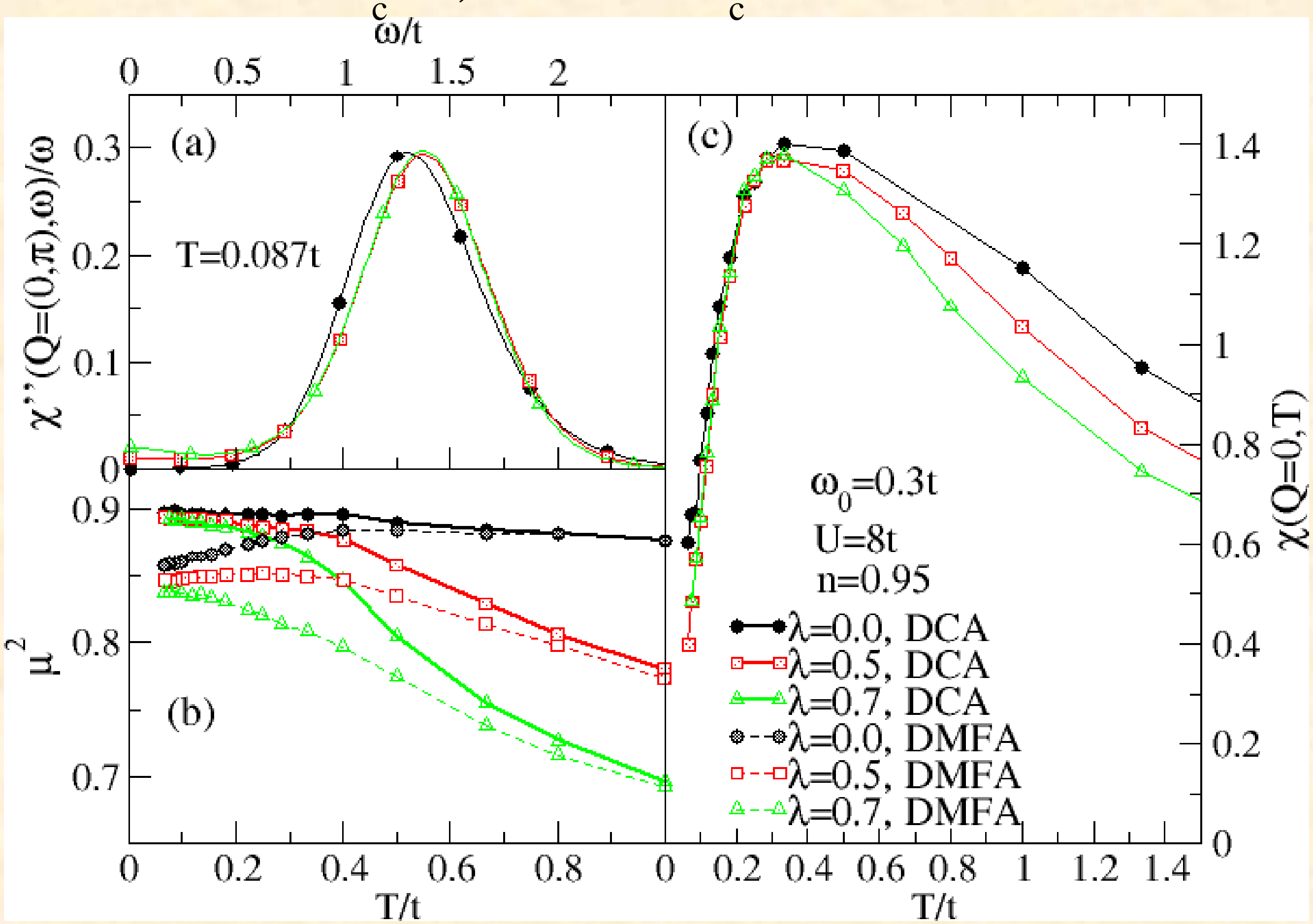
$$\alpha_O = -\frac{d\ln(T_c)}{d\ln(m_O)}$$



G.M. Zhao Nature 385 236

Spin Properties

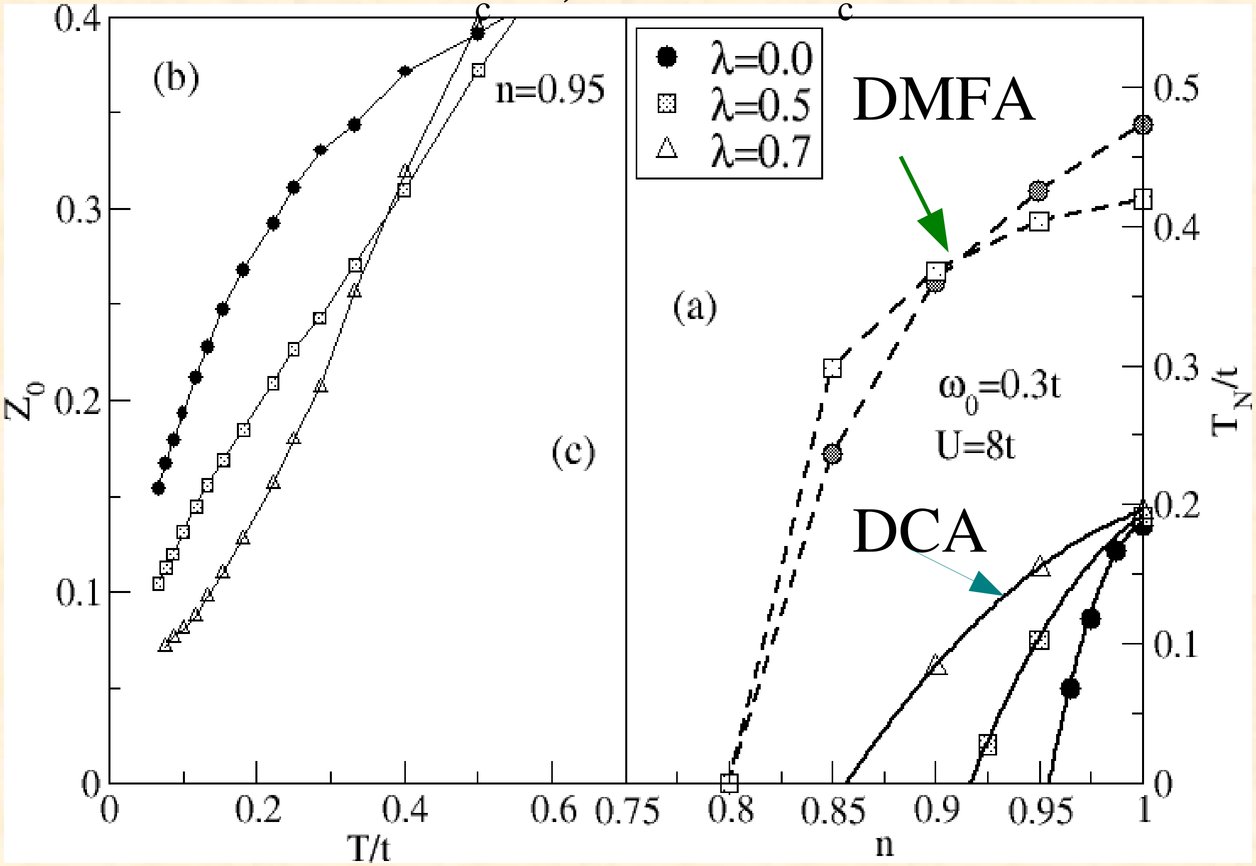
DCA N_c=4, DMFA N_c=1



- **Phonons don't change**
  - **J**
  - **unscreened moment**
  - **T* (much)**
- **μ^2 gives more evidence of polarons**

Neel Transition and Quasiparticle Fraction

DCA N_c=4, DMFA N_c=1



- **Phonons suppress hole motion**
- **Enhance T_N at finite doping**

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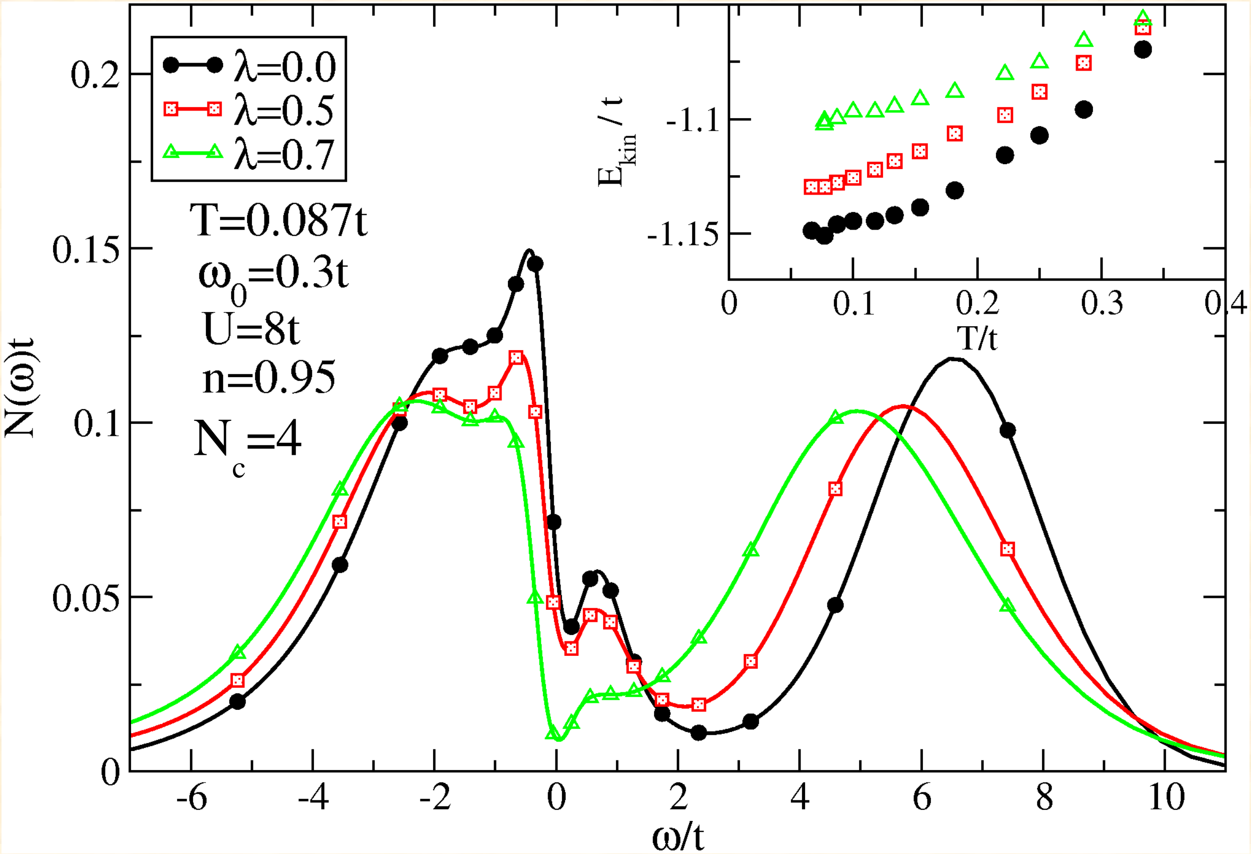
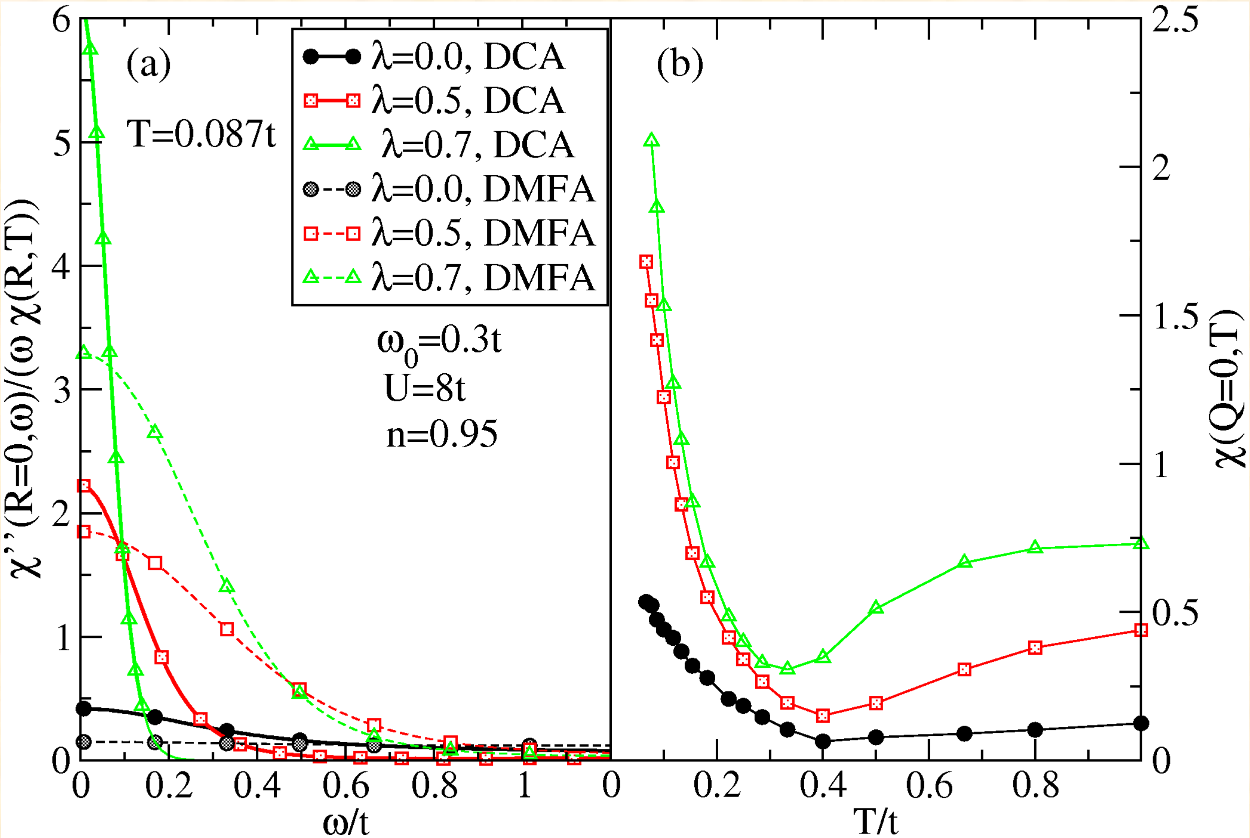
Single-Particle Properties



- Holstein Phonons suppress
  - N(0)
  - U_{eff}
  - kinetic energy gain at low T
- PG doesn't change much

Charge Susceptibility

DCA N_c=4, DMFA N_c=1



- **Phonons Enhance the charge susceptibility**
- **phase separation for λ > 0.7**
- **Narrow band of charge carriers in the dynamic susceptibility**
  - **polarons**
  - **dramatically enhanced by non-local correlations**

Outline

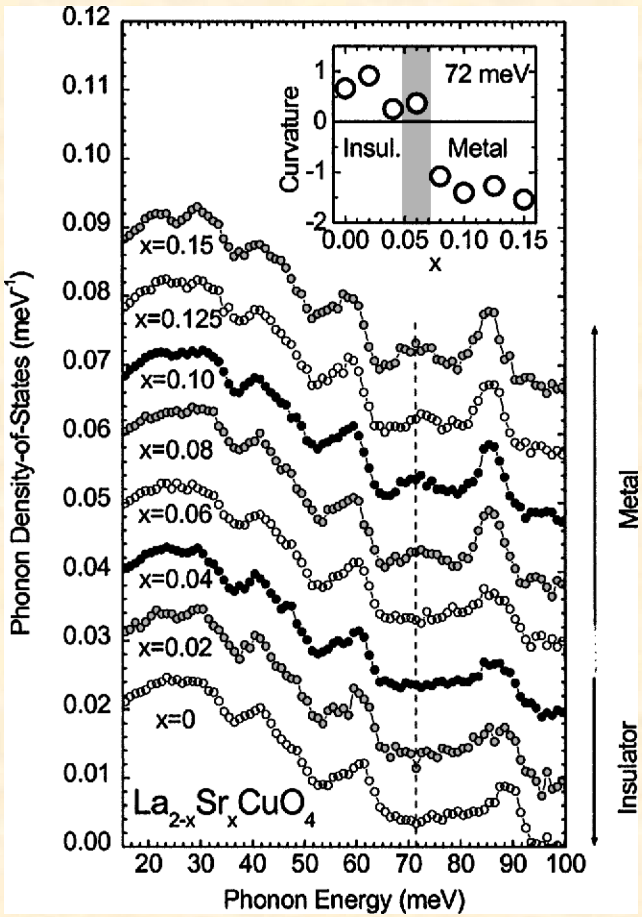
- Cuprates + Hubbard Model
- Hubbard Model
  - N_c=4
  - Larger Clusters?
  - What is the pairing mechanism?
- Hubbard-Phonon Model
  - Phonon-Enhanced spin Polarons
  - **Phonon Suppression of T_c**
- Conclusions and Outlook

What About Pairing

- **Phonons strongly enhance AFM at finite doping**
  - **Should enhance the spin mediated paring interaction**
- **Phonons suppress the QP fraction Z_0 and N(0)**
  - **Should suppress T_c**
- **Which effect wins?**

Breathing and Buckling Phonon modes

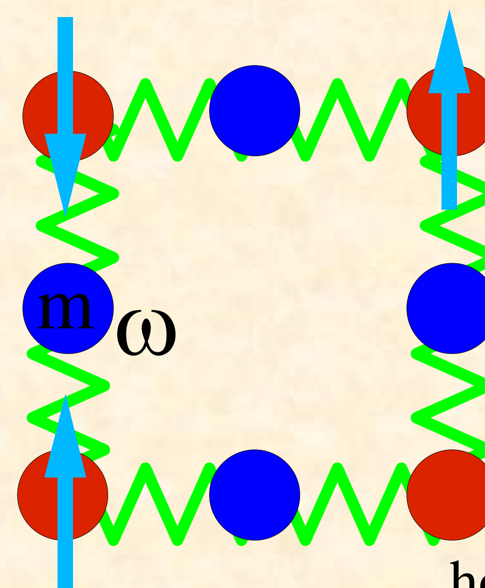
Phonon in DOS



R.J. McQueeney, PRL,87 077001

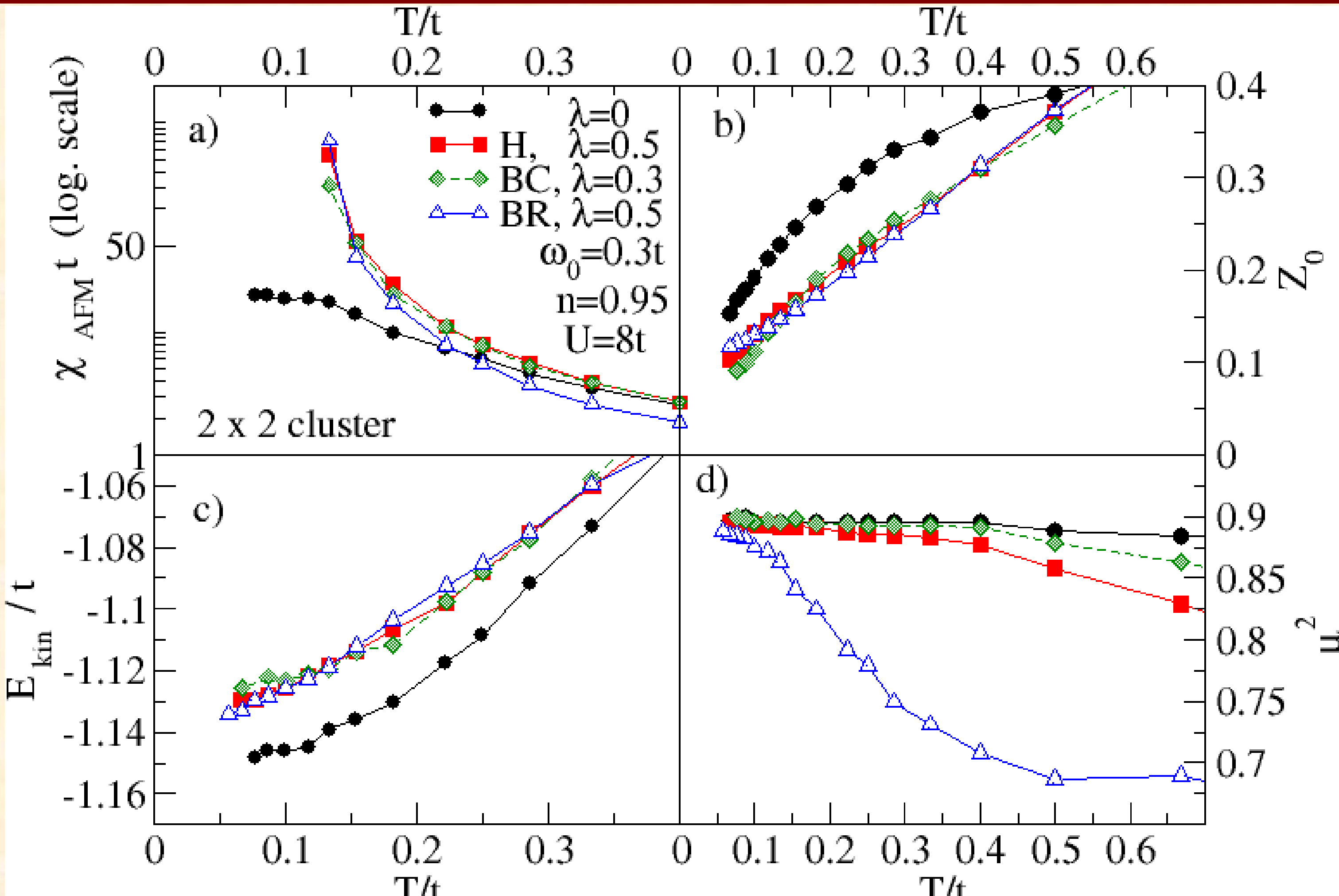
- **Breathing and buckling modes**
  - **breathing +-**
  - **buckling ++**
- **Identified in experiment**
- **Found to couple strongly to doped carriers**

$$\lambda = g^2/(2tm\,\omega^2)$$



hole

Same evidence of polaron formation



$N_c=4$

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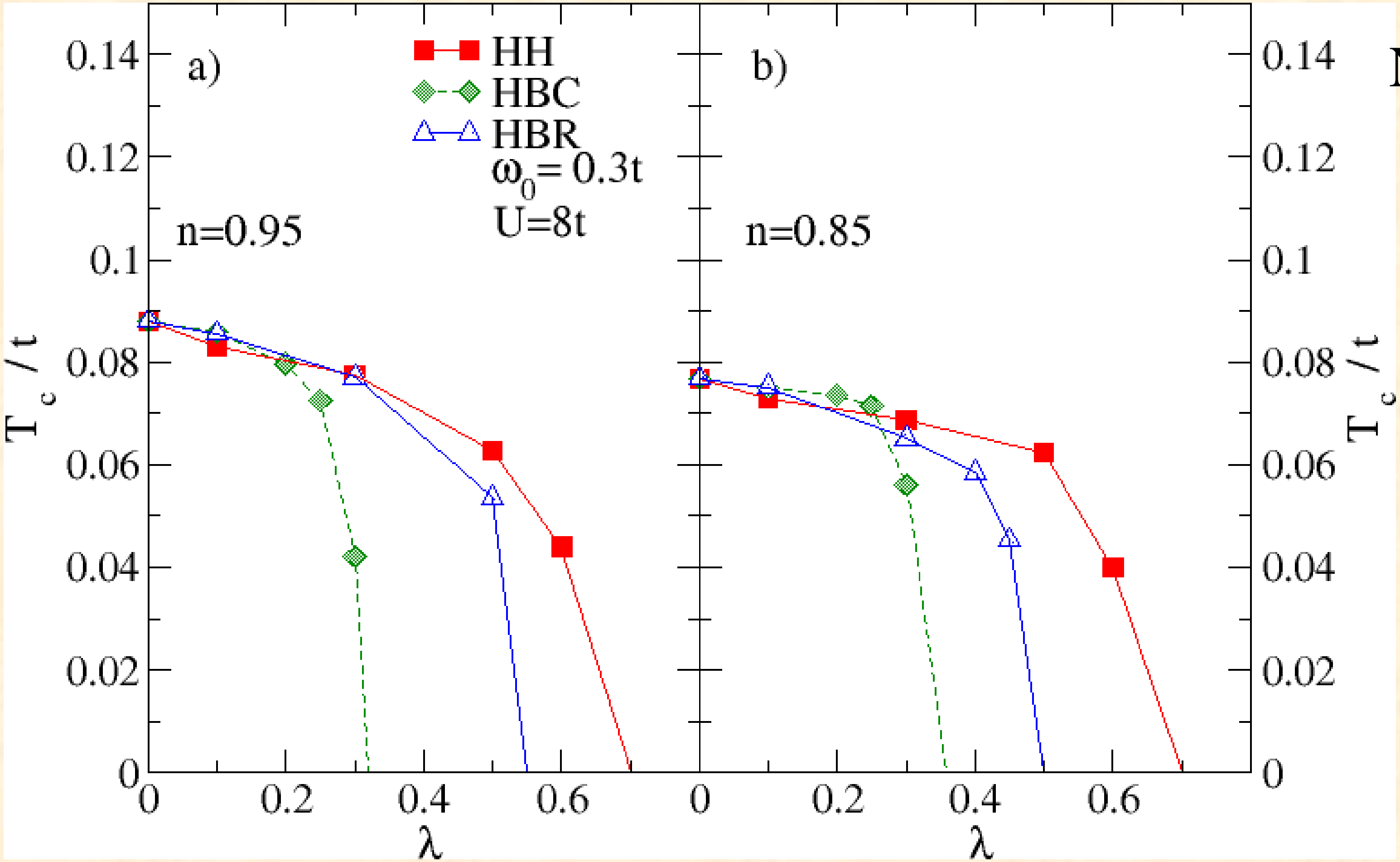
H=Holstein, BC=Buckling, BR=Breathing

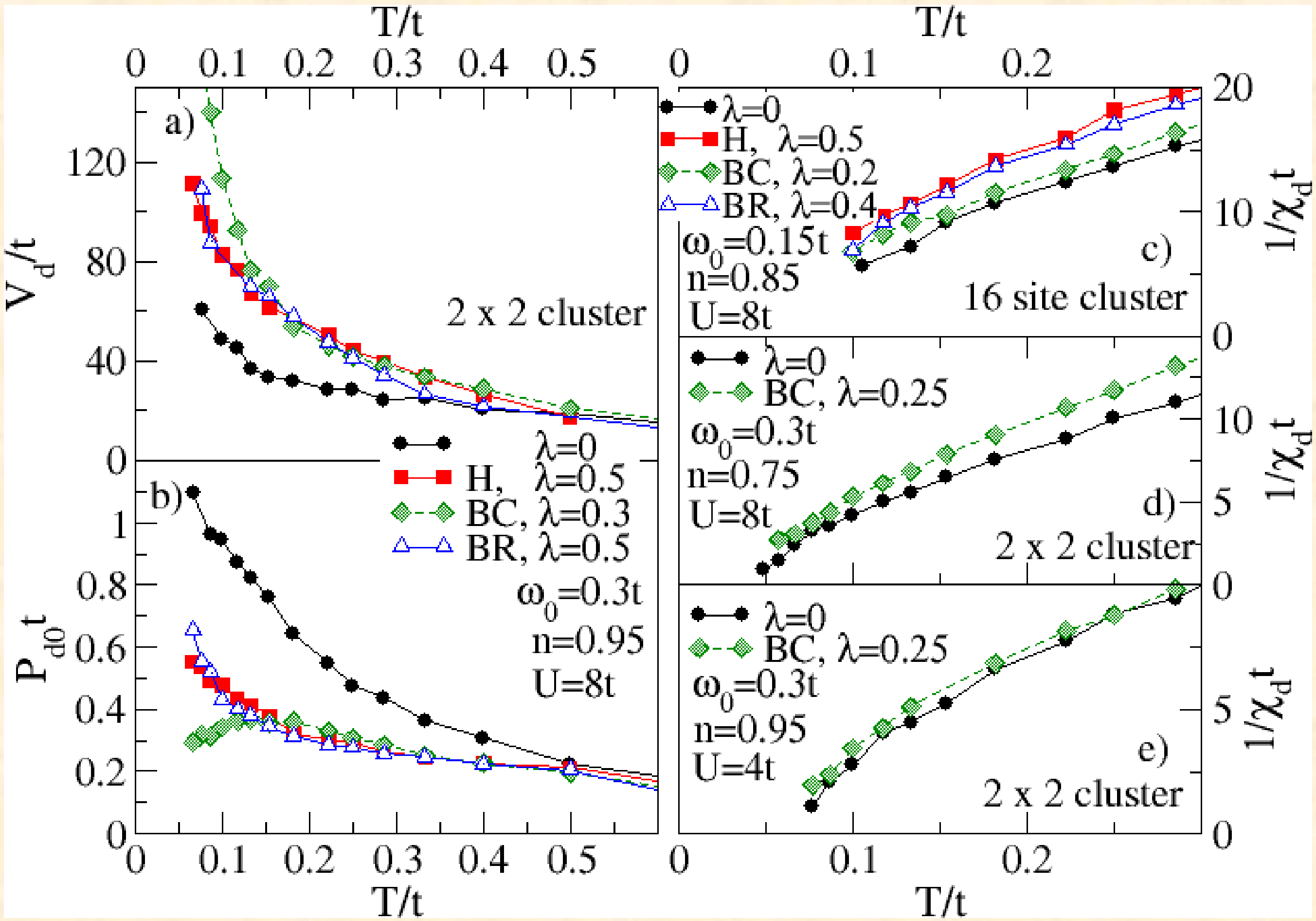
Phonons Appear to Suppress Pairing



$N_c=4$

HH=Holstein, HBC=Buckling, HBR=Breathing

Why do phonons suppress Tc?



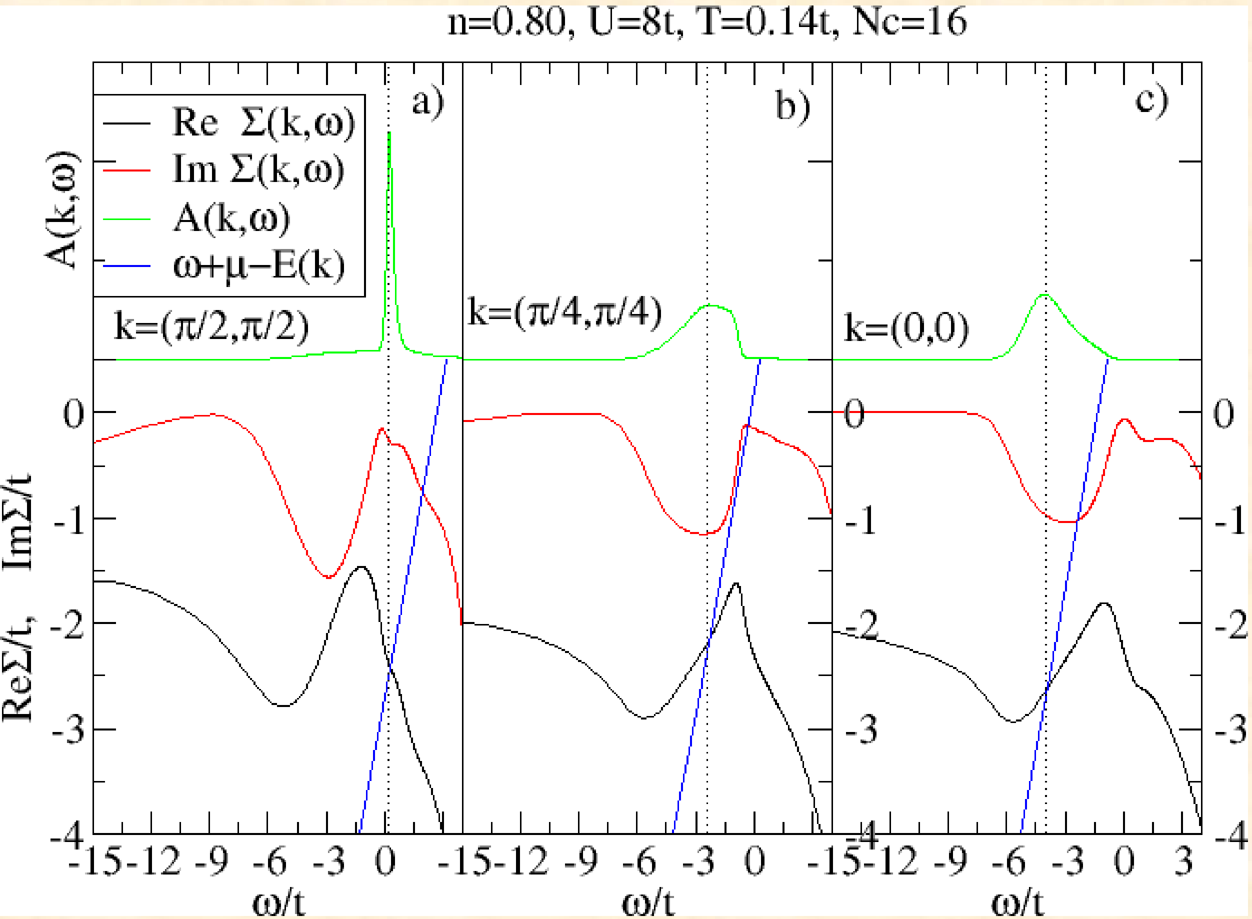
- **Enhance the d-wave pairing interaction V_d**
- **Suppress N(0) (Z_0)**
- **The latter appears to win!**

H=Holstein, BC=Buckling, BR=Breathing

Conclusions

- **Hubbard Model Captures Cuprate Phenomena**
- **N_c=4 mean field = qualitative description of cuprates.**
- **Larger (Betts) clusters.**
  - **$T_c(N_c) \approx$ constant within error bars.**
  - **Pairing from Spin channel.**
- **Local Phonons**
  - **enhance AFM and d-wave pairing interaction V_d**
  - **suppress Z_0, N(0), ... polarons**
  - **suppress T_c**

High Energy Kink in the Self Energy



- Features below kink energy E_{kink} depend weakly on K
- QP Peaks in A(k,ω) when Re(ω +μ - E(k) - Σ(k,ω))=0
  - intersection of black and blue lines
- -ImΣ(k,ω) large for $\omega < E_{kink}$
- Abrupt change in slope of ReΣ(k,ω) for $\omega < E_{kink}$ signals the start of the waterfall structure in spectra.
- Dispersion for large |ω| falls below bare result by causality. Here, ReΣ(k,ω) ~ a/ω, where a=∫dω (-1/π) ImΣ(k,ω) >0

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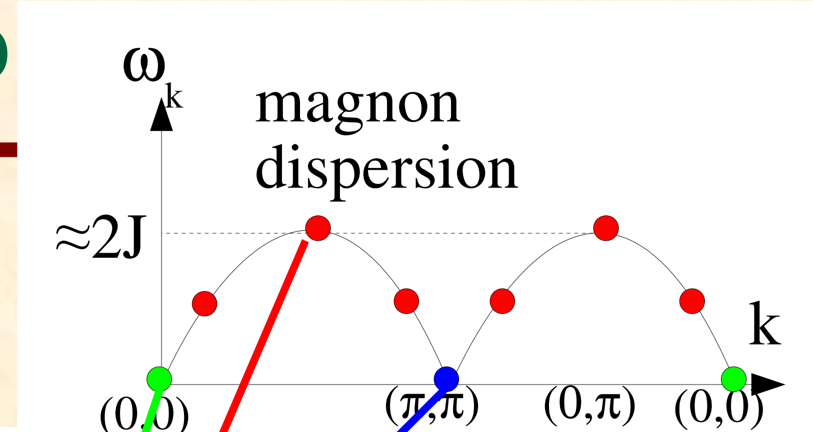
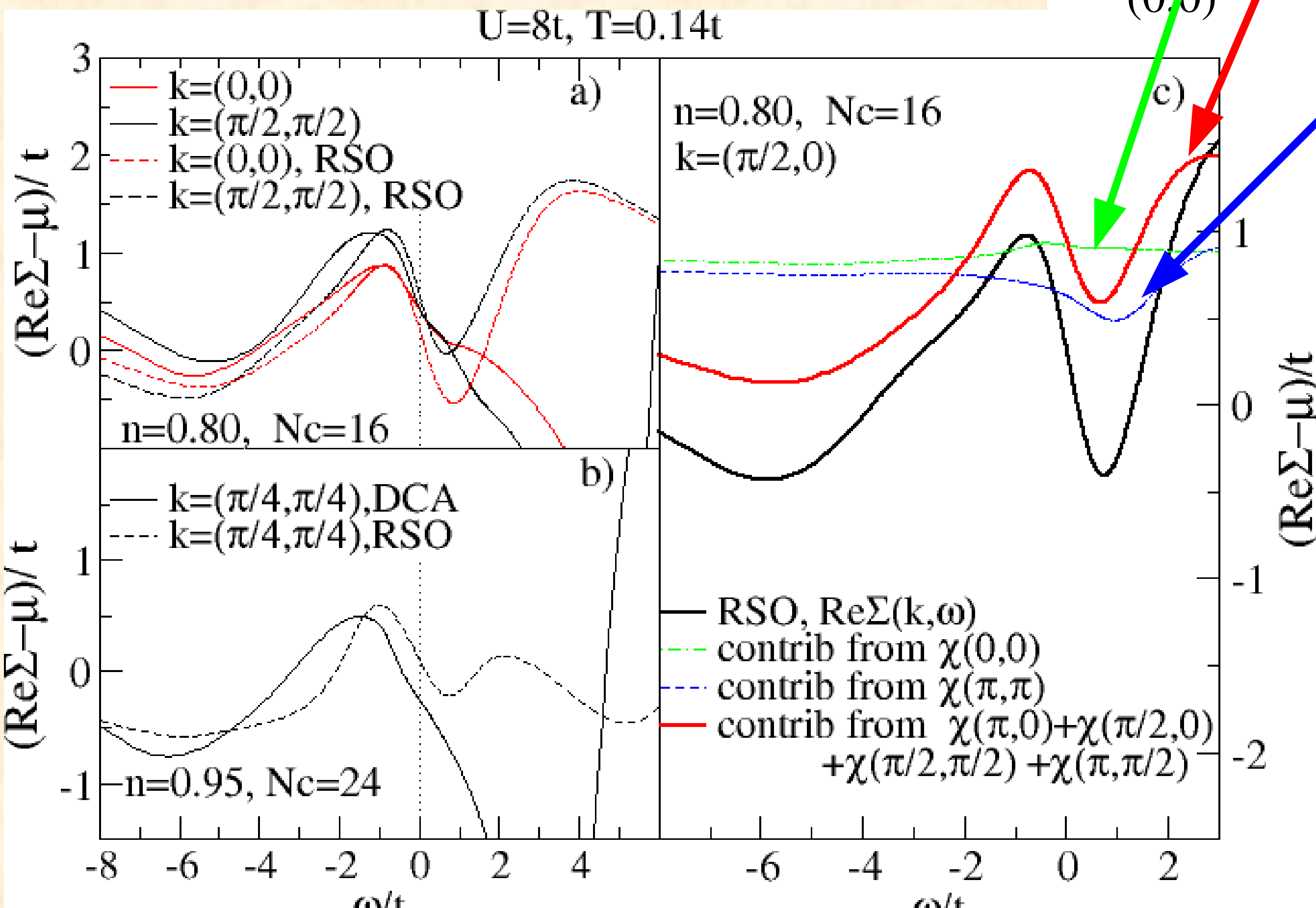
Origin of the Kink in RSO





- **RSO and DCA/QMC self energies agree for ω<0.**
- **HE kink comes from QP scattering from high energy spin fluctuations.**

A. Macridin
PRL to appear

HE Spin Excitations and doping