Nodal/antinodal dichotomy in cuprates : *a valence-bond dynamical mean-field approach*

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http://www.cpht.polytechnique.fr/cpht/correl/mainpage.htm

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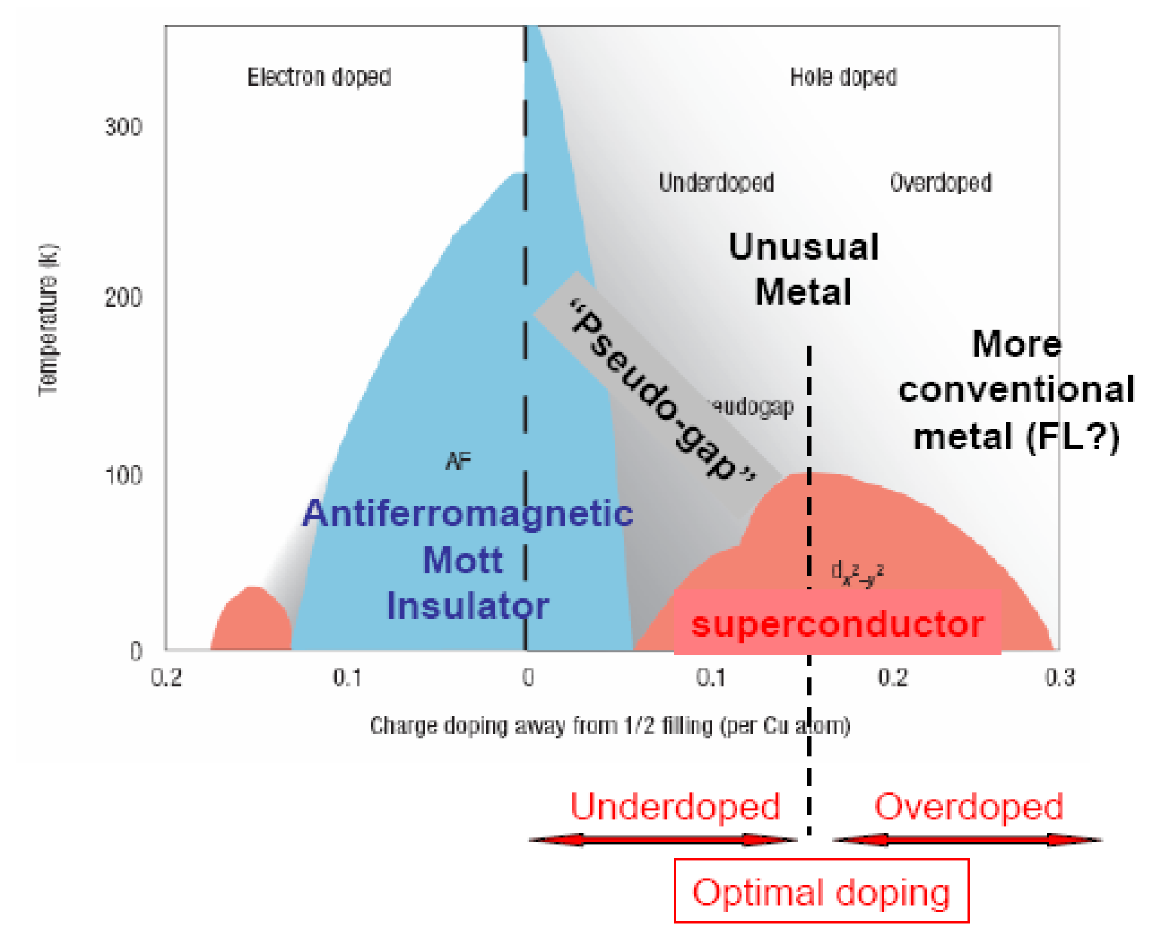
Momentum-space differentiation

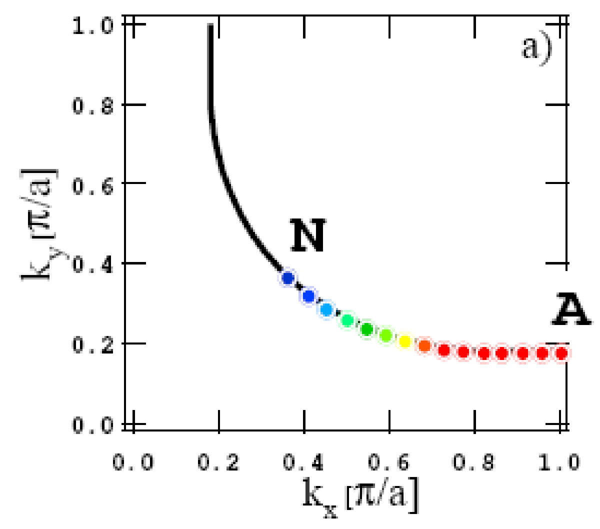
A key phenomenon in underdoped cuprates

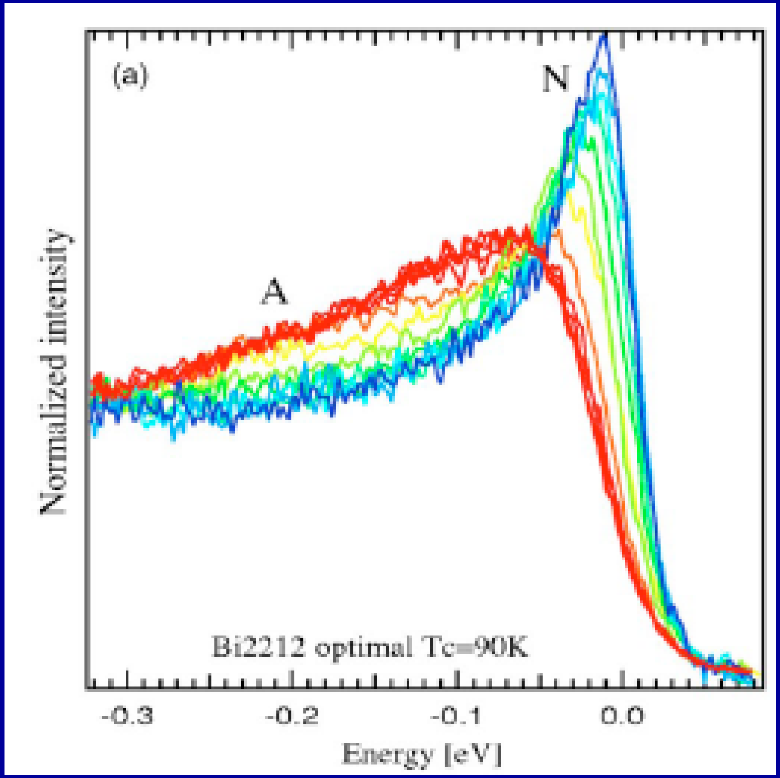


NORMAL state:

- ``Nodal'' regions display reasonably coherent quasiparticles
- In contrast, excitations in the ``antinodal'' regions e.g. (0,π) are much more incoherent

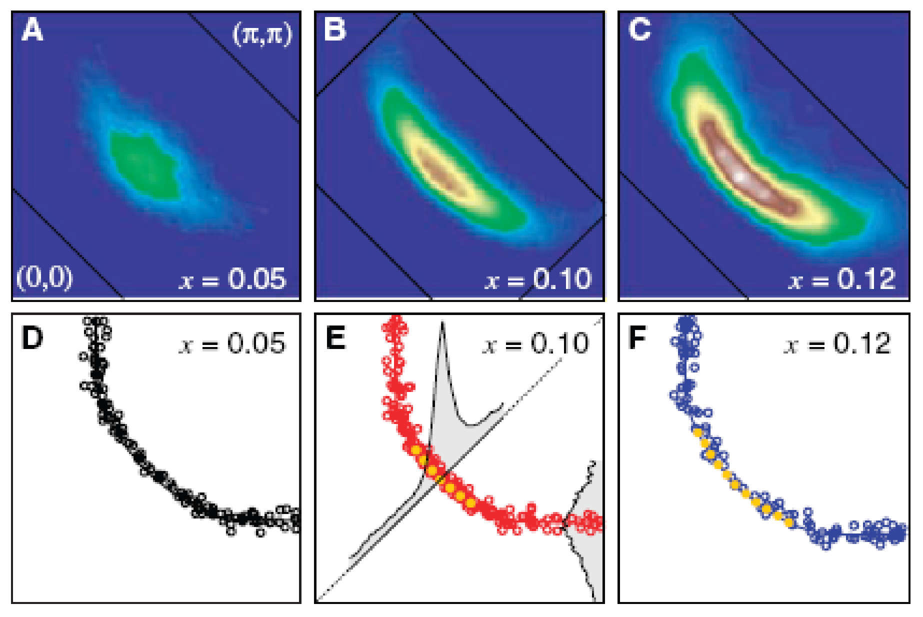
  AND they are (pseudo-) gapped below T*





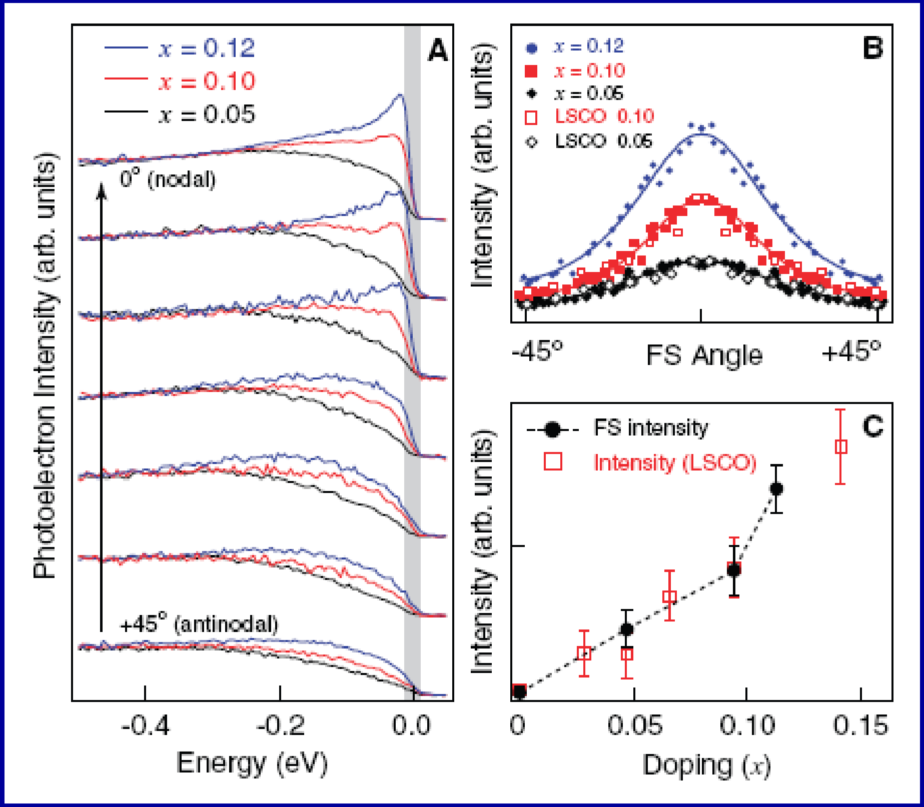
Kaminski et al., 2004 Bi2212
Tc=90K@T=140K

ARPES sees « Fermi arcs »



$Ca_{2-x}Na_xCuO_2Cl_2$

K.Shen et al. Science 2007



SUPERCONDUCTING state:

* Antinodal quasiparticles make a comeback

(Note: still they remain somewhat fragile at very low doping…)

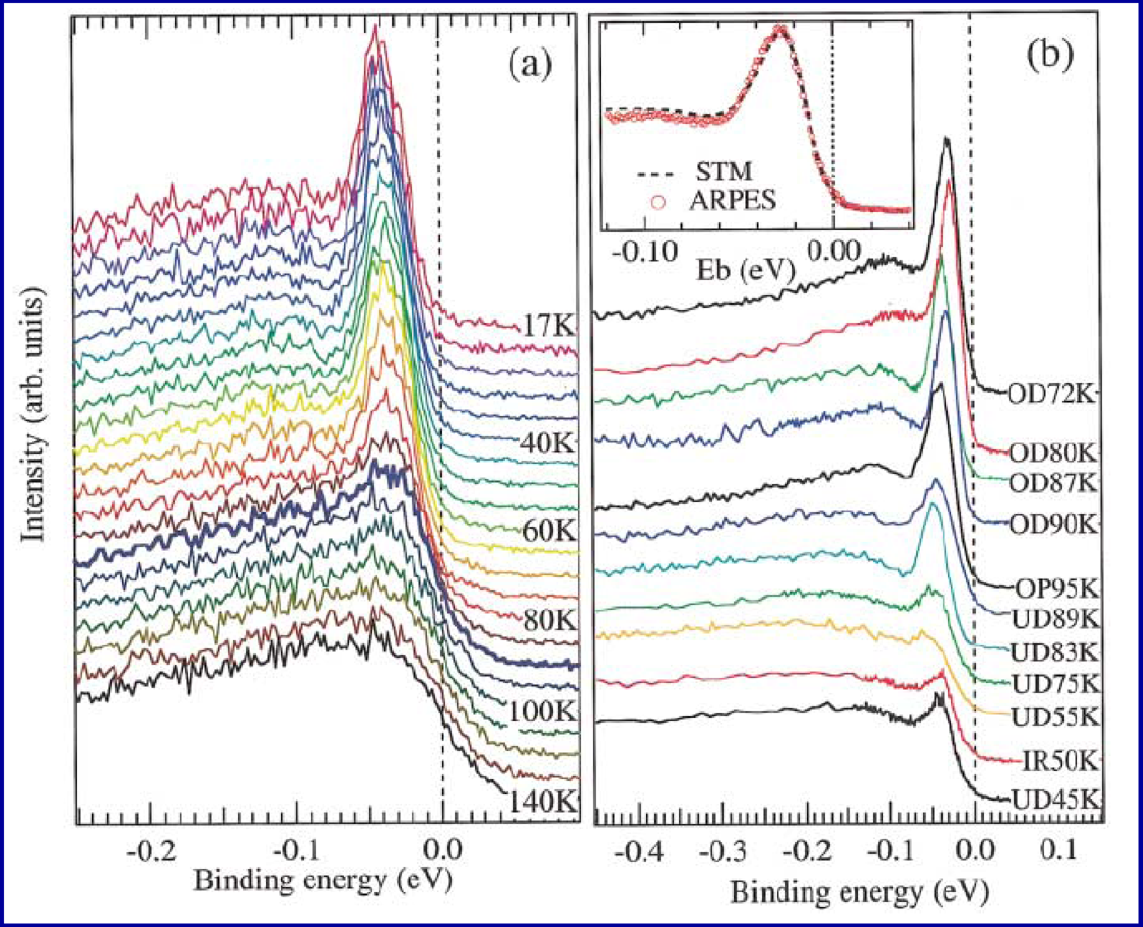


FIG. 1 (color). (a) ARPES spectra at $(\pi, 0)$ of slightly overdoped Bi2212 ($T_c = 90$ K) for different temperatures ($T = 17$, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, 95, 100, 110, 120, 130, and 140 K). (b) Spectra at $(\pi, 0)$ at low T (14 K) of differently doped Bi2212 samples (OD—overdoped; OP—optimally doped; UD—underdoped; IR—300 MeV electron irradiated, followed by the value of T_c). Intensity of the spectra is normalized at a high binding energy where the spectral intensity shows a minimum (~ -0.5 eV). Inset: Comparison between low-T ARPES at $(\pi, 0)$ and STM for the same OD72K sample.

Ding et al. PRL 2001

Why is this challenging for theory ?

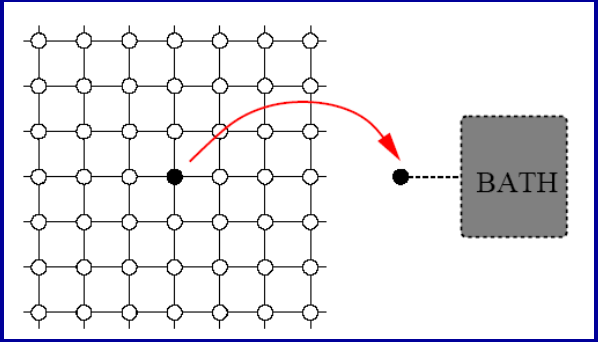
- Approach to the Mott insulator: *quasiparticle coherence scale*
- Brinkman-Rice/Slave bosons/DMFT: *Uniform scale along Fermi surface* (of order δt)
- Need to take into account inter-site superexchange (J)

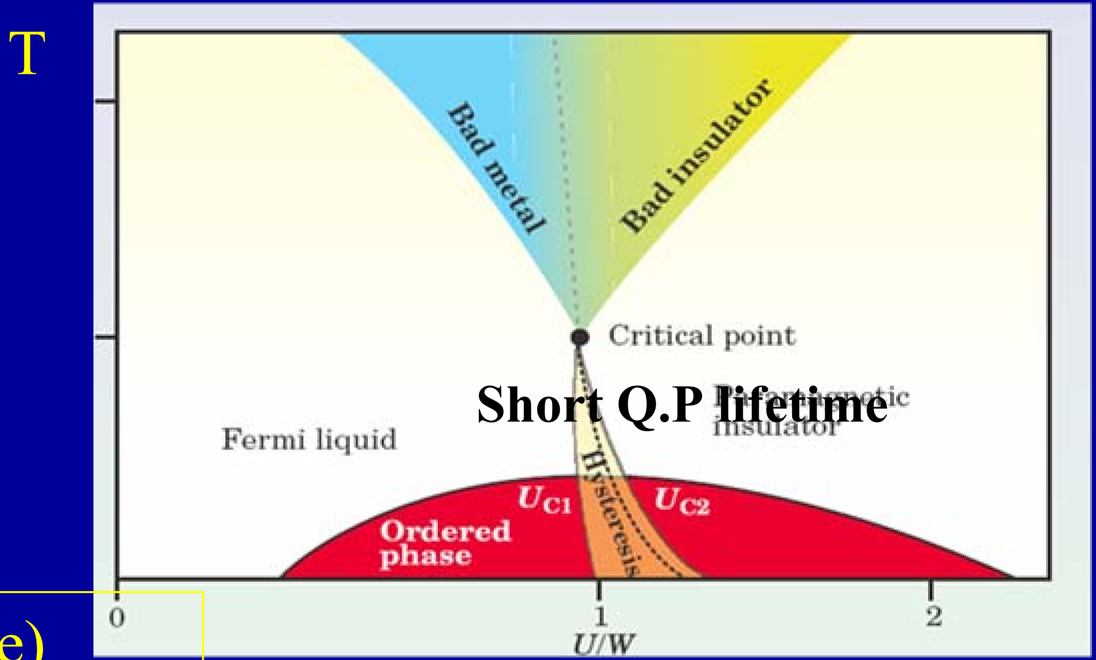
→ singlet formation/spatial correlations

Brinkman-Rice/DMFT leads e.g. to a large effective mass ~1/δ
while in fact ~ 1/J is expected for J < δt
(Indeed: spin entropy released at scale J)

Dynamical mean-field theory (single-site)

- Provides a simple theory of the proximity of the Mott transition
- Good at describing **the destruction of coherent quasiparticles** (small QP coherence scale, short lifeime near Mott transition)

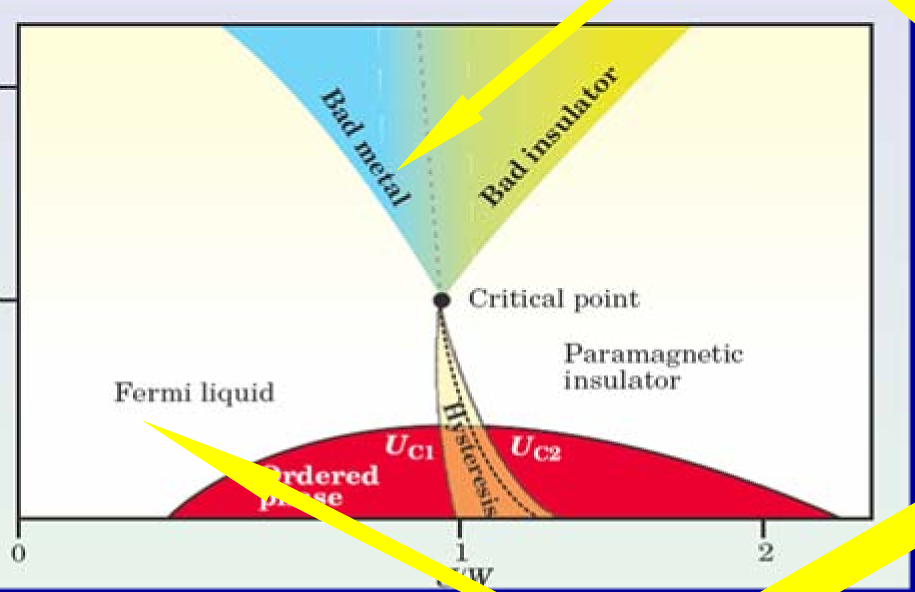


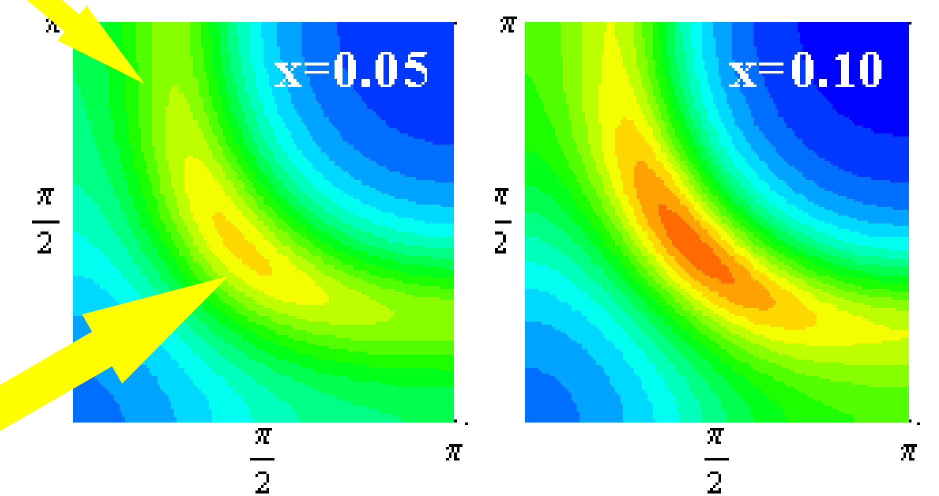


Coherent exc.: k-space (wave)
Incoherent exc: real space (particle)

Qualitative ideas :

Antinodal Region





Region near (π,0) has higher scattering

Nodal Region

Civelli et al., PRL 2005

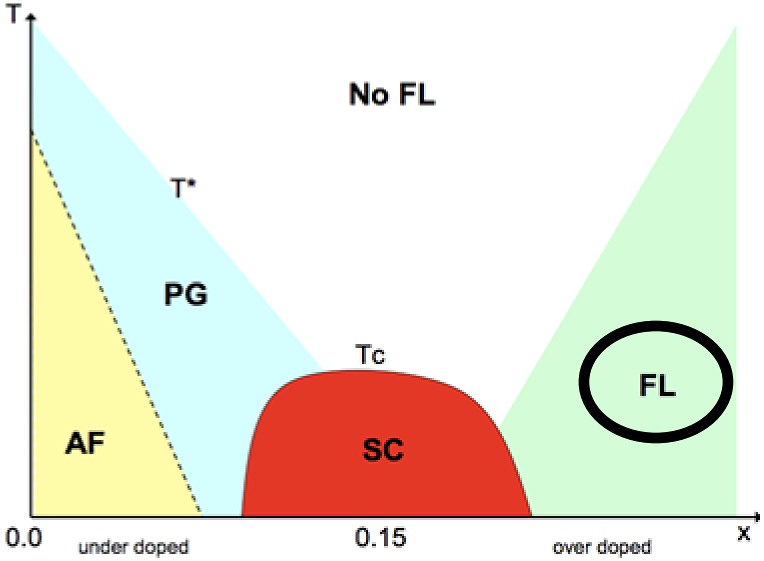
1) Build in singlet correlations from the start

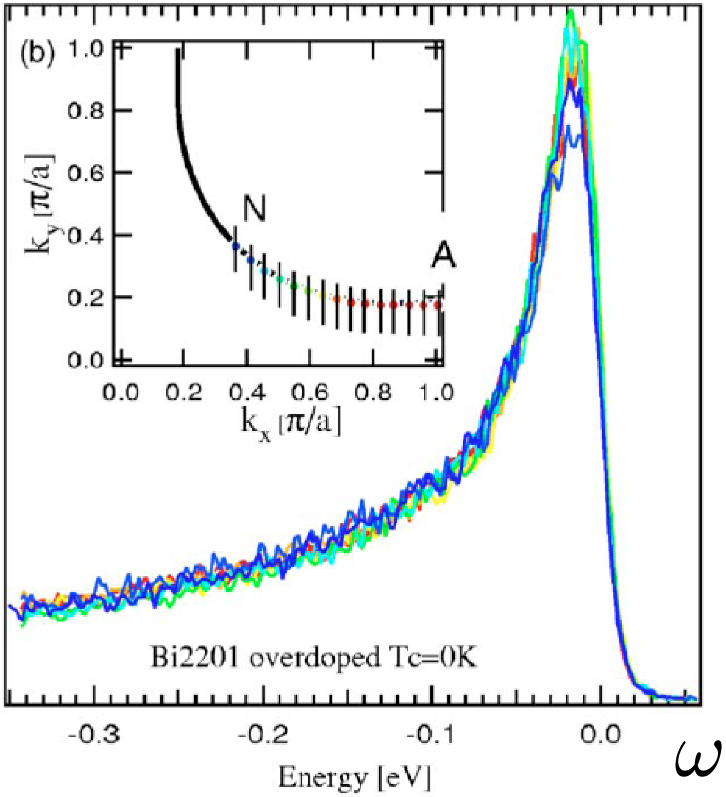
2) View nodal and antinodal regions
as two different types
of ``orbitals'' seeing different degrees of correlations

« Plain vanilla » cluster extension of DMFT

A « compass » to orient ourselves,
Starting from:
- High-temperature/
- High-energy/
- High-doping level …

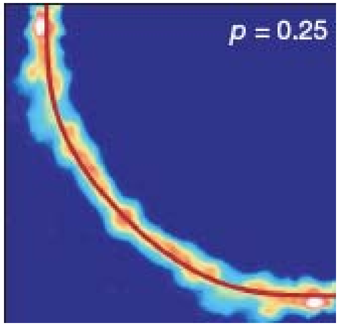
Overdoped regime: ~ uniform in momentum space





ω

Kaminski et al., PRB (2005)



$$A(k,\omega=0)$$

Platé et al., PRL (2005)
Tl2201 OD

Spectral properties are isotropic along the Fermi surface

2D Hubbard model (t,t’,U)

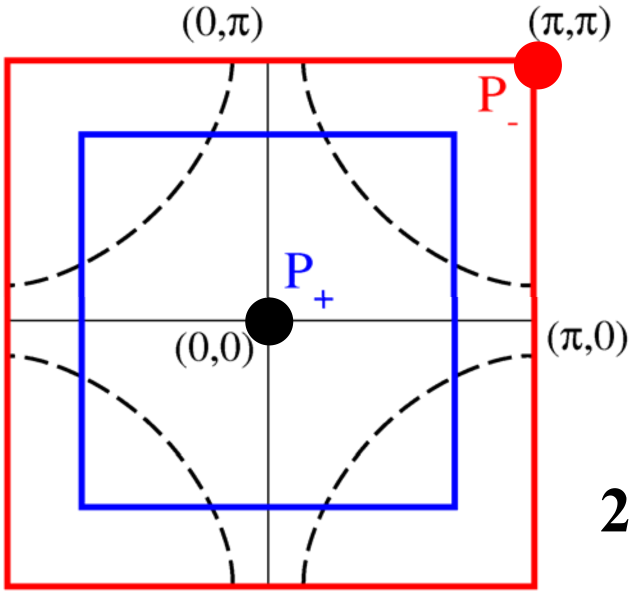
$$H = \sum_{\mathbf{k},\sigma=\uparrow,\downarrow} \varepsilon_{\mathbf{k}} c^{\dagger}_{\sigma\mathbf{k}} c_{\sigma\mathbf{k}} + U \sum_{i} n_{i\downarrow} n_{i\uparrow}$$

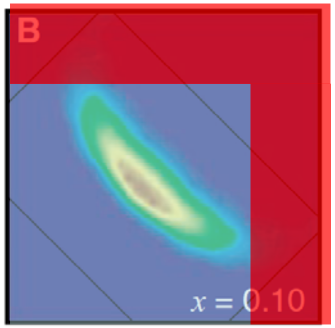
$$\varepsilon_{\mathbf{k}} = -2t\left(\cos(\mathbf{k}_x) + \cos(\mathbf{k}_y)\right) - 4t' \cos(\mathbf{k}_x)\cos(\mathbf{k}_y).$$

In the following:

U/t = 10
t’/t = -0.3
Hole-doped
Unit of energy: 4t (= 1)

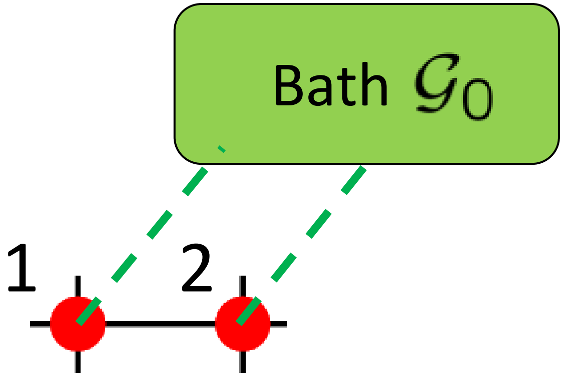
Valence-bond DMFT: bond-in-a bath





One patch covers the nodal part of the BZ. The other covers the antinodal part

2-patch DCA construction

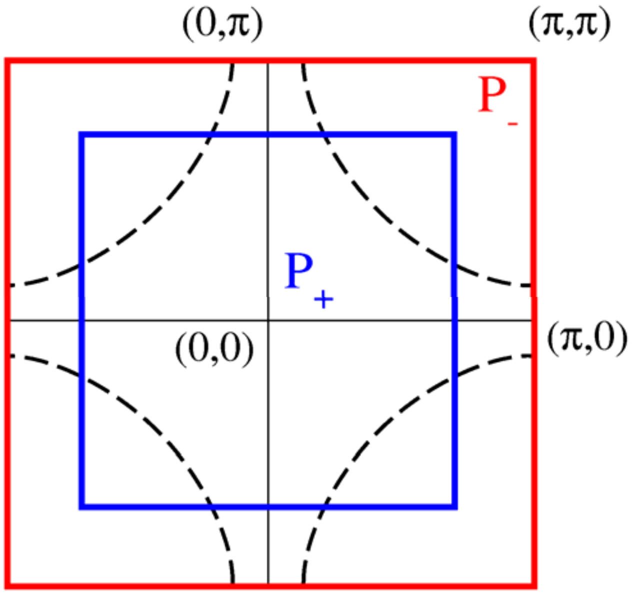


Two-site Anderson impurity model

In the even/odd basis:

- The even (bonding) orbital 1+2 is associated with the central (nodal) patch
- The odd (antibonding) orbital 1-2 is associated with the border (antinodal) patch

Self-consistency condition:

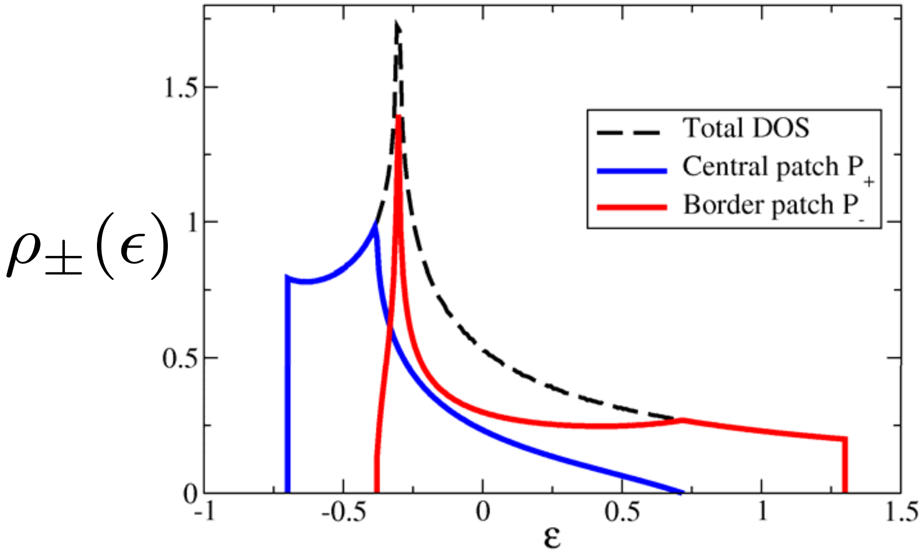


In DCA, the lattice self-energy is constant over the patches and equal to

$$\Sigma_{\text{lattice}} = \begin{cases} \Sigma_+ & \text{in the central patch} \\ \Sigma_- & \text{in the border patch} \end{cases}$$

$$\boxed{G_\pm(i\omega_n) = \int \frac{\rho_\pm(\epsilon)}{i\omega_n + \mu - \epsilon - \Sigma_\pm(i\omega_n)}}$$

$$G_\pm(i\omega_n) = \sum_{k \in P_\pm} G_{\text{lattice}}(i\omega_n, k)$$

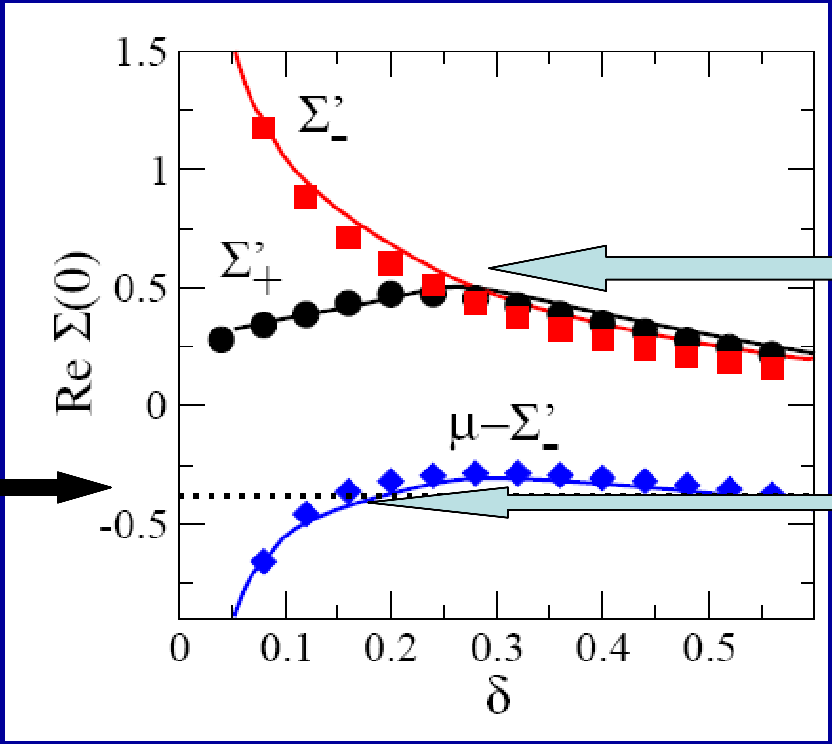


Solver: CT-QMC
(P.Werner et al.)

Main findings …

… emphasizing a few take-home qualitative aspects

1. *Mott transition selectively removes antinodal states at low doping:*



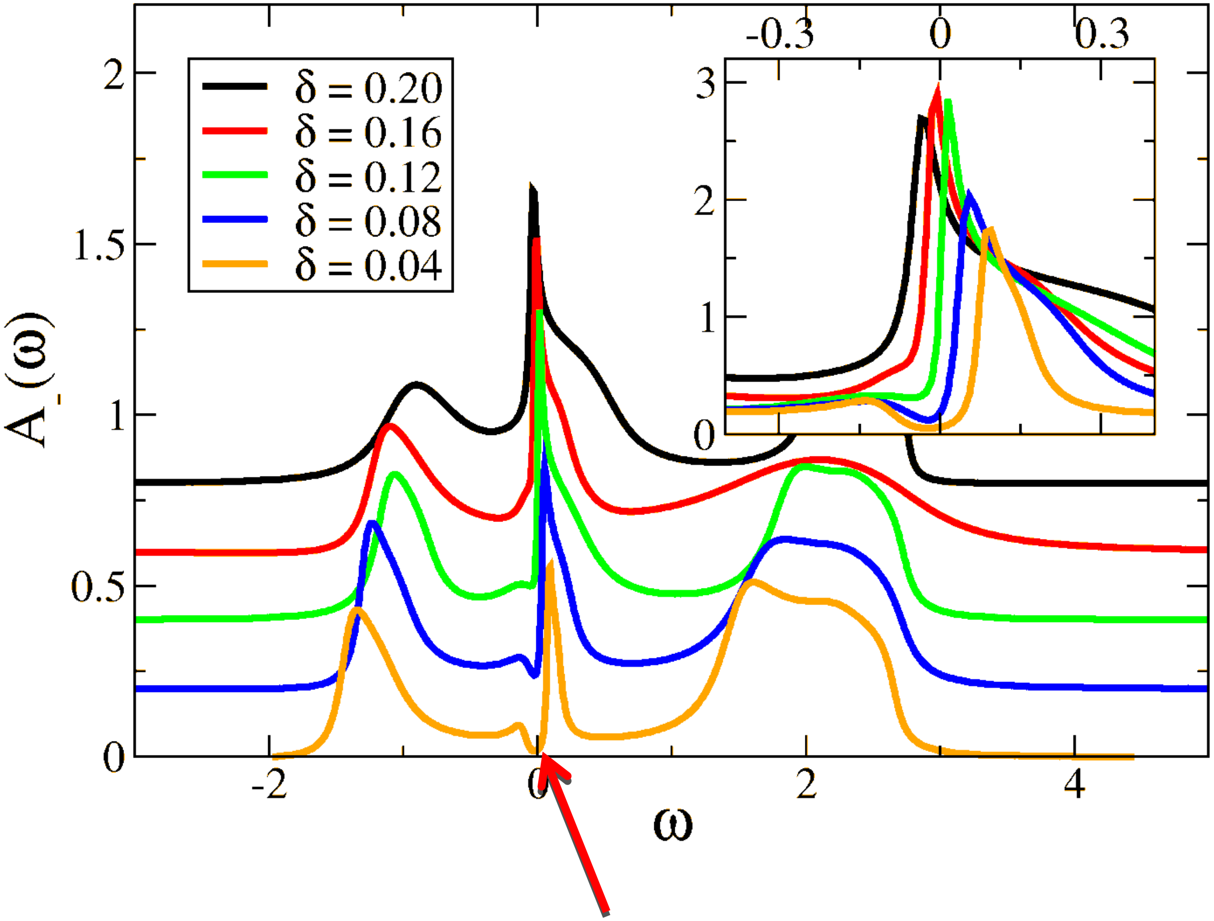
Onset of differentiation

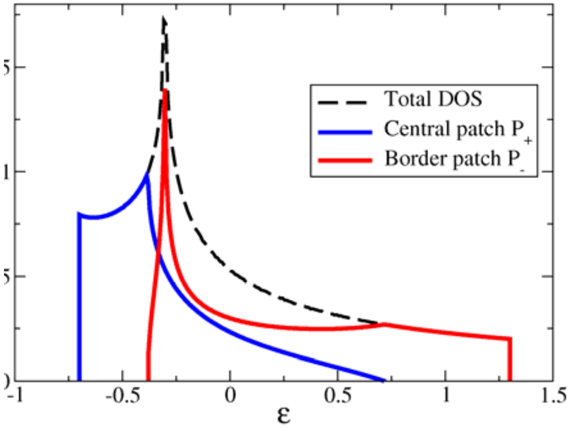
Band edge of outer patch d.o.s

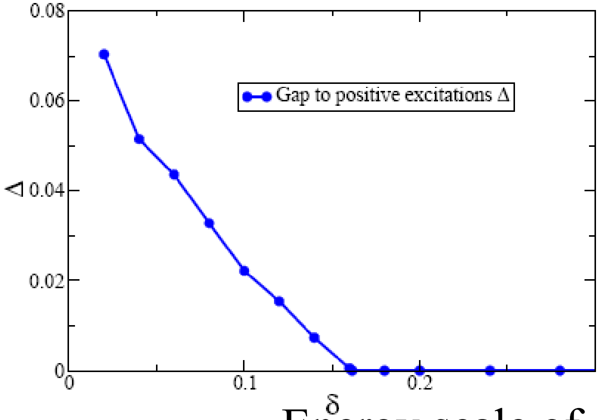
Outer/odd Orbital gets (pseudo-) gapped

Zero-frequency self-energies vs. doping

Antinode: not a sharp gap, a pseudogap!







Energy scale of
pseudogap on positive
energy side

At the antinode, a pseudogap appears below the transition.

Correlations have a strong effect (e.g. prominent Hubbard bands)

Pseudogap opening upon cooling:

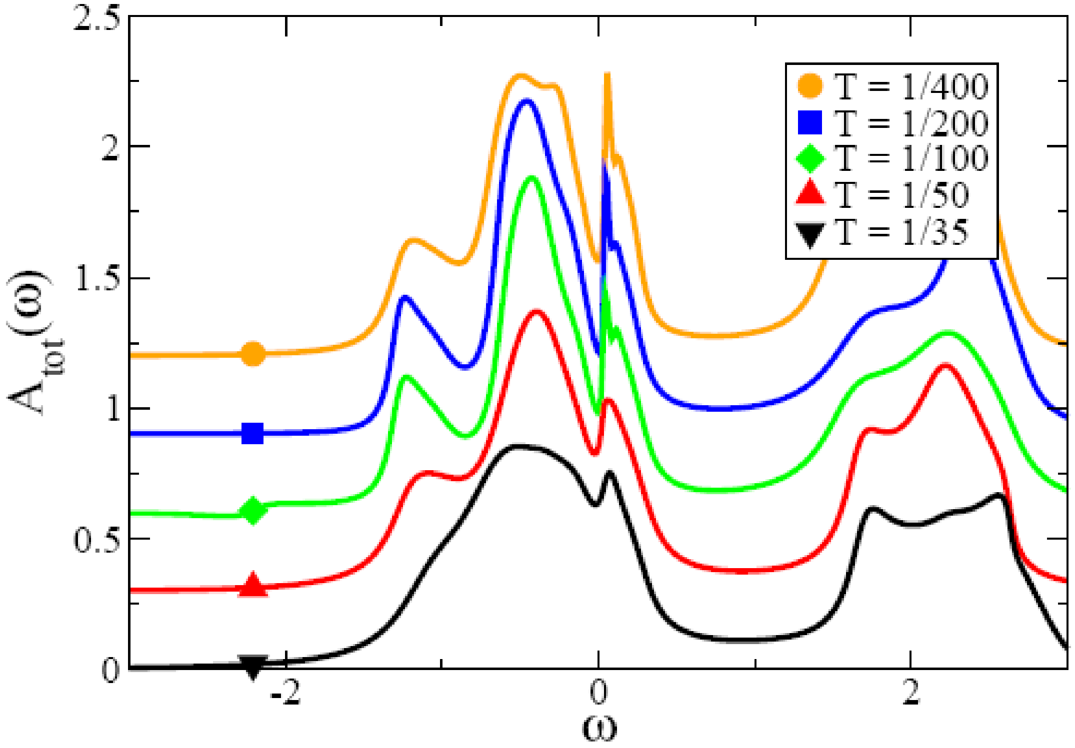
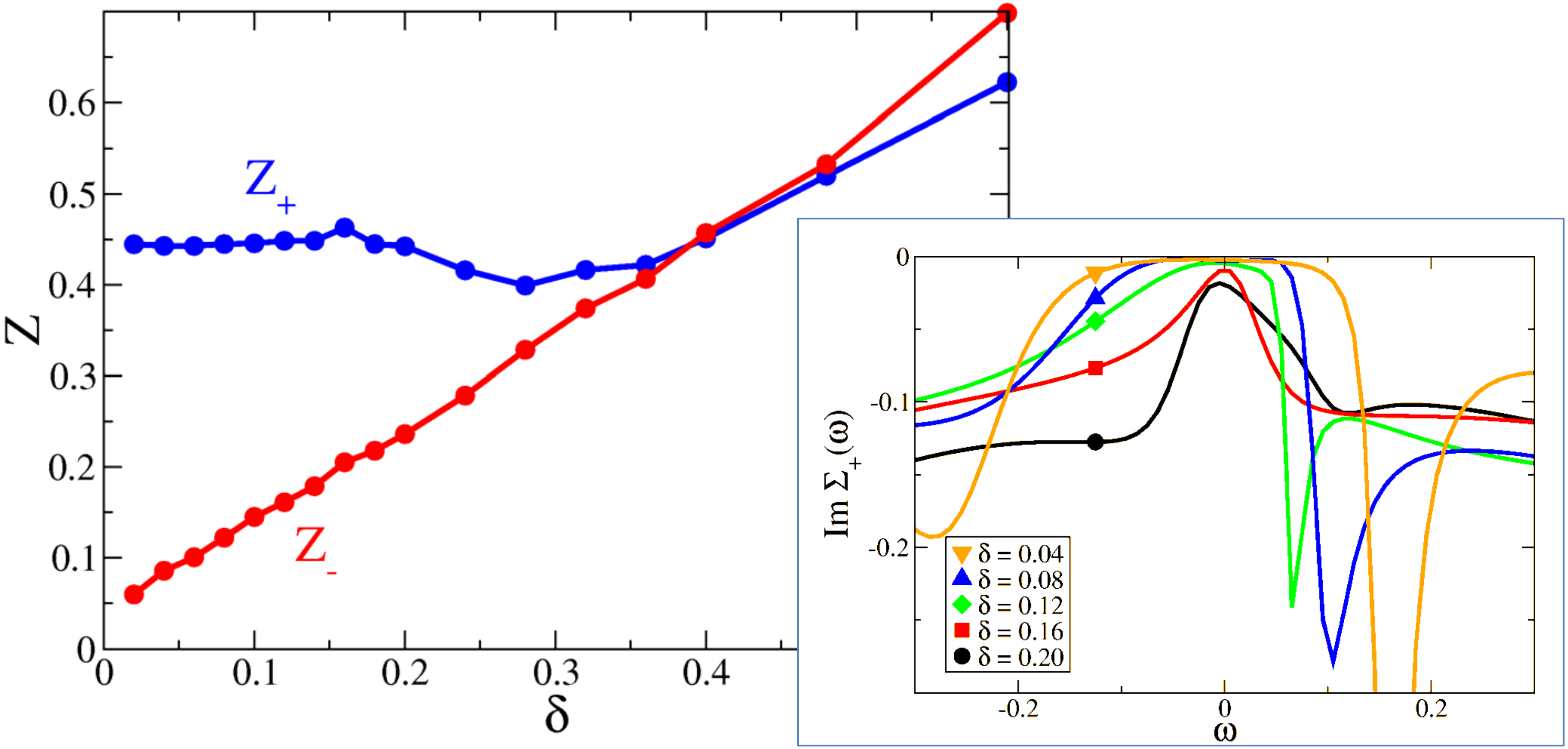


FIG. 10: (Color online) Total spectral function $A_{\rm tot}(\omega)$ for various temperature at $\delta = 0.08$. A shift of 0.3 has been added between each curves for clarity.

(Curves shifted upwards relative to one another, for clarity)

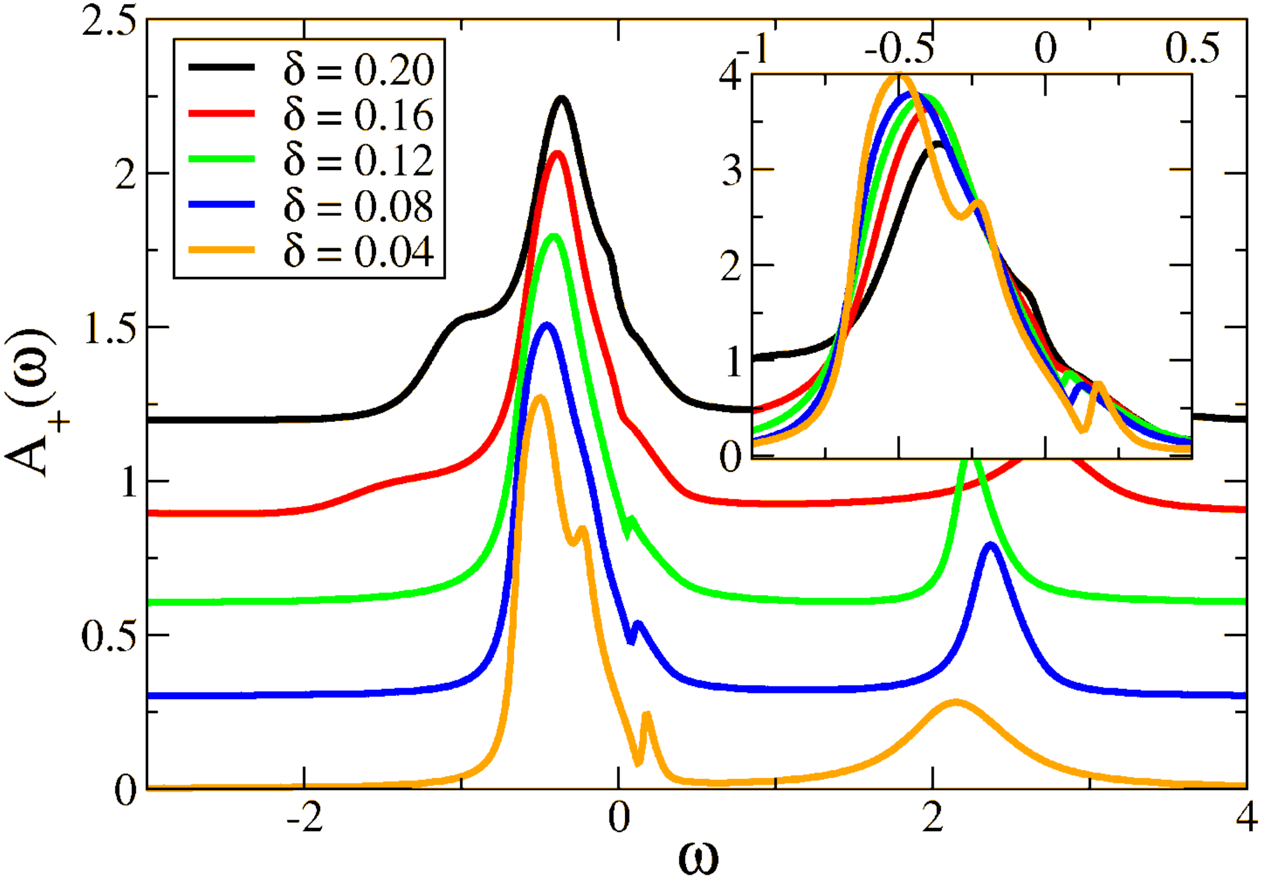
Opening of pseudogap leads to PROTECTION of nodal quasiparticles…

Quasiparticle weights and lifetime: a protected node



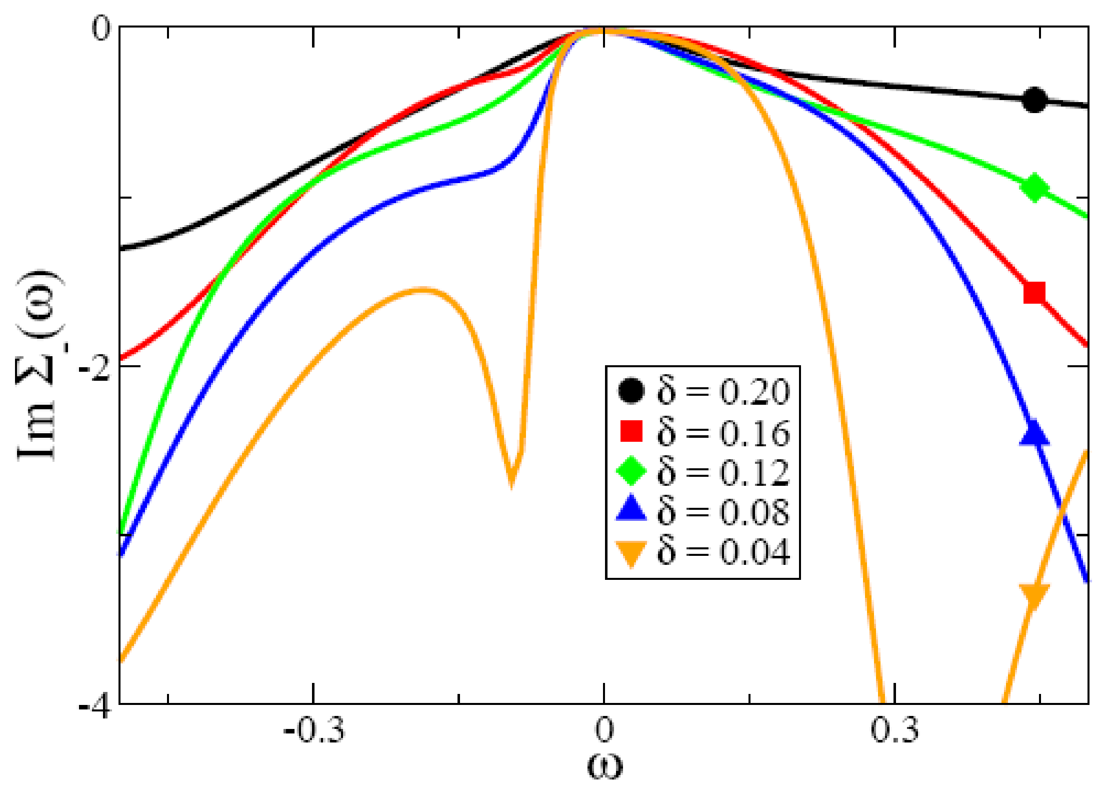
Below the critical doping, when the odd orbital is insulating, the even (nodal) orbital has a roughly constant quasiparticle residue: it is protected

Node: weaker correlations



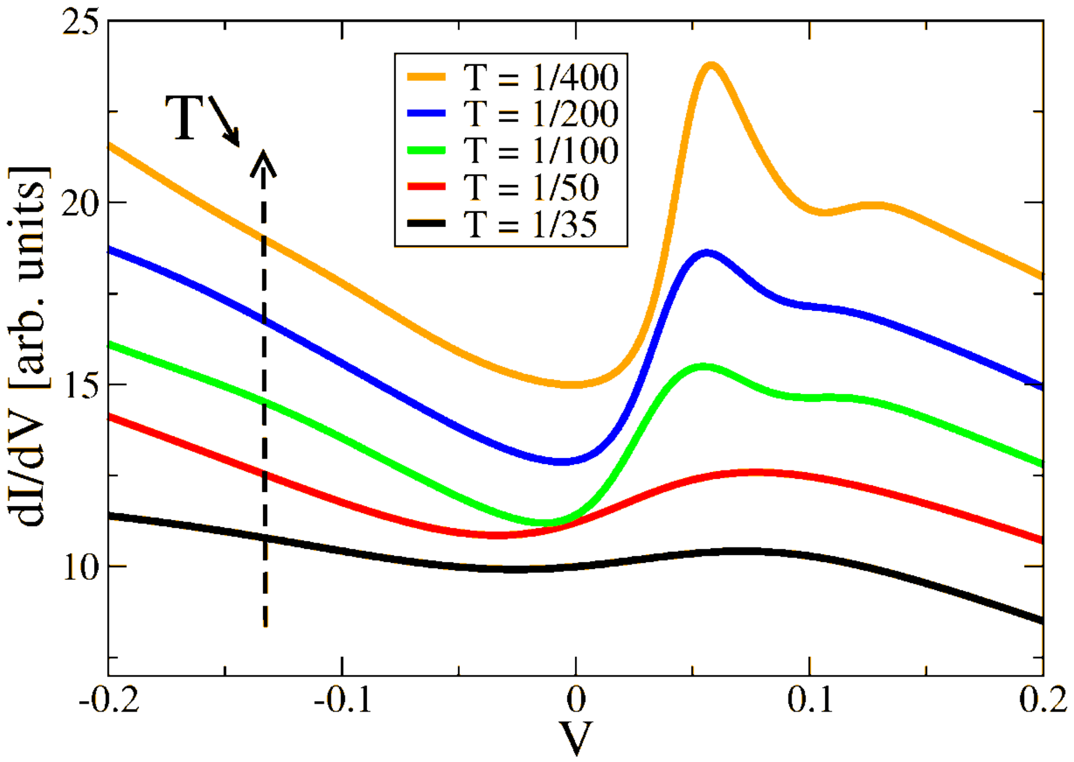
At the node, there are well-defined quasiparticles. The Hubbard bands are not very prominent. The correlations have a weak effect at the node

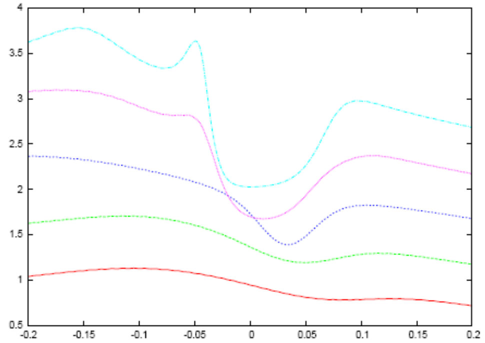
In contrast, antinodal scattering rate dramatically increases as doping level is reduced:

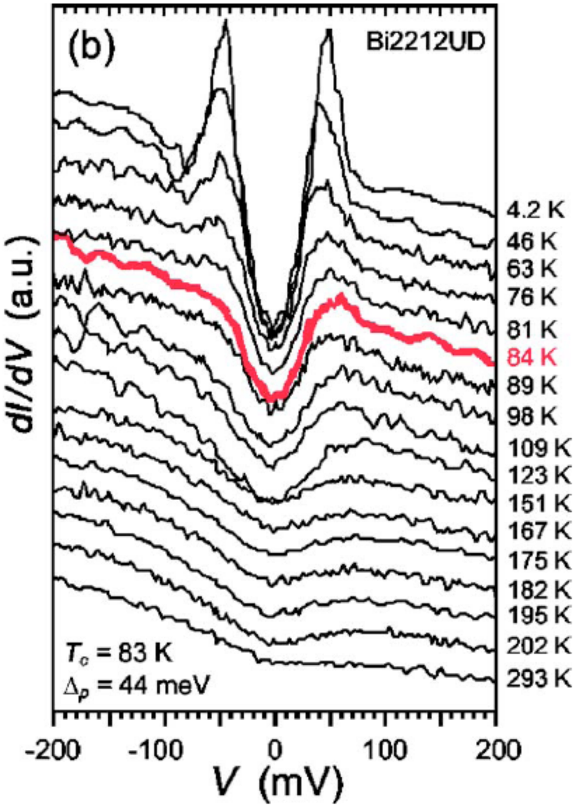


(In a somewhat stronger manner for occupied states)

Tunneling spectra (normal state)





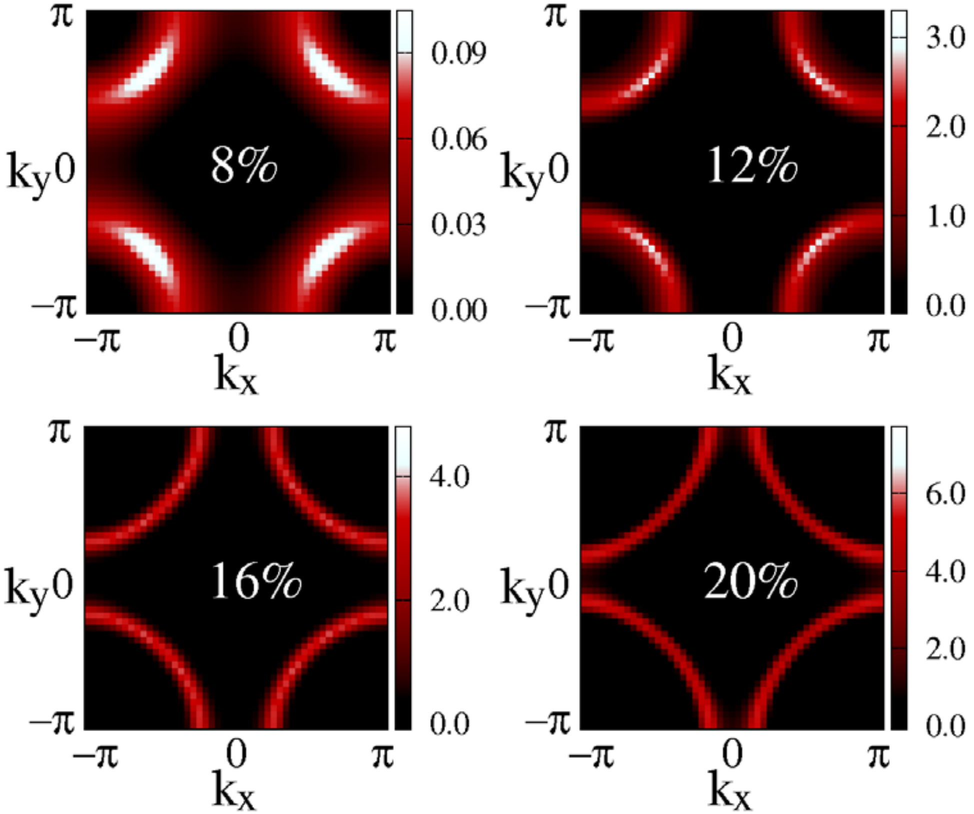


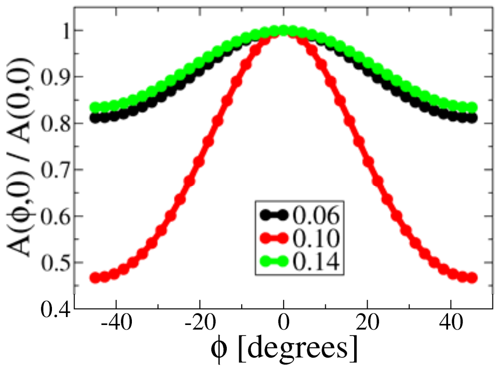
Renner et al., PRL (1998)

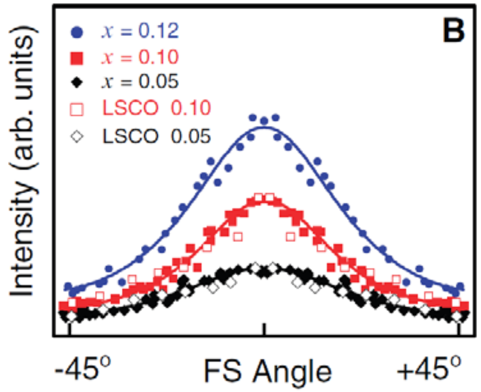
Main features:

- **A dip at low voltage (pseudogap)**
- **A peak at small positive voltage**
- **An overall particle-hole asymmetry**

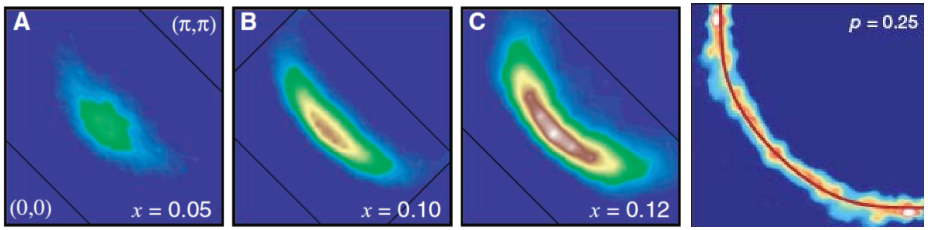
Calculated ARPES intensity maps







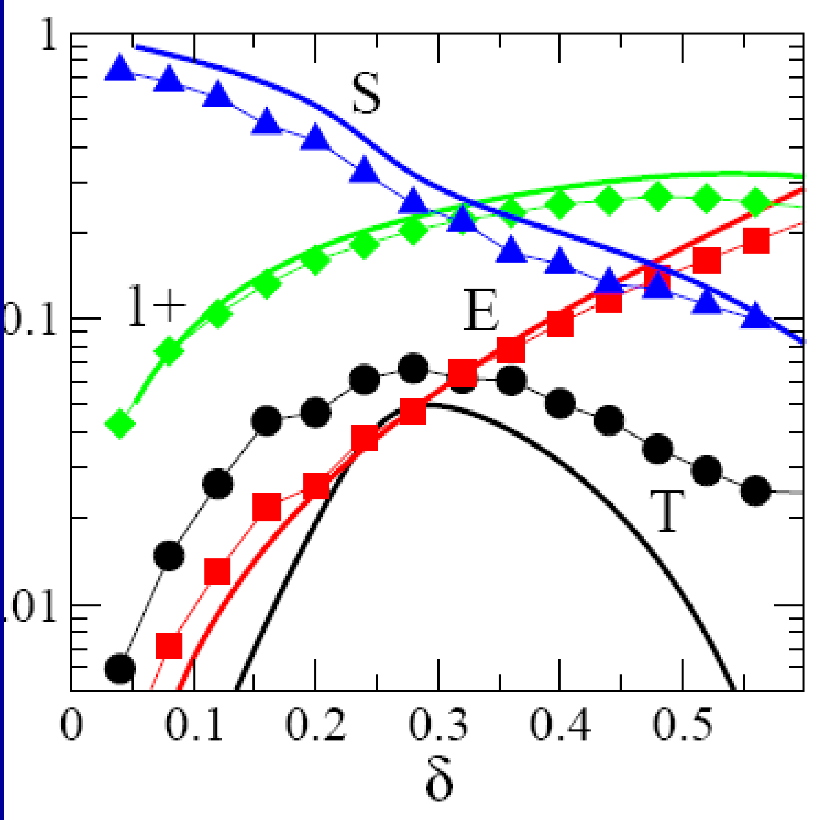
Shen et al., Science (2005)



Maximum contrast around 10%

With an (cumulant-) interpolation over the Brillouin zone…

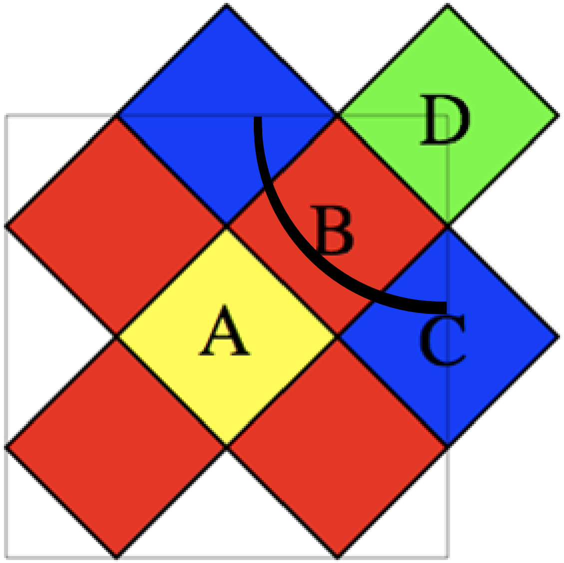
- Low doping regime is dominated by formation on singlets on bonds (gradually evolves to ~ Brinkman-Rice at higher doping)



Statistical weights of the singlet (S) and 1-particle (1+) state Vs. doping

Consistent with larger clusters?

- Is this picture compatible with larger clusters?
- In 8-site cluster: 2-step transition as a function of doping:
  - Patch C becomes insulating first
  - Patch B becomes insulating after



8 sites: P. Werner, E. Gull, O. Parcollet and A. J. Millis, arXiv:0903.3012 (2009)

Take–home messages

- Proximity to Mott transition destroys antinodal quasiparticles
- Pseudogap opening protects the nodal quasiparticles
- Low-dopin regime is dominated by the buildup of short-range singlet correlations
- Minimal cluster-extension of DMFT accounts for nodal/antinodal differentiation