Correlated Superconductivity in the Copper Oxide Planes a Cluster DMFT perspective

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Support: NSF

Gabriel Kotliar, Rutgers

Outline

- Some general comments on mean field theories for strongly correlated materials.
- Slave boson mean field theories and cluster Dynamical Mean Field Theory.
- Some generic properties of superconductivity near the Mott transition. [Pseudogap, coherence, incoherence-crossover, mechanism of Tc]
- Bridging structure property relation. On the strength of correlations in different cuprates.

Why do we want a MFT of correlated materials ?

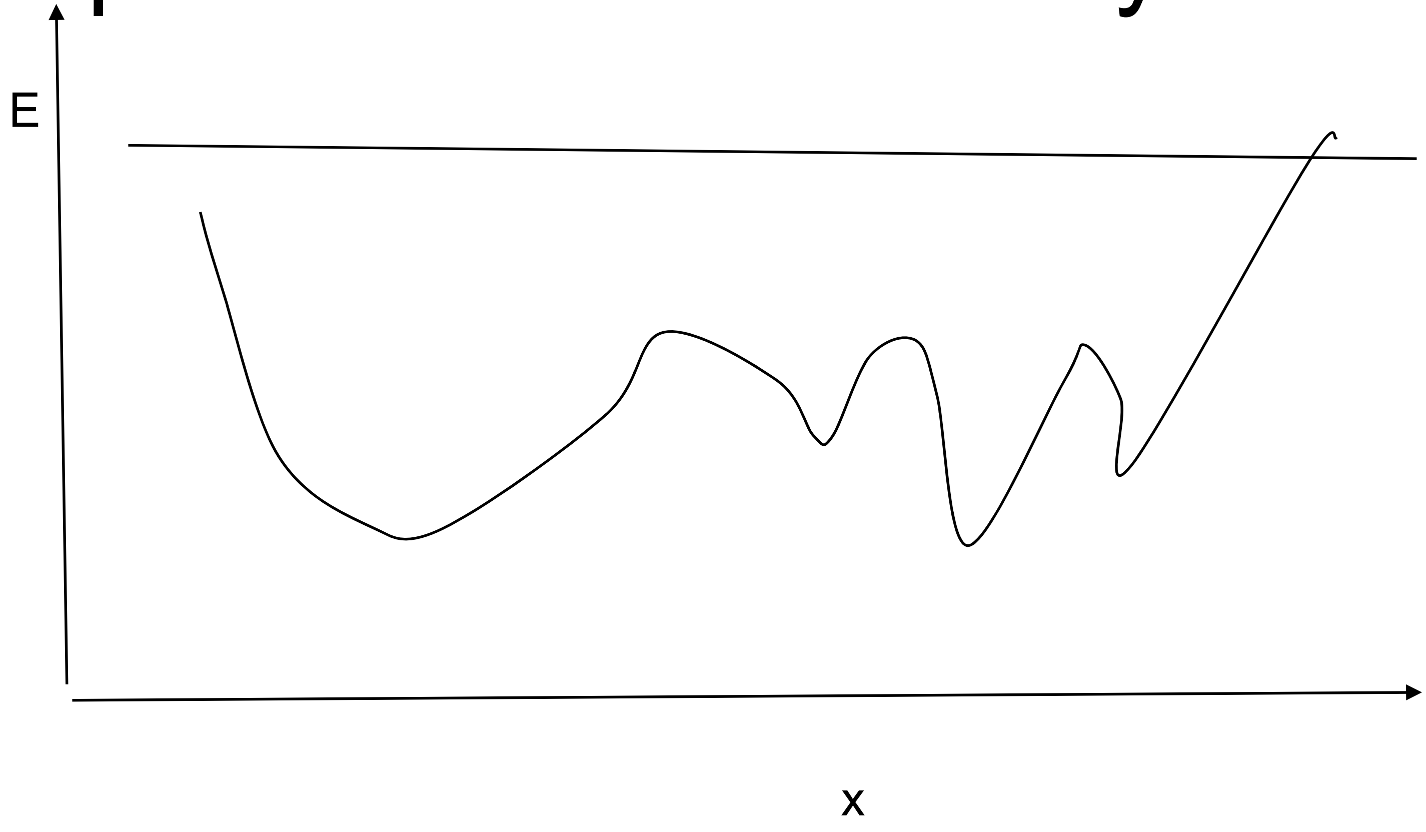
- Difficulties of solving exactly 2d models, realistic or not, at low temperatures.
- Need for understanding the solutions →design.
- Separate long wavelength (fluctuations, collective modes, diffects) effects from local physics.
- CDMFT Proceeds from high temperatures where single site is accurate. Captures short range orders in an unbiased fashion.
- Separates the study of the evolution of mean field solutions from the evaluation of their energies.

- Understand how the proximity to the Mott transition affects the “normal “ and superconducting state. Follow different states as a function of parameters T.
- Second step, computation of the free energies in specific models, study other ordered phases. Additional terms in the Hamiltonian can stabilize them.

- Realistic implementations (e.g. LDA+DMFT) makes material specific studies, has been successful for many systems with 3d, 4f and 5f electrons.

Almost (but not quite yet) parameter free.
Understand trends. Predict trends.

Energy Landscape of Correlated Materials. At low T. Many solutions to the DMFT equations with broken symmetries.



P. W. Anderson, *Science* **235**, 1196 (1987) Mott insulator→ high Tc

$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + J \sum_{\langle ij\rangle} (S_i S_j - \frac{1}{4} n_i n_j)$$

Slave Boson Formulation: Baskaran Zhou Anderson (1987) Ruckenstein Hirschfeld and Appell (1987)

$$c_{i\sigma} = f_{i\sigma} b^{\dagger}{}_{i}$$

$$\kappa_{ij} = \langle f^{\dagger}{}_{i\uparrow} f_{j\uparrow} \rangle + \langle f^{\dagger}{}_{i\downarrow} f_{j\downarrow} \rangle$$

$b^{+}i\ bi + f^{+}\sigma i\ f\sigma i = 1$

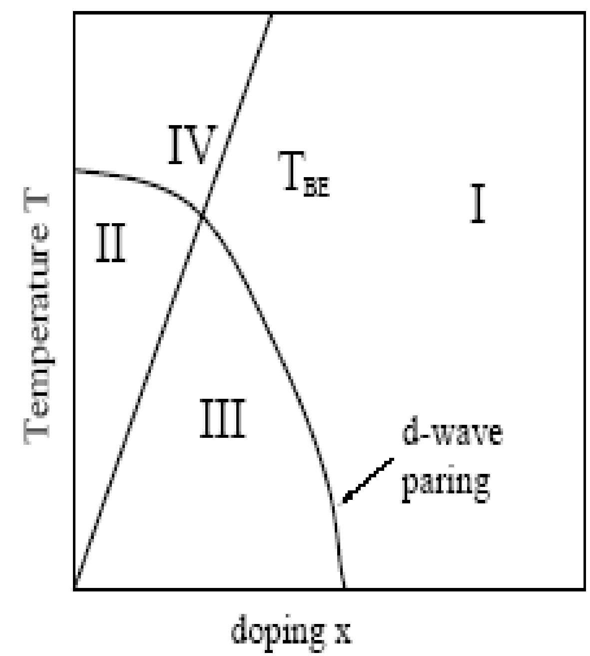
$$\Delta_{ij} = \langle f_{i\uparrow} f_{j\downarrow} \rangle - \langle f_{i\downarrow} f_{j\uparrow} \rangle$$

Other RVB states with d wave symmetry. Flux phase or s+id (G. Kotliar (1988) Affleck and Marston (1988) . Spectrum of excitation have point zeros like a a d –wave superconductor. Many other states ! Dimer states……….

RVB phase diagram of the Cuprate Superconductors. Superexchange.

- Tc controlled by J.
- Trvb, onset of spin pairing.
- < b>, T_{BE} , coherence temperature, formation of QP
- Superconducting dome. Pseudogap evolves into SC
- Problems: a) poor description of the incoherent part b) MFT too uniform c) other states i.e. AF.
- Restricted form of the electron self energy.

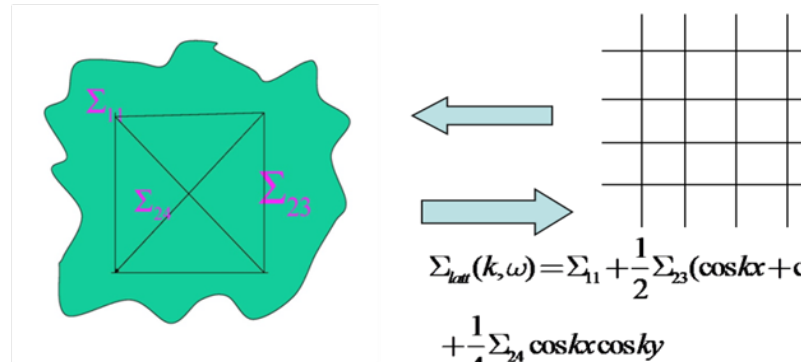
G. Kotliar and J. Liu Phys.Rev. B 38,5412 (1988)



Related approach using wave functions:T. M. Rice group. Zhang et. al. Supercond Scie Tech 1, 36 (1998, Gross Joynt and Rice (1986) M. Randeria N. Trivedi , A. Paramenkanti PRL 87, 217002 (2001)

Single Site and Cluster Dynamical Mean Field Theory

- Map lattice model to impurity in a medium.
- “Metallicity” Itineracy order parameter->Weiss field.
- Generate impurity quantities lattice quantities



$$\Sigma_{latt}(k,\omega)=\Sigma_{11}+\frac{1}{2}\Sigma_{23}(\cos kx+\cos ky)+\frac{1}{4}\Sigma_{24}\cos kx\cos ky$$

- Single site DMFT is unique but cluster extensions are not. Various approaches DCA, CDMFT,Edmft, Ecdmft, etc. (self energy, cumulant, GF periodization)…..
- The mean field theory is still a non trivial problem! Various impurity solvers (QMC, CTQMC, NCA, ED…)

Can study various solutions AF , SC, AF+SC as a function of parameters (i.e. normal and superconducting state). Removes many of the shortcomings of SB MFT.

$$\Sigma_n \; \Sigma_a \;, \Sigma(k,i\omega) \approx \Sigma \; (i\omega) = \Sigma \; (i\omega)[G(i\omega)]$$

Migdal Eliashberg theory, simplest example of a single site DMFT. Electron phonon problem, local self energy, perturbative solver.

Formal extension of DMFT to superconduting state, odd frequency pairing for very large overdoping using Fye Hirsch QMC . *A. Georges, G. Kotliar, and W. Krauth, Z. Phys. B 92 313-321 (1993)*. (see arXiv:0904.2788 T. H. Geballe, M. Marezio)

Cluster DMFT includes d wave, and removes many of the shortcomings of RVB MFT.

Early studies of plaquette and links DMFT

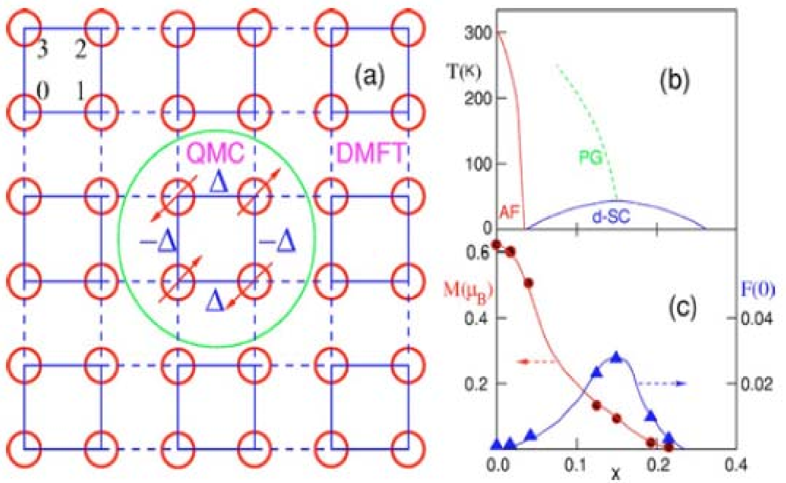


FIG. 39. (Color in online edition) Four-site cluster calculation for the 2D Hubbard model: (a) Schematic representation of an antiferromagnetic d-wave 2×2 periodically repeated cluster. (b) Generic phase diagram of high-temperature superconductor. (c) Magnetic (M) and d-wave superconducting (F) order parameters versus hole doping in the 2D Hubbard model at $\beta t=15$, $t'=-0.15t$, $U=4.8t$ calculated with a four-site cluster approach similar to the DCA/QMC method. From Lichtenstein and Katsnelson, 2000.

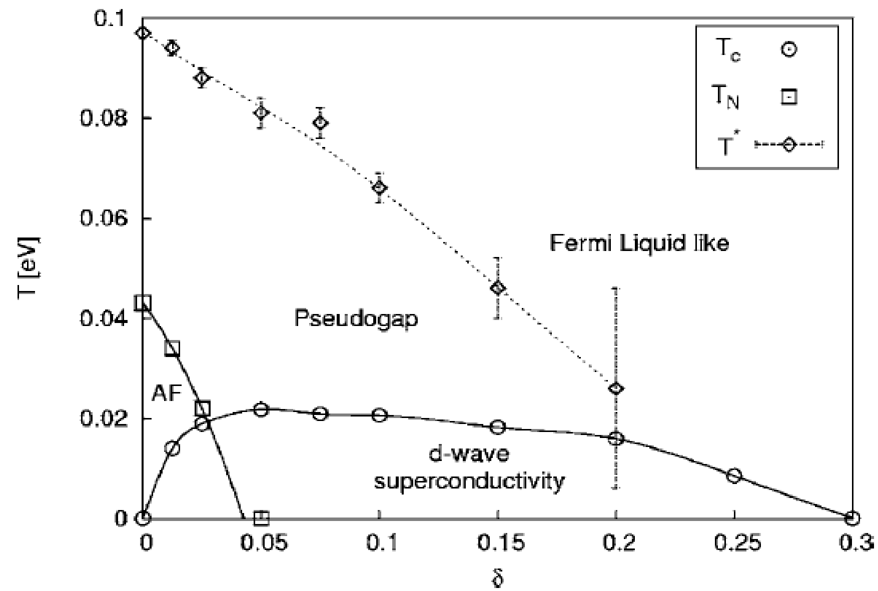
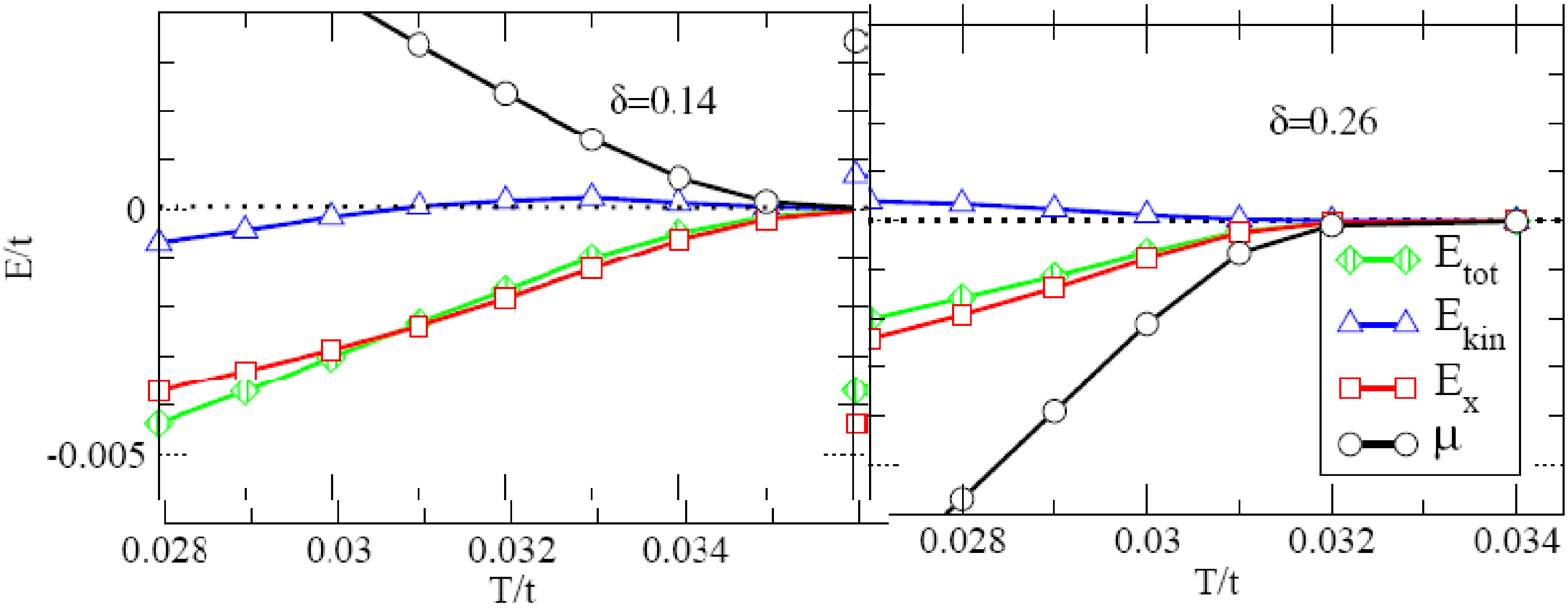


FIG. 40. Temperature-doping phase diagram of the 2D Hubbard model when $U=8t$ calculated with DCA/QMC for a four-site cluster, $N_c=4$. The error bars on T^* result from the difficulty in locating the maximum in the uniform spin susceptibility. Regions of antiferromagnetism, d-wave superconducting, and pseudogap behavior can be seen.

Stanescu, T. D., and P. Phillips, 2003, Phys. Rev. Lett. **91,**017002. DCA in 2x2

Jarrell, M., T. Maier, et. al. 2001, Europhys. Lett. **56, 563.**

E Energy difference between the normal and superconducing state of the t-J model. K. Haule (2006)



Optics and RESTRICTED SUM RULES

$$H \ \ hamiltonian, \ \ J \ electric\ current, \ P \ polarization$$

$$\int_0^\infty \sigma(\omega)\, d\omega = \frac{\pi}{iV} < [P, J] > = \frac{\pi n e^2}{m}$$

Below energy Λ

$$\int_0^\Lambda \sigma(\omega) d\omega = \frac{\pi}{iV} < [P_{eff}, J_{eff}] >$$

$$H_{eff}, \ J_{eff}, \ P_{eff}$$

$$-\sum_k n_k \frac{\partial^2 \varepsilon_k}{\partial^2 k}$$

Low energy sum rule can have T and doping dependence . For nearest neighbor it gives the kinetic energy. Use it to extract changes in KE in superconducing state

Optics and RESTRICTED SUM RULES

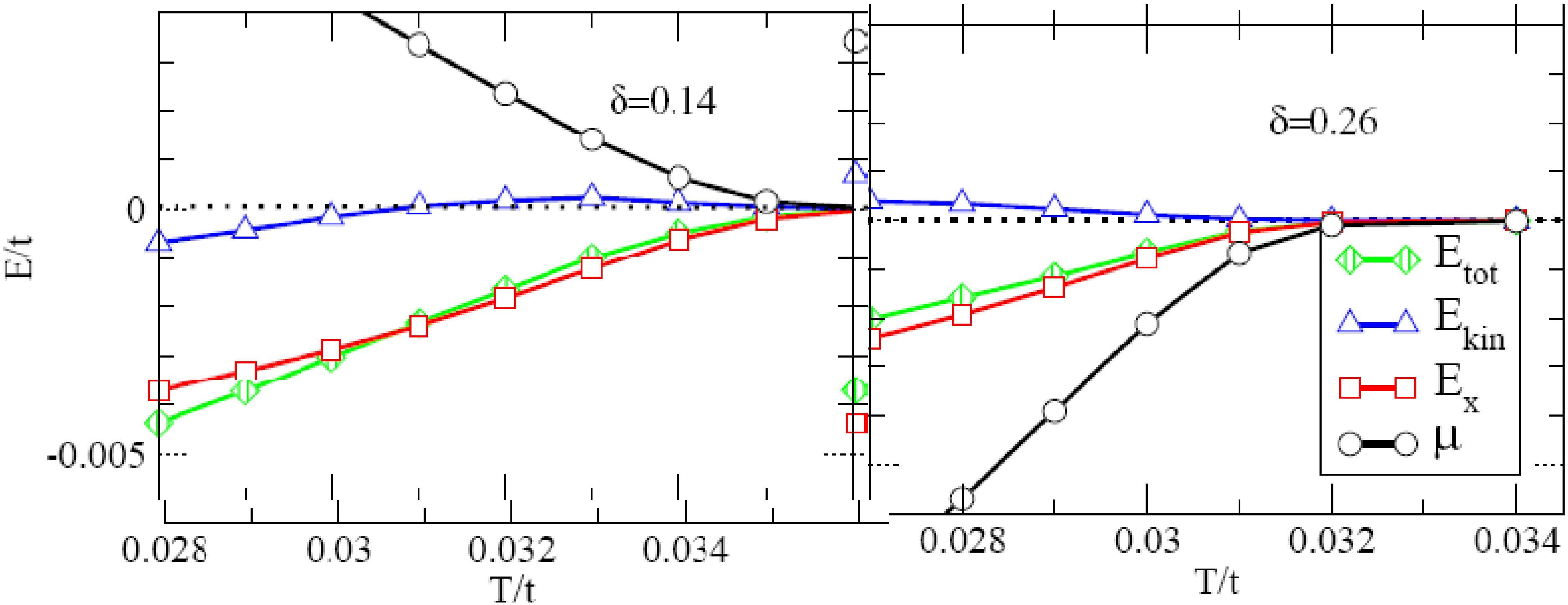
$$\int_0^\Lambda \sigma_n(\omega) - \sigma_s(\omega)\, d\omega = < -T >_n(T) - < -T >_s(T)$$

<T>n is only defined for T> Tc, while <T>s exists only for T<Tc

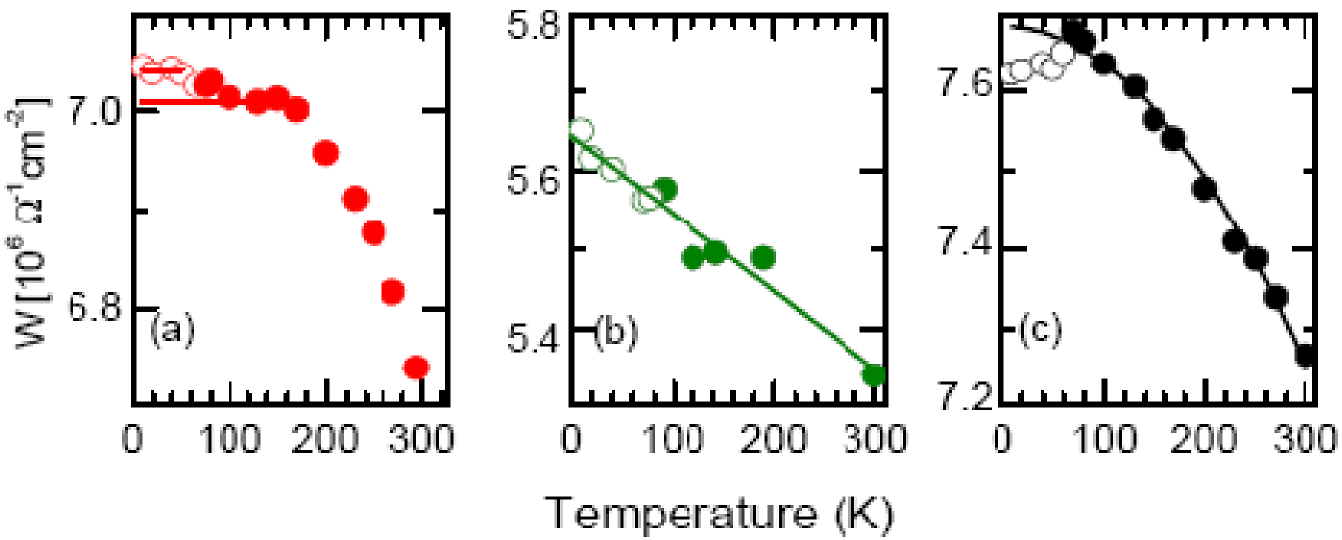
Experiment: use of this equation implies extrapolation.

Theory : use of this equation implies of mean field picture to continue the normal state below Tc.

E Energy difference between the normal and superconducing state of the t-J model. K. Haule (2006)

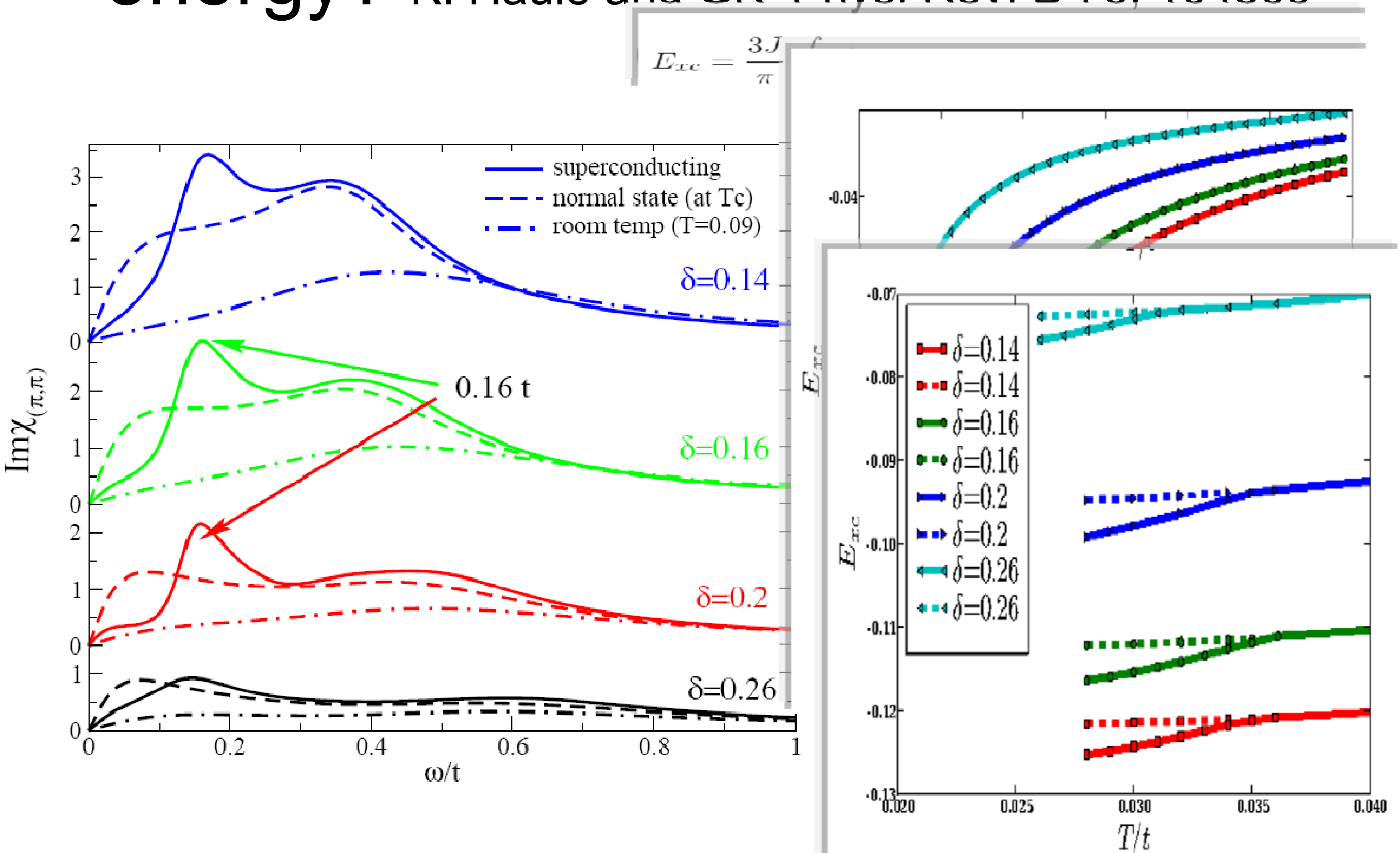


. Spectral weight integrated up to 1 eV of the three BSCCO films. a) under-
doped, Tc=70 K; b) ~ optimally doped, Tc=80 K; c) overdoped, Tc=63 K; the full
symbols are above Tc (integration from 0+), the open symbols below Tc, (integrationfrom 0, including th

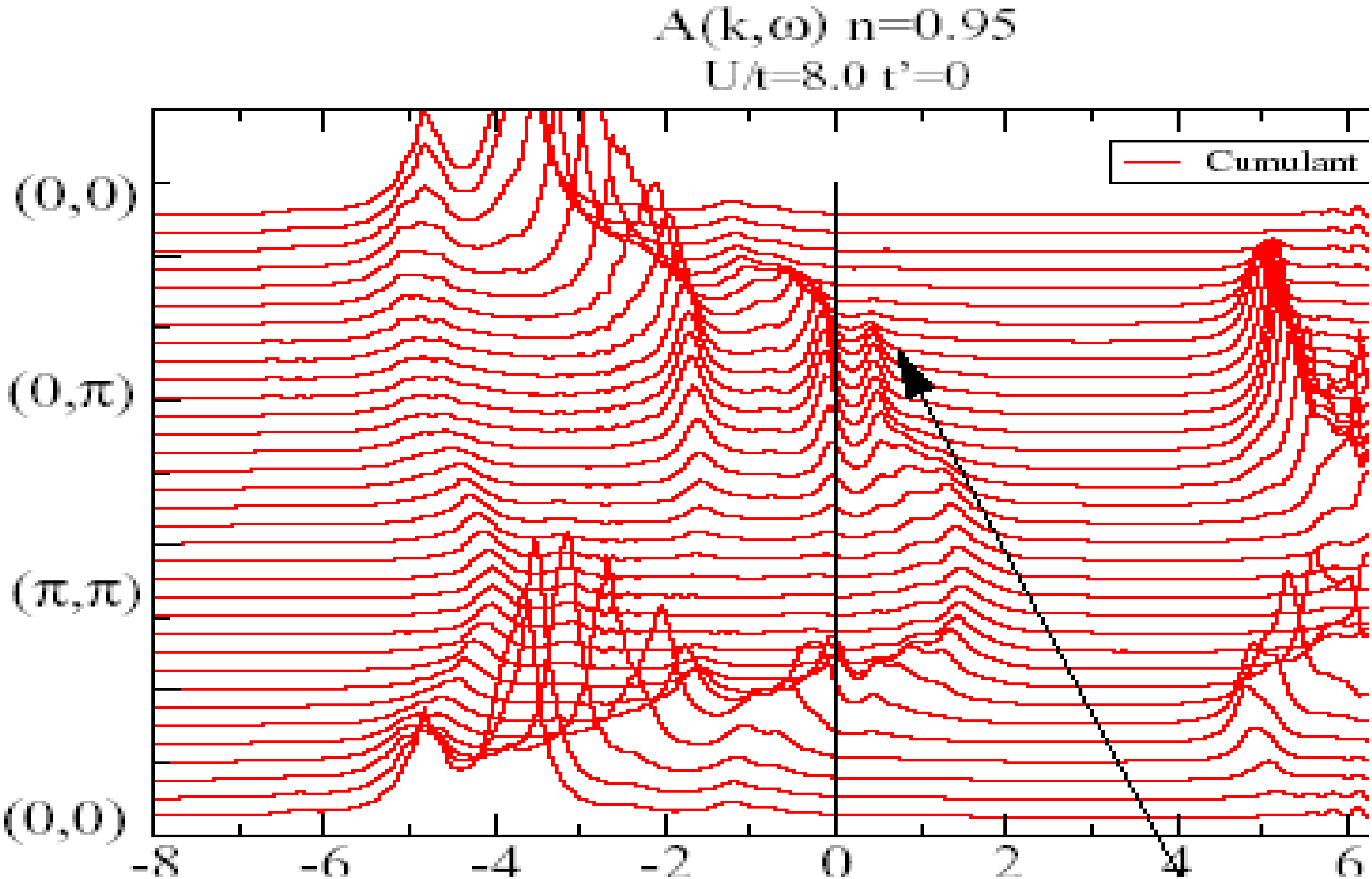


H.J.A. Molegraaf et al., Science 295, 2239 (2002).
A.F. Santander-Syro et al., Europhys. Lett. 62, 568 (2003).
Cond-mat 0111539. G. Deutscher et. A. Santander-Syro and N. Bontemps. PRB 72, 092504(2005) . Recent review:

Where is the change of exchange energy? K. Haule and GK Phys. Rev. B 76, 104509



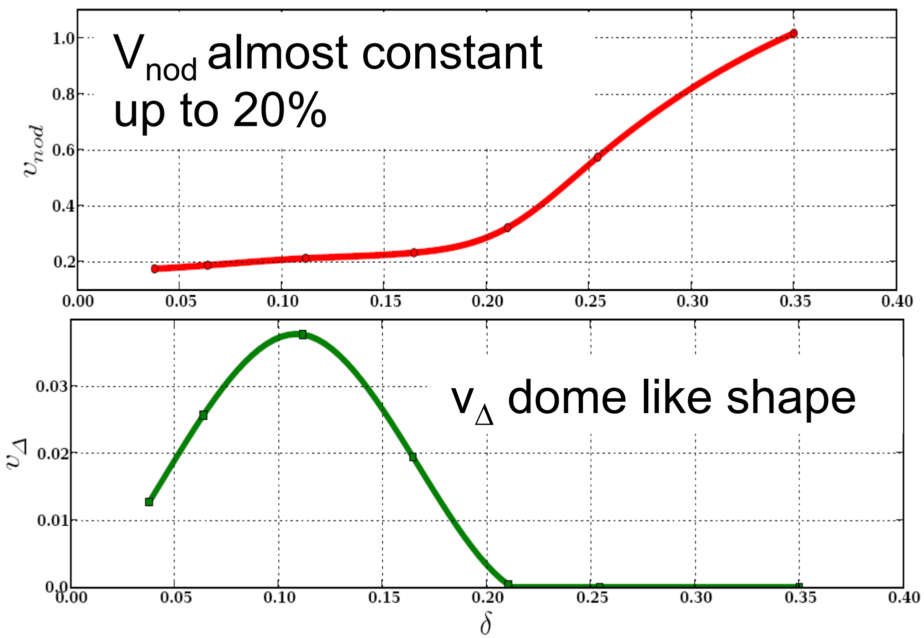
Nodal Antinodal Dichotomy and pseudogap in CDMFT T. Stanescu and GK Phys. Rev. B 74, 125110 (2006), B. Kyung et.al. PRB 73, 165114 (2006)

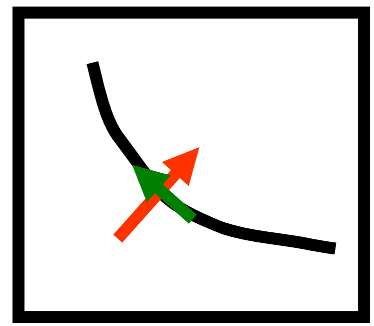


Nodal quasiparticles

$$v_{nodal} = Z_{nodal}\left(\frac{d\epsilon_{\mathbf{k}}}{dk_{\perp}} + \frac{d\Sigma_{\mathbf{k}}}{dk_{\perp}}\right)$$

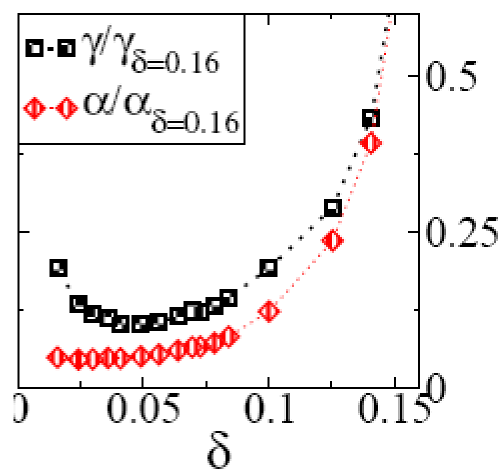
$$v_{\Delta} = Z_{nodal}\frac{\Sigma_{\mathbf{k}}^{anomal}}{dk_{||}}$$





the slope=v$_{nod}$
almost constant

N(ω) = ωγ   γ= Znod/(vnod vΔ)



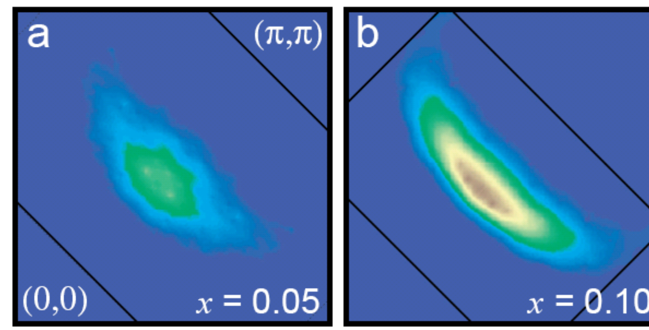
Superconducting gap tracks Tc!

M. Civelli, cond-mat 0704.1486 PRL (2008)

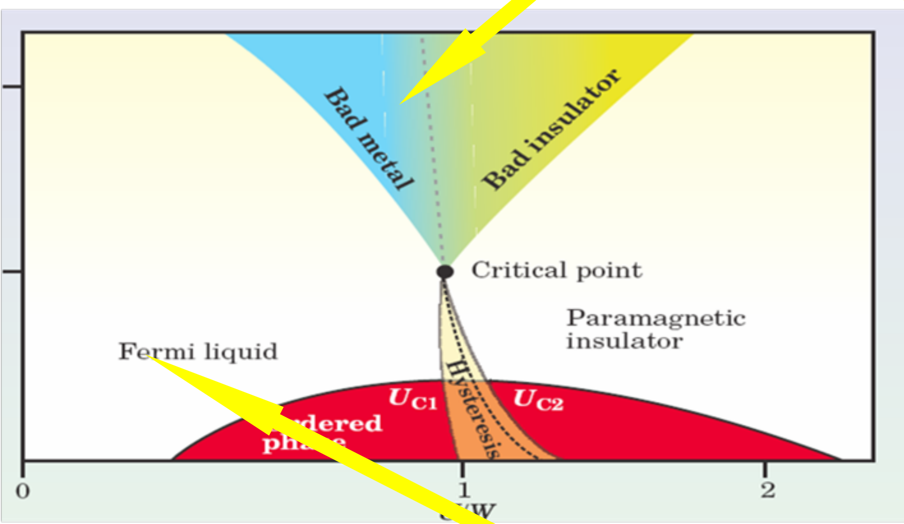
Pseudogap and Fermi arcs, in CDMFT
U=16 t=1, t'=-.3 , Hubbard model

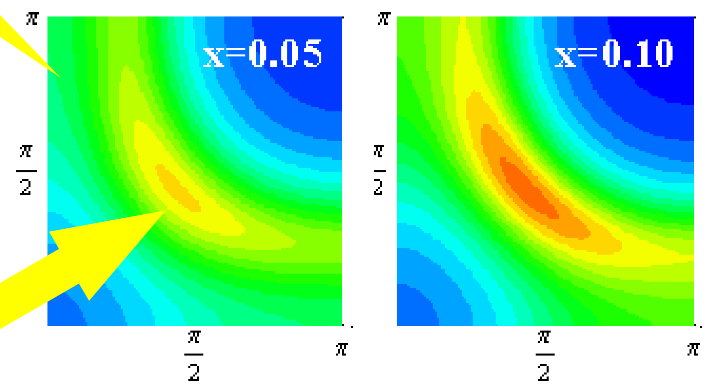
Spectral Function $A(k,\omega \to 0) = -1/\pi\, G(k, \omega \to 0)$ vs k

K.M. Shen et.al. 2004



Antinodal Region





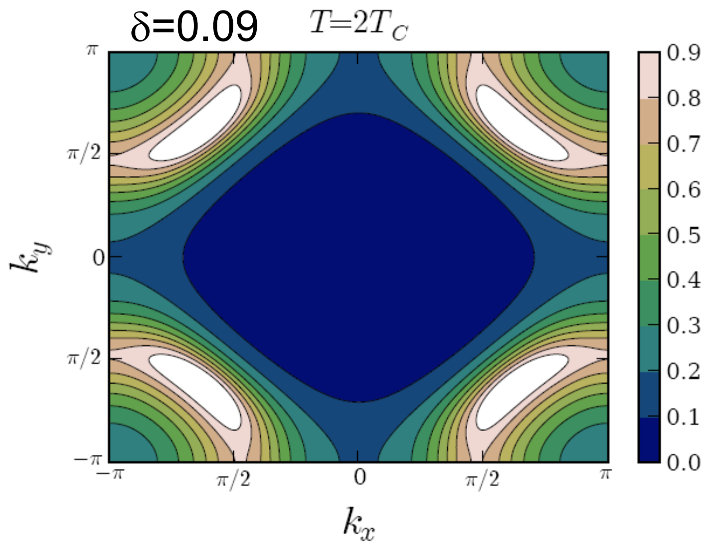
2X2 CDMFT

Senechal et.al
PRL94 (2005)

Nodal Region

Civelli et.al. PRL 95 (2005)

Fermi surface



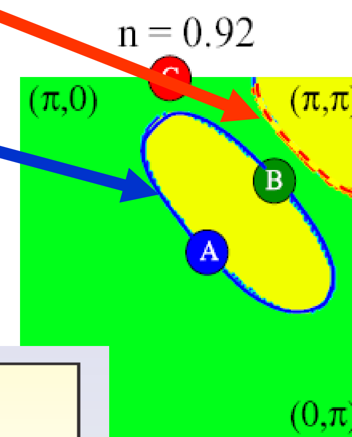
T.D. Stanescu and G. Kotliar, Phys. Rev. B **74**, 125110(2006)

Cumulant $M = (\omega + \mu - \Sigma)^{-1}$rt in ranged:

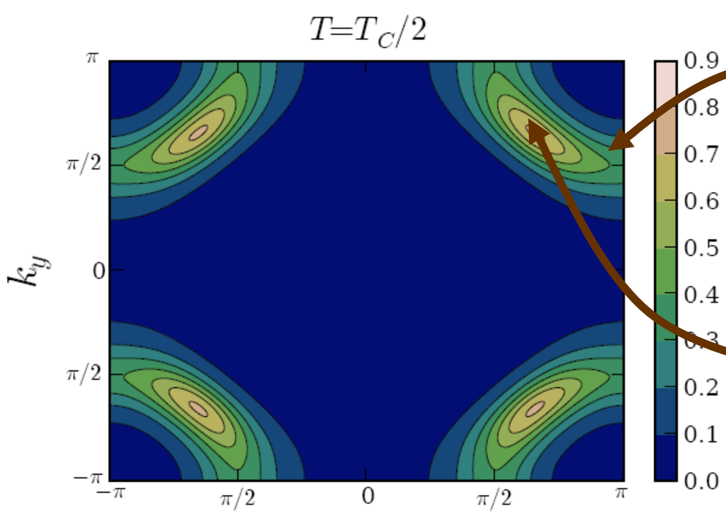
$$M_{\mathbf{k}} = M_{11} + M_{12}(\cos k_x + \cos k_y) + M_{13} \cos k_x \cos k_y$$

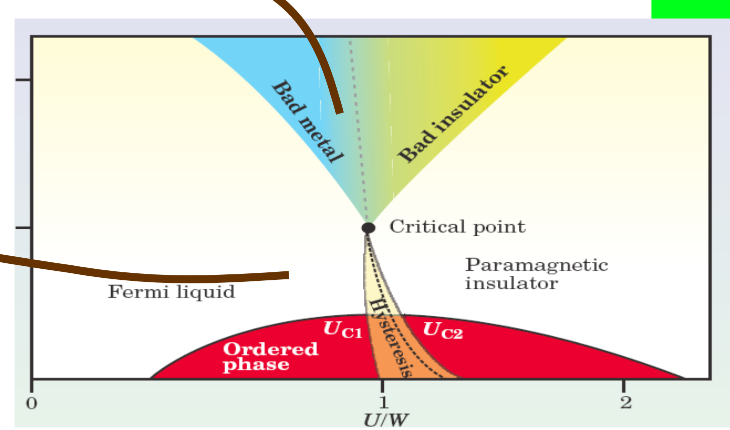
Arcs FS in underdoped regime

pockets+lines of zeros of G == arcs

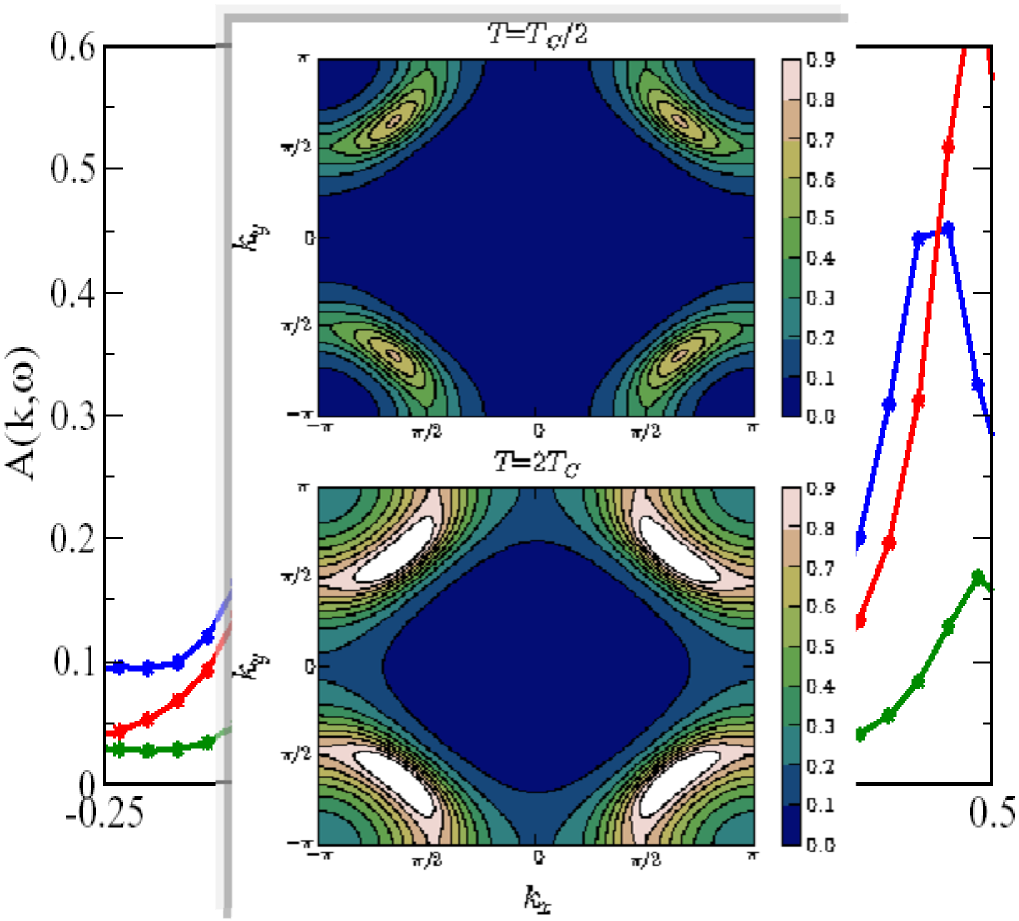


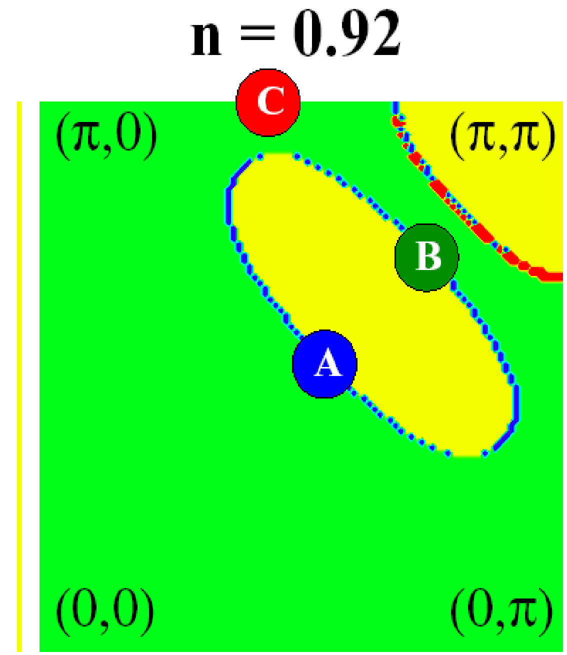
Arcs shrink with T!





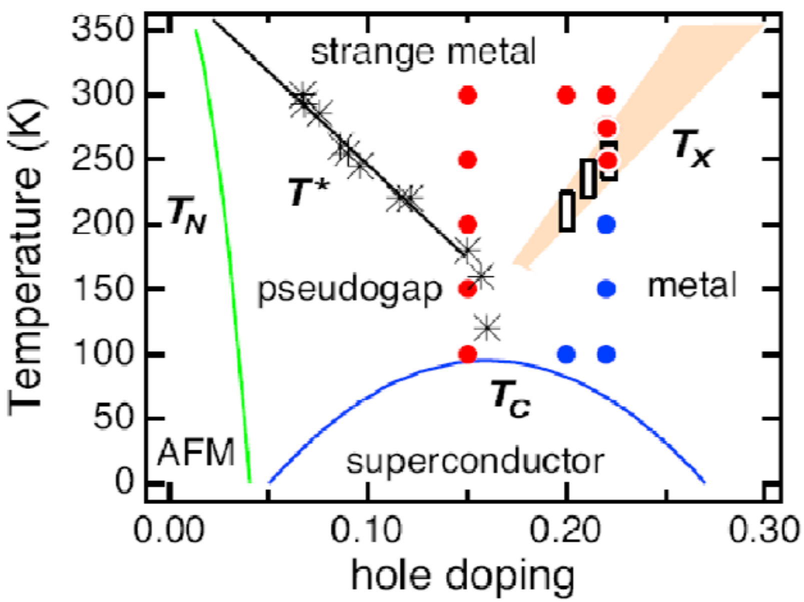
T. Stanescu and GK Phys. Rev. B **74**, 125110 (2006) Pseudogap state pockets + lines of zeros that screend them.

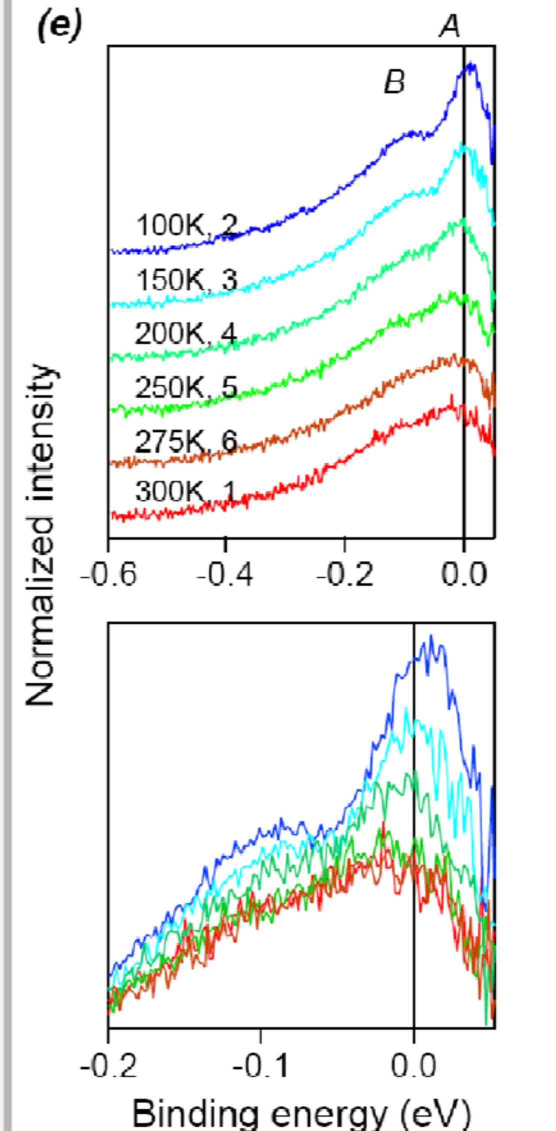




Some similiarities with phenomenological approach developed around the same time. Yang Rice and Zhang PRB 73 174501 (2006). R. M. Konik, T. M. Rice, A. M. Tsvelik, Phys. Rev. Lett96, 086407 (2006).

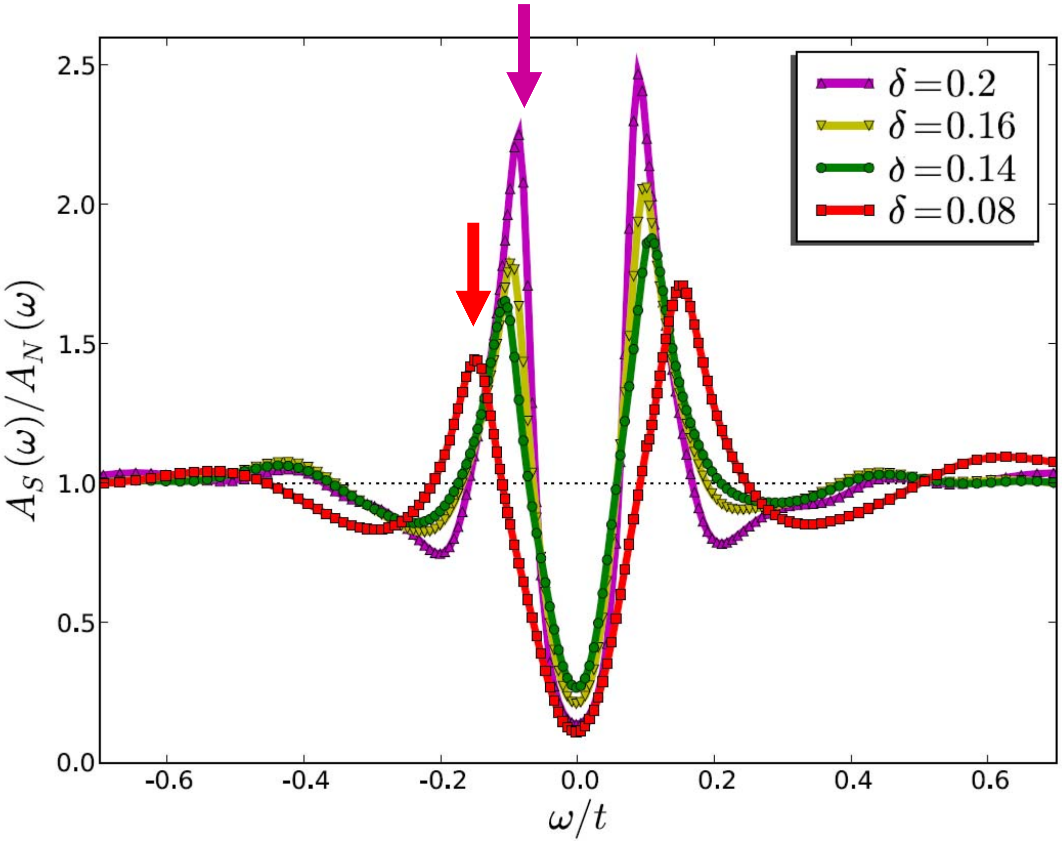
OVERDOPED REGIME : Coherence Incoherence crossover. Kaminski et. al. Phys. Rev. Lett. **90**, 207003





(e) Spectrum at $(\pi, 0)$ (divided by the Fermi function) at various temperatures. All curves are overlapped on the bottom of the panel to demonstrate lack of temperature dependence of the lineshape above 250K.

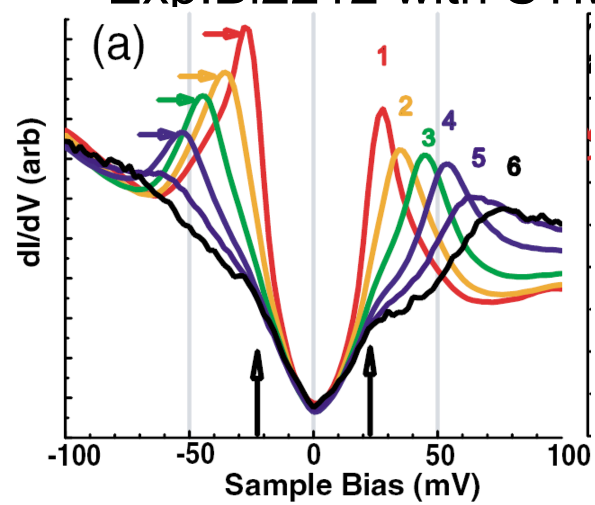
Ratio A_S/A_N



Ratio more universal, more symmetric

With decreasing doping gap increases, coherence peaks less sharp->Non BCS

Exp:Bi2212 with STM



Alternative explanation Fang, et.al. **PRL** vol 96, 017007 (2006).

McElroy,.. JC Davis,
Sa PRL 94, 197005 (2005)

Nodal quasiparticles

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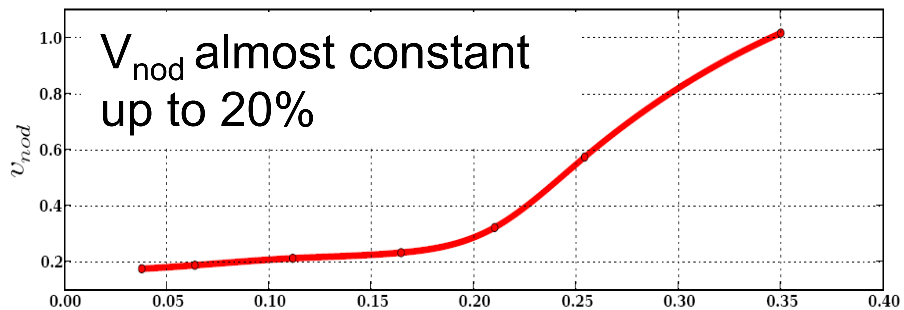
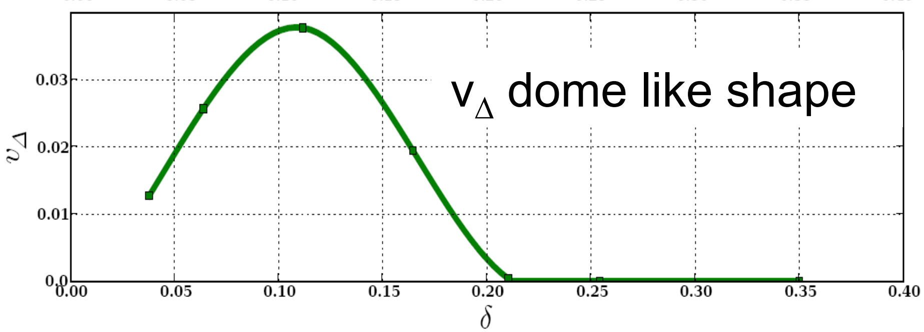
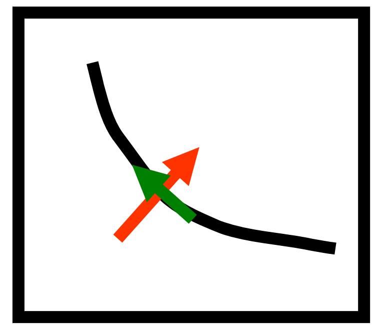
$$v_{\Delta} = Z_{nodal}\frac{\Sigma^{anomal}_{\mathbf{k}}}{dk_{||}}$$

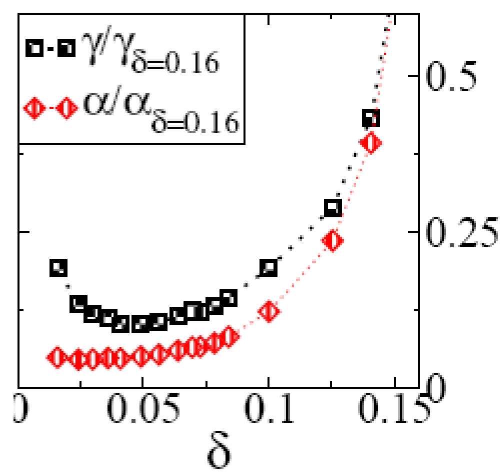






the slope=v_{nod} almost constant

$N(\omega) = \omega\gamma \quad \gamma = Z_{nod}/(v_{nod}\, v_\Delta)$



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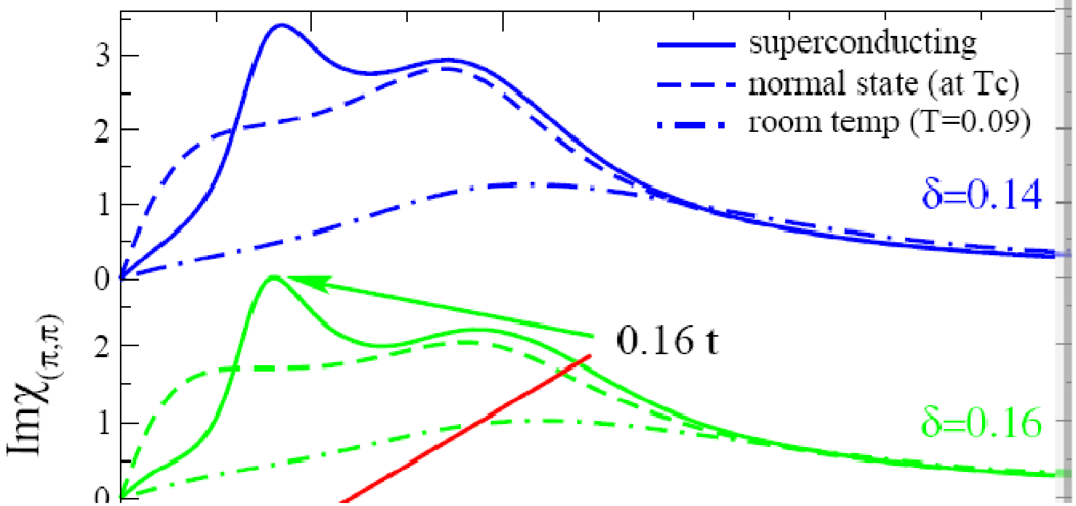
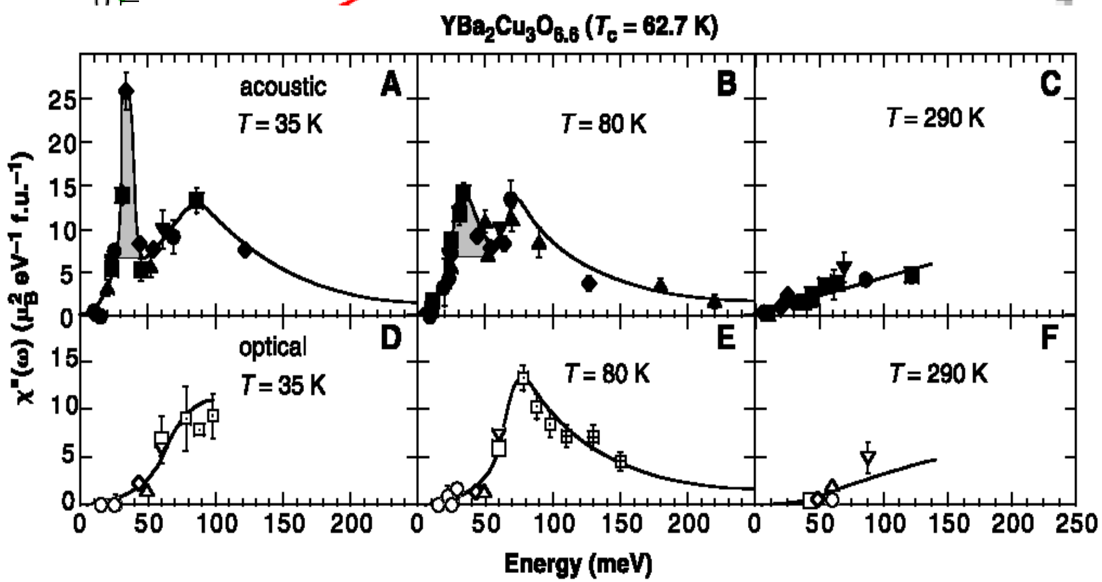
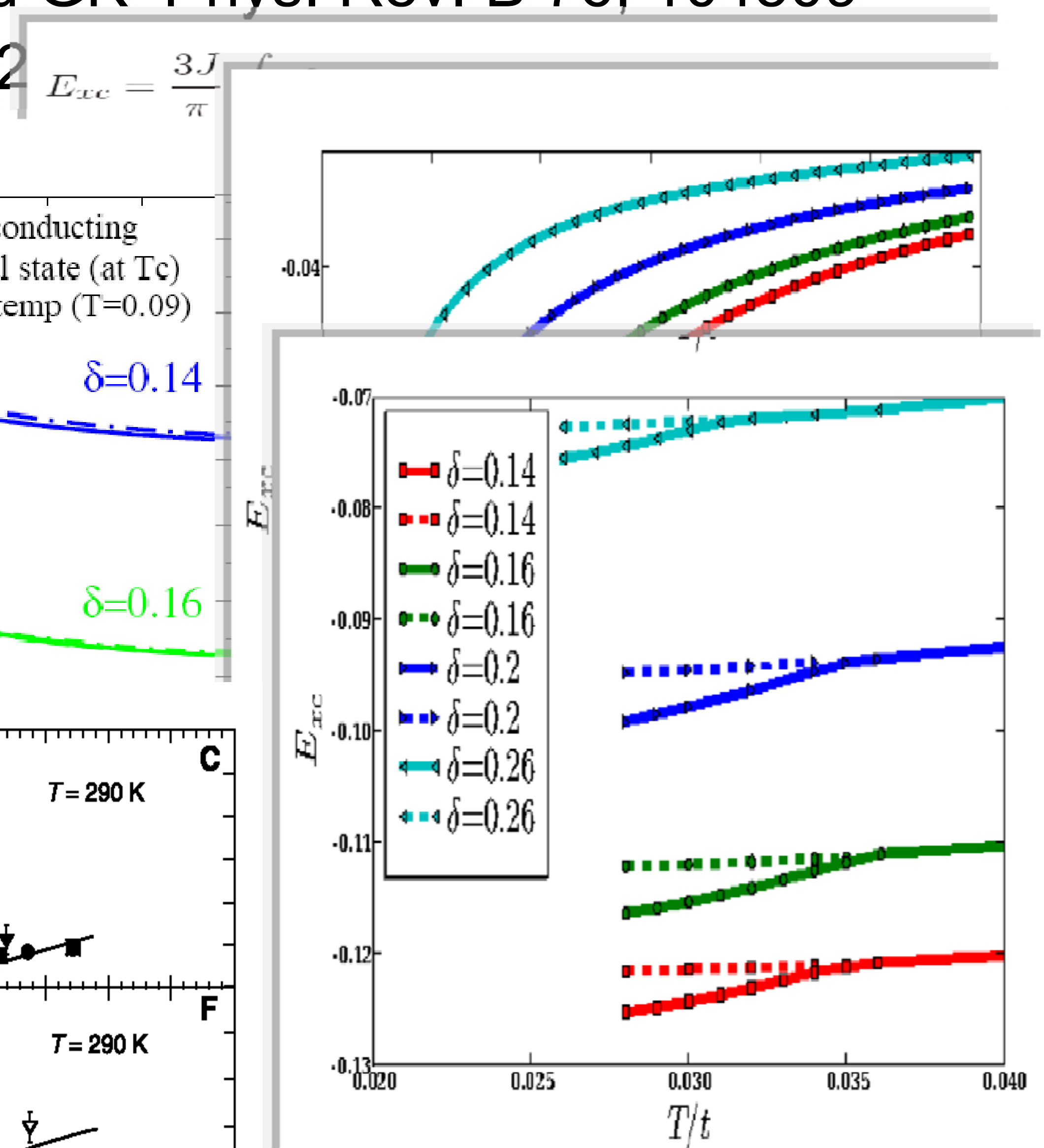
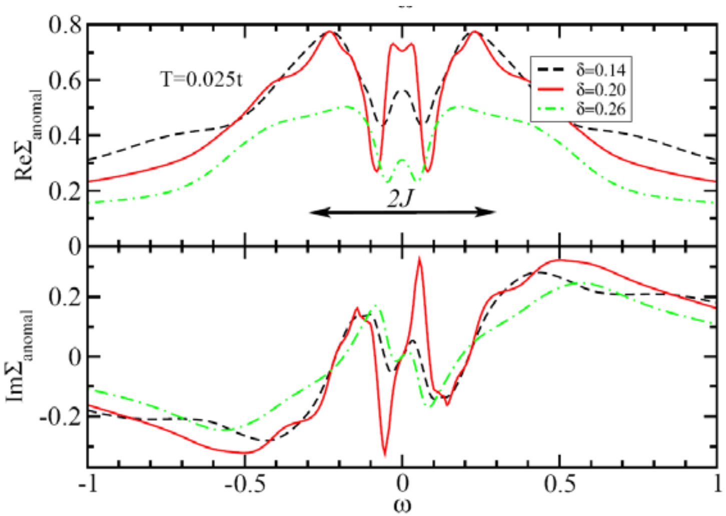
Where is the change of exchange energy? K. Haule and GK Phys. Rev. B 76, 104509 (2

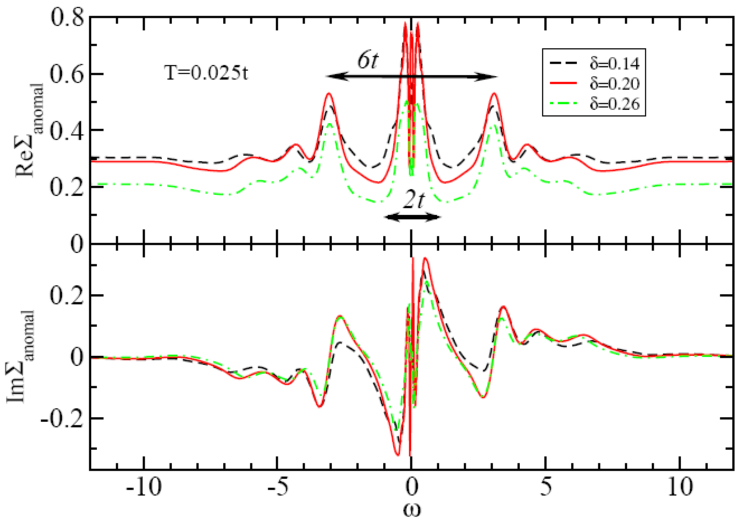






Anomalous self-energy on real axis





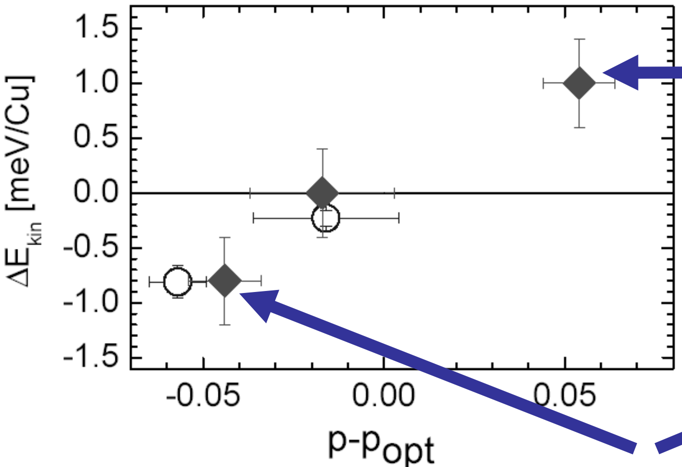
- Many scales can be identified
  J,t,6t

$$.\Sigma_a(\infty) / \int d\omega' \Sigma''_a(\omega') \frac{}{\omega'} = .3$$

$$\Sigma_a(i\omega) = -\int d\omega' \Sigma''_a(\omega') \frac{}{i\omega_n - \omega'} + \Sigma_a(\infty)$$

Computed by the NCA for the t-J model
K Haule and GK (2006)

Kinetic energy change



Kinetic energy increases

Kinetic energy decreases

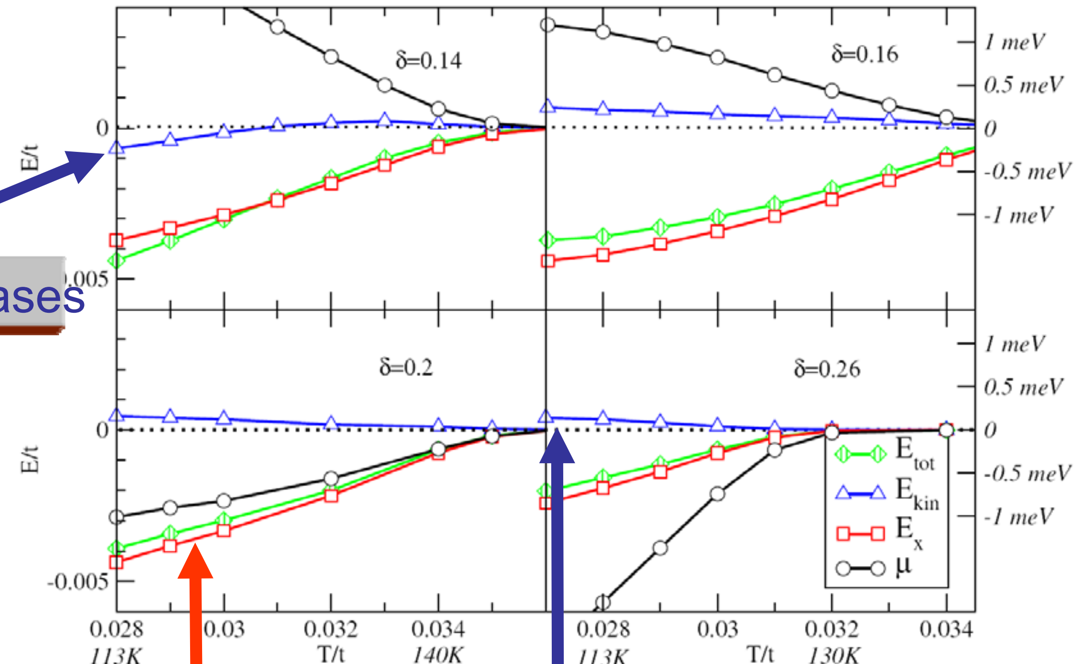
FIG. 2: Change ΔE_{kin} of the kinetic energy, in meV per copper site, calculated from equations (1) and (3), versus the charge p per copper with respect to p_{opt} (Eq.6). Full diamonds: data from Ref.[3], high frequency cut-off 1 eV. Open circles: data from Ref.[1], high frequency cut-off 1.25 eV. Error bars: vertical, uncertainties due to the extrapolation of the temperature dependence of the normal state spectral weight down to zero temperature; horizontal, uncertainties resulting from $T_c/T_{c,max}$ through Eq.6 (see text). We have taken $T_{c,max} = (83 \pm 2)$ K for films and (91 ± 2) K for crystals.

Guy Deutscher[1], Andrés Felipe Santander-Syro[2] and Nicole Bontemps[3]

cond-mat/0503073

Phys Rev. B **72**, 092504 (2005)

cluster-DMFT, cond-mat/0601478



Kinetic energy increases

Exchange energy decreases and gives **largest contribution** to condensation energy

Accuracy of DMFT? Remarkable advances in optical lattices. [compressiblity, double occupancy] Good agreement with DMFT in the (high) temperature range.

Science 5 December 2008:
Vol. 322. no. 5907, pp. 1520 - 1525
DOI: 10.1126/science.1165449

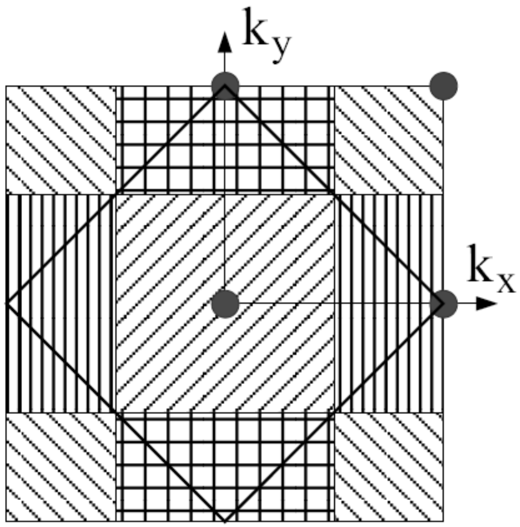
RESEARCH ARTICLES

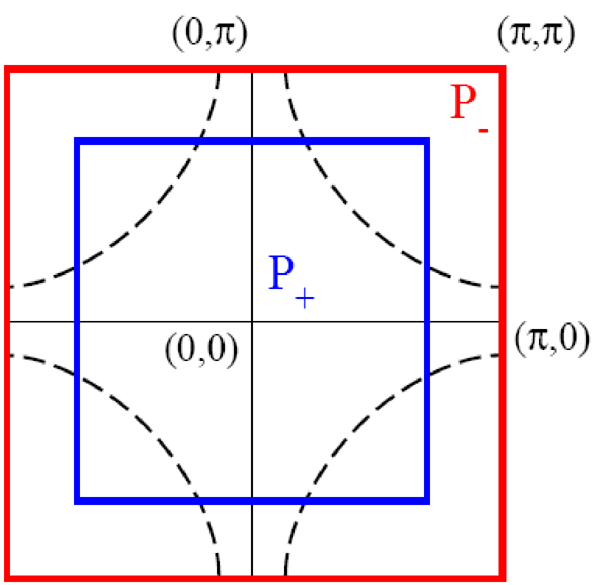
Metallic and Insulating Phases of Repulsively Interacting Fermions in a 3D Optical Lattice

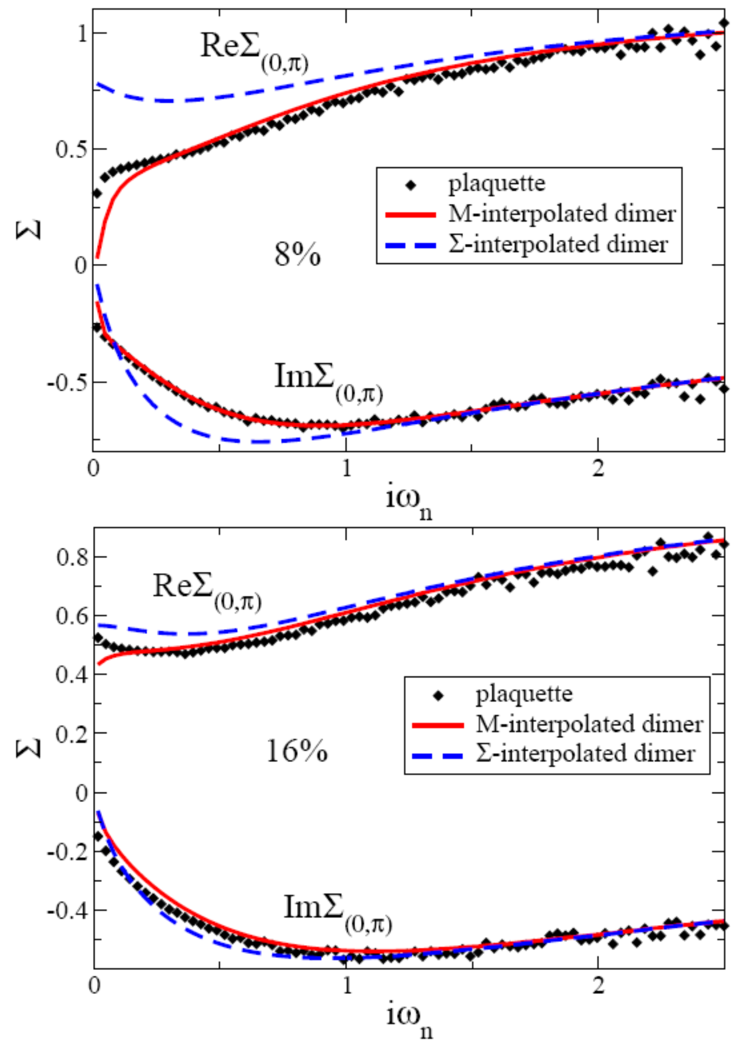
U. Schneider,[1] L. Hackermüller,[1] S. Will,[1] Th. Best,[1] I. Bloch,[1,2*] T. A. Costi,[3] R. W. Helmes,[4] D. Rasch,[4] A. Rosch[4]

See also De Leo et. al. PRL.

Two site vs four site. Ferrero et. al.

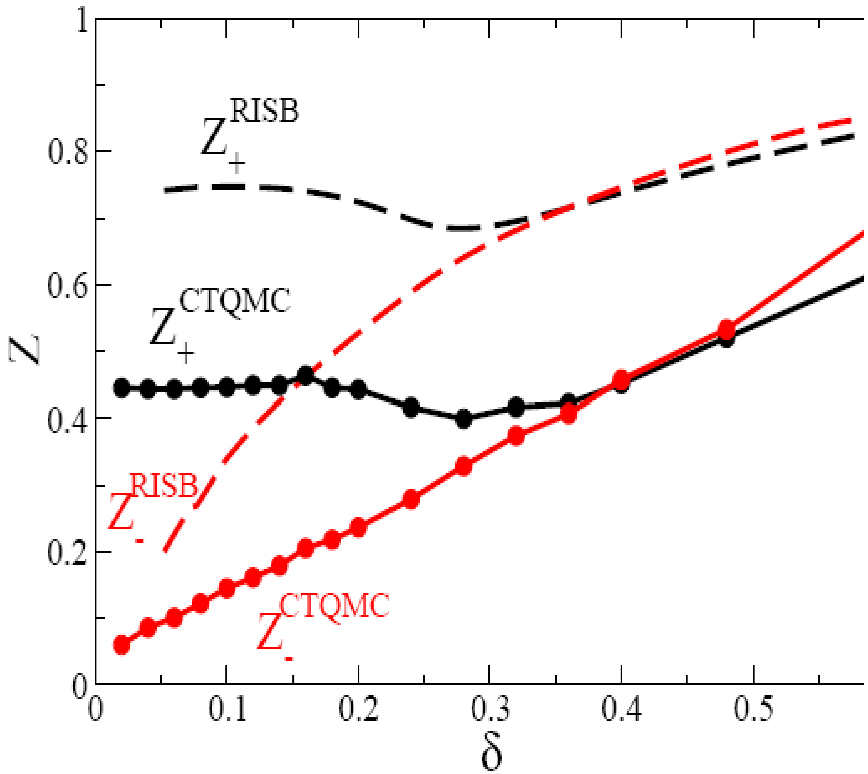






Ferrero Cornaglia DeLeo Parcollet Kotliar Georges (2009)

RI Slave bosons vs CTQMC (Ferrero et. al.). Spin pairing.



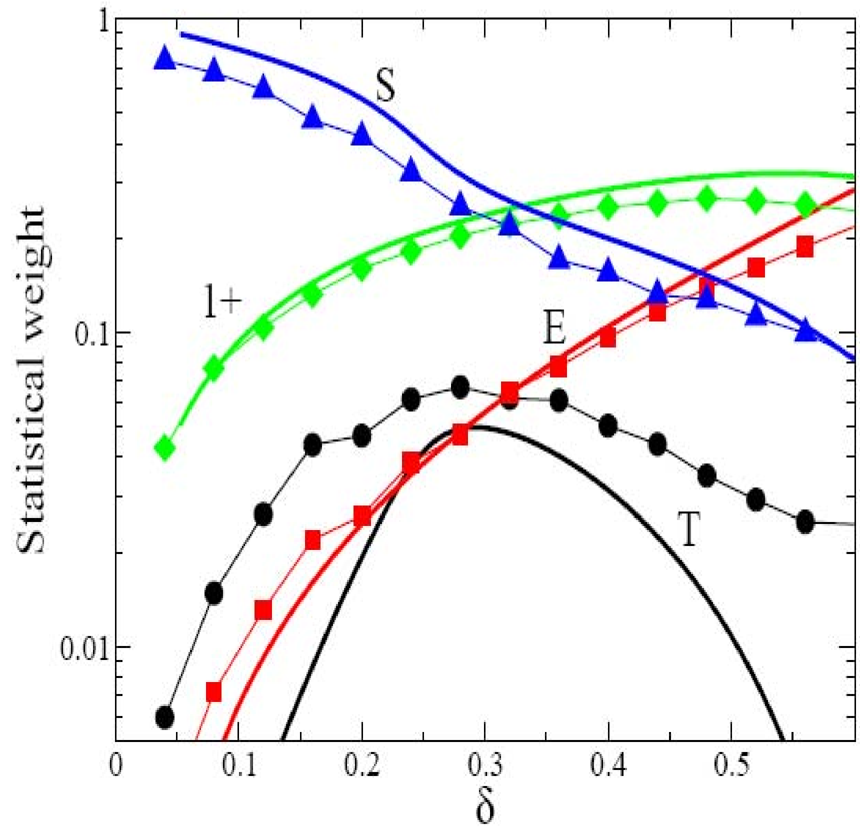


FIG. 15: (Color online) Statistical weights of the various dimer cluster eigenstates (labeled as in Table I). S is the intra-dimer singlet, 1+ the (spin-degenerate) state with one electron in the even orbital, E the empty state and T the intra-dimer triplet. $\beta = 200$.

Correlated Superconductivity

- New concepts and techniques to treat highly incoherent normal state and the superconductivity that emerges from it.
- Coherence incoherence crossover, lines of zeros, momentum space differentiation, ……
- Proximity to the Mott transition, accounts for many observations in correlated superconductors.
- Still further developments are needed to improve the formulation and solution of the cluster DMFT eqs.
- Material specific properties. Normal State OK. Tc ‘s ?
- DMFT material databases to help the search. Many properties can be “designed”.

Discussion questions

- What have we learned on what makes high Tc high from the cuprates and other materials ?
- What makes a material be high Tc ? Chemistry ? Dimensionality ? Luck ?
- More is different ?
- What can theory reasonably (and honestly) say about Tc and how to raise or lower it ?

Discussion questions:

1) What are the prospects for direct Eliashberg-style 1st principles computation of pairing interaction in electronic pairing systems with weak-intermediate (and why not large)strength correlations? In the absence of such tools, how can theory guide the search for higher Tc?

1) Do we need to abandon our cherished precept that atomic-scale phenomena are irrelevant for superconductivity?

3) In cuprates and other strongly correlated materials, are there issues where traditional DFT calculations can contribute, where strong correlations play a less important role?

4) What are the prospects of applying current methods to problems of inhomogeneous superconductivity in real materials: surfaces, grain boundaries, & Josesphson junctions...

5) If you look into the future 5 years and assume continued improvement in computer speed and memory, what superconductivity problems could one tackle which are out of reach now?