A DCA Study of the High Energy Kink Structure in the Hubbard Model Spectra

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Thanks to T. Devereaux, A. Lanzara, W. Meevasana, B. Moritz, G. A. Sawatzky, and F. C. Zhang

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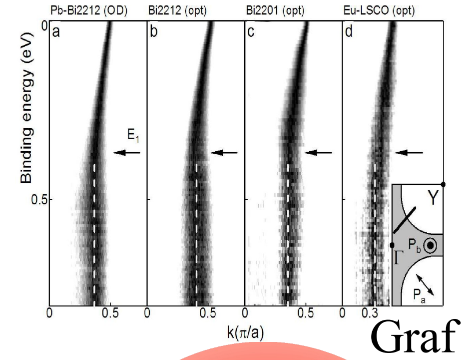
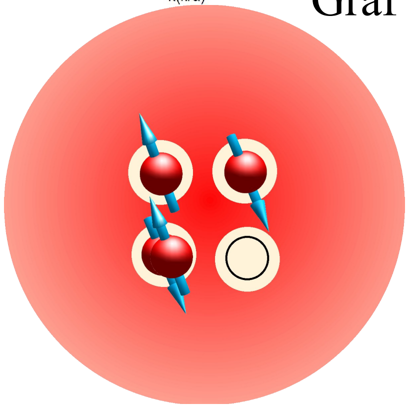
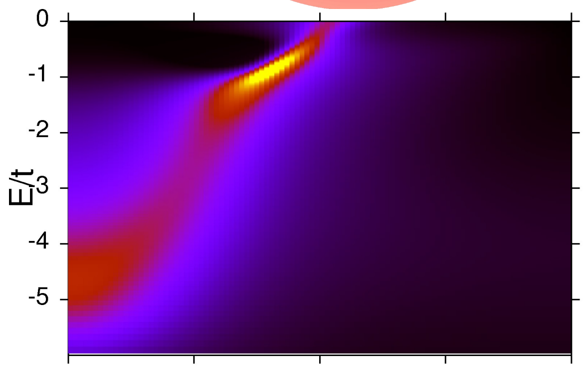
Dresden, April 07

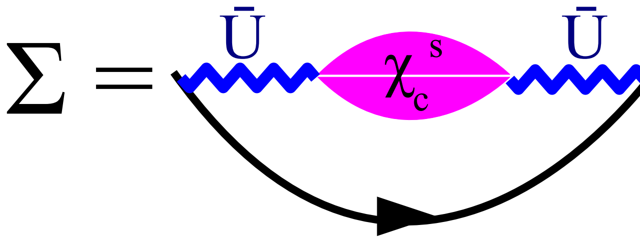
Outline

- HE kink
- Model + DCA
- Results for Spectra
- Possible Method to Analyze Cuprates
- Conclusion









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Some High Energy Kink References

J. Graf, et al., preprint, cond-mat/0607319.
W. Meevasana, et al., preprint, cond-mat/0612541.
T. Valla, et al., preprint, cond-mat/0610249.
J. Chang, et al., preprint, cond-mat/0610880.
B. P. Xie, et al., preprint, cond-mat/0607450.
Z.-H. Pan, et al., preprint, cond-mat/0610442.6
Q.-H. Wang, et al., preprint, cond-mat/0610491.
C. Grober, et al., Phys. Rev. B 62, 4336 (2000).
S. Odashima, et al., Phys. Rev. B 72, 205121 (2005).
F. Ronning, et al., Phys. Rev. B 71, 094518 (2005).
E. Manousakis, preprint, cond-mat/0608467.
K. Byczuk, et al., Nature Physics, cond-mat/0609594.
A. Macridin, et al. preprint, cond-mat/0701429.

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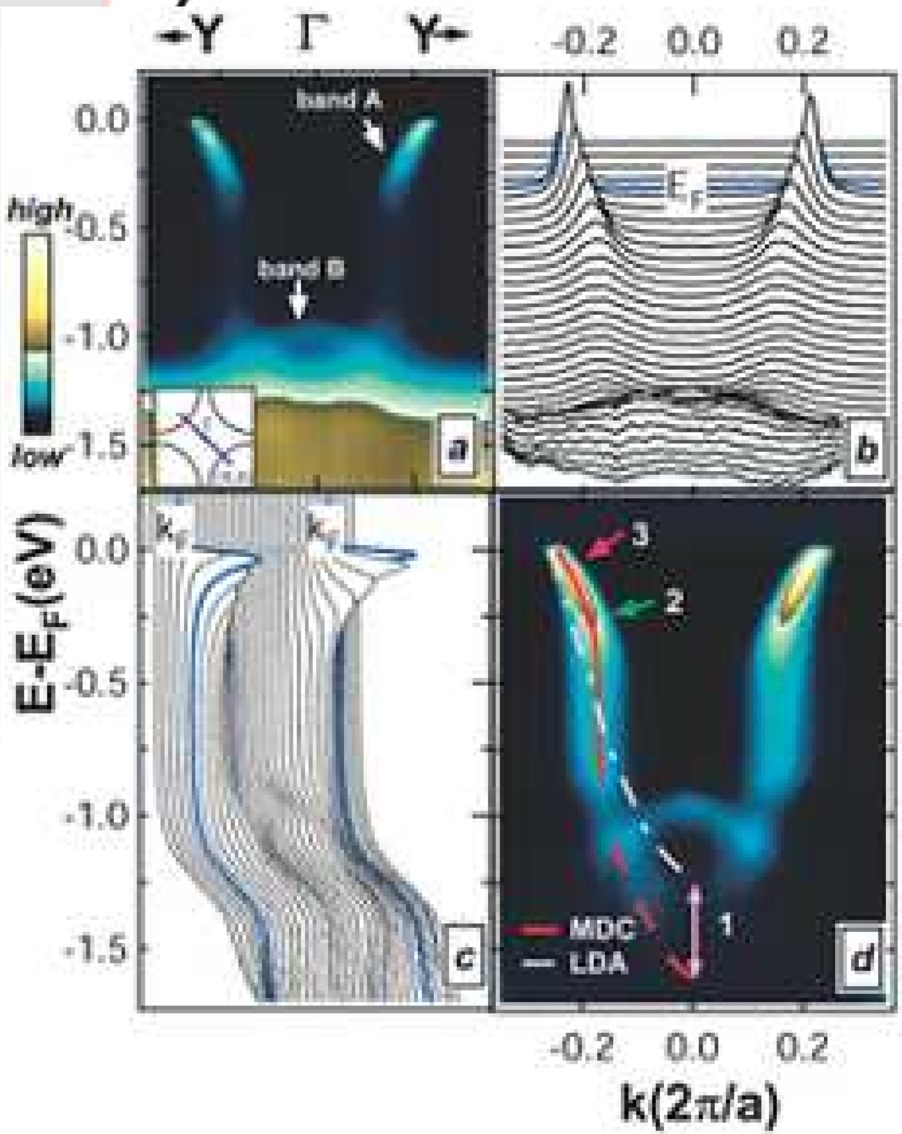
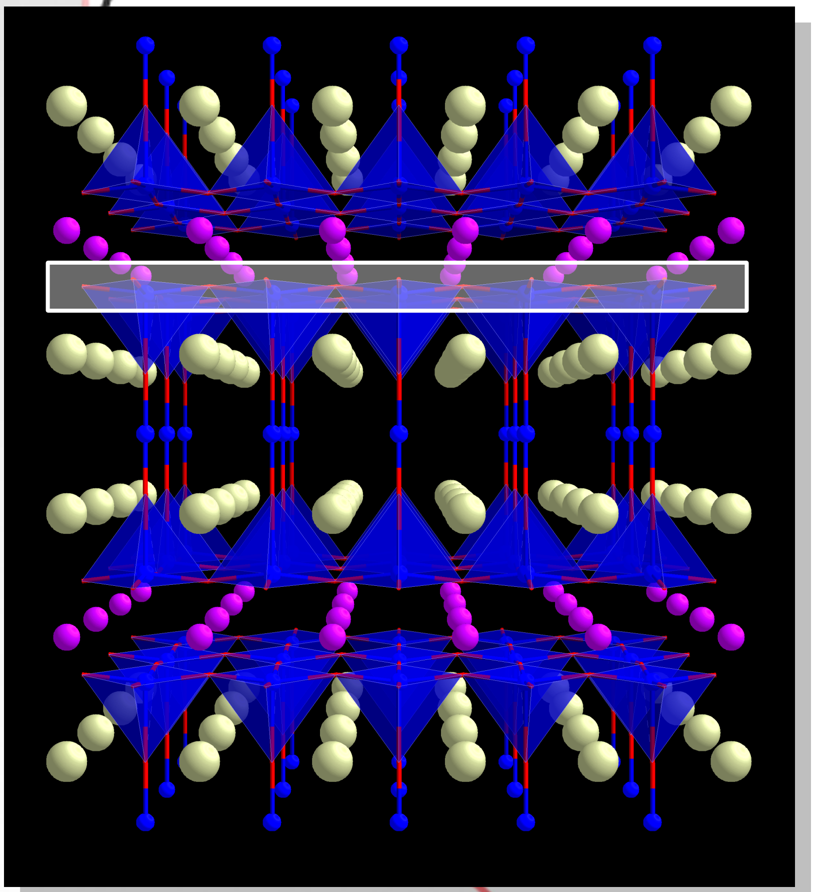
High-Energy Kink (overdoped Bi2201)

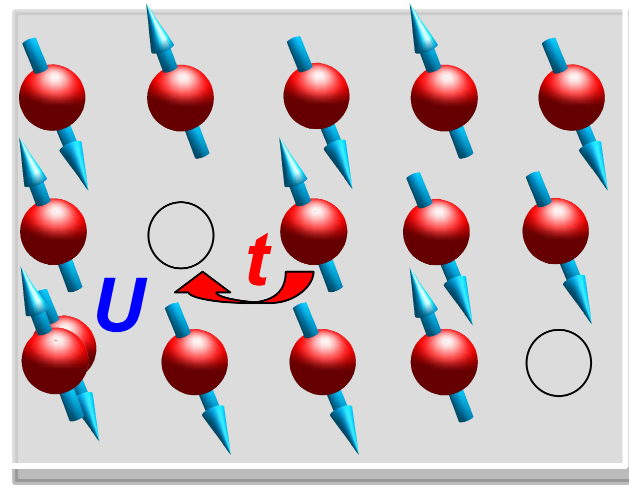


- HE kink beginning at about 0.25-0.3 eV
- High energy band (bottom) falls below LDA

Meevasana et al., cond-mat/0612541

Modelling The Cuprates





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

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

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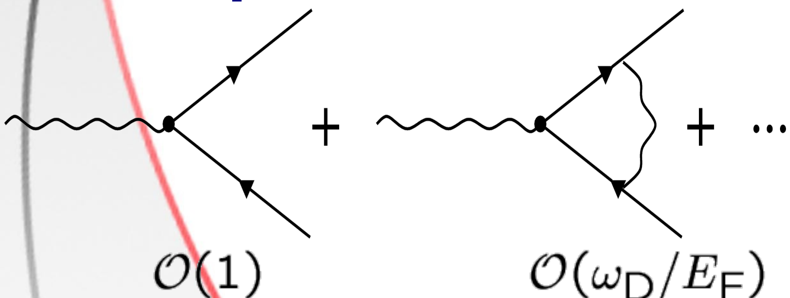
Small Parameter?

BCS (conventional) SC:

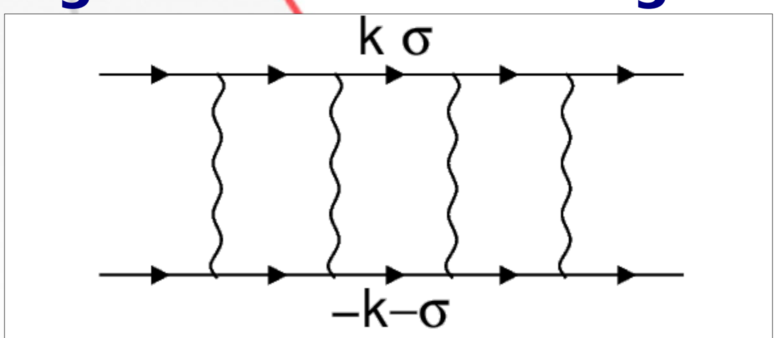
Small parameter:

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

Electron-phonon vertex:



Neglect classes of diagrams:



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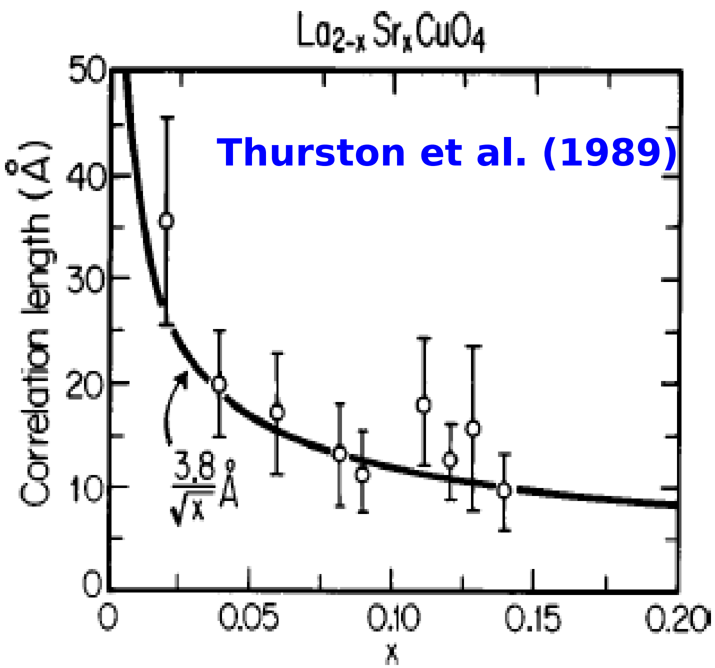
Cuprate (unconventional) SC:

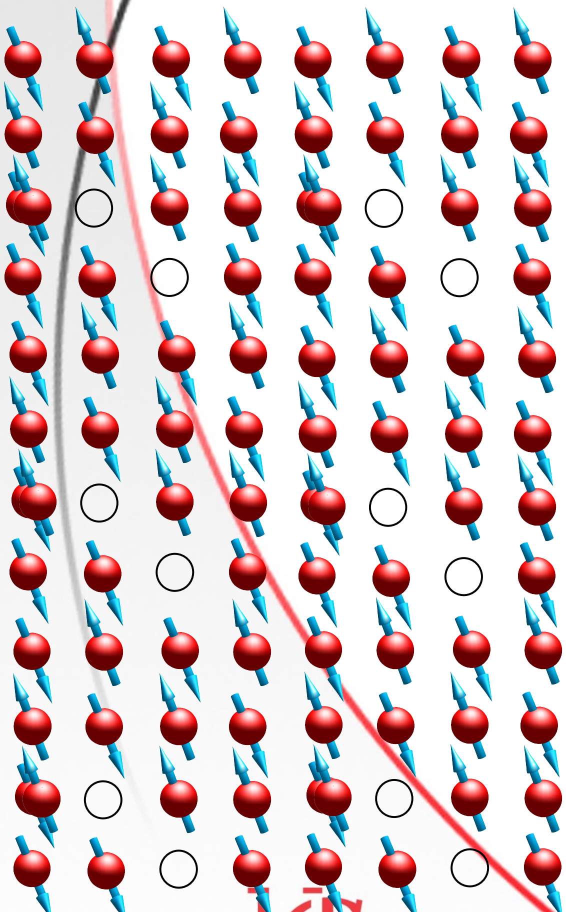
No small energy scale: $U/W \approx 1$

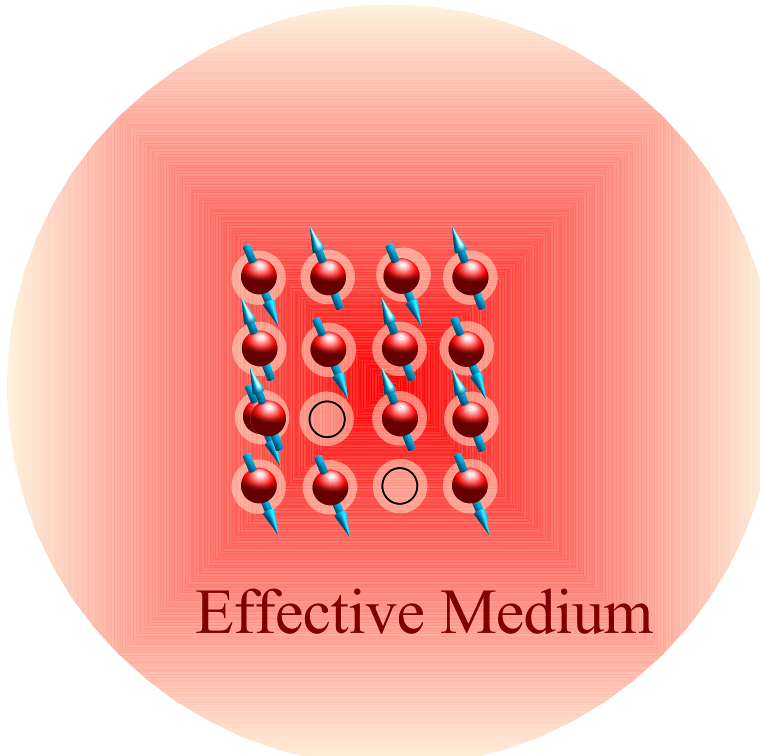
But in Cuprates:



Short-ranged AF correlations

Dynamical Cluster Approximation





Short length scales, within the cluster, treated explicitly.

Long length scales treated within a mean field.

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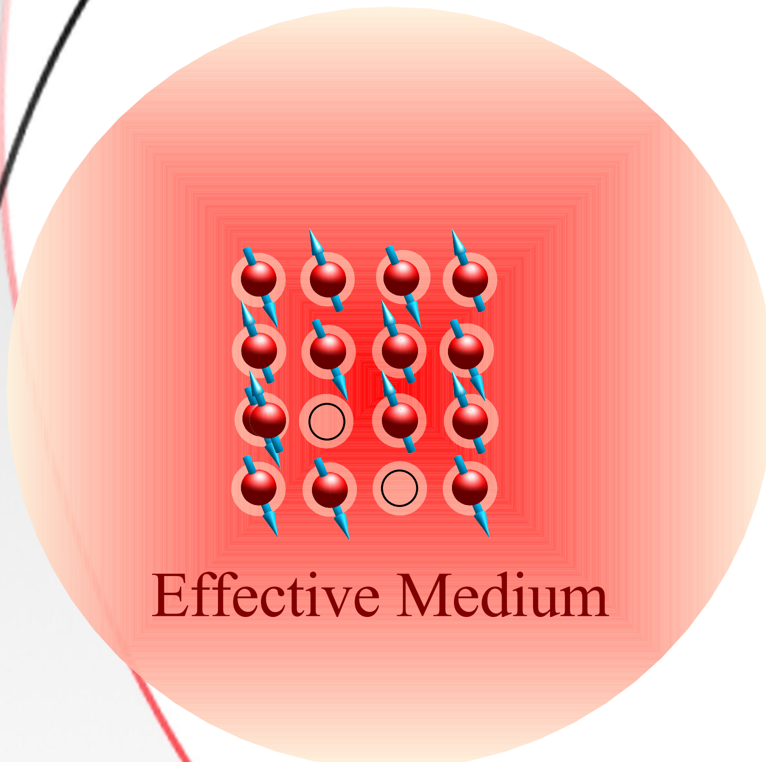
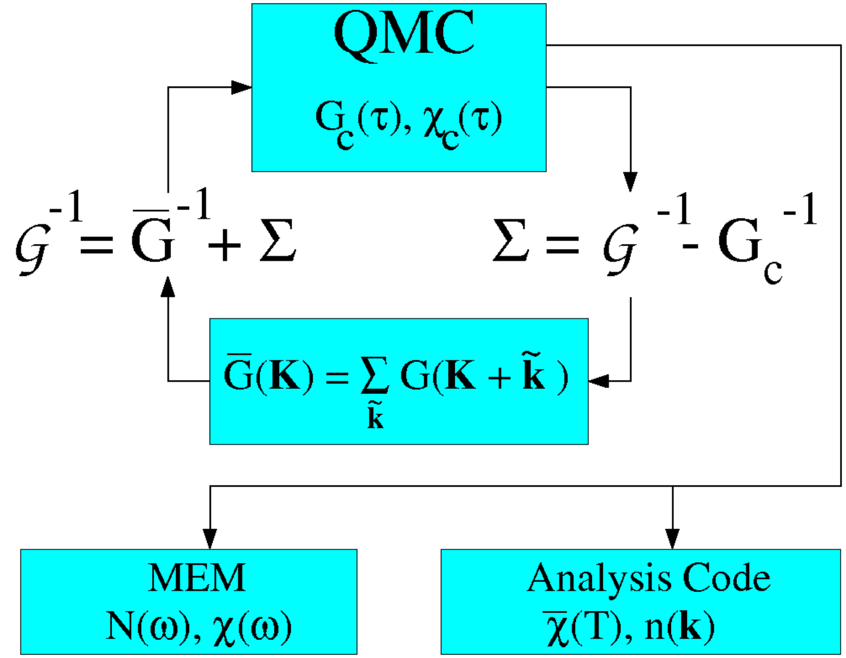
For a review of quantum cluster approaches: Th. Maier *et al.*, *Rev. Mod. Phys. 77, pp. 1027 (2005).*

QMC Cluster Solver





10^2—10^4 procs.

ORNL/CES X1e, Xt3

★QMC in the Infinite Dimensional Limit, M. Jarrell, QMC Methods in CM Physics, Ed. M. Suzuki, (World Scientific, 1993), p221-34.
★The Hubbard Model in Infinite Dimensions: A QMC Study, Mark Jarrell, Phys. Rev. Lett. 69, 168-71 (July 1992).
★A QMC Algorithm for Non-local Corrections to the Dynamical Mean-Field Approximation, M. Jarrell, PRB 64, 195130/1-23 (2001).

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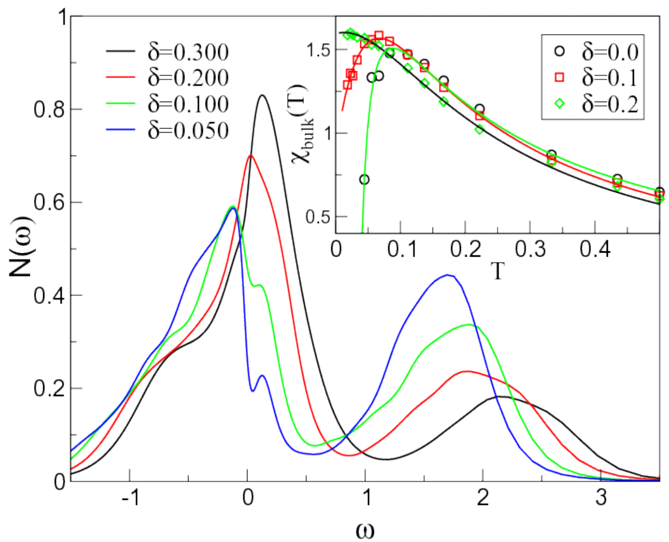
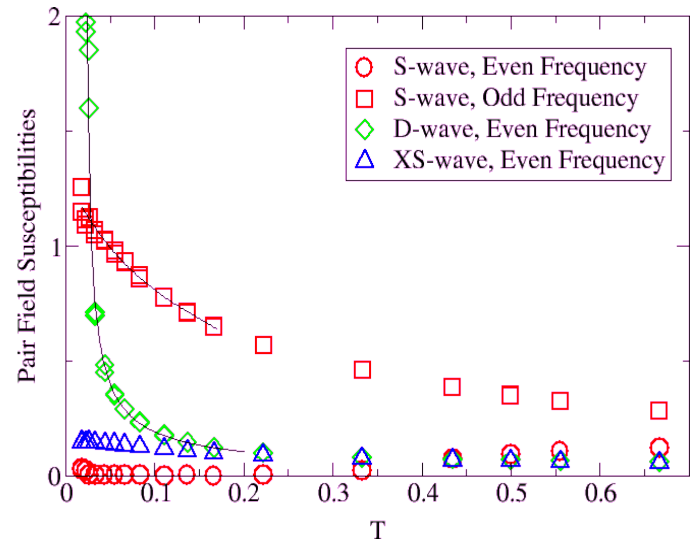
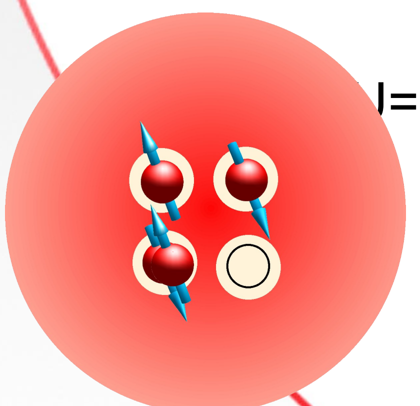
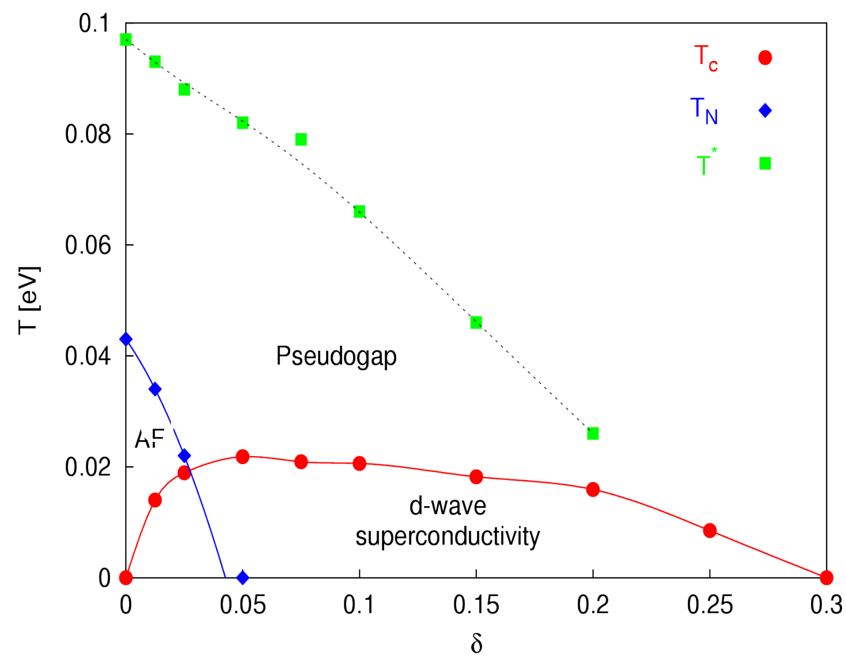
4-site cluster DCA - 2D Hubbard model







U=8t



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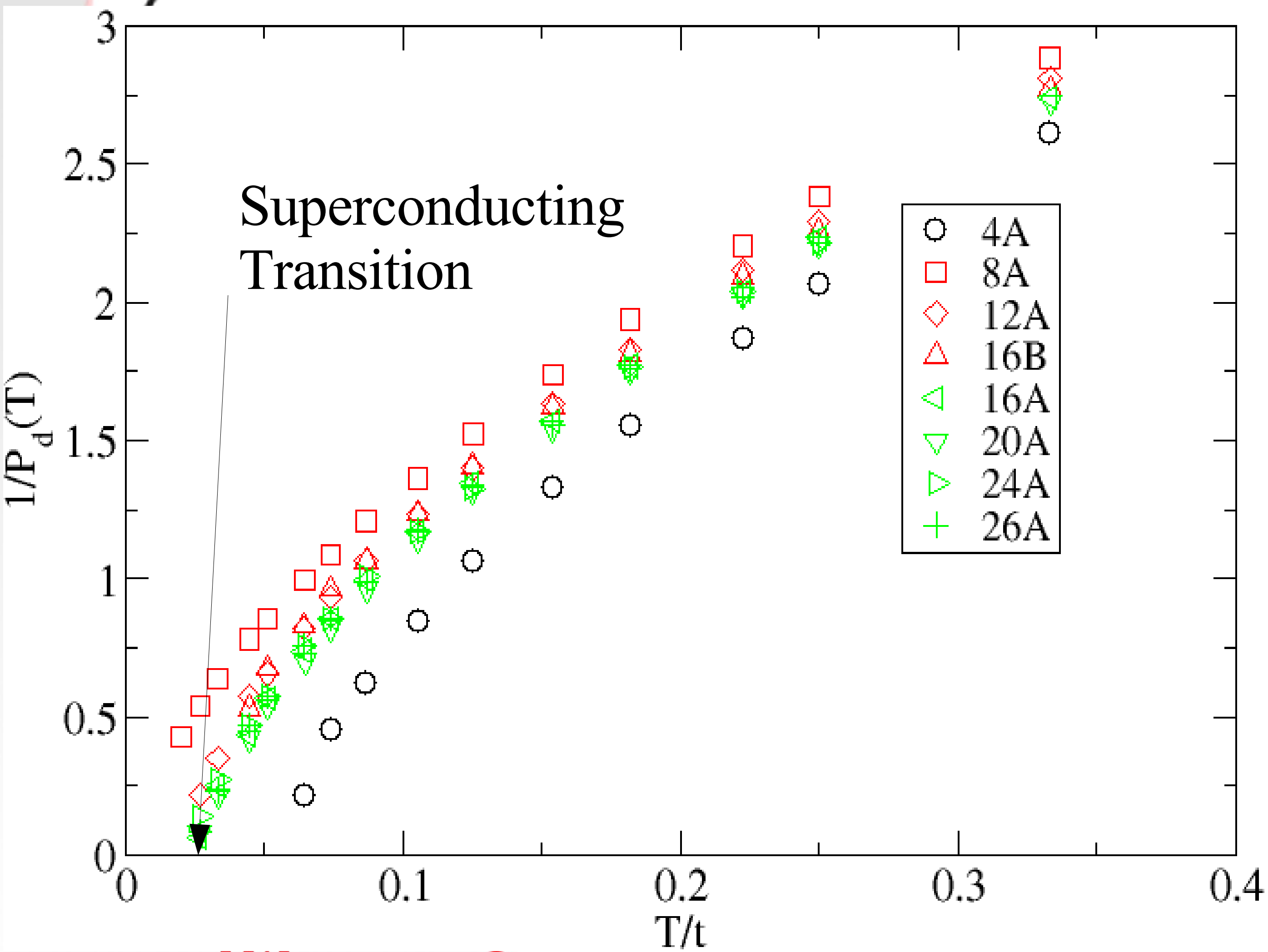
MJ, EPL, 2001

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



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

Th. Maier, PRL

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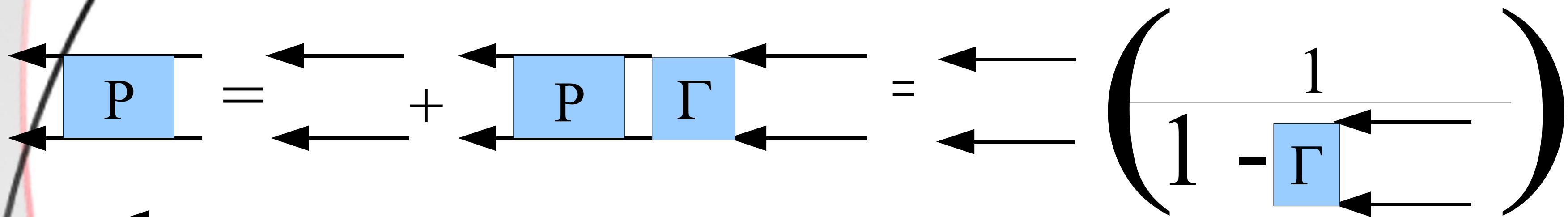
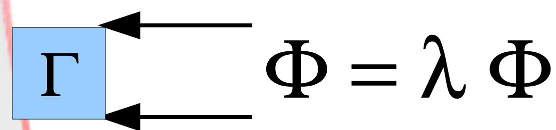
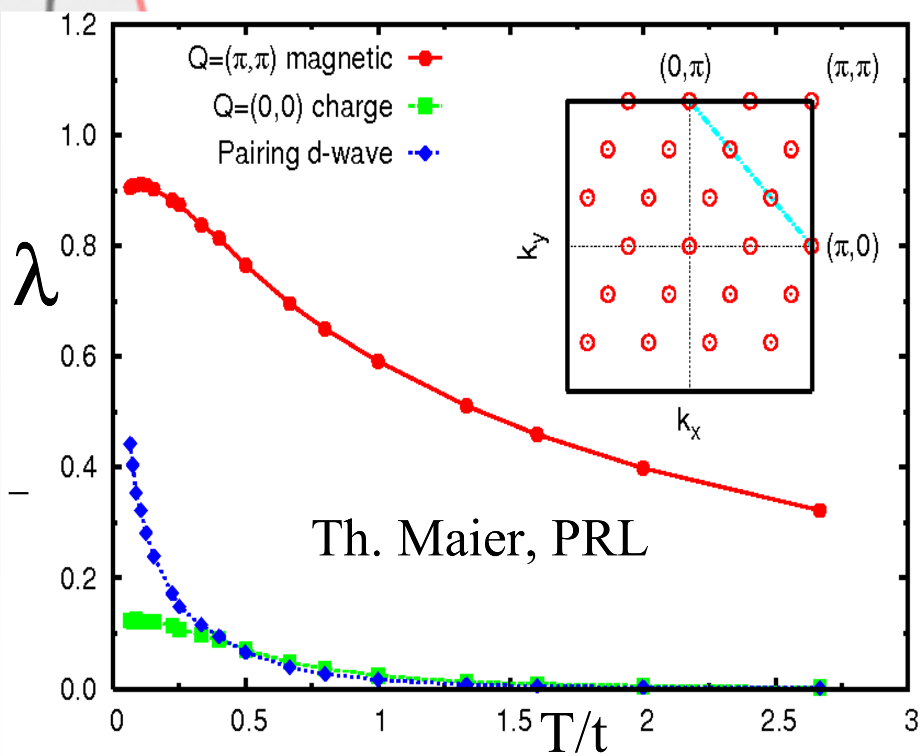
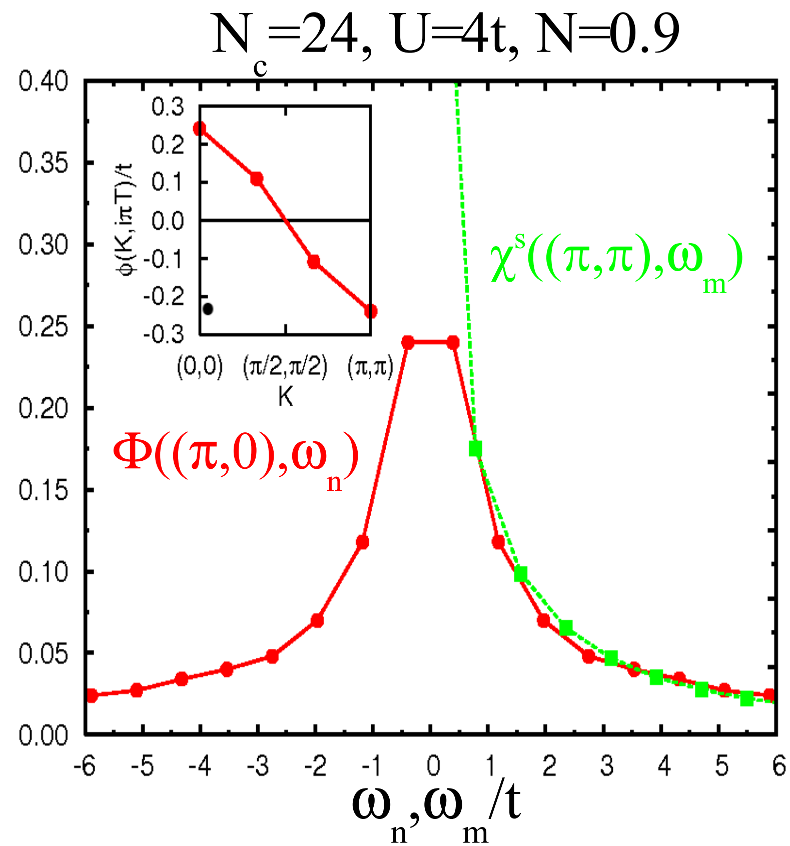
The Mechanism: Clues from the pairing matrix



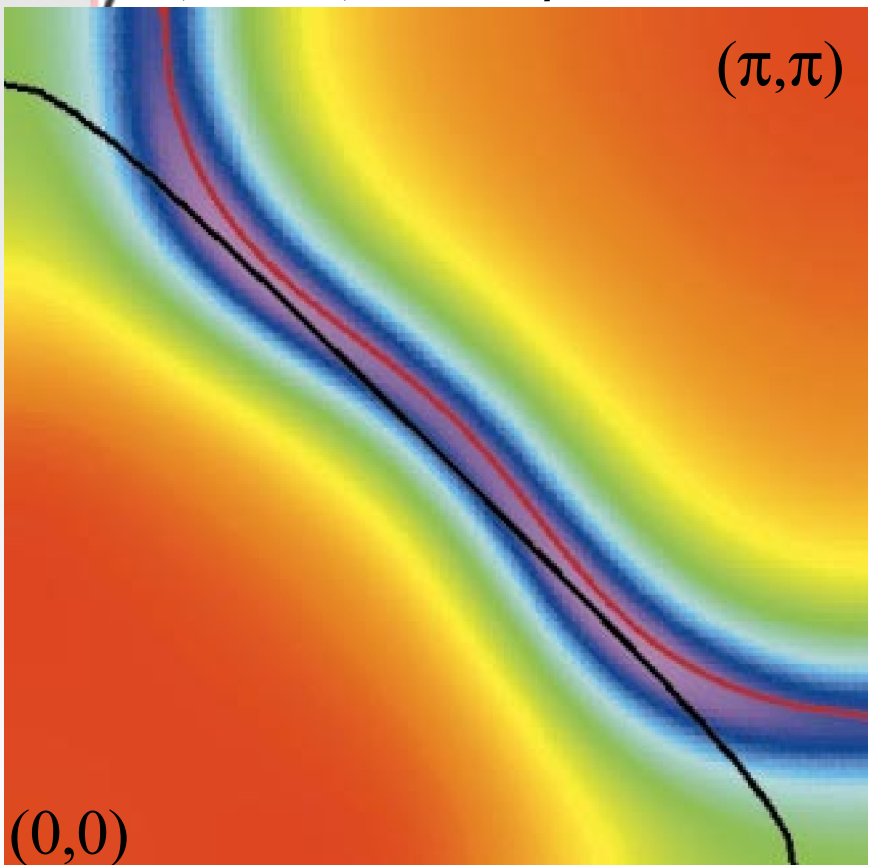






Nonlocal corrections in spectra

A(k,ω=0) U=8t, βt=8



- —— DMF
- —— DCA (Nc=16)
- Non-local corrections to DMF distort the Fermi surface.
- Act like t' (t'')
- Phys. Rev. B 66, 075102 (2002).

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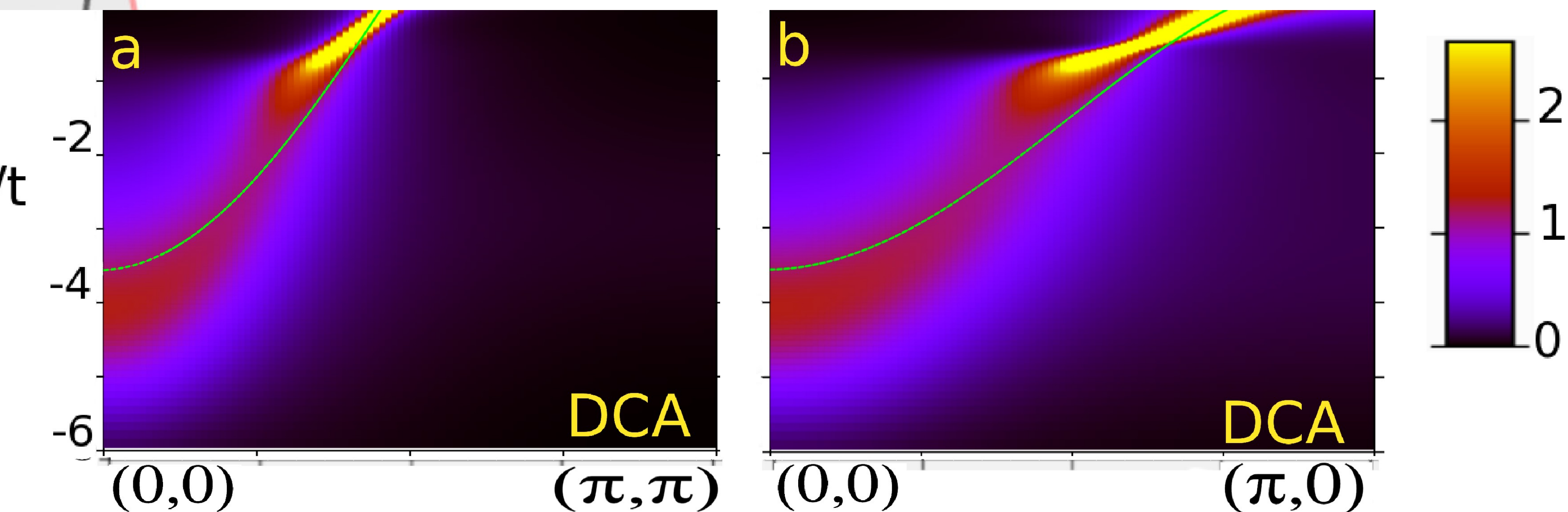
High-Energy Kink in the 2D Hubbard Model

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



- Kink at $E_{kink}\approx$-t
- (0,0) Dispersion below bare band

A. Macridin unpublished

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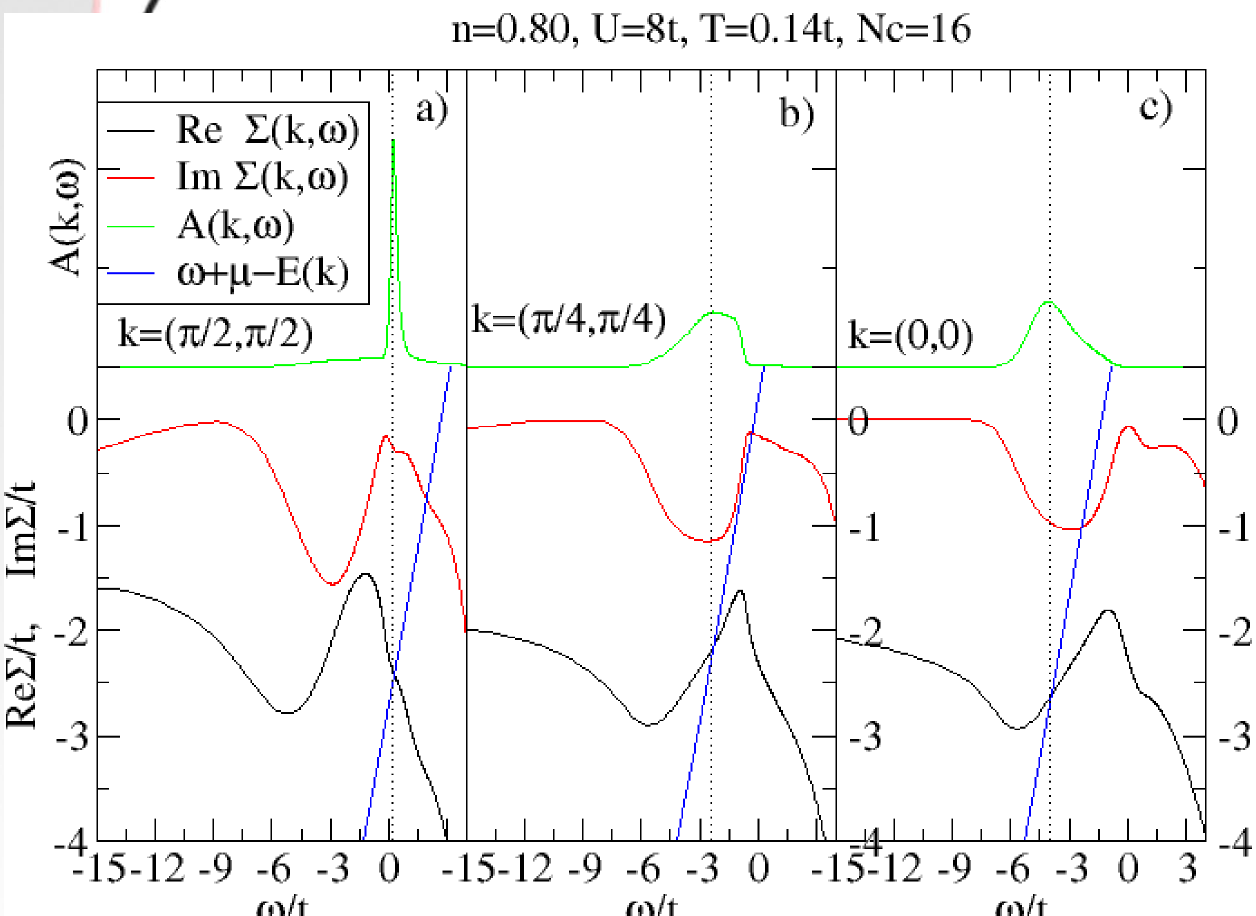
High Energy Kink in the Self Energy



- 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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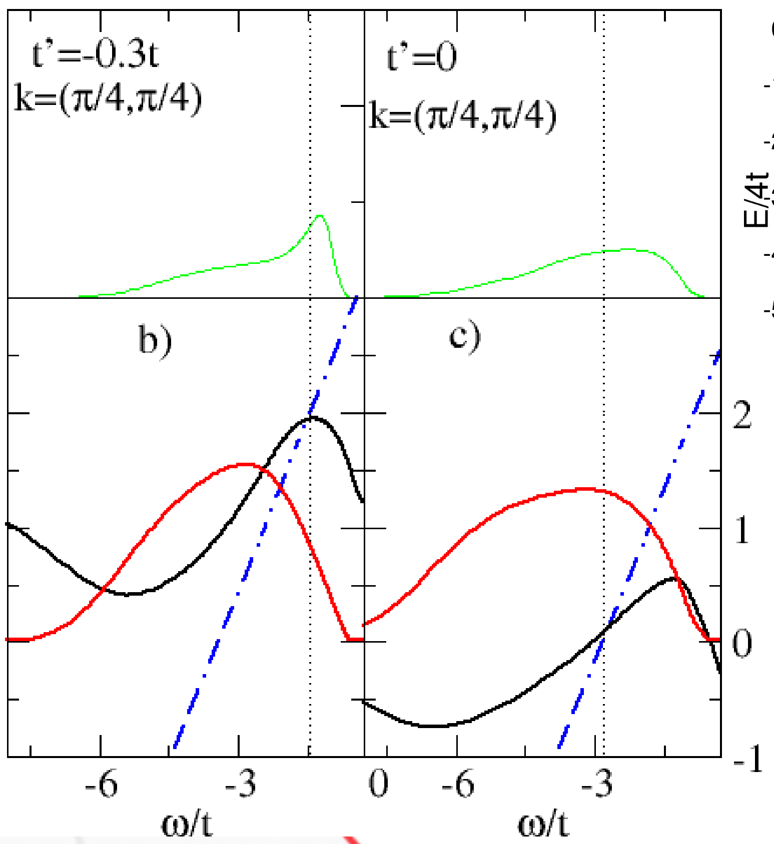
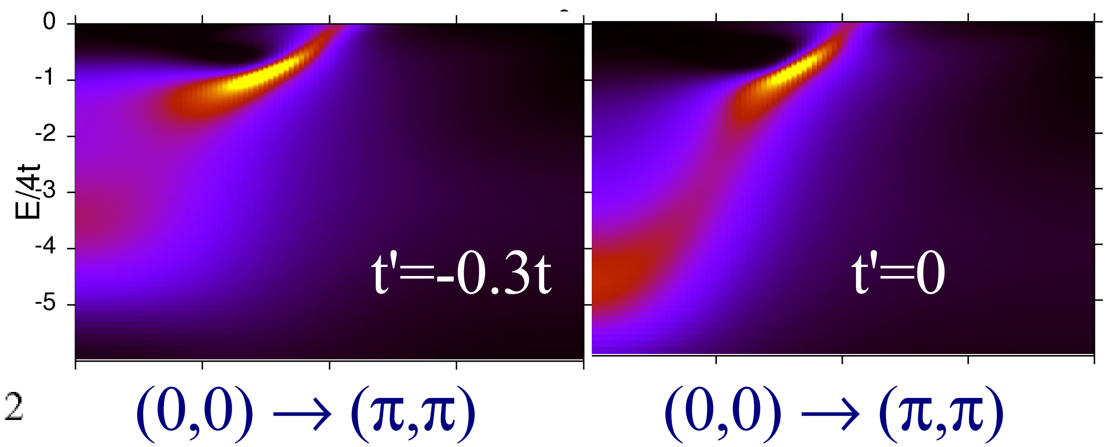
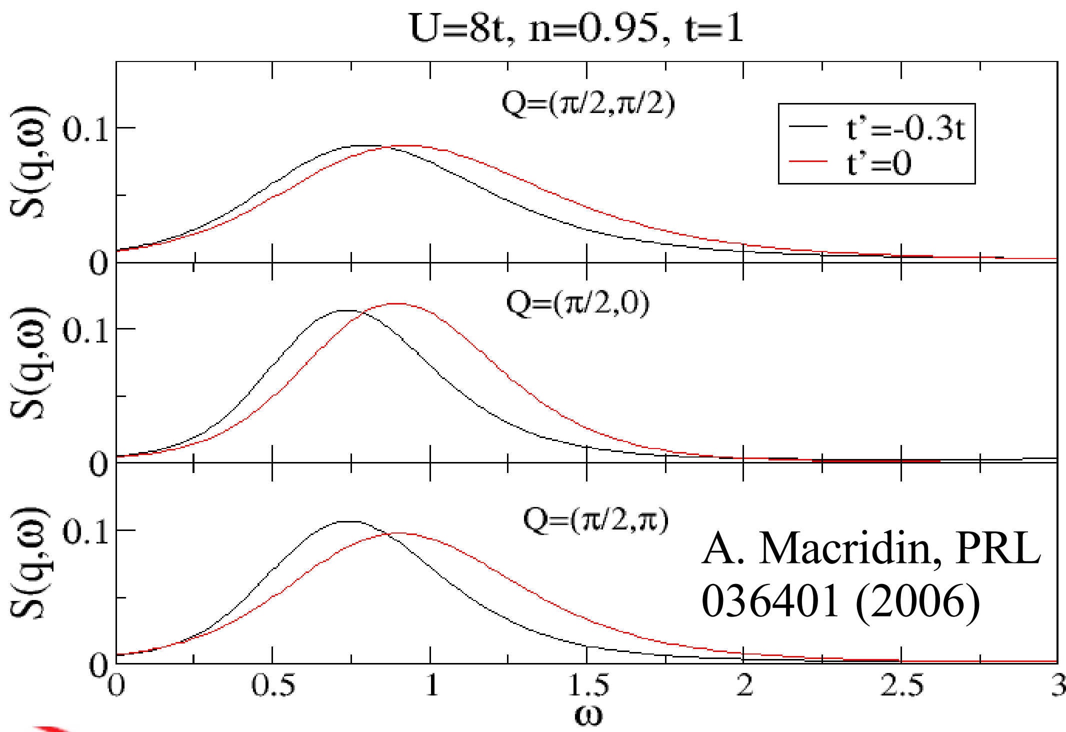
Bandstructure (t') changes waterfall

n=0.95, U=8t, T=0.13t, Nc=16



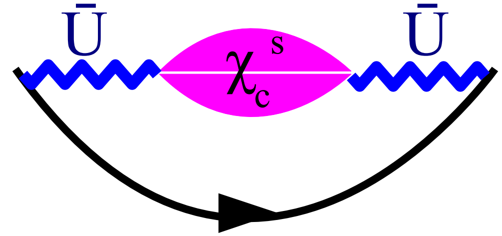




A. Macridin, PRL 036401 (2006)

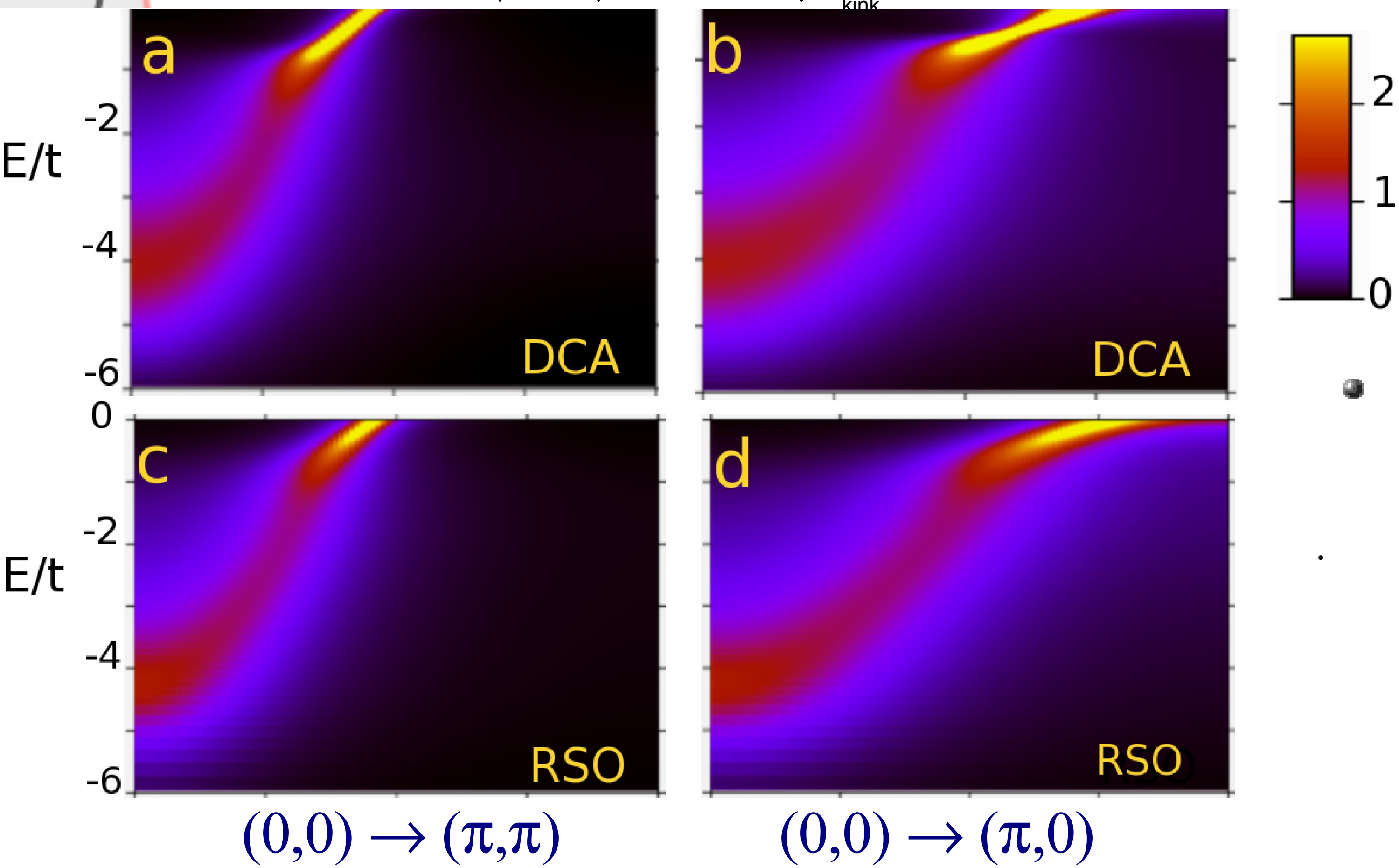
- dive more steep for h-doped (t'<0)
- less steep for e-doped (t'>0, but AF)

Origin of the HE Kink

$\Sigma =$ 

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

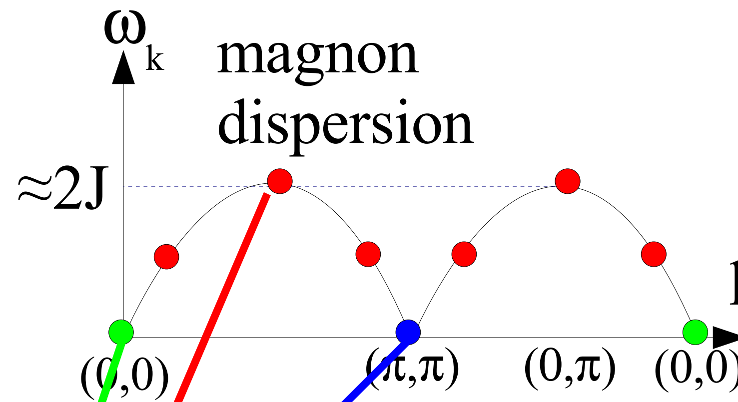
n=0.8, U=8t, cluster 16B, E_{kink} = - t

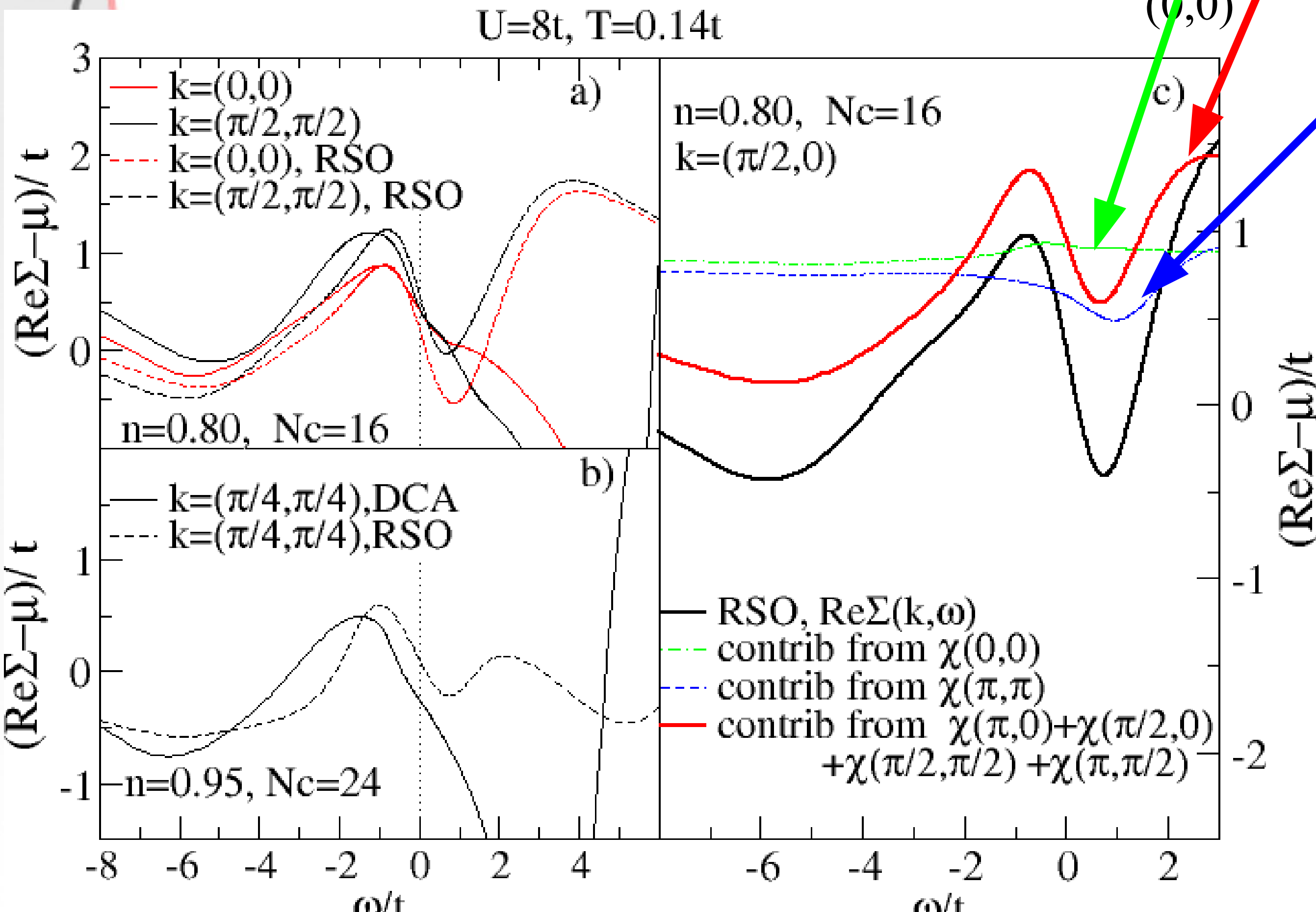


- Spin, charge, and pair terms (different χ).
- Spin dominates
- $\bar{U}$<U due to QP renormalization.

- 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.

Origin of the Kink in RSO

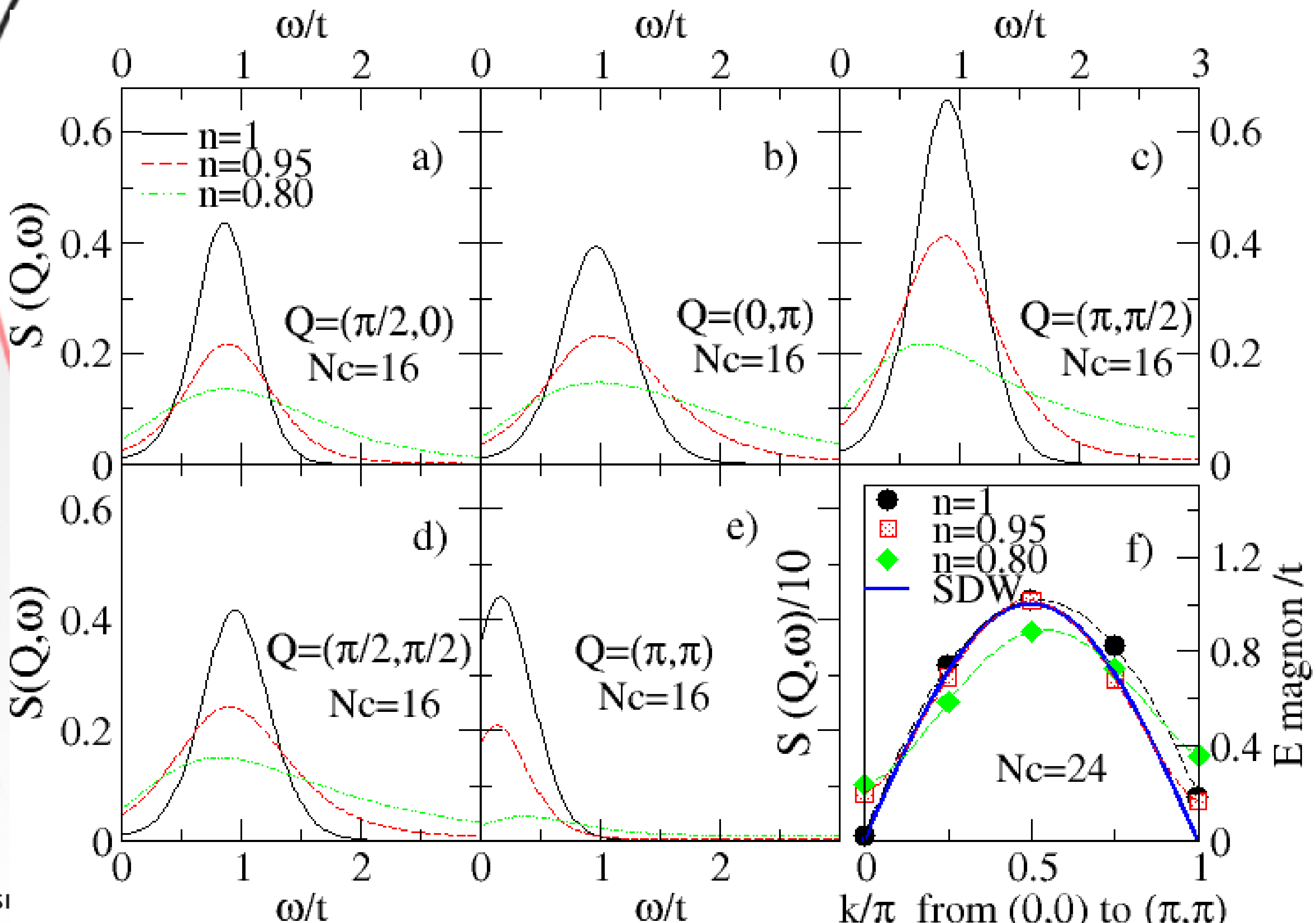




- RSO and DCA/QMC self energies agree for ω<0.
- HE kink comes from QP scattering from high energy spin fluctuations.

A. Macridin
unpublished
cm-0701429

HE Spin Excitations and doping



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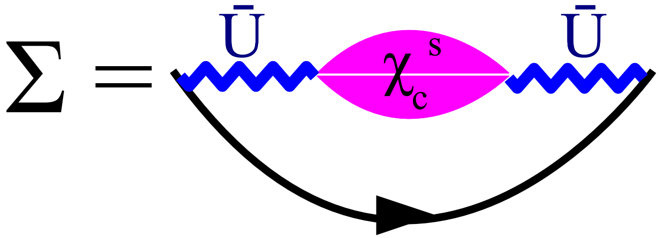
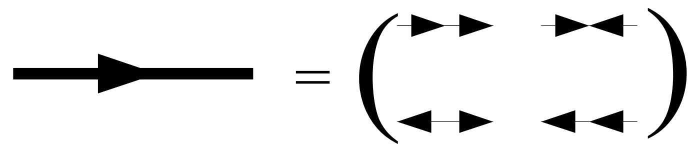
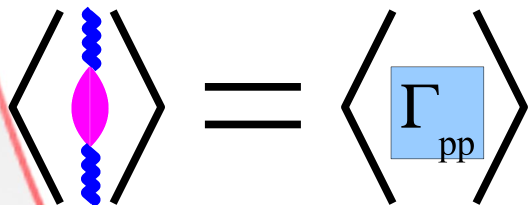
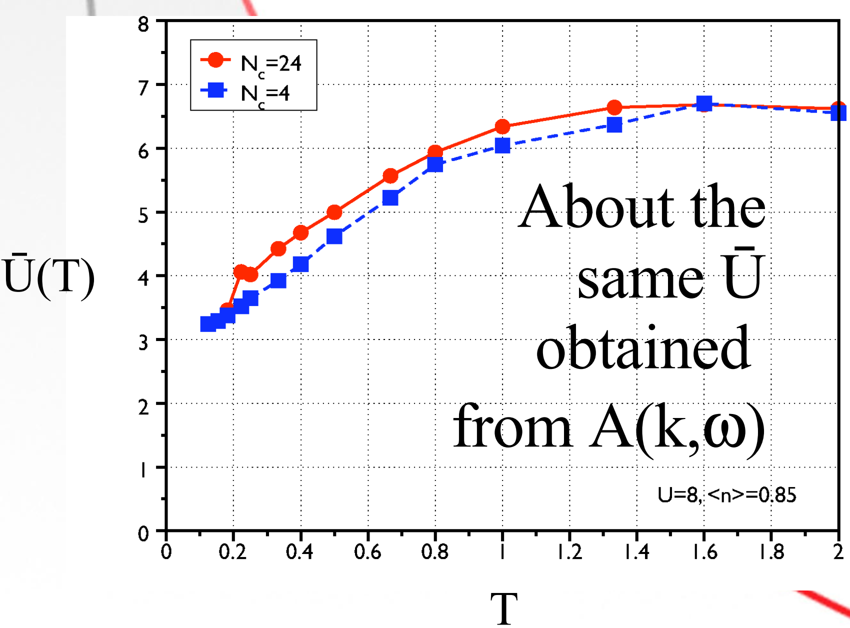
RSO Applied to Superconductivity

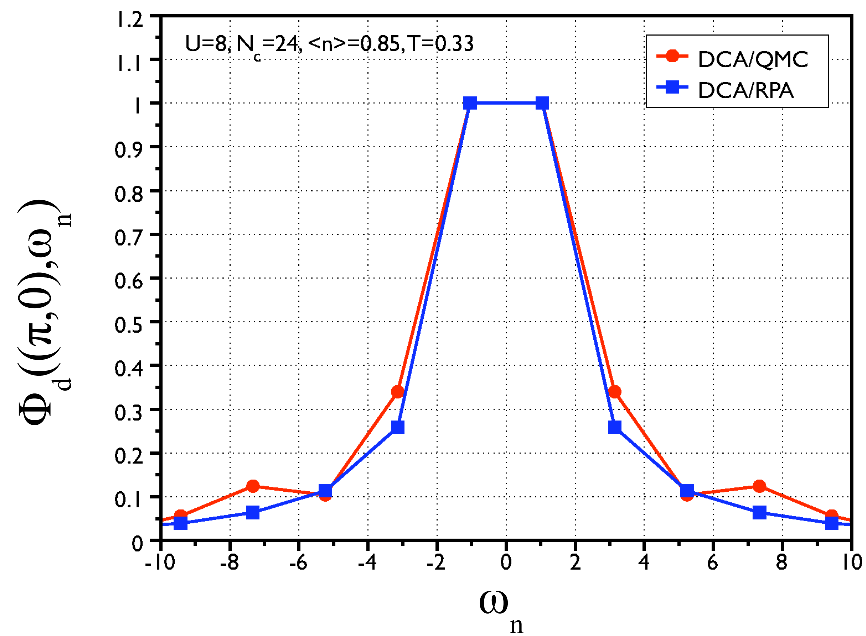


where now

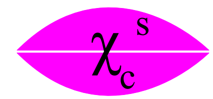


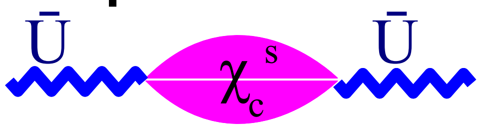


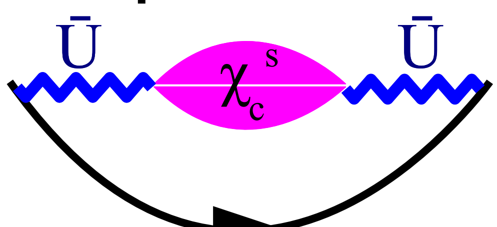




Possible method to analyze experiment

- Extract spin $S(q,\omega)$ from neutron scat.
  - use to calculate $\chi(k,\omega)=$ 

- Compare to ARPES to determine $\bar{U}$
  - 

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

  -
  - Test 1-band model and spin-fluctuation mediated pairingfor the cuprates.

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Conclusion

- DCA-QMC simulations of 1-band model captures many cuprate features
- HE kink in 2D HM due to coupling to HE spin fluctuations
  - Features $\omega<0$ are well described by coupling quasiparticle to spin fluctuations.
  - Same approximation captures superconducting properties.
- Contributes to the method used to analyze experiment

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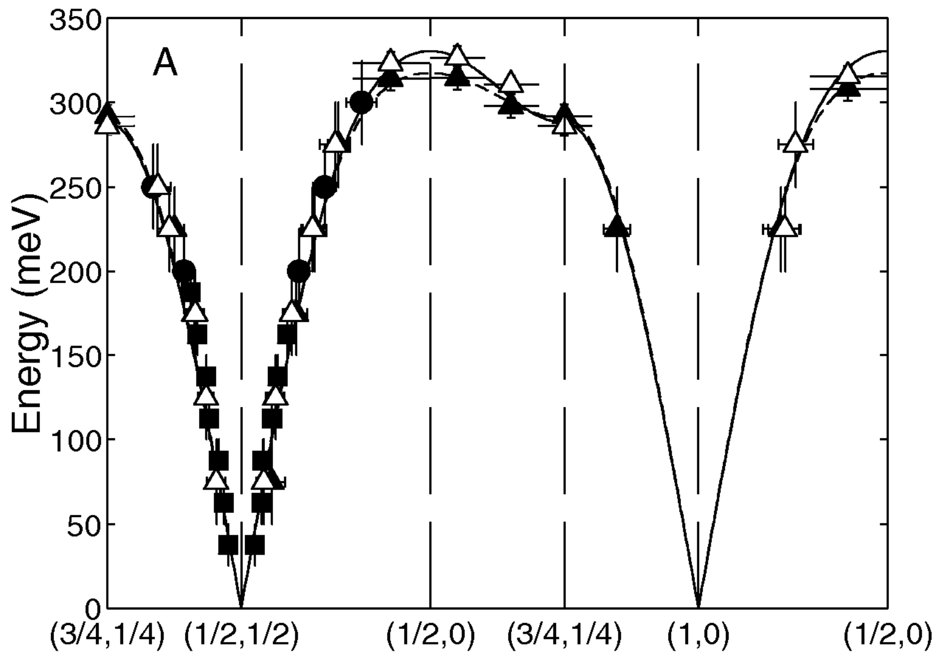
Magnons in 214

VOLUME 86, NUMBER 23 PHYSICAL REVIEW LETTERS 4 JUNE 2001

R. Coldea,[1,2] ... and Z. Fisk[6]

intensities. The extracted nearest-neighbor exchange $J = 111.8 \pm 4$ meV is antiferromagnetic, while the next-nearest-neighbor exchange $J' = -11.4 \pm 3$ meV across the diagonal is *ferromagnetic*. A wave-vector-independent quantum renormalization factor [12] $Z_c = 1.18$ was used in converting spin-wave energies into exchange couplings. The zone-boundary dispersion becomes more pronounced upon cooling as shown in Fig. 3A, and



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