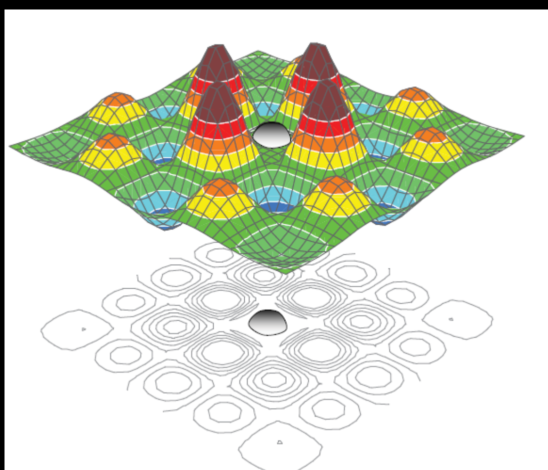
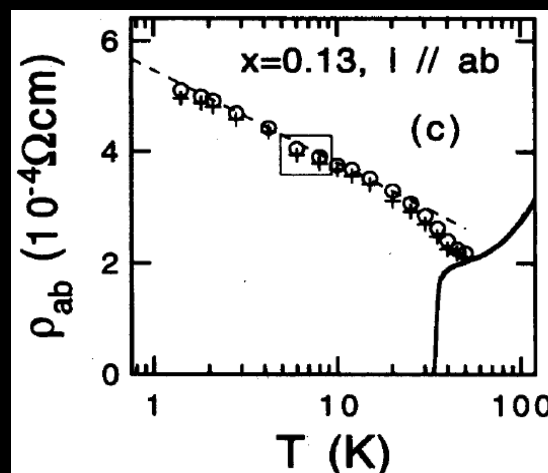
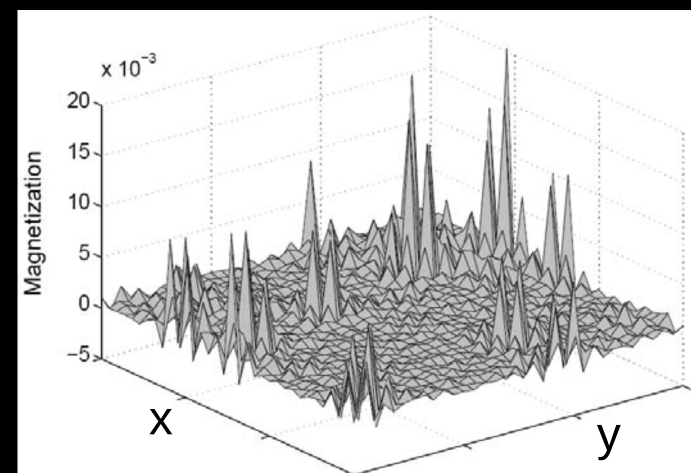
Defects in strongly correlated metals and superconductors

P.J. Hirschfeld, U. Florida







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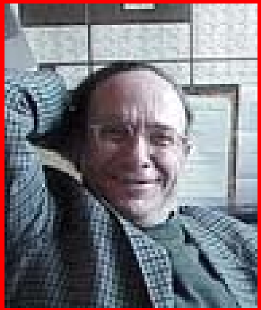
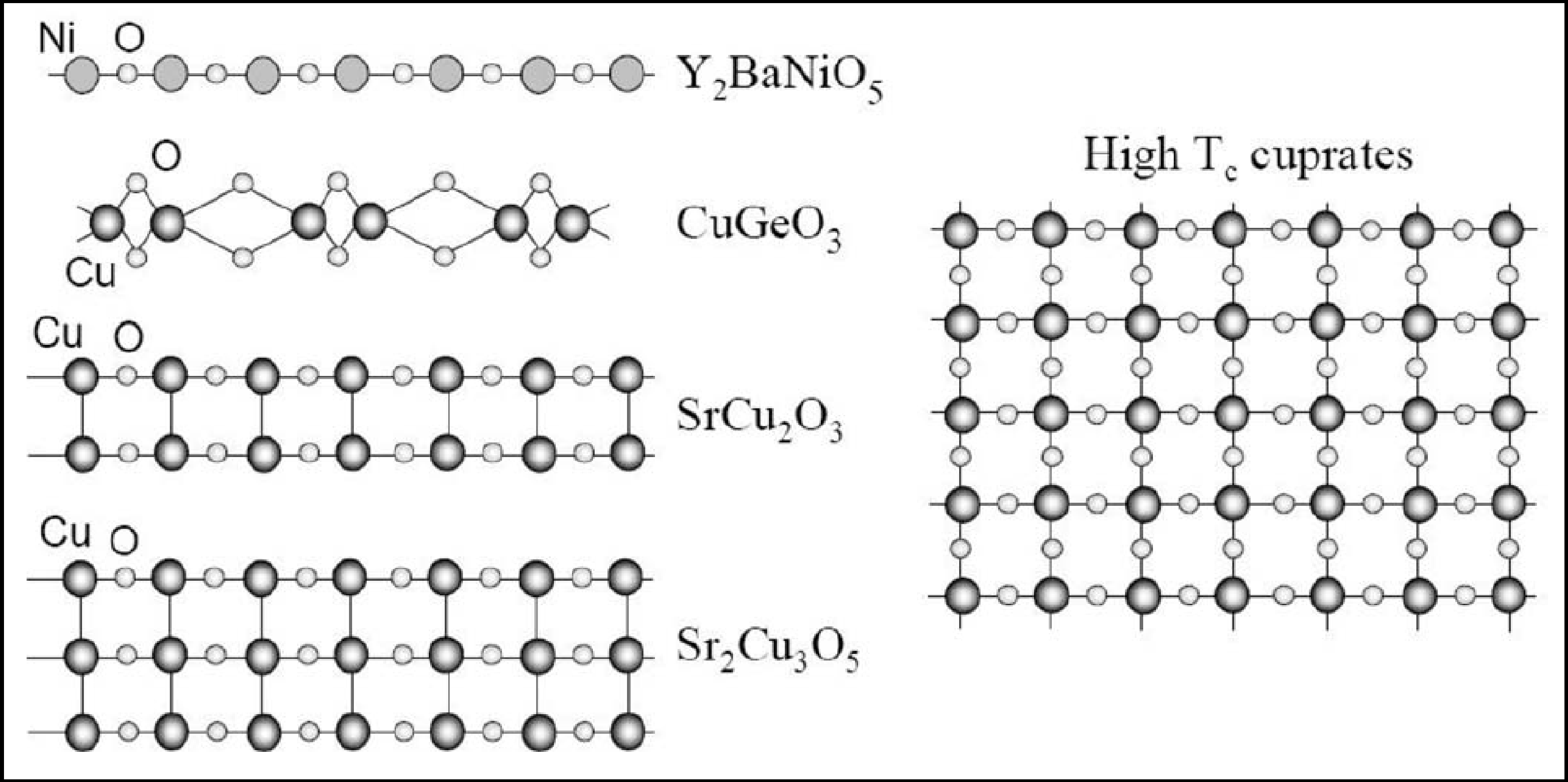


Henri Alloul

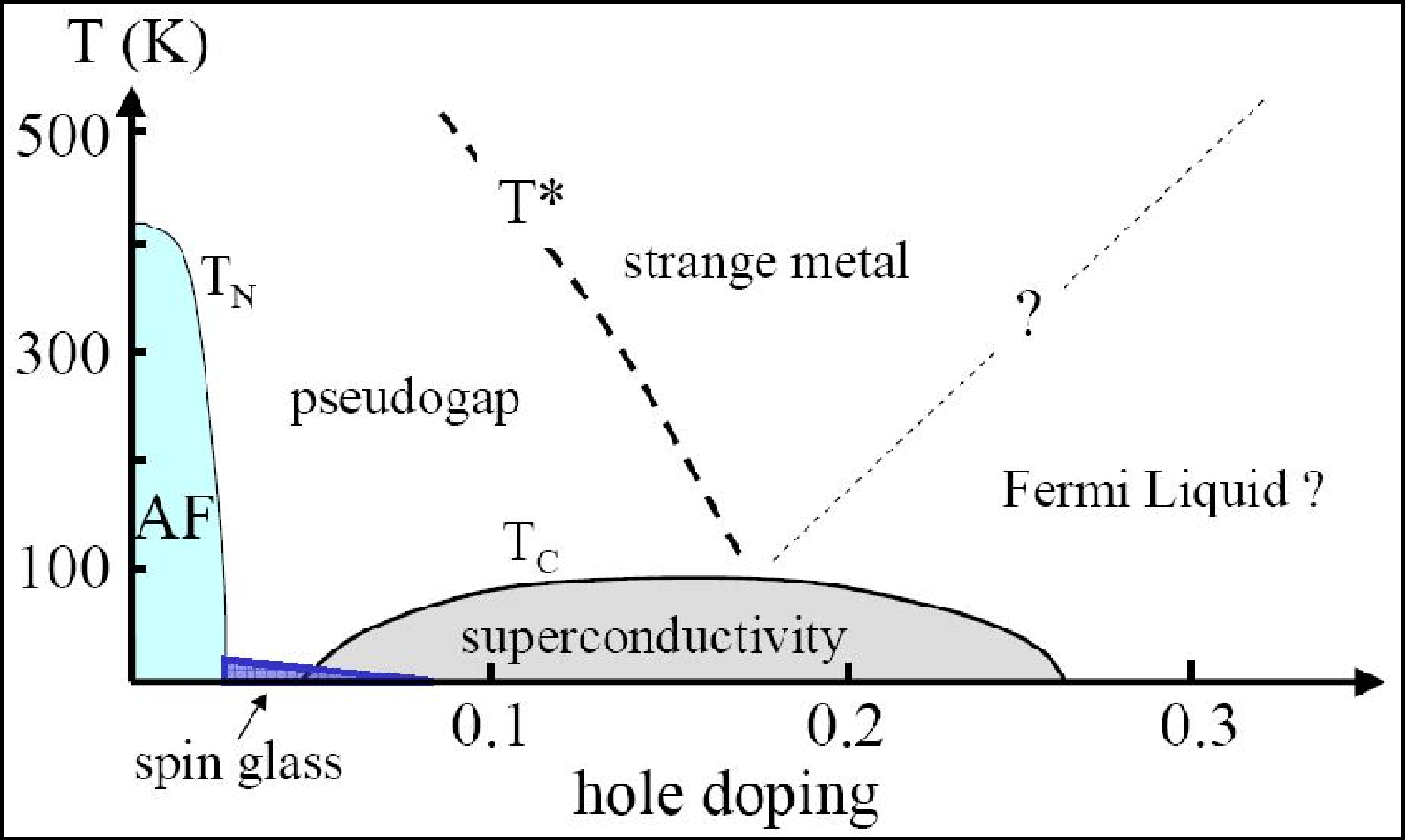
Outline

- Impurity induced magnetism
- AF/SC coexistence in cuprates: stripes/droplets?
- YBCO/dirty cuprates "dichotomy"
- NMR linewidths
- Neutrons: order from disorder?
- Quasiparticle properties:
  - thermal conductivity
  - resistivity
  - STM

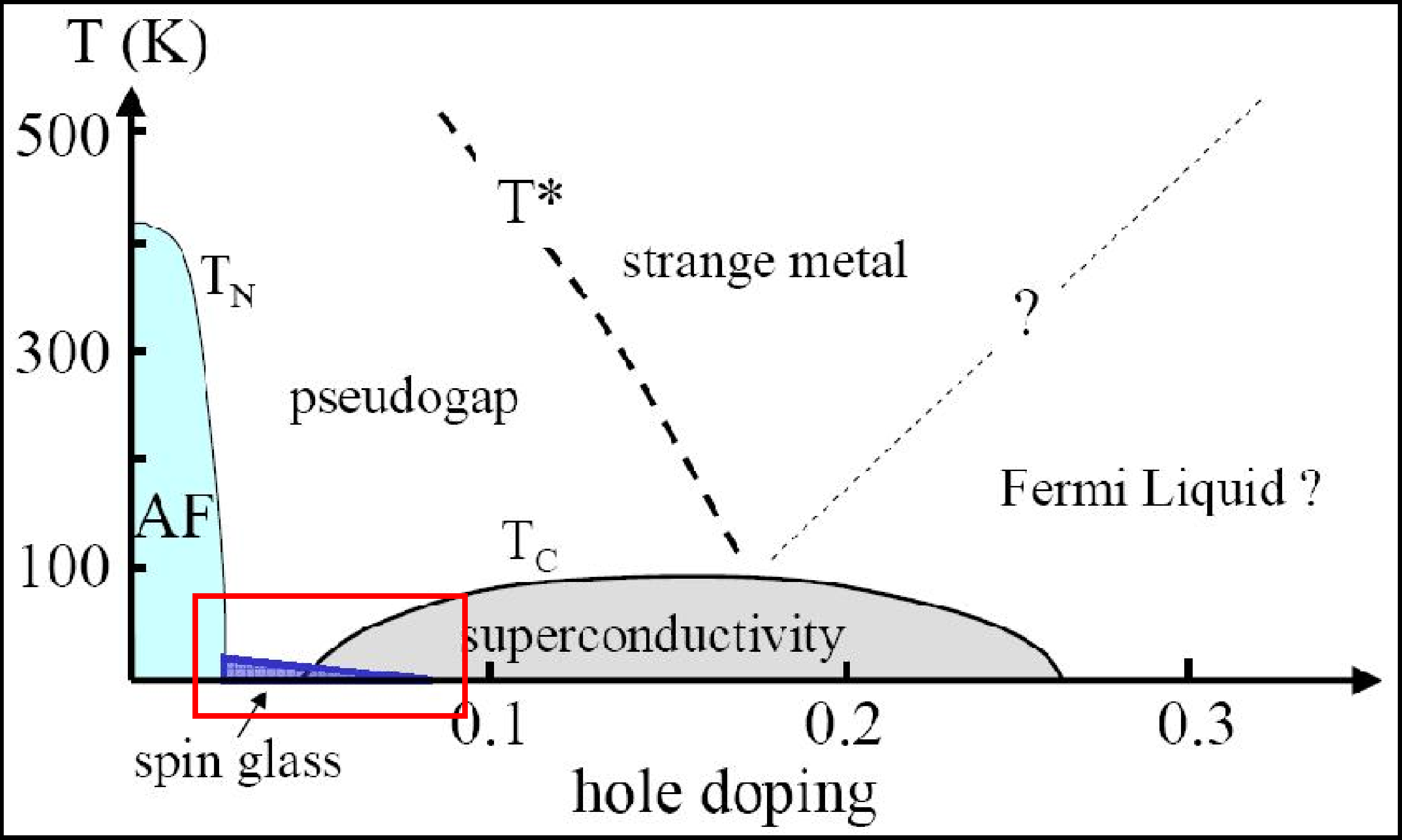
Some inorganic strongly correlated materials



Cuprate phase diagram



Cuprate phase diagram



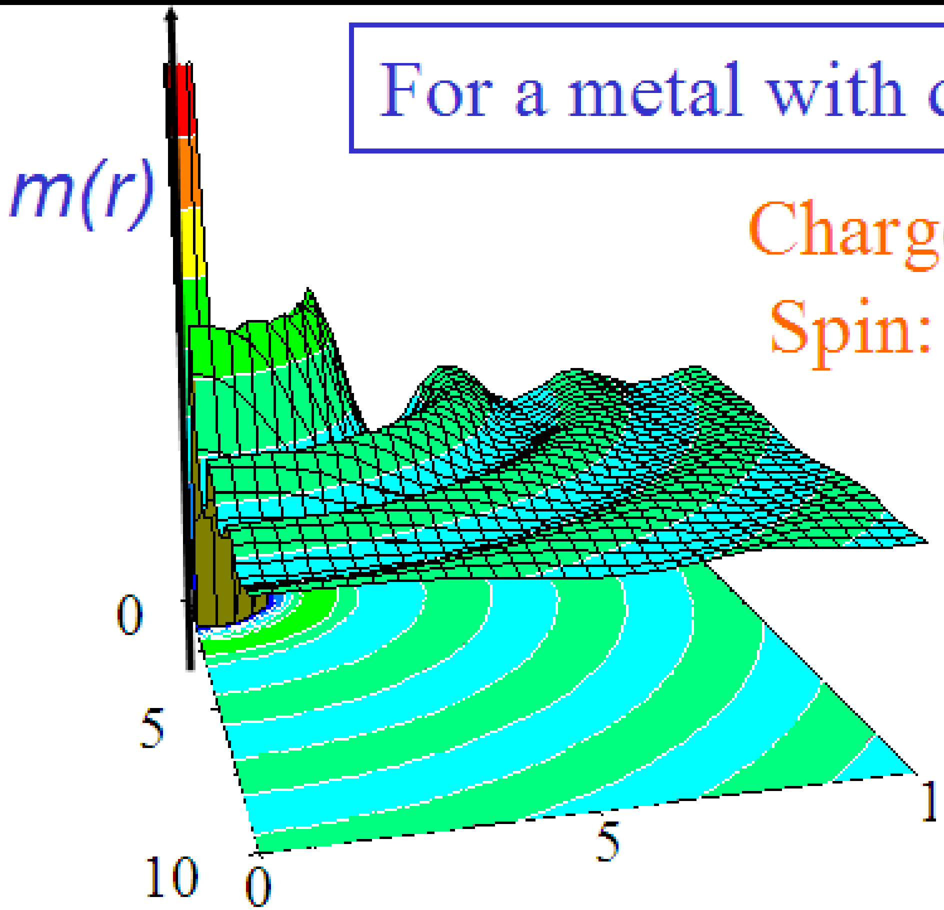
phase separation/competition of AF, etc. and SC regions?

consequences for d-wave quasiparticles?

Friedel response of free Fermi gas to magnetic moment

(J. Friedel 1958)

For a metal with dilute impurities



Charge : Friedel oscillations

Spin: RKKY Spin polarization

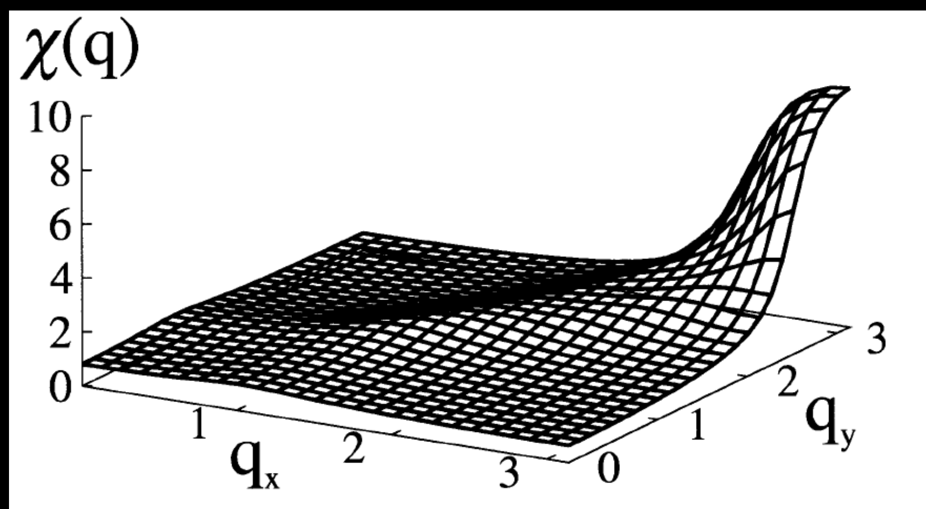
$$m(r) = \cos(2k_F r) / r^2$$

(2D)

What will happen in a *correlated* gas when a *nonmagnetic* impurity is inserted?

Simplest approach: describe background correlations with RPA

$$\chi = \frac{\chi_0(T)}{1 - U\chi_0(T)}$$



Magnetic susceptibility peaked near π,π enhances *staggered* magnetic response in real space

Generation of *staggered* response to *uniform* field

may include disorder

RPA for general system:

$$\chi(\mathbf{r},\mathbf{r}') = \chi_0(\mathbf{r},\mathbf{r}') + U\sum_{\mathbf{r}''}\chi_0(\mathbf{r},\mathbf{r}'')\chi(\mathbf{r}'',\mathbf{r}')$$

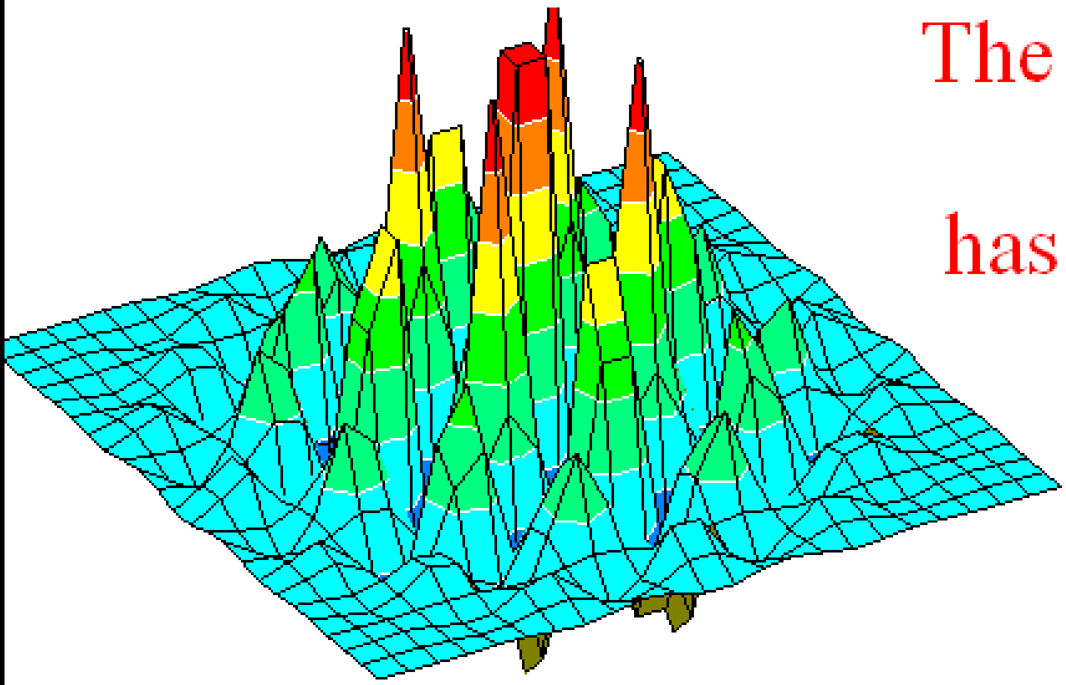
1) homogeneous system

$$\chi(\mathbf{q}) = \chi_0(\mathbf{q})(1 - U\chi_0(\mathbf{q}))^{-1}$$

2) impurity: all q's are *coupled.* In particular, a uniform (q=0) magnetic field now couples to q=π,π and induces staggered response if $\chi(q)$ is large there

So…

In a magnetic system with AF correlations



The induced polarization

$\chi'(r)$

has a staggered behavior

Poilblanc Scalapino Hanke 95,96…Martins, Dagotto, Riera: 96,97

Impurity-induced spin excitations in quasi-1D systems: theory

- 1D systems are testing grounds for these ideas because we can do calculations exactly.

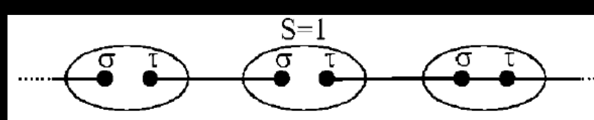
- Excitation spectrum of spin 1/2, 3/2, … Heisenberg chains gapless
  “ “ 1,2, 3…. “ “ gapped

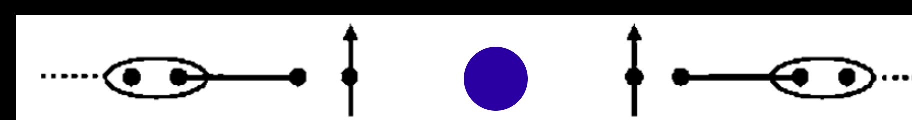
- Impurities cut chains into segments of even or odd numbers of spins.

- Response to impurity knows about correlations of pure chain!

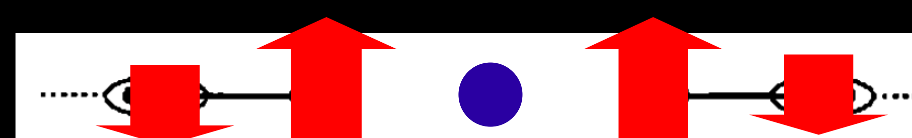
Ex.: Ground state of spin-1 chain: with impurity

H=0:



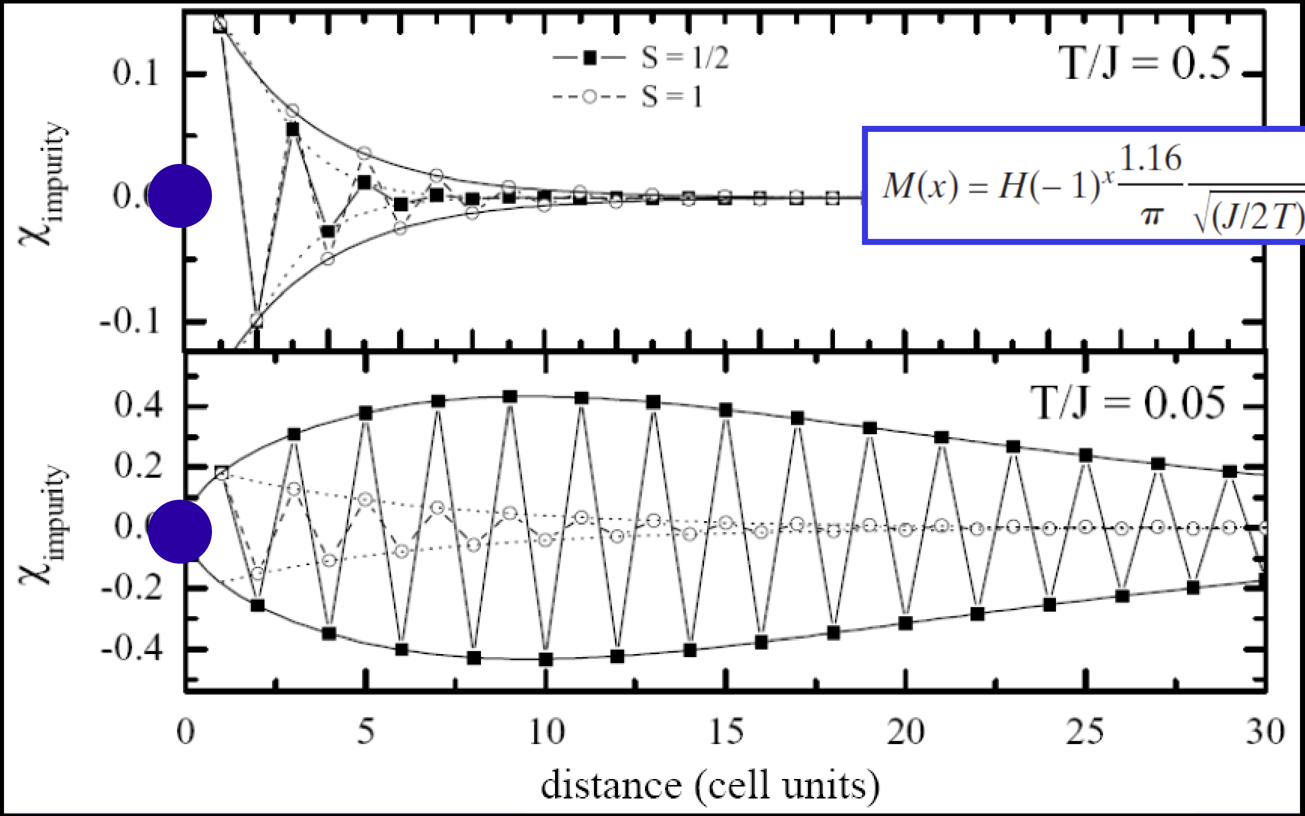


H>0:



Impurity-induced spin excitations in quasi-1D systems: theory

Spin-1/2 or spin-1 Heisenberg chains with end defect



$$M(x) = H(-1)^x \frac{1.16}{\pi} \frac{x}{\sqrt{(J/2T)\sinh(4Tx/J)}}$$

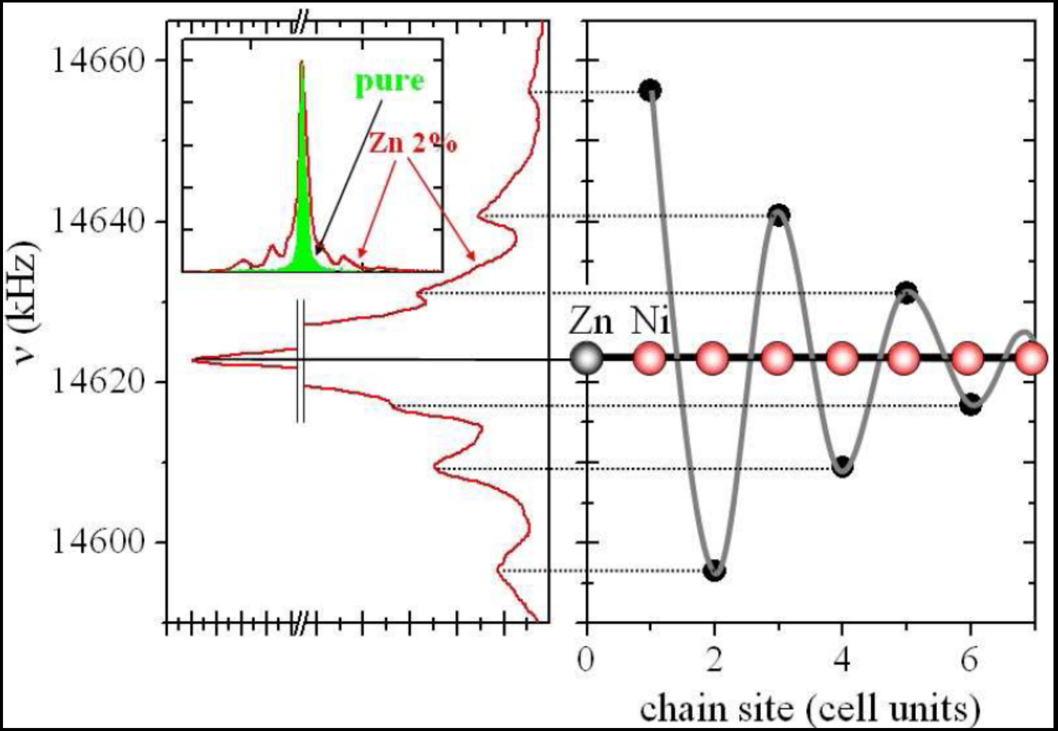
Miyashita & Yamamoto 1993; Sorensen & Affleck 1995; Kim et al 1998; Alet & Sorenson 2000…

Impurity-induced spin excitations in quasi-1D systems: experiment

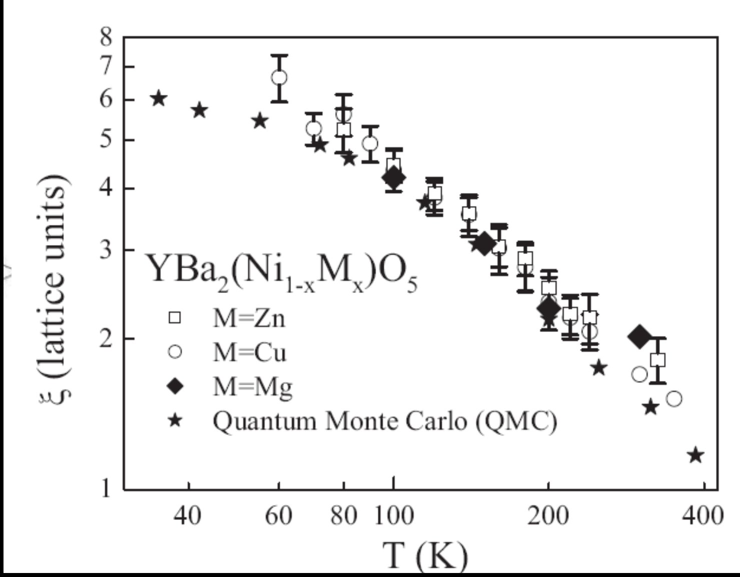
Tedoldi et al 1999
Das et al 2004

(YBa_2NiO_5)

(spin-1 Heisenberg chain)



Tedoldi et al 1999
Das et al 2004



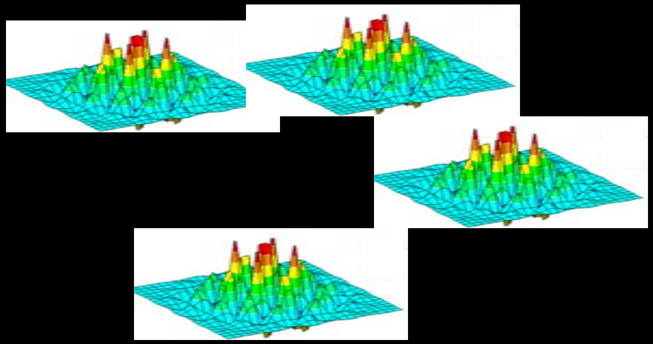
Impurity probes coherence length of pure system (theory!)

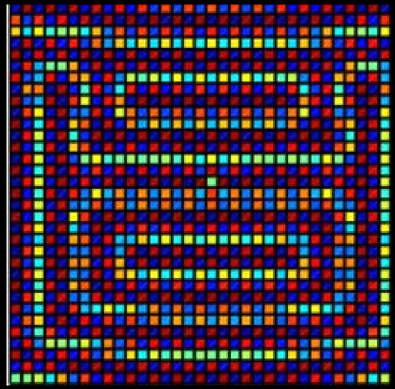
How about 2D? Cuprates

Does such impurity-induced magnetism exist, and how does it show up?

Is it always induced by a magnetic field, or can it exist spontaneously?

Is the induced magnetism from random impurities phase-incoherent, or can it cause long range order when “droplets” overlap?

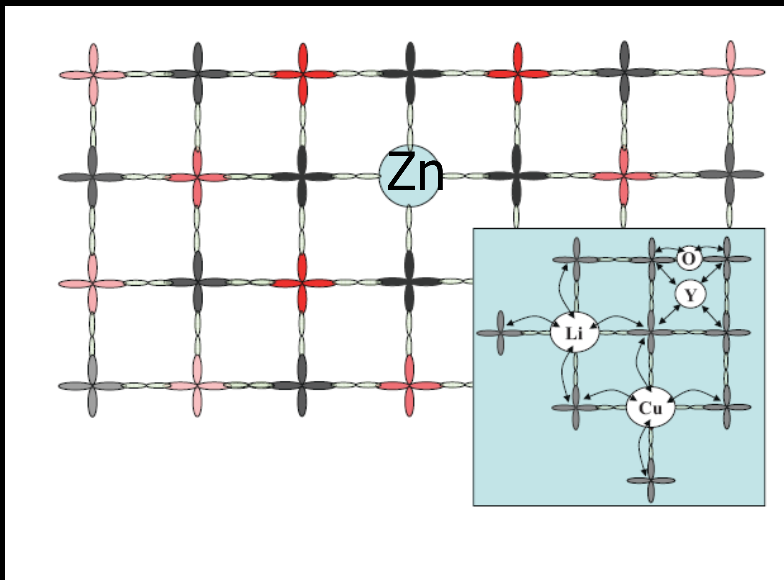




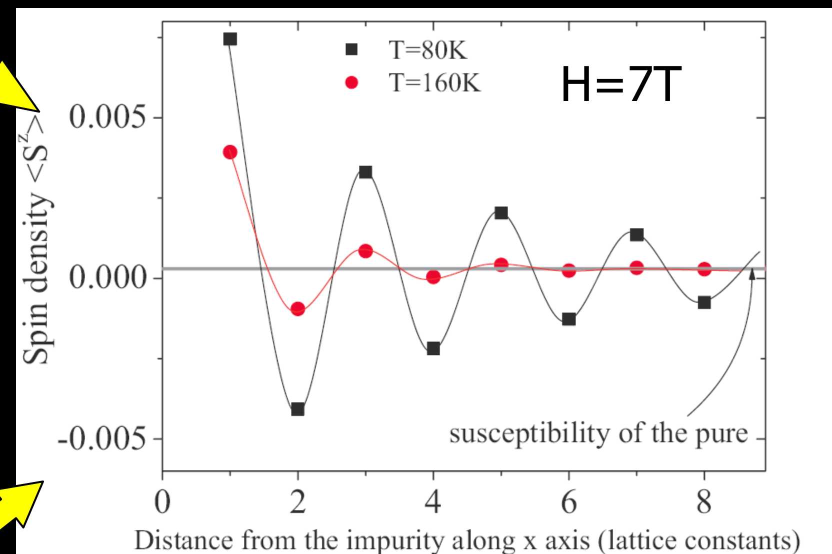
Is this the same thing as “stripes” pinned by disorder?

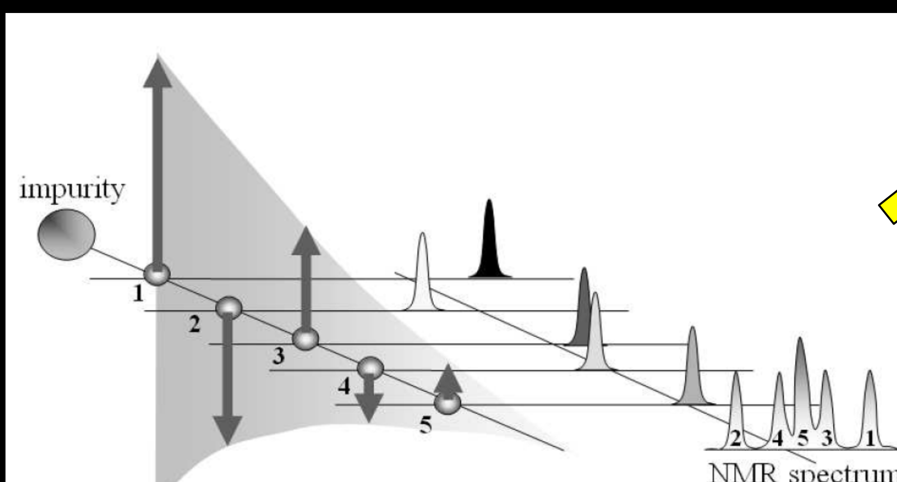
Magnetism at non-magnetic impurity sites in cuprates

NMR expts.: in-plane impurities in YBCO (Alloul group, …)



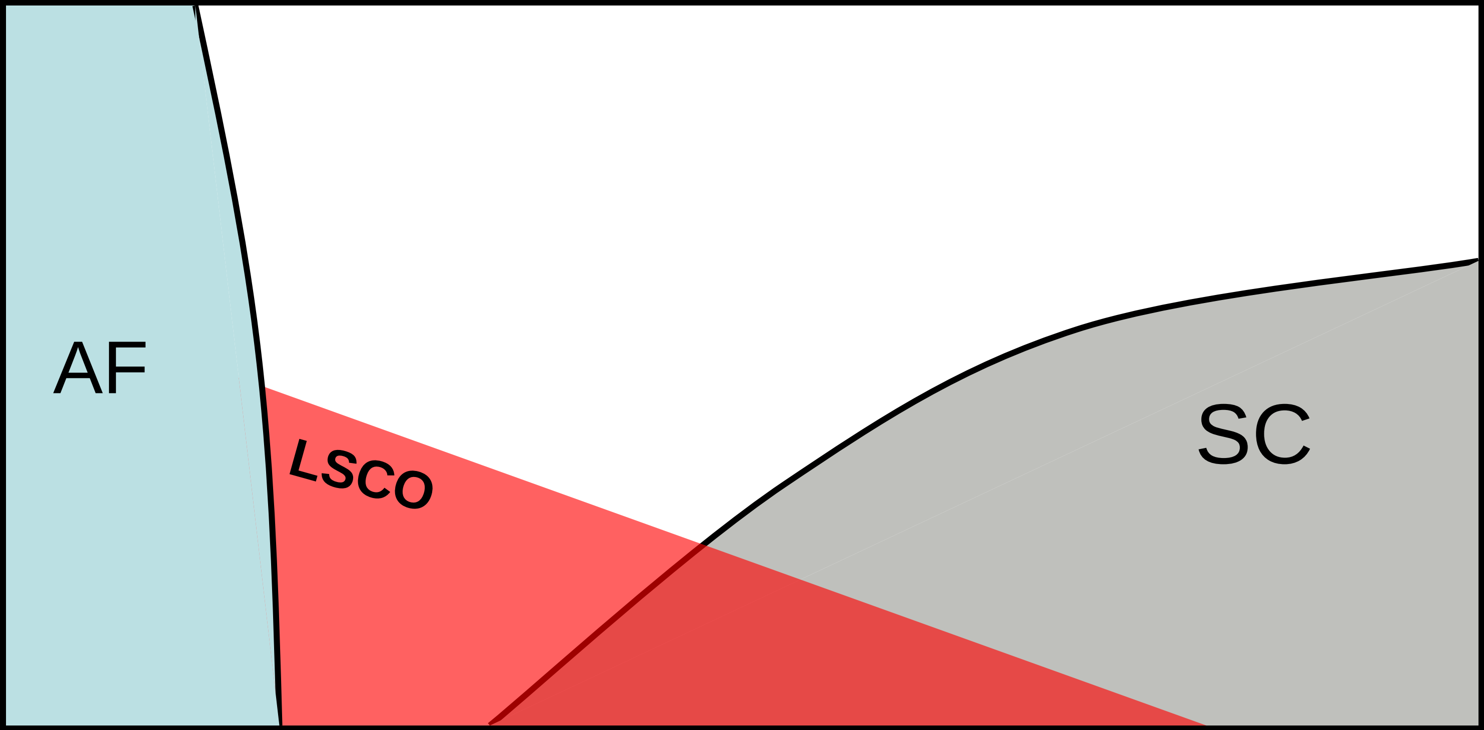
alternating polarization induced near Zn, Li, …



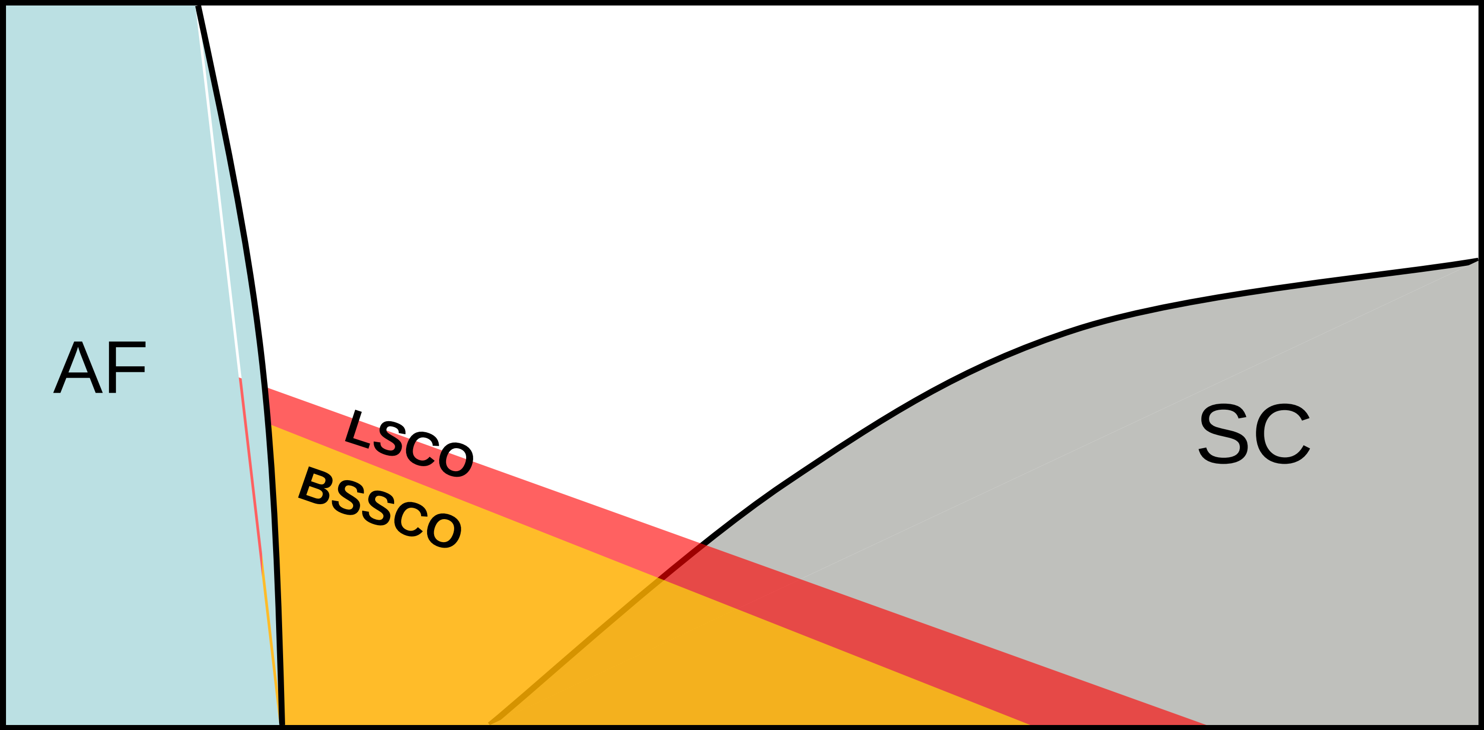


"moments" are *paramagnetic,*
↑S⇧→0 as H→0

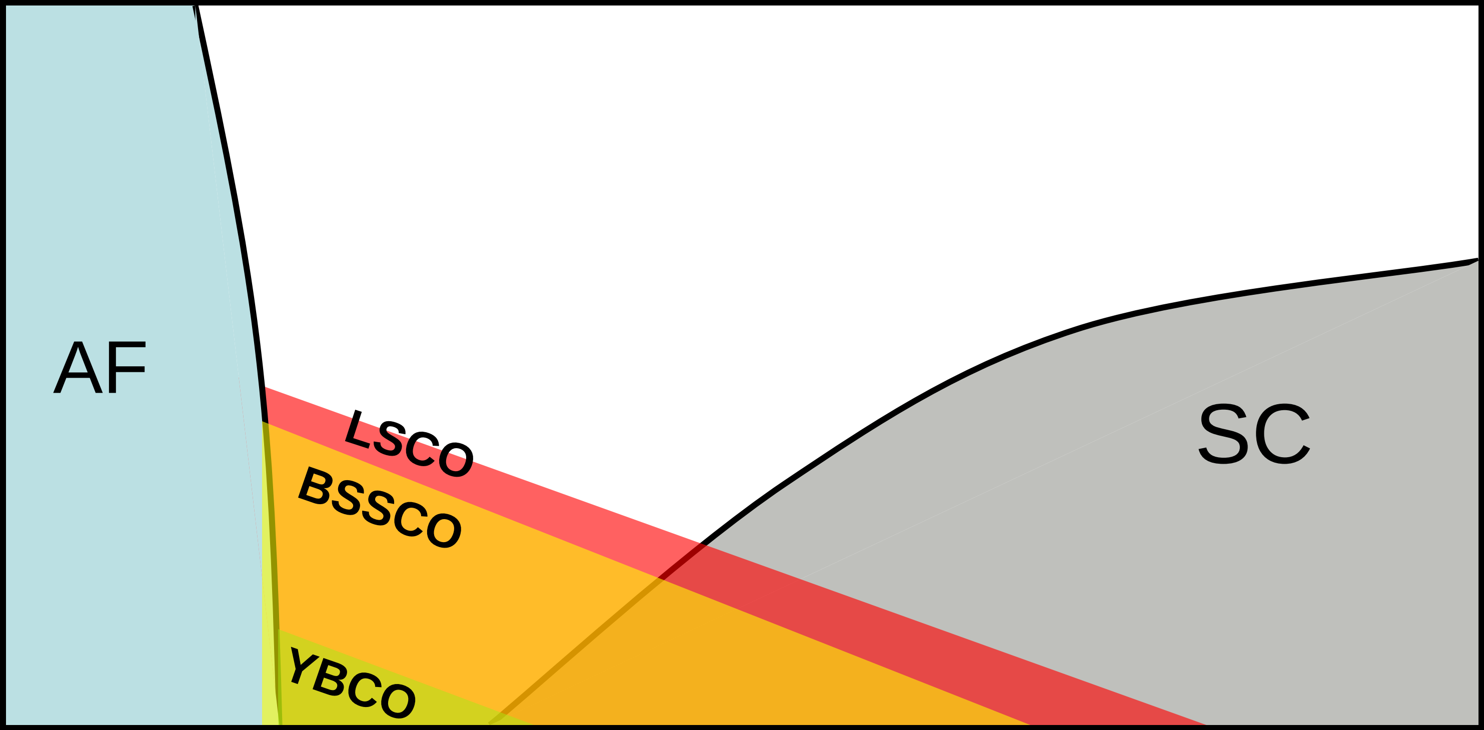
“spin glass” phase diagrams



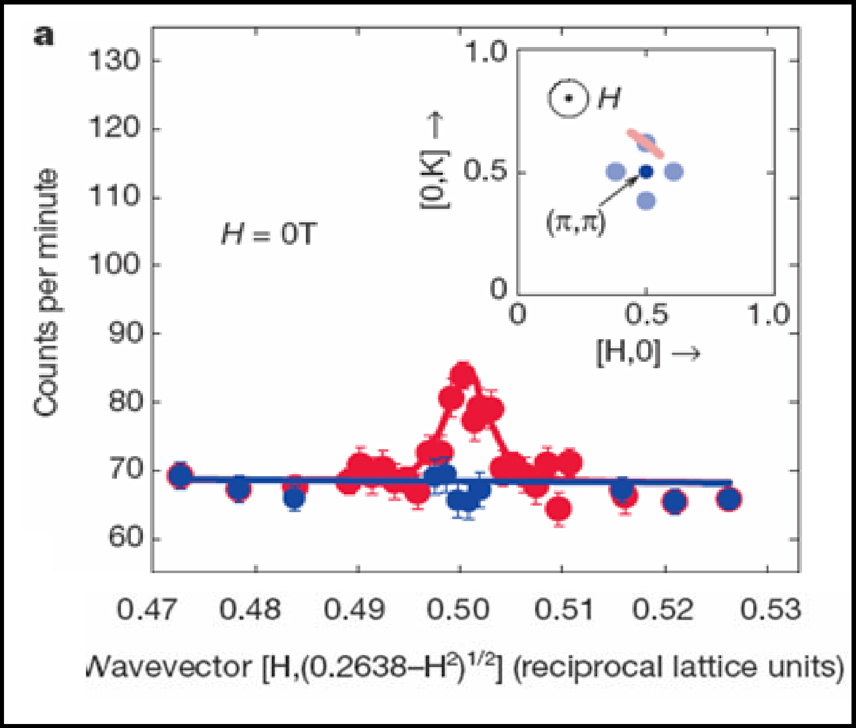
“spin glass” phase diagrams

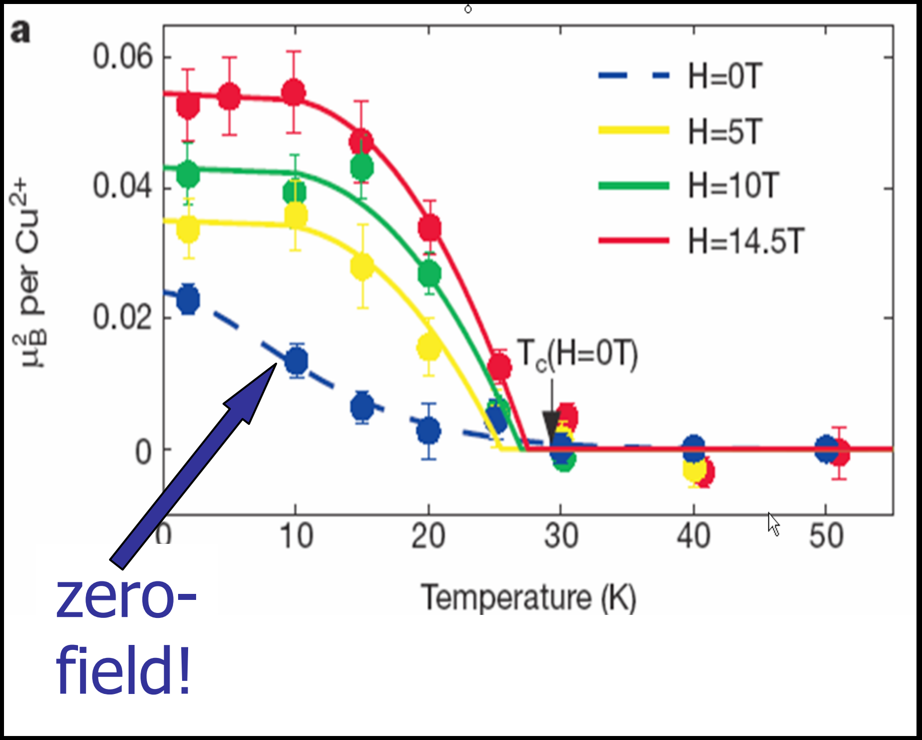


“spin glass” phase diagrams



Frozen "ordered" magnetism in superconducting LSCO, enhanced by field



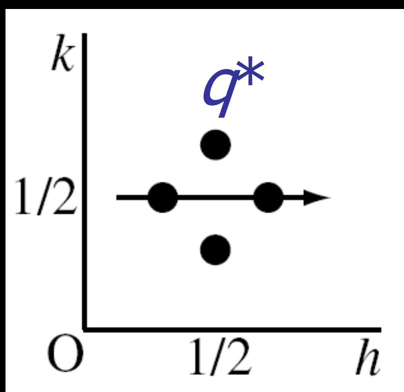


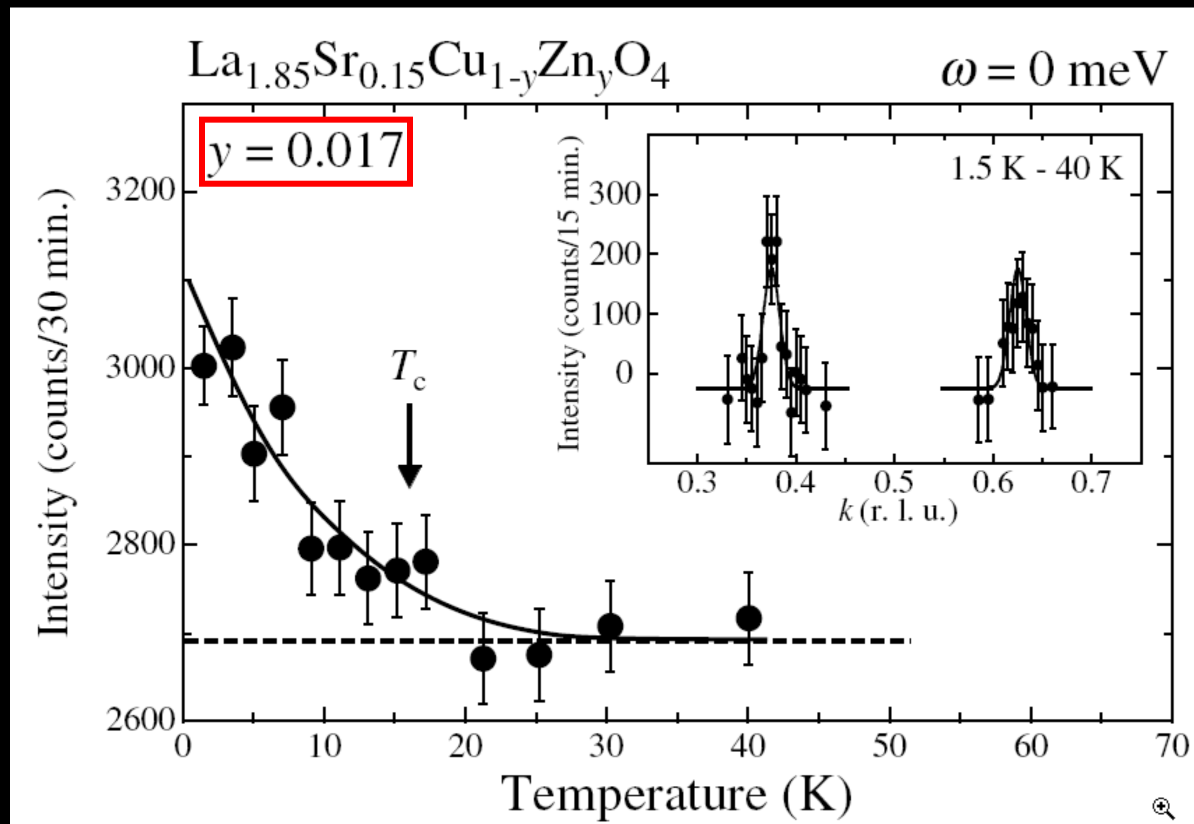
Lake et al 2002:

Static ordered magnetism in underdoped LSCO (x=7.5%)

Kimura et al 2003: disorder can create ordered magnetic state

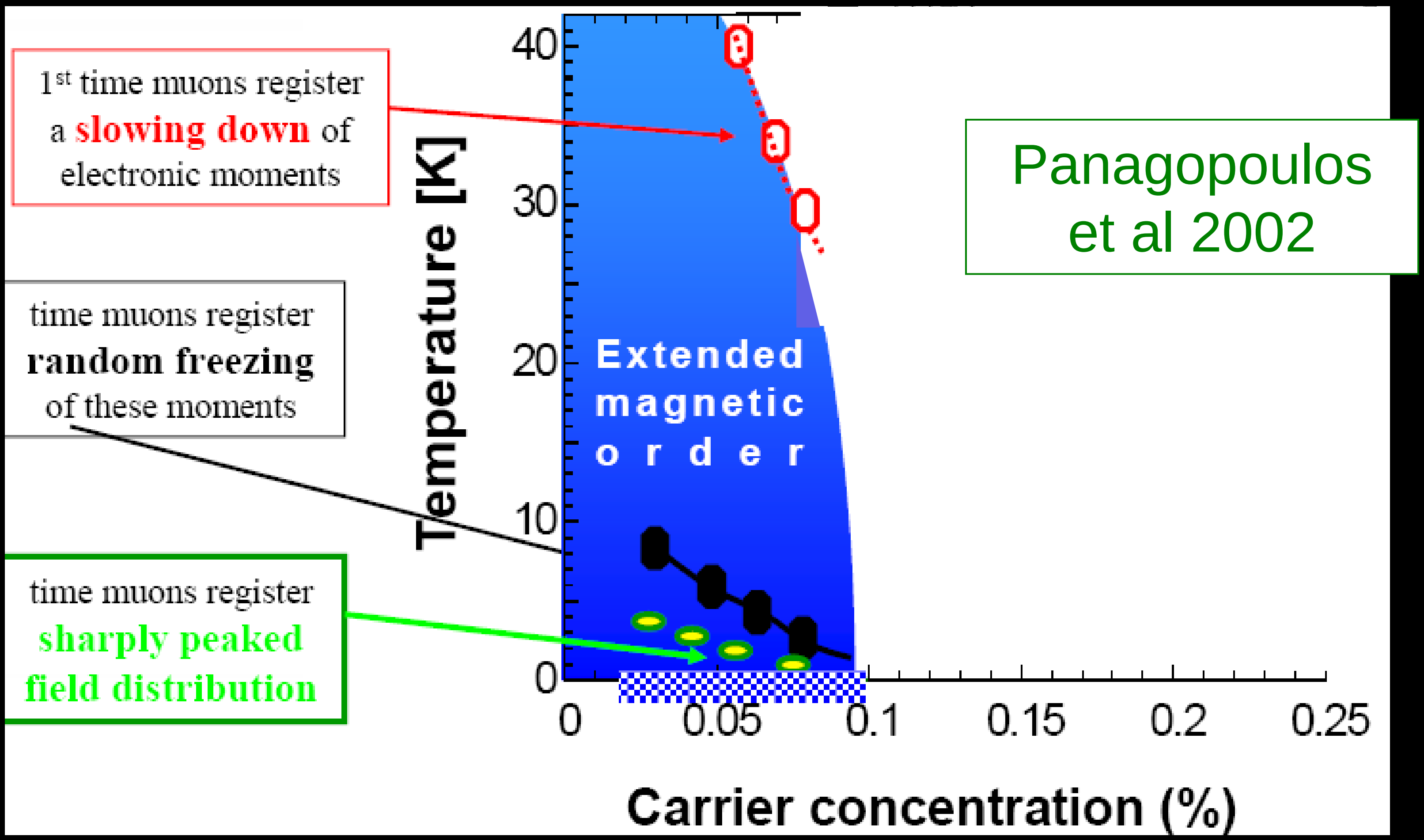
optimally doped LSCO
(x=15%)



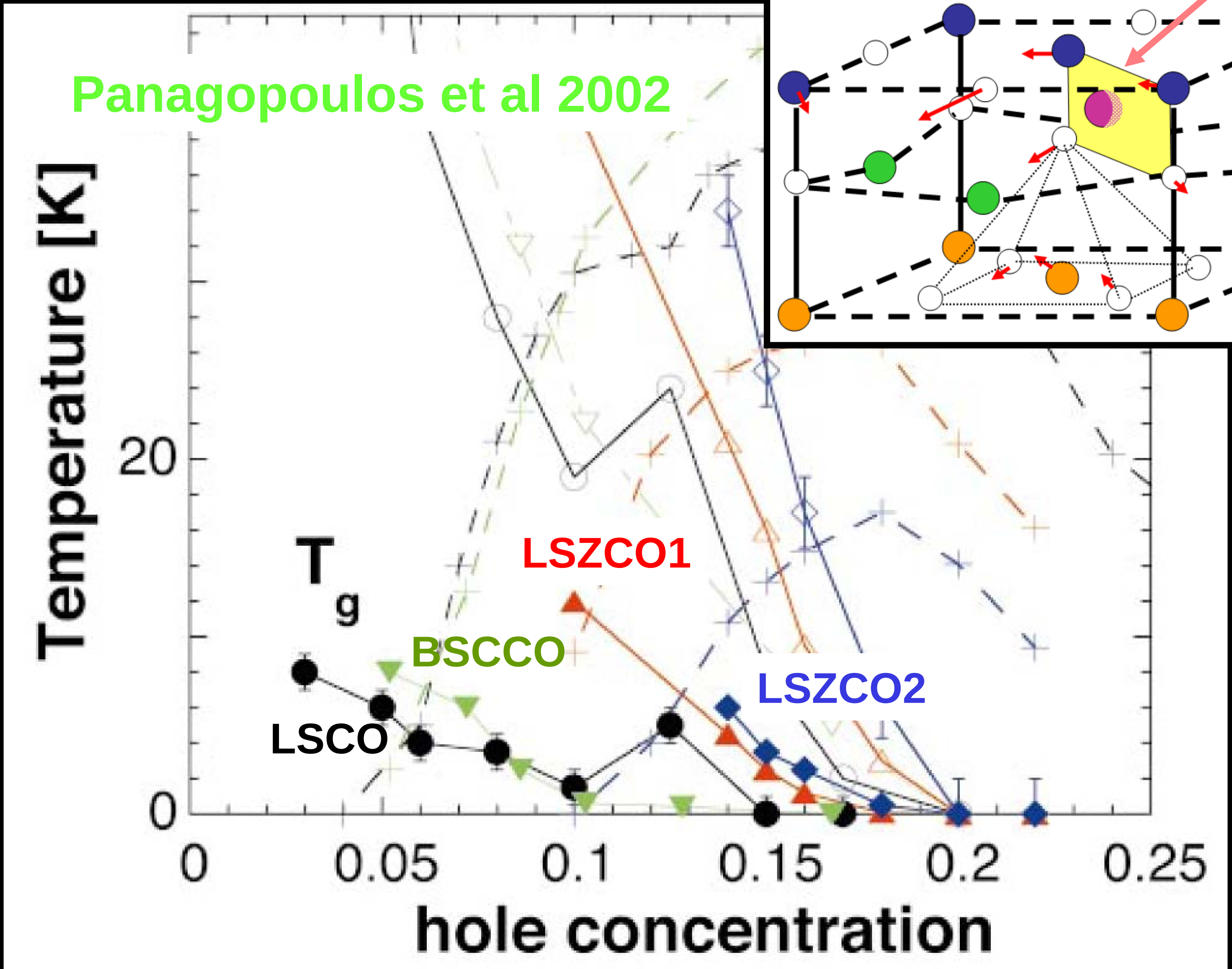


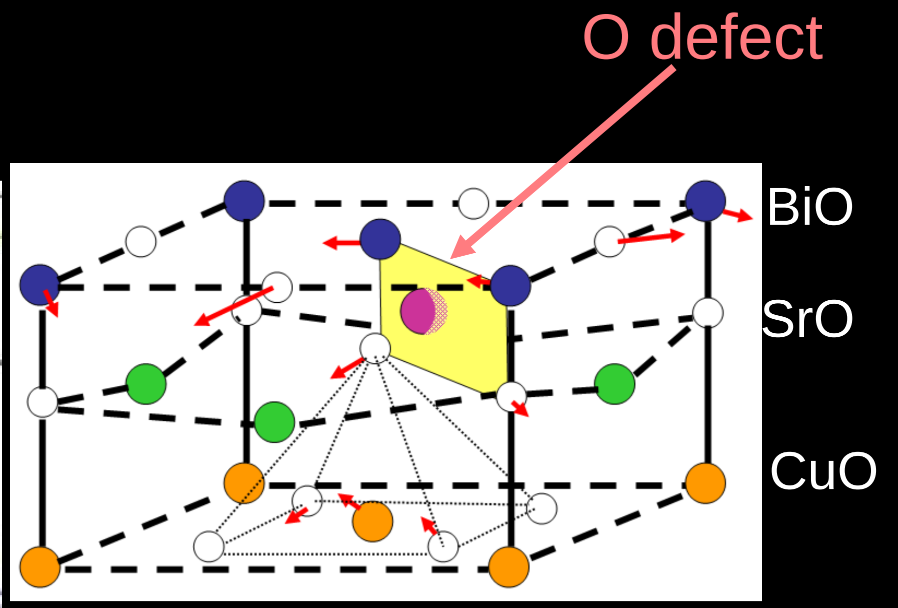
- No static magnetism observed in “pure” sample
- None observed when 1% Zn was added
- Signal at *q** with 1.7% Zn

μSR in LSCO, BSCCO: spin freezing

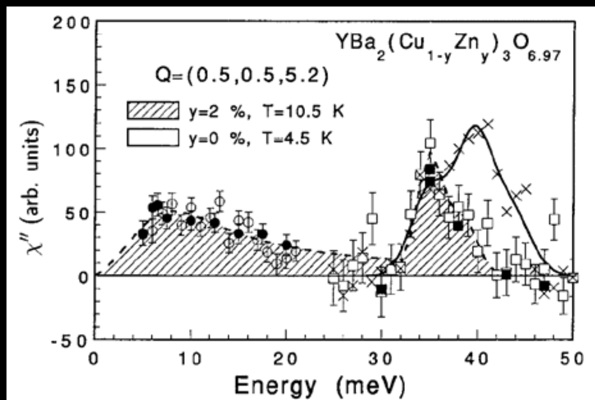


μSR: BSCCO, LSCO





YBCO is different (neutrons & μSR)



Optimal doping: Zn shifts spectral weight to low ω, no static ordering Sidis et al 1996, 2000

Sidis et al 2001:

pure $YBCO_{6.5}$: quasistatic magnetic ordering

The circumstance that this is clearly not observed implies that the magnetic moments fluctuate on a time scale longer than the one of the neutron scattering experiment (10^{-10} s) but much shorter than the one of the μSR experiment (10^{-6} s).

(dirty sample – B. Keimer, priv. comm.)

Same group: $YBCO_{6.45}$ (T_c=35K) displays static order aXv: 0902.3335

Controversy over coexistence at very low doping O6.35:
Sanna et al 2004, Stock et al 2006, R. Miller et al 2006

YBCO/LSCO "dichotomy"

YBCO:

- only paramagnetic impurity moments, even with Zn. No static magnetism in H=0.
- universal qp transport in underdoped samples

clean! Especially ortho-I,II

LSCO (BSCCO, etc.):

- static ordered magnetism in pure underdoped samples x<15%, induced by extra disorder at optimal doping
- qp transport suppressed at underdoping

dirty! Dopants always disordered

Try to understand differences with simple theory of impurity-induced magnetism

Superconductivity +AF correlations+disorder

Can we understand expts. at low doping in superconducting state by simple mean-field theory, accounting for finite disorder?

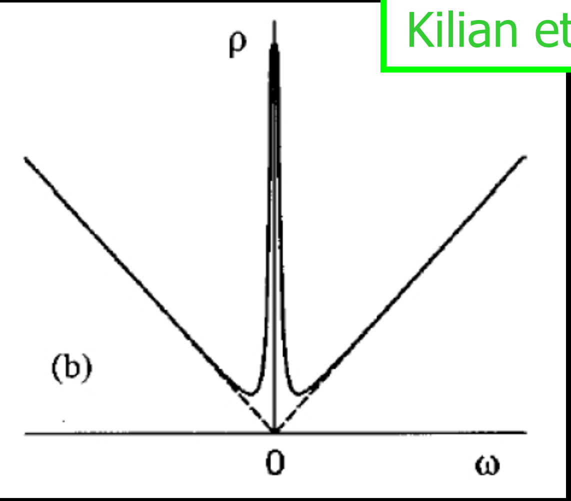
Theories of moment formation in 2D correlated systems

see Alloul et al, Rev Mod Phys 81, 45 (2009)

strong coupling:

- Poilblanc, Scalapino Hanke 1994
- Gabay 1994
- Khaliullin, Fulde… 1995, 97,…
- Dagotto,… 1996,97
- Tsuchiura,… 2000*
- Wang Lee 2002*

⋮



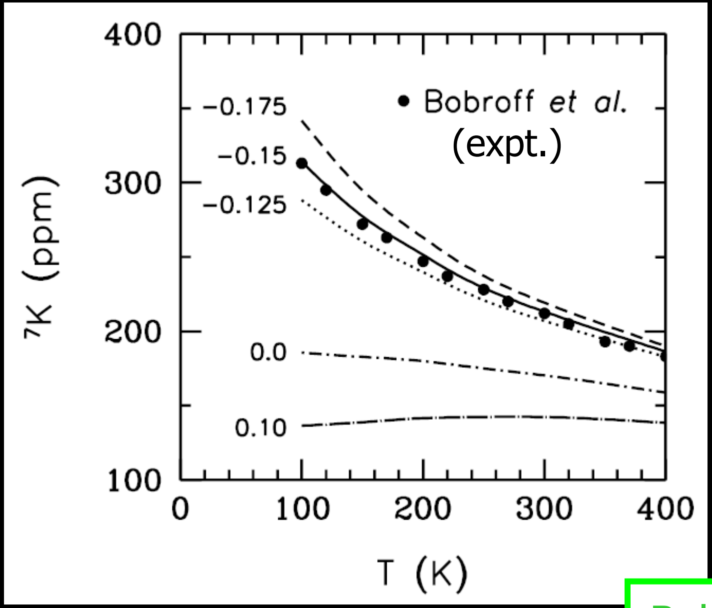
Kilian et al 1999

weak coupling:

- Early "local paramagnon" theories: Lederer, Beal Monod, …Schrieffer…

- Bulut 2000, 2001
- Ohashi 2001, 2002*
- Ting, … 2004*

* dwSC state



Bulut 2001

Hamiltonian (weak-coupling approach)

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma}$$

Kinetic Energy (Lattice Hopping)

$$+ \sum_{i\sigma} \left(V^{imp}_{i\sigma} - \mu \right) \hat{n}_{i\sigma}$$

Impurity Potential & Chemical Potential

$$+ U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

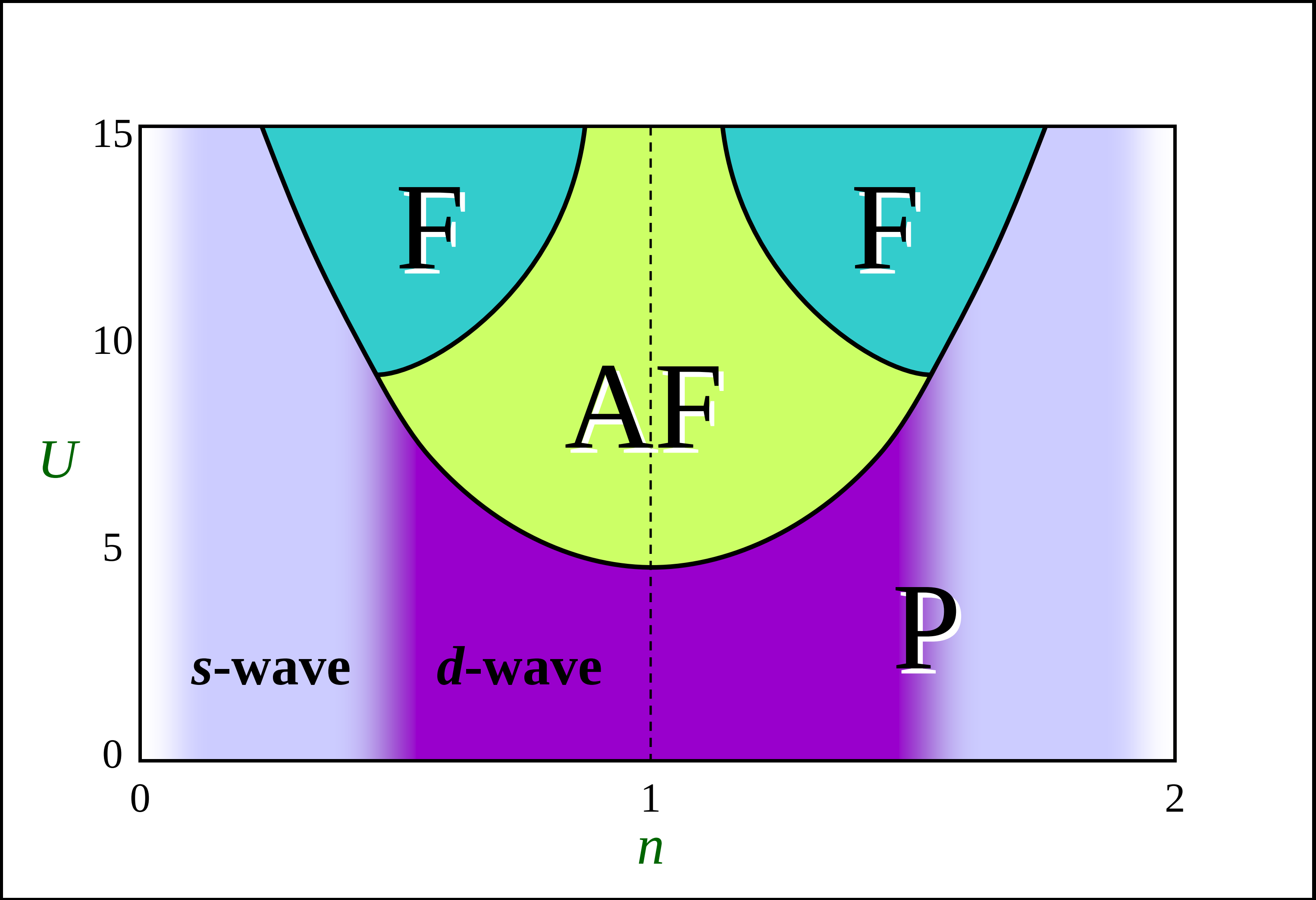
Magnetic Correlations

$$+ \frac{V_1}{2} \sum_{\langle ij \rangle \sigma\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'}$$

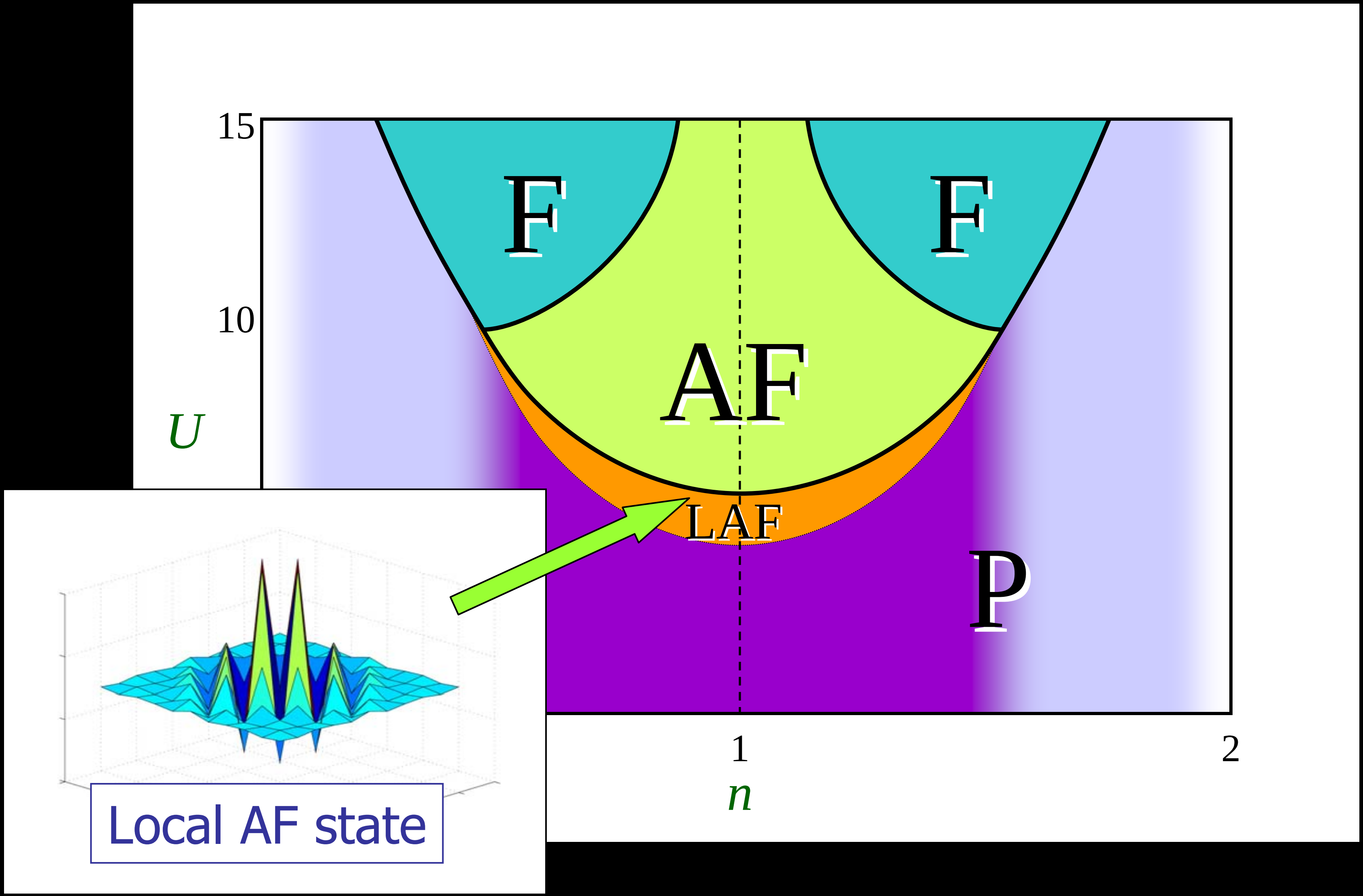
d-wave Pairing

with Hartree-Fock factorization

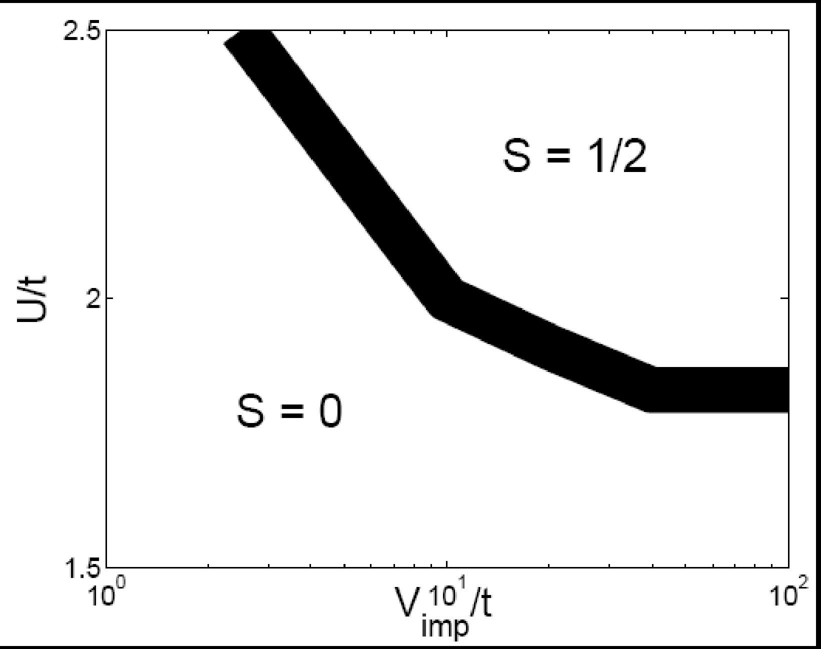
Homogeneous phase diagram



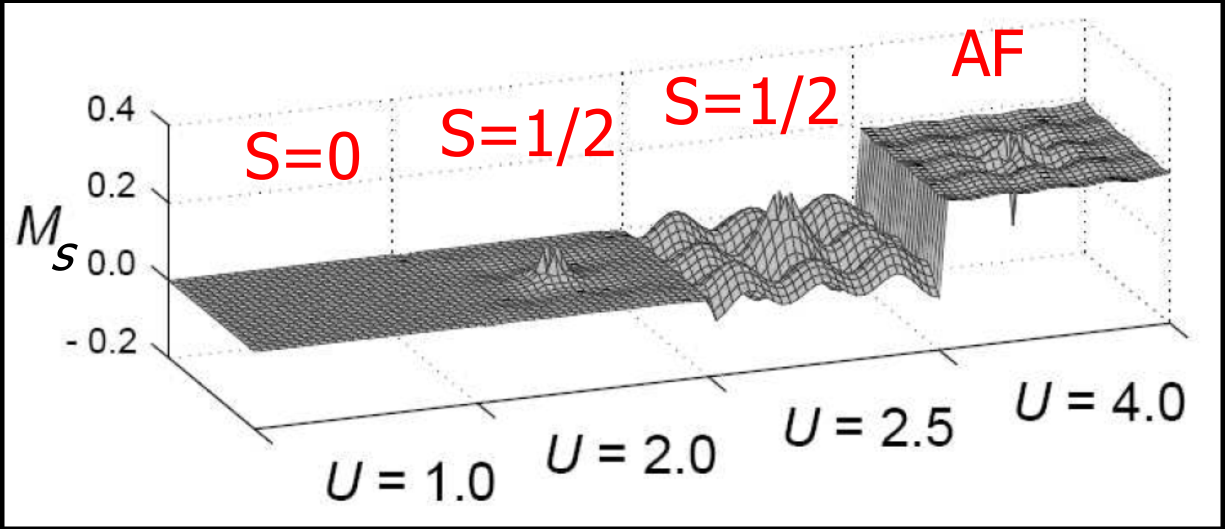
Local magnetic droplet around 1 nonmagnetic impurity



Local magnetic state depends on V_{imp} and U

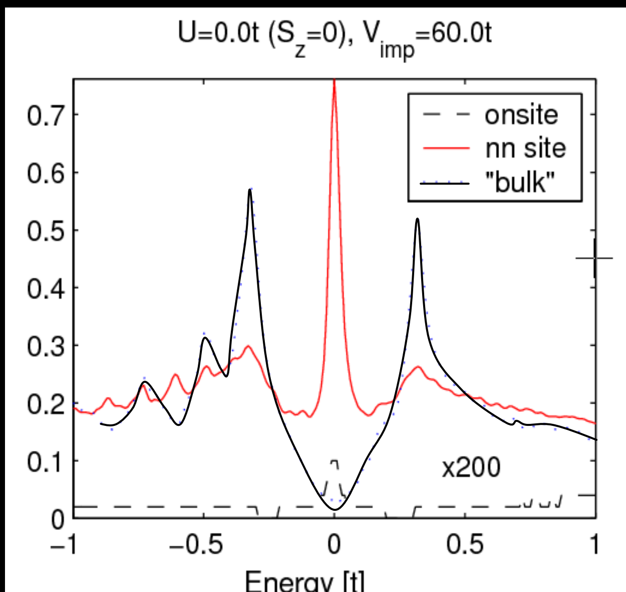


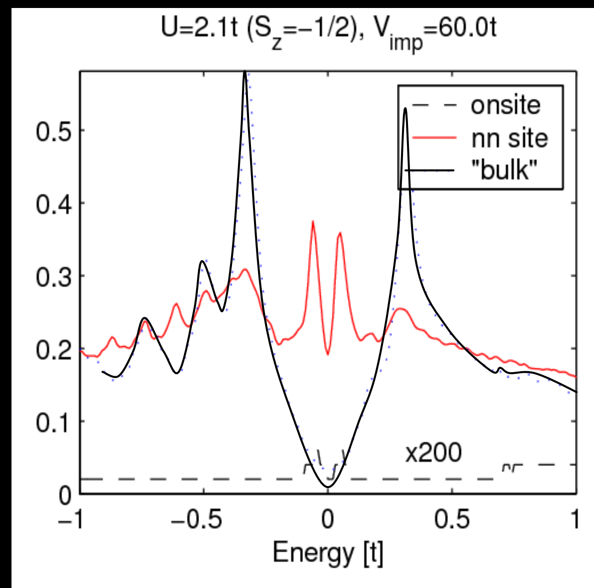
"phase transition" similar to
Salkola Balatsky Schrieffer 1997
for s-wave

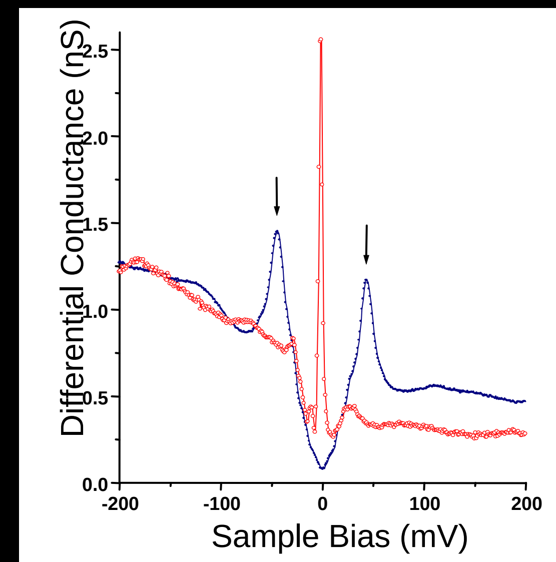


Magnetism from splitting of impurity resonance

Recall: Pan et al 2000







* Optmal doping: all resonances unsplit ⇒paramagnetic state

* Underdoped: some split resonances observed (?)

Is disorder-induced magnetism = phase competition?

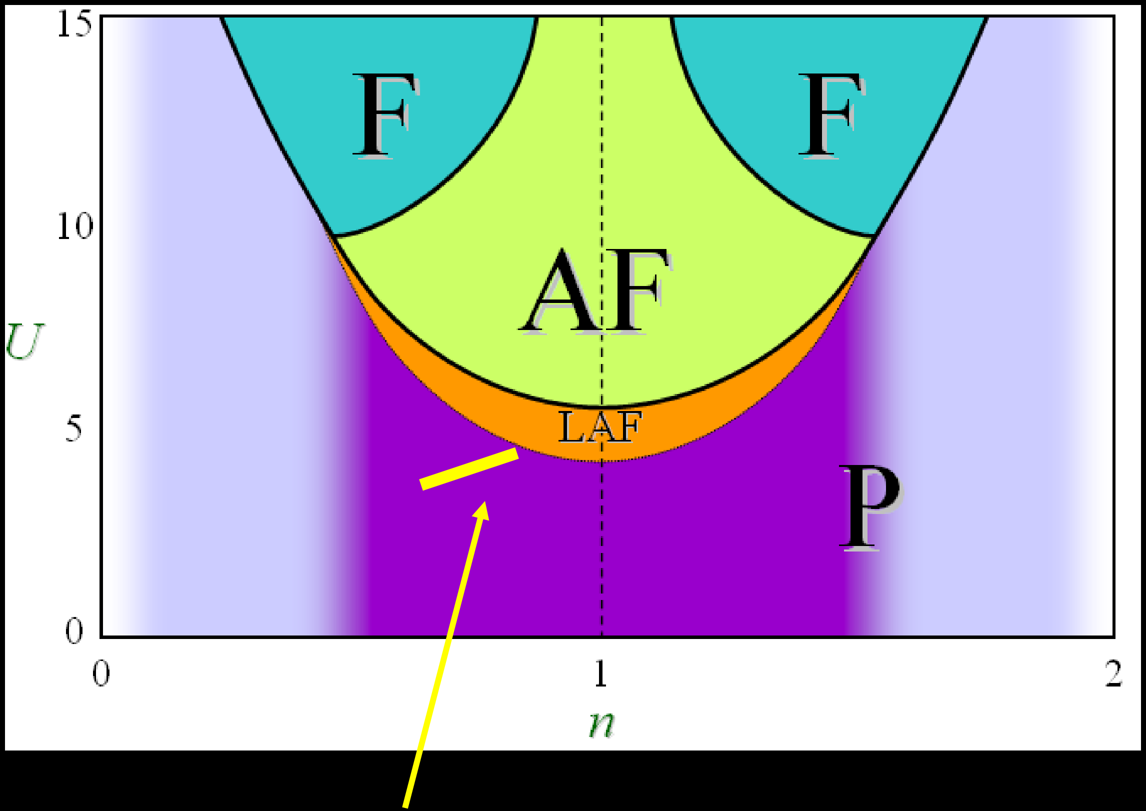
$$S = \int d^2x \int_0^{1/T} d\tau \Big\{ \frac{1}{2}\{(\partial_\tau \phi_\alpha)^2 + c^2(\nabla_x \phi_\alpha)^2 + [r + v|\psi(x)|^2]\phi_\alpha^2\} + \frac{u}{2}(\phi_\alpha^2)^2 \Big\},$$

e.g. Demler et al 2001

No:

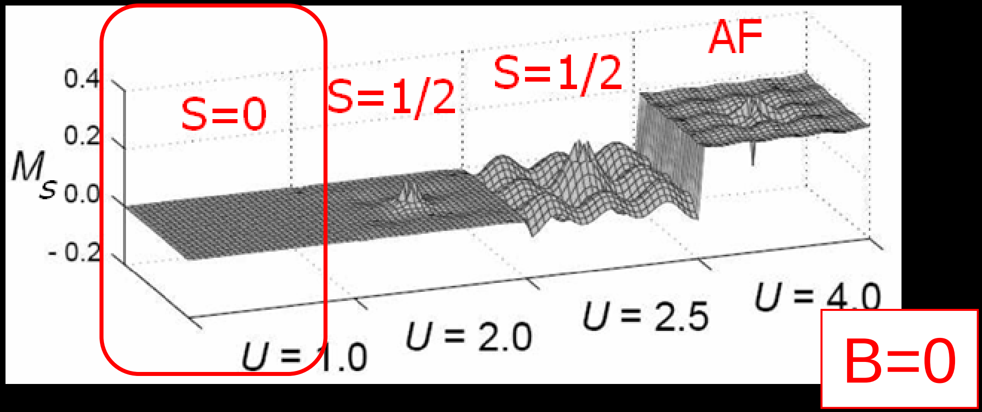
- In SC state, bound states leading to magnetism are found to be formed & split by field even if SC order parameter is artificially held constant.
- Similar phenomenology in N state, although no bound state without pseudogap

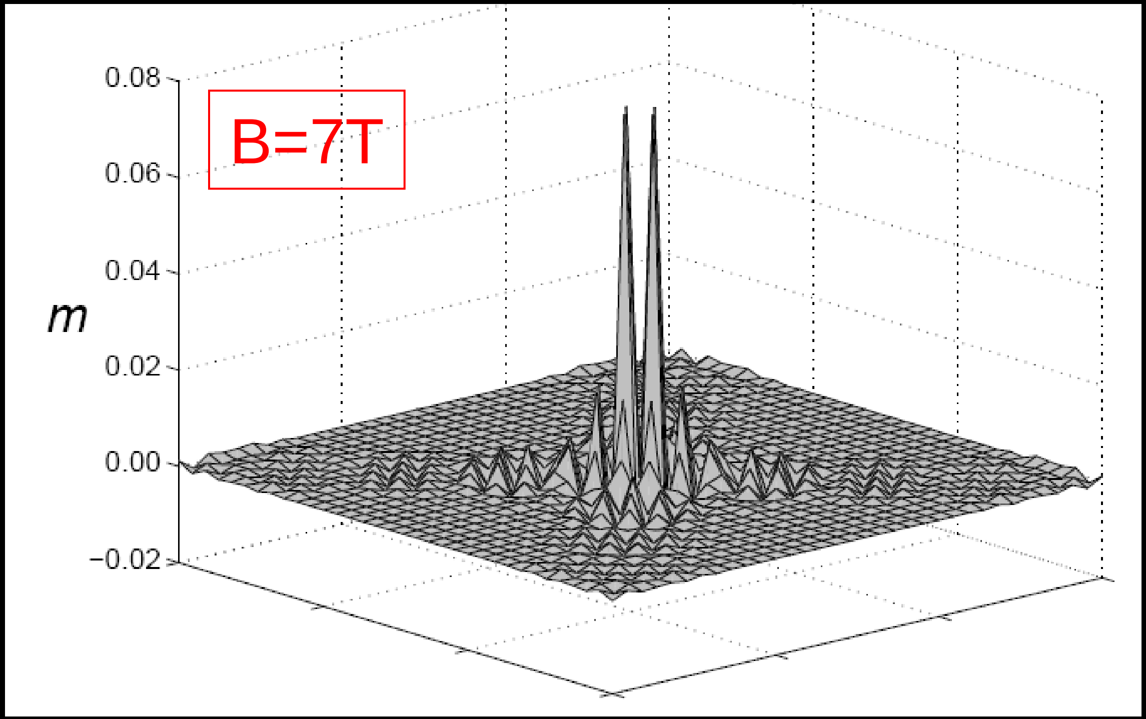
YBCO



YBCO: “no” static magnetism
assume: clean except for Zn

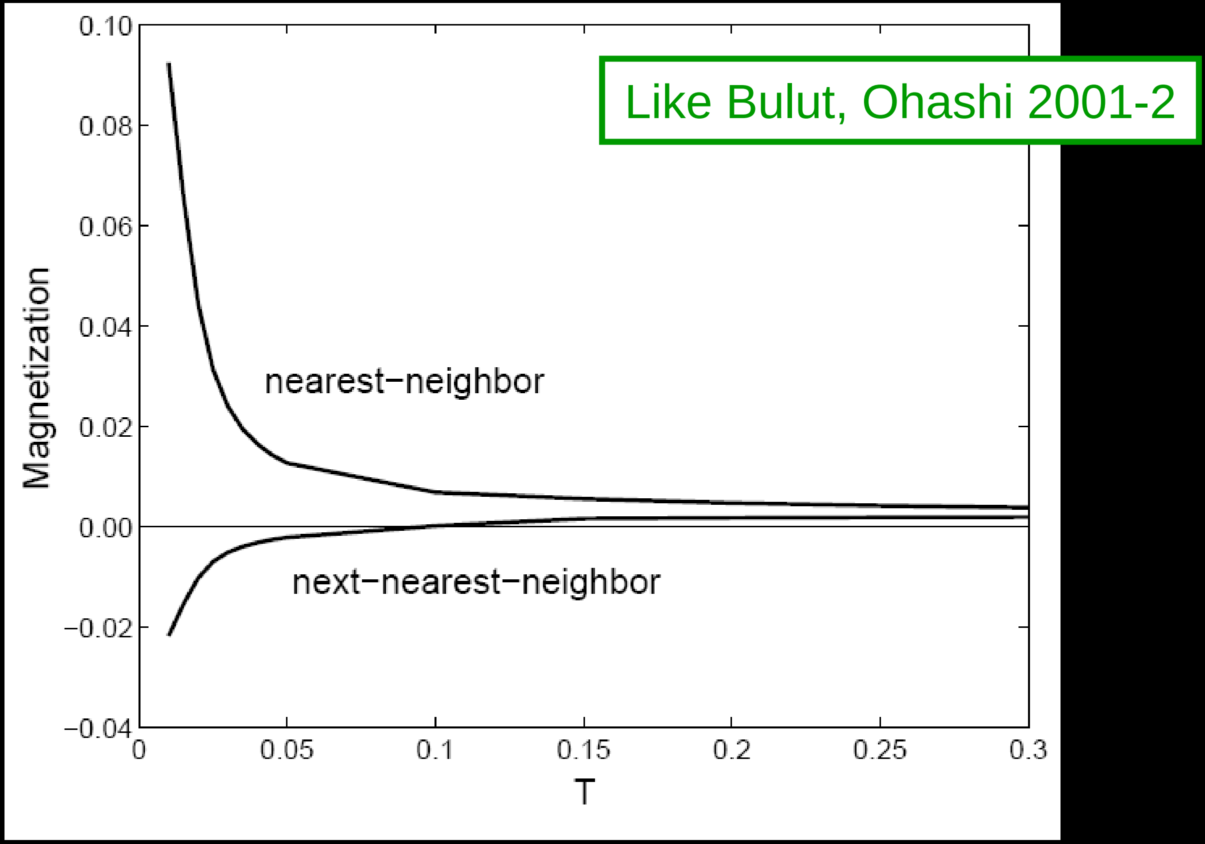
Zn impurity induced magnetization pattern in magnetic field





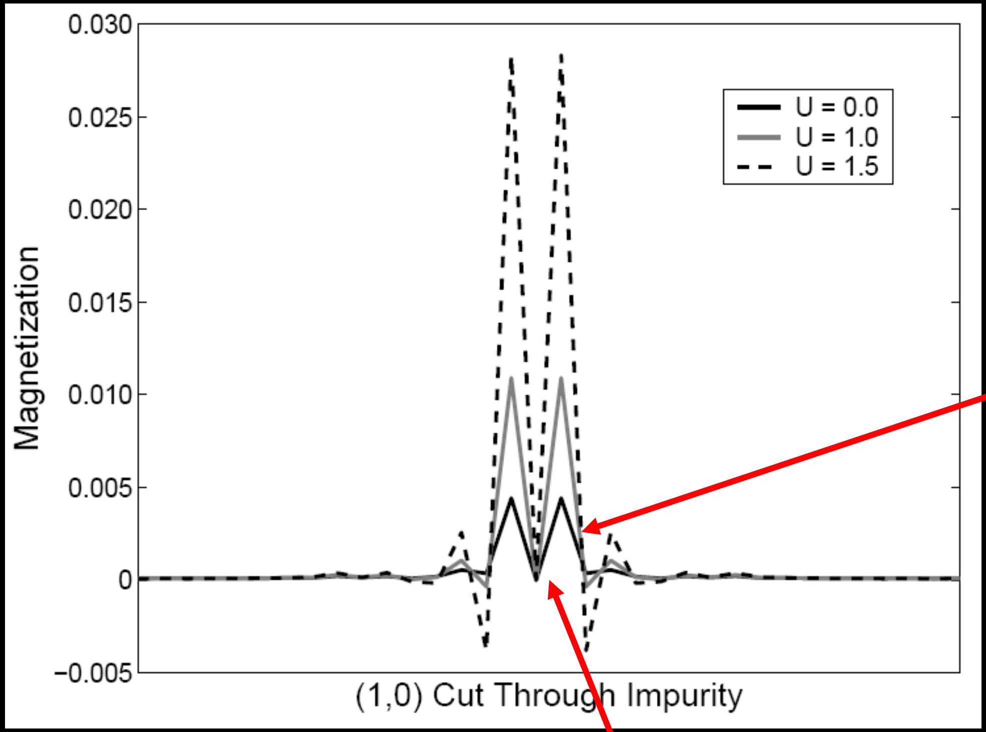
paramagnetic moment!

T-dependence for single impurity in field



strong enhancement of impurity magnetism at low T

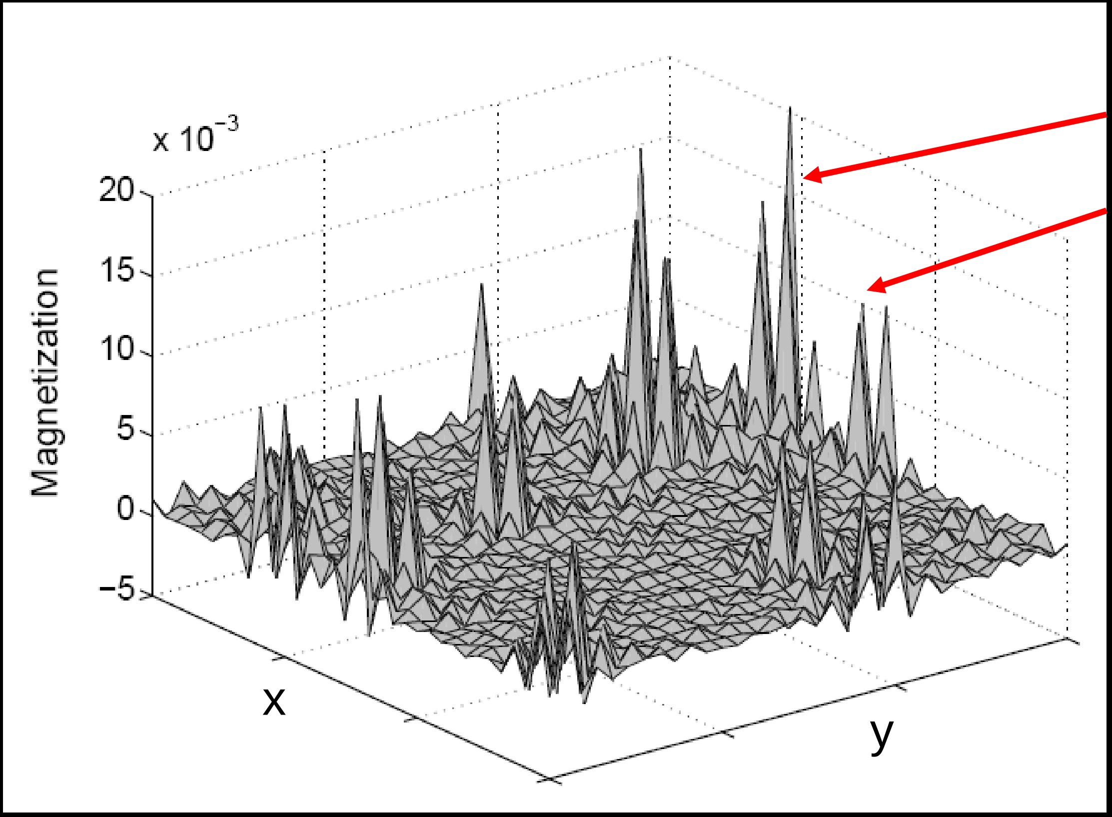
Importance of correlations



ordinary Friedel oscillations

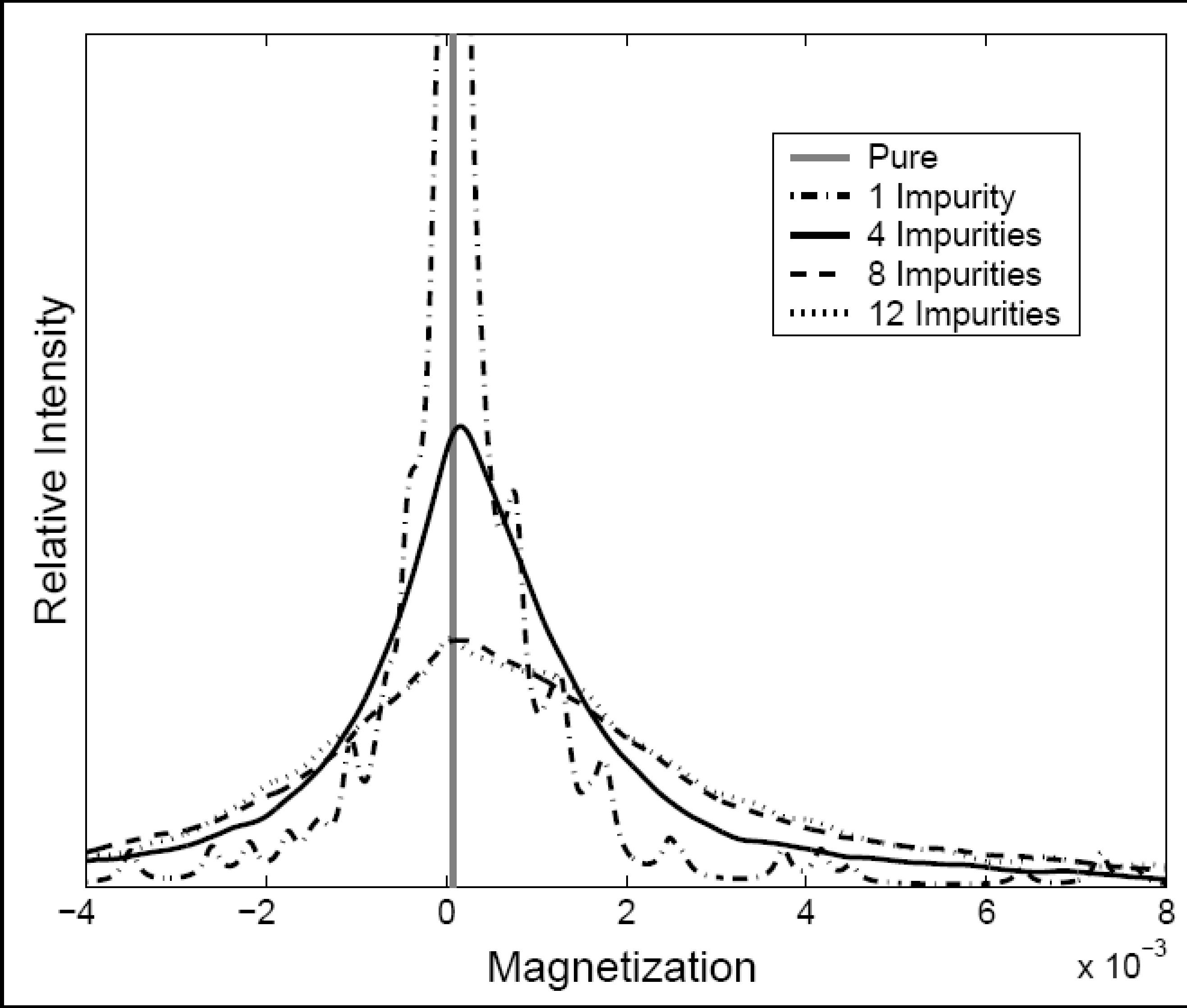
U=0 results give modulated magnetization (Friedel), *but* a) m>0 always; b) too small ⇒ disagrees with "LDOS-only" explanation (Tallon, Xiang, …)

Interference of many impurities

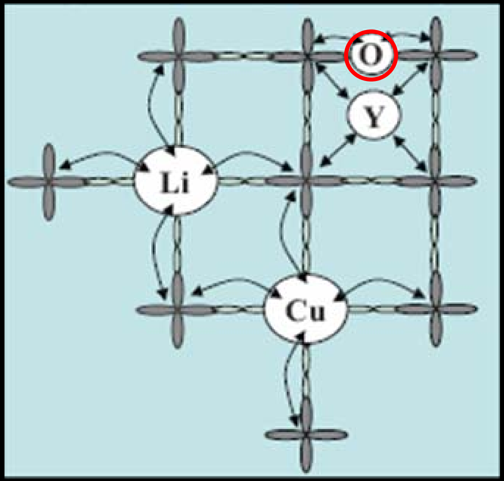


Magnetization depends on local disorder environment

Effect of interference on m-histogram



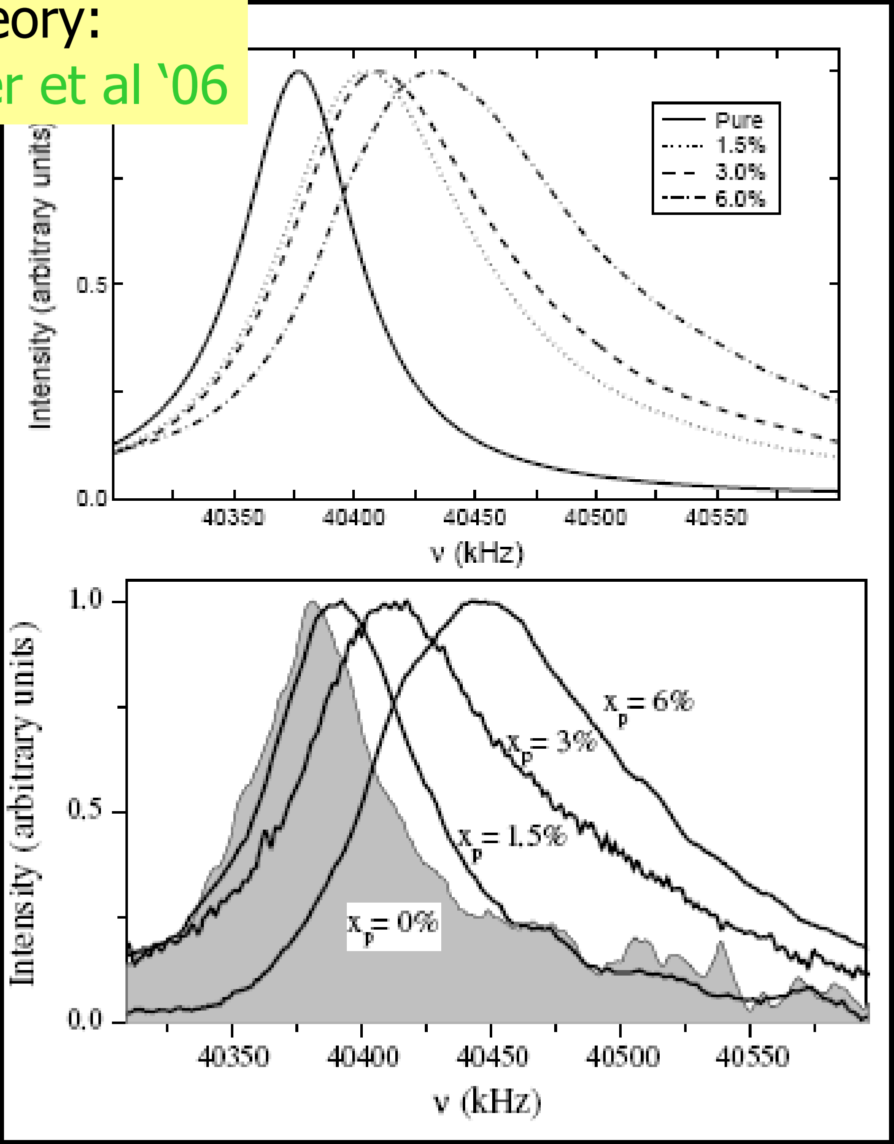
^{17}O NMR: comparison of line for 0,1.5,3,6% Zn



Fix T=15K, U=1.75t, t'/t=-3.5, x=15%, V_{imp}=10t

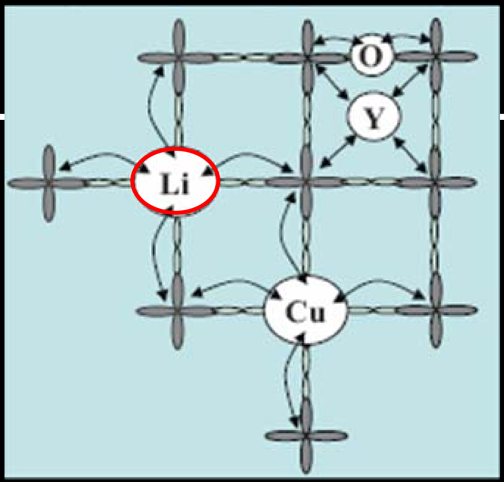
vary n_{imp}

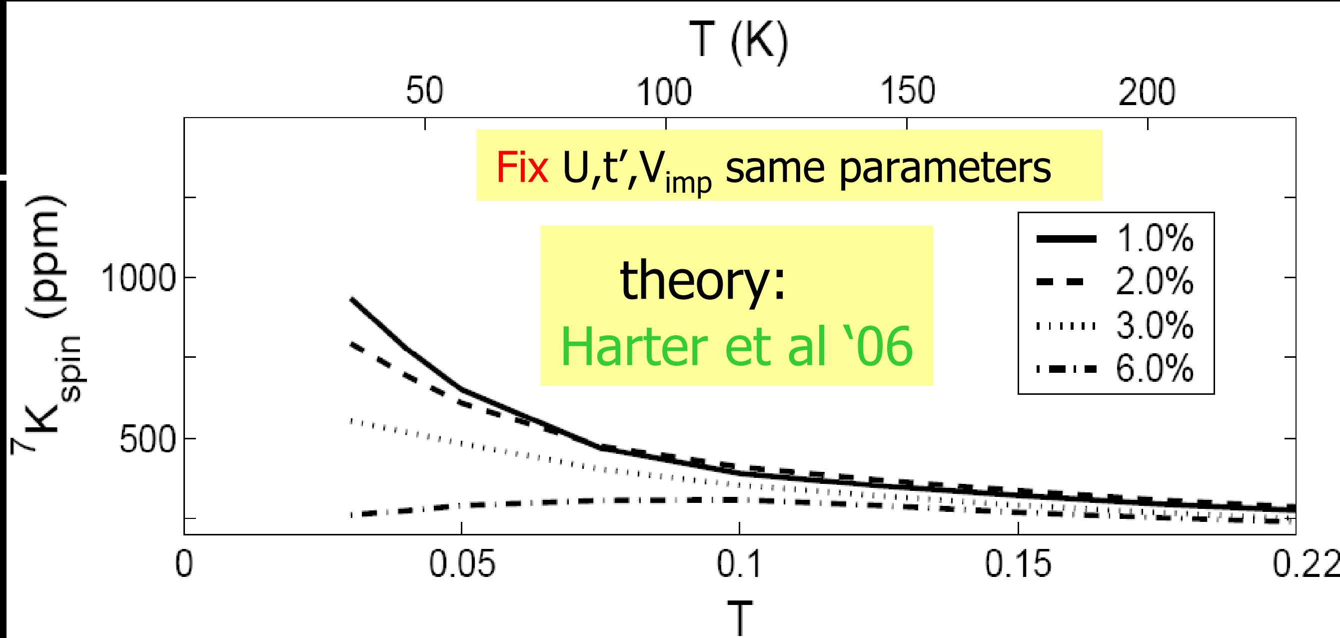
theory: Harter et al '06

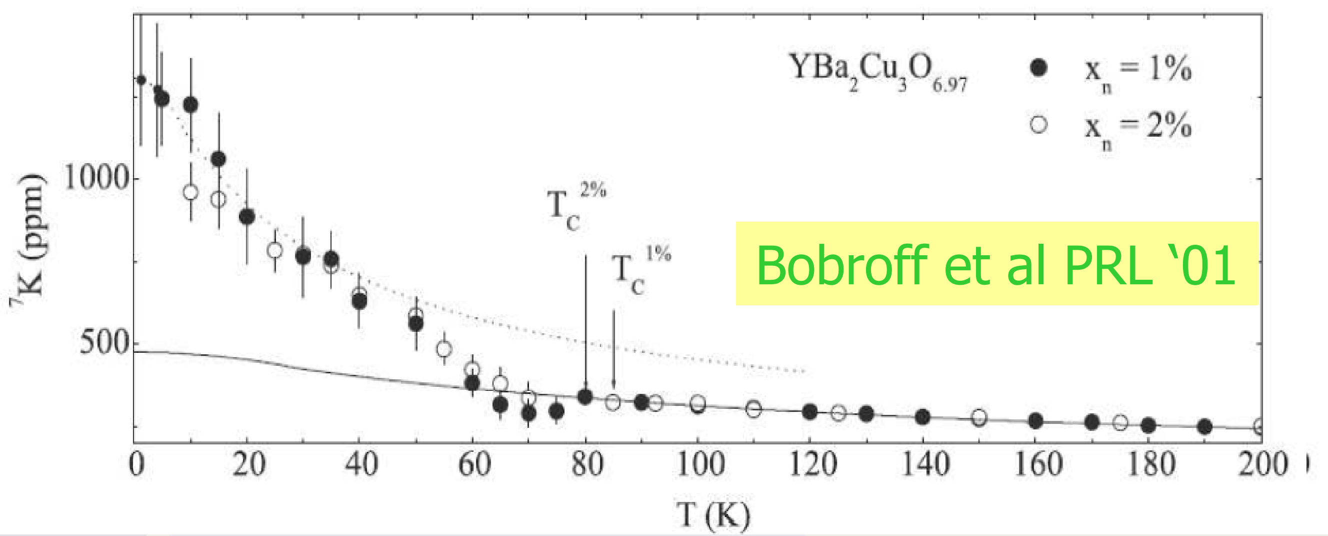


expt: Ouazi et al PRL '06

Short distances: ^{7}Li NMR

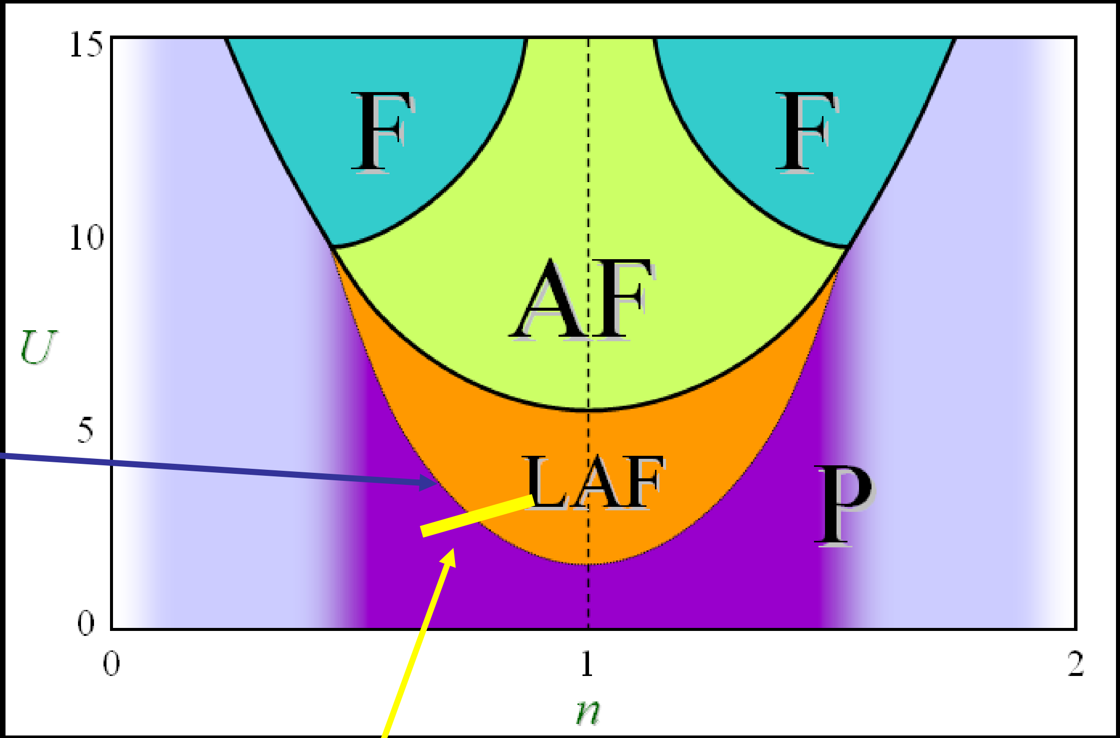






LSCO
(and other intrinsically disordered cuprates)

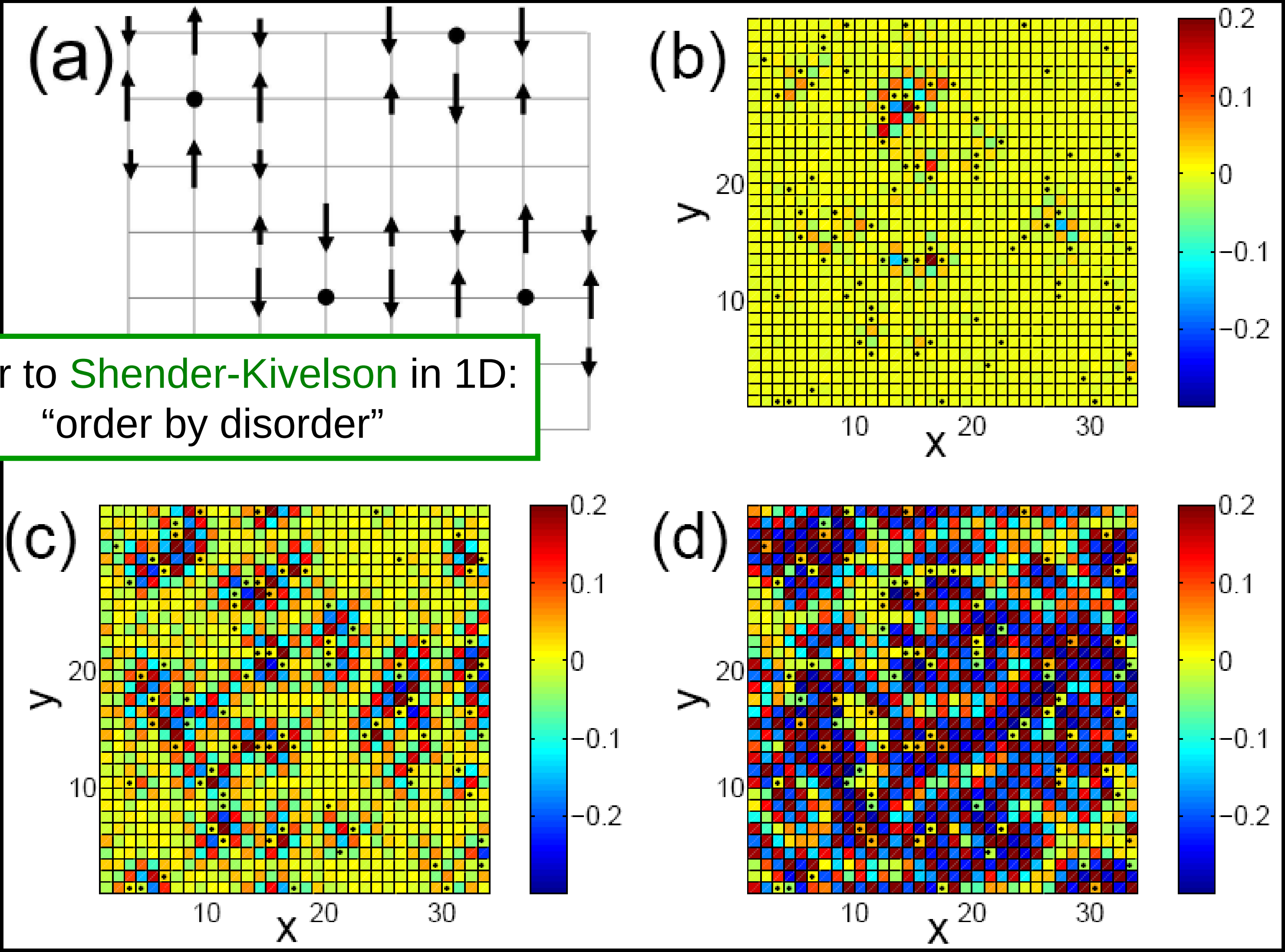
disorder
enlarges
Local AF
phase



LSCO: static ordered magnetism exists
assume: "intrinsically dirty" due to Sr dopant disorder

Andersen, Schmid, Kampf, PH PRL 2007

Formation of magnetic order: x=7.5%

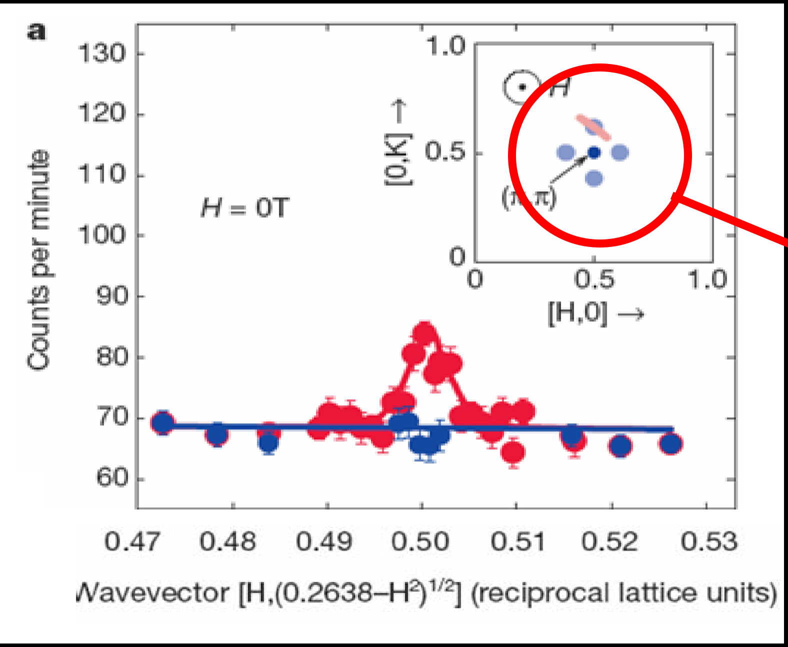


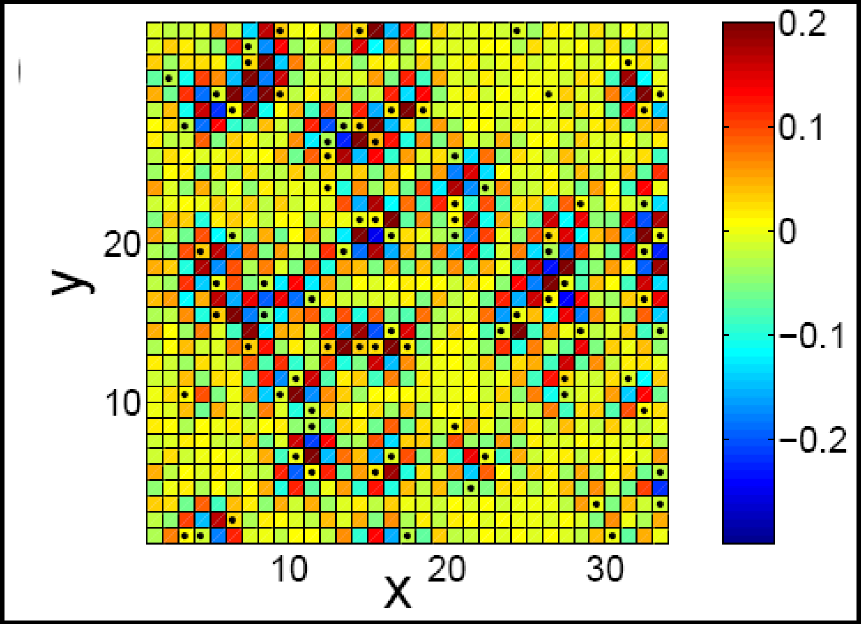
Similar to Shender-Kivelson in 1D: "order by disorder"

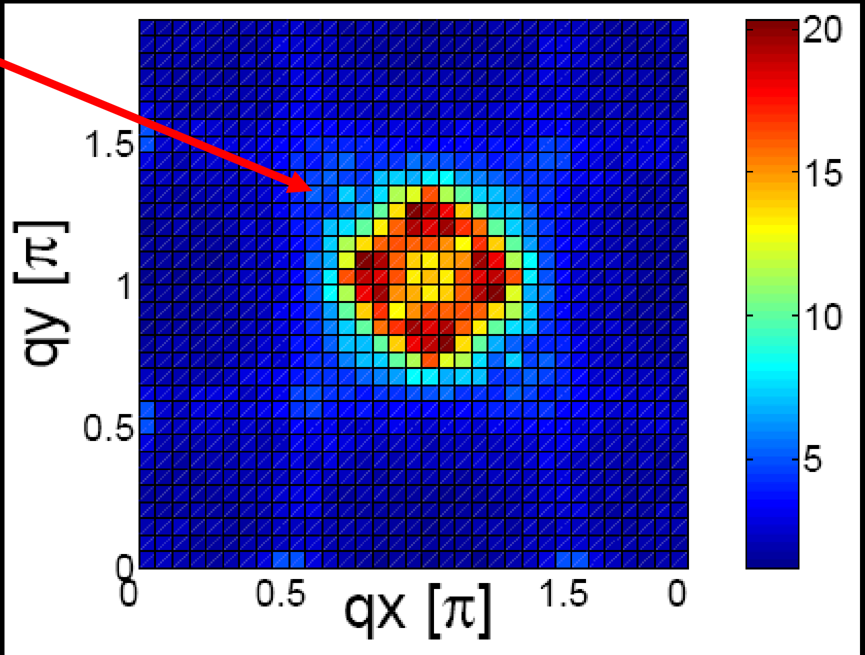
$U = 2.8t$ (b), $U = 3.2t$ (c), and $U = 3.6t$ (d)

Real space/q-space magnetism (underdoped)

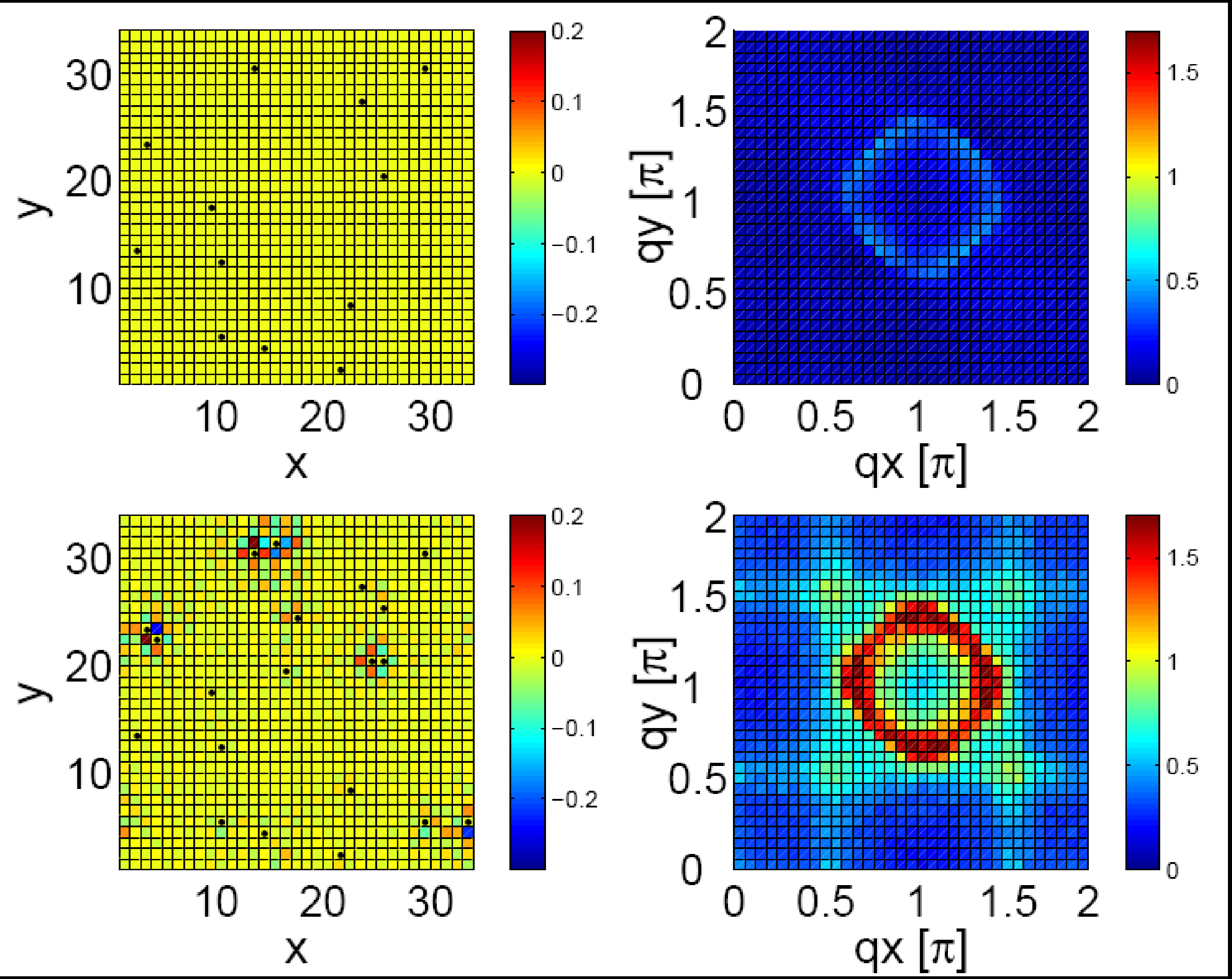
Lake et al 2002







tuning transition with Zn a la Kimura 2003 (opt. doping)



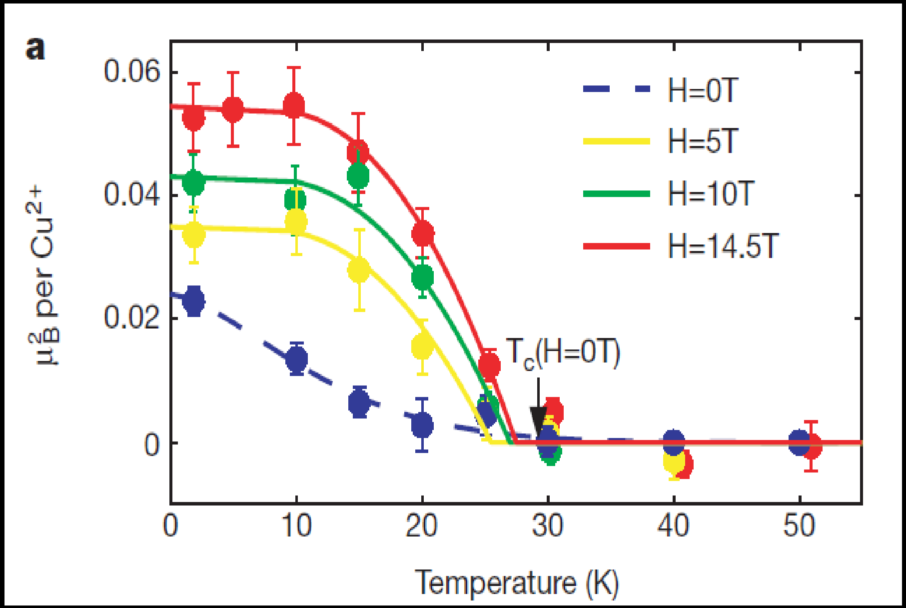
1%

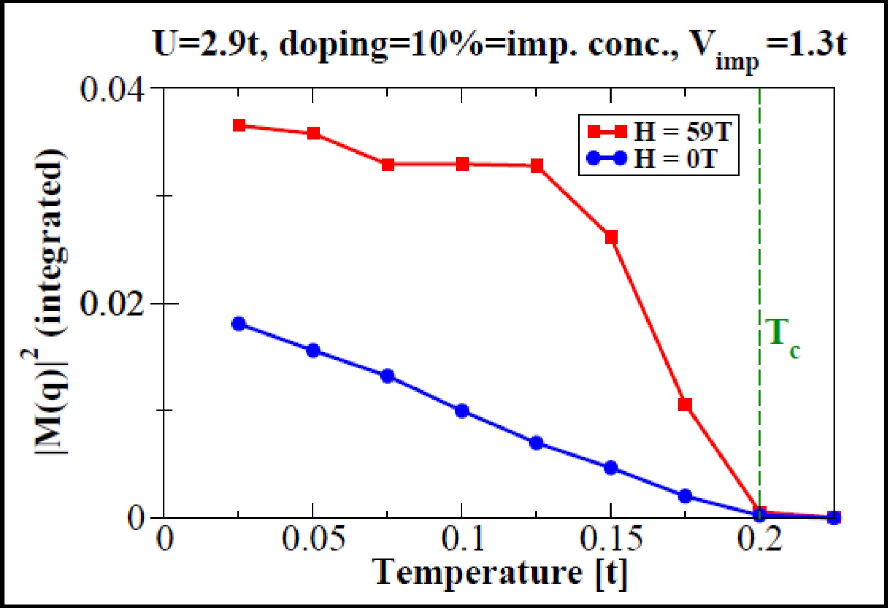
2%

U=3.2; V_{imp}=100t

T,H dependence

Expt: 7.5% doped LSCO: Lake et al 2002 Theory: Schmid, Kampf, PH & Andersen 2009





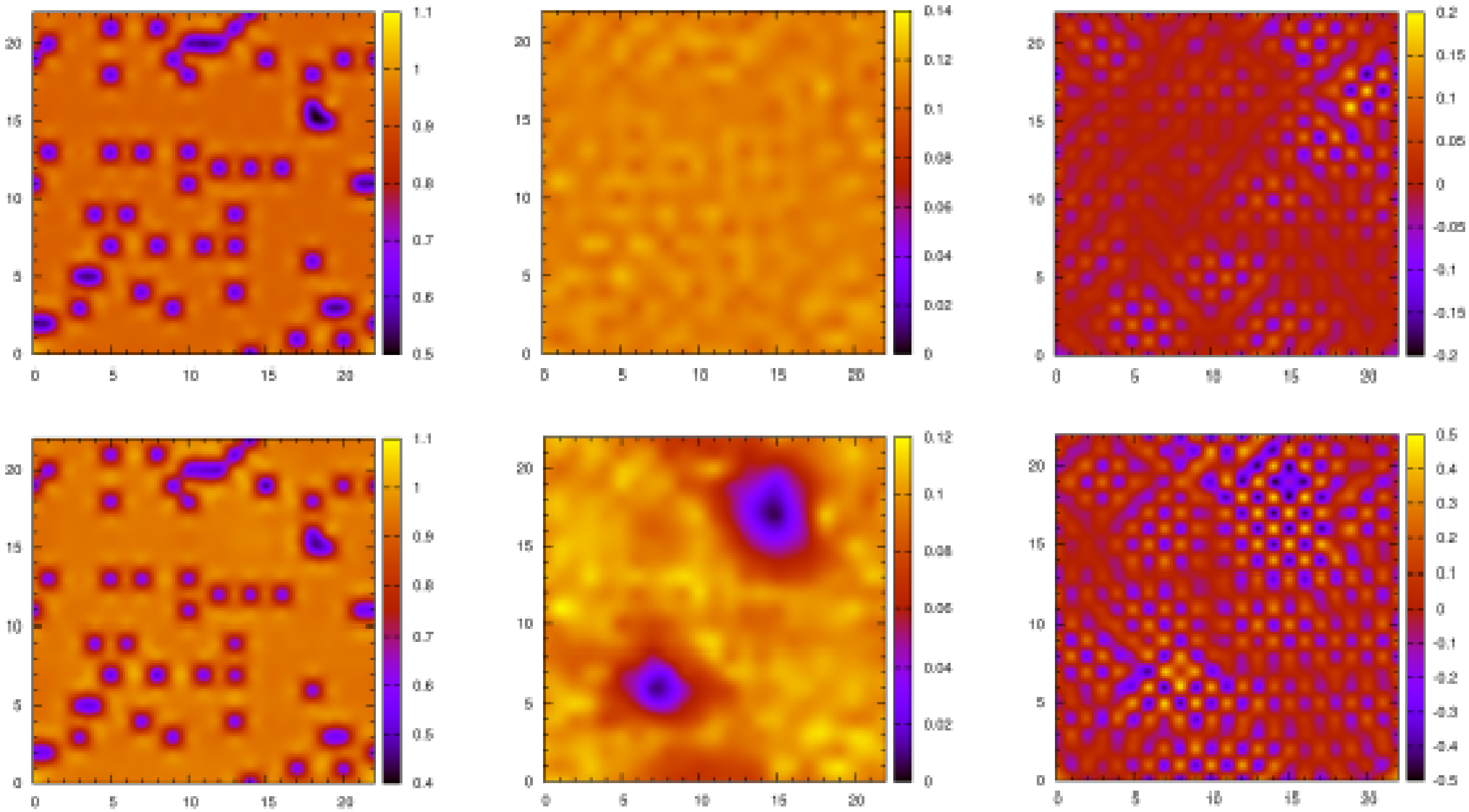
"Ordered" magnetic signal begins at T_c due to bound state formation

Combined Disorder & Field-Induced Antiferromagnetism

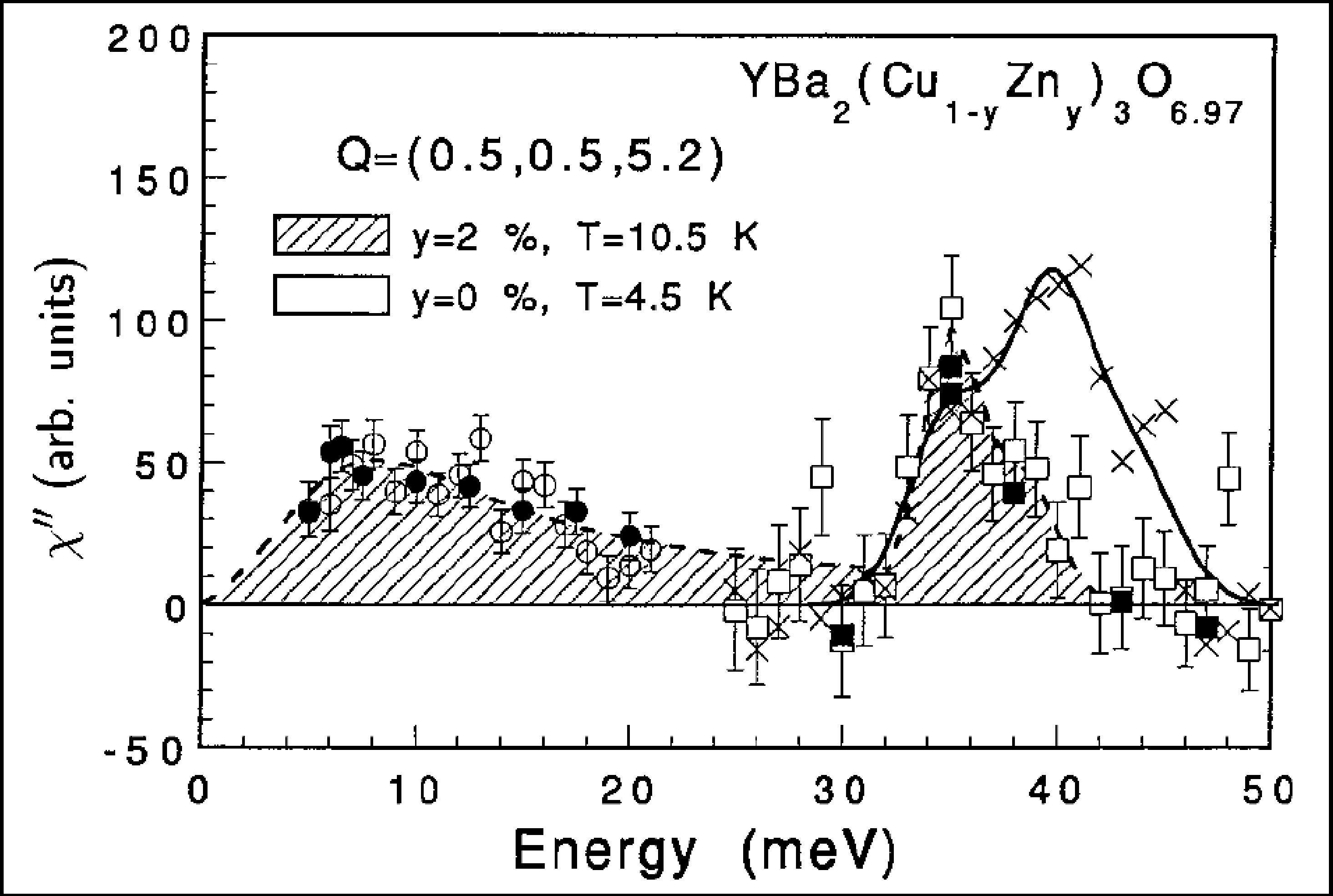
Charge Density | Order Parameter | Magnetization

$\Phi = 0$

$\Phi = 2\Phi_0$



Neutron response: freezing of spin fluctuations by disorder



Optimal doping: Zn shifts spectral weight to low ω,
no static ordering in YBCO Sidis et al 1996, 2000, 2001

Theory: freezing of spin fluctuations by disorder

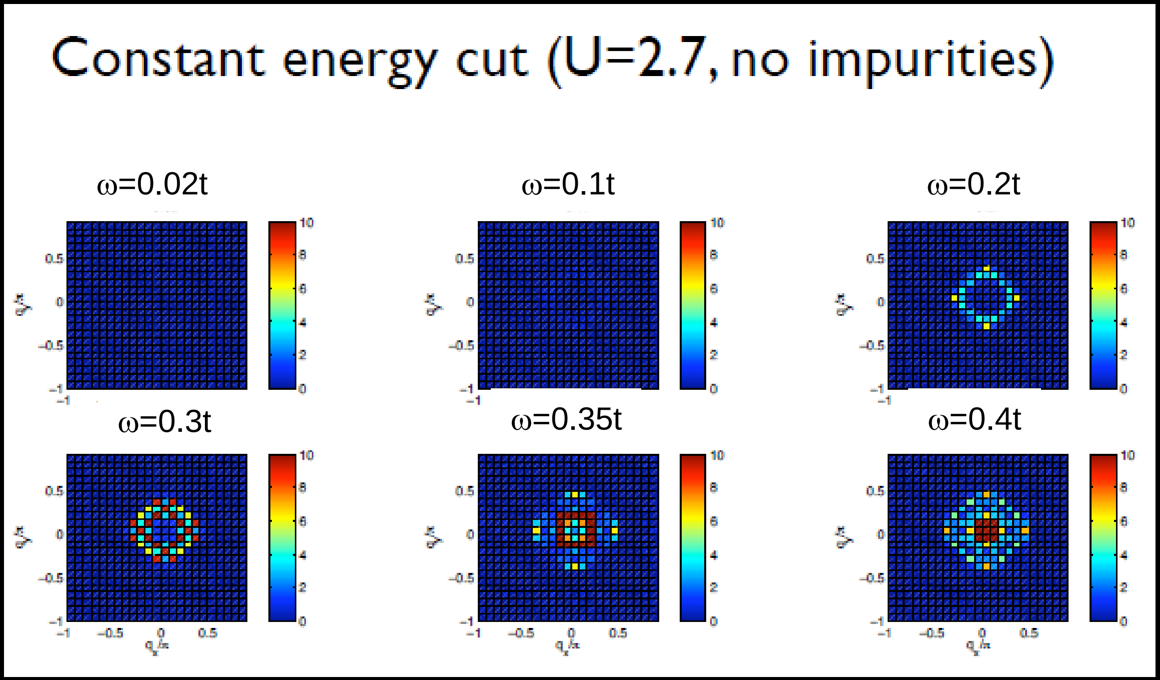
Dynamical susceptibility from BdG eigenvalues and eigenfunctions:

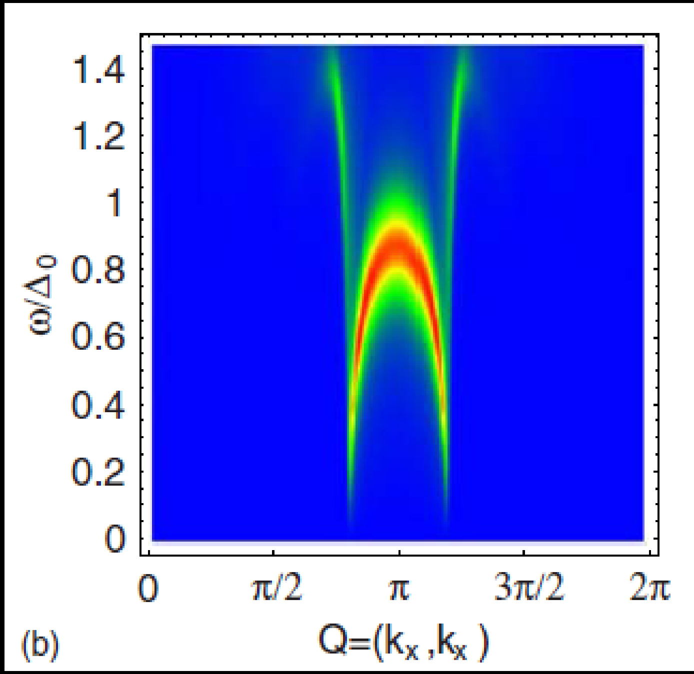
Graser, PH, Andersen 2009

$$
\begin{aligned}
&\chi(\vec{r}_i,\vec{r}_j) = \\
&\sum_{m,n,\sigma} u^*_{m,i\sigma} u_{n,i\sigma} \left(u^*_{n,j\sigma} u_{m,j\sigma} + v_{m,j\bar{\sigma}} v^*_{n,j\bar{\sigma}}\right) \frac{f(E_{m,\sigma}) - f(E_{n,\sigma})}{\omega + E_{m,\sigma} - E_{n,\sigma} + i0^+} \\
&- \sum_{m,n,\bar{\sigma}} v_{m,i\bar{\sigma}} v^*_{n,i\bar{\sigma}} \left(v_{n,j\bar{\sigma}} v^*_{m,j\bar{\sigma}} + u^*_{m,j\sigma} u_{n,j\sigma}\right) \frac{f(E_{m,\bar{\sigma}}) - f(E_{n,\bar{\sigma}})}{\omega + E_{n,\bar{\sigma}} - E_{m,\bar{\sigma}} + i0^+} \\
&+ \sum_{m,n,\sigma} v_{m,i\sigma} u_{n,i\sigma} \left(u^*_{n,j\sigma} v^*_{m,j\sigma} + u^*_{m,j\bar{\sigma}} v^*_{n,j\bar{\sigma}}\right) \frac{1 - f(E_{m,\sigma}) - f(E_{n,\sigma})}{\omega - E_{n,\sigma} - E_{m,\sigma} + i0^+} \\
&- \sum_{m,n,\sigma} u^*_{m,i\sigma} v^*_{n,i\sigma} \left(v_{n,j\sigma} u_{m,j\sigma} + v_{m,j\bar{\sigma}} u_{n,j\bar{\sigma}}\right) \frac{1 - f(E_{m,\sigma}) - f(E_{n,\sigma})}{\omega + E_{n,\sigma} + E_{m,\sigma} + i0^+}
\end{aligned}
$$

Neutron response: theory

Graser, PH, Andersen 2009

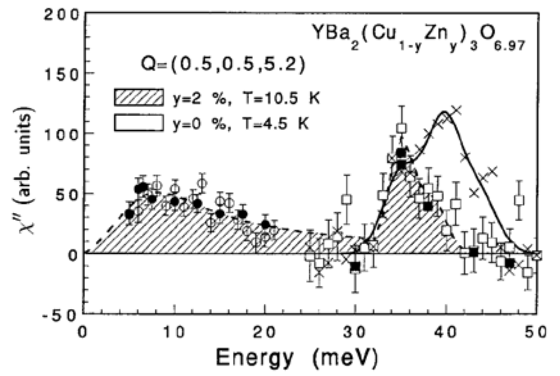




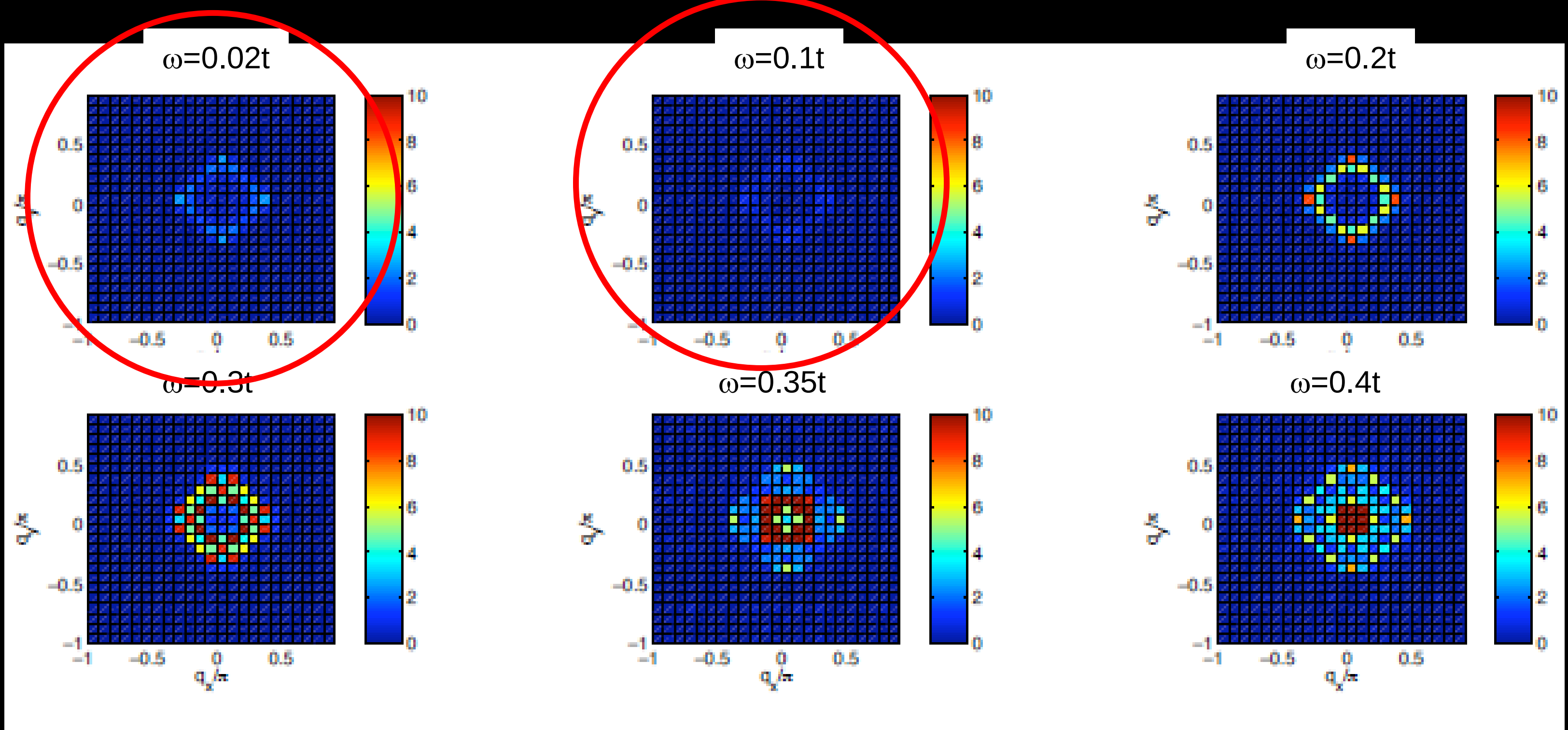
See e.g Eremin 2008

Neutron response: theory

Graser, PH, Andersen 2009



freezing of spin fluctuations by 1 impurity V=100t



Quasiparticles in presence of disordered magnetism

- qp’s may scatter with small q from weak magnetic fluctuations

- qp’s may reconstruct, or suffer intense Umklapp scattering, if sizeable regions of quasi-LR order are present

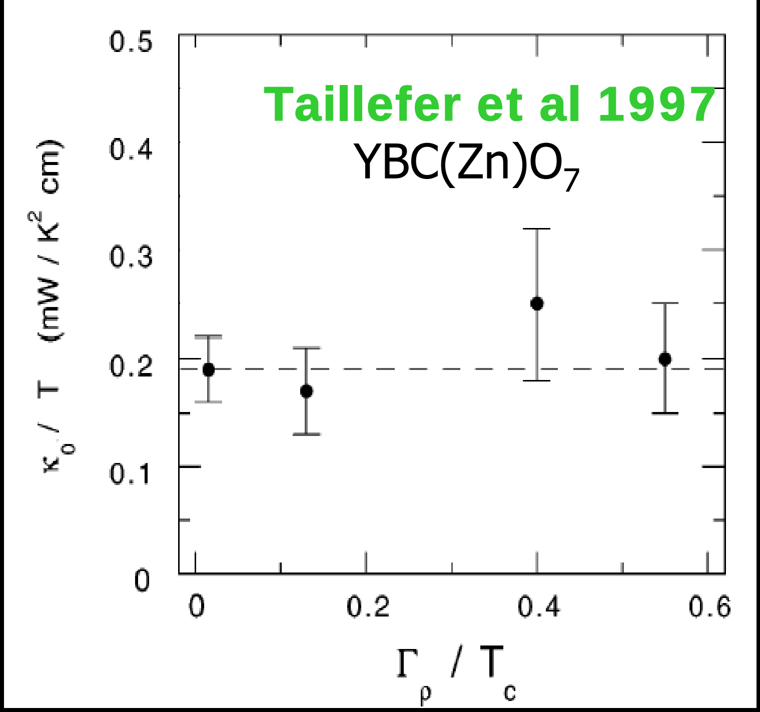
- Q: mean field theory overestimates order.

  Is the picture qualitatively the same for slow fluctuations?

Transport: breakdown of "universal" thermal conductivity

P.A. Lee 1993; Graf et al 1995

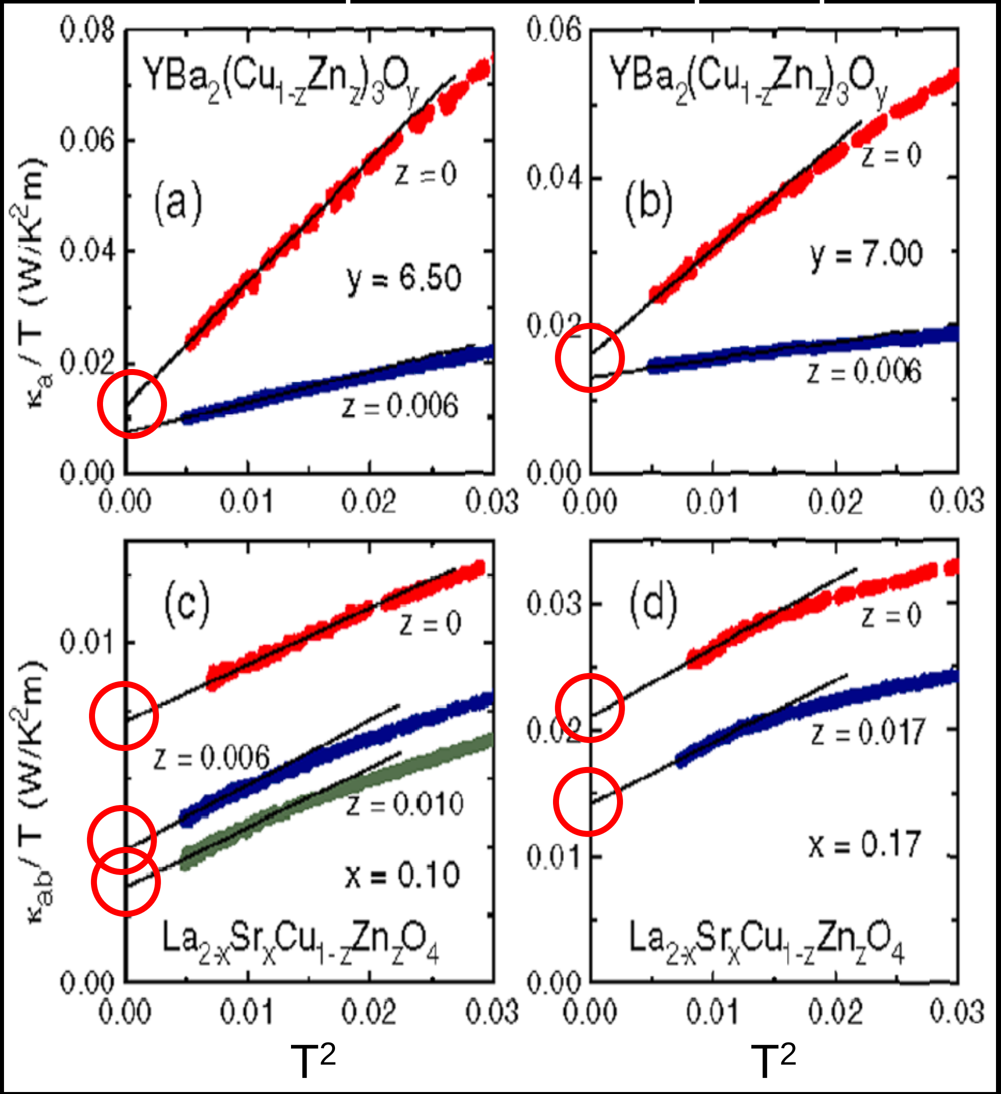
$$\frac{\kappa_0}{T} = \frac{k_B^2}{3\hbar}\,\frac{n}{c}\left(\frac{v_F}{v_2} + \frac{v_2}{v_F}\right)$$



Sun et al 2006

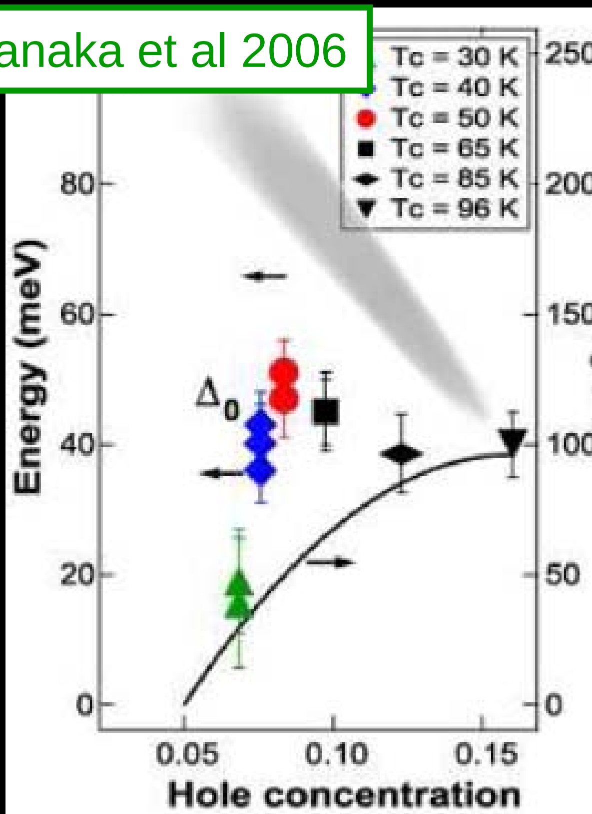
underdoped

~ opt. doped

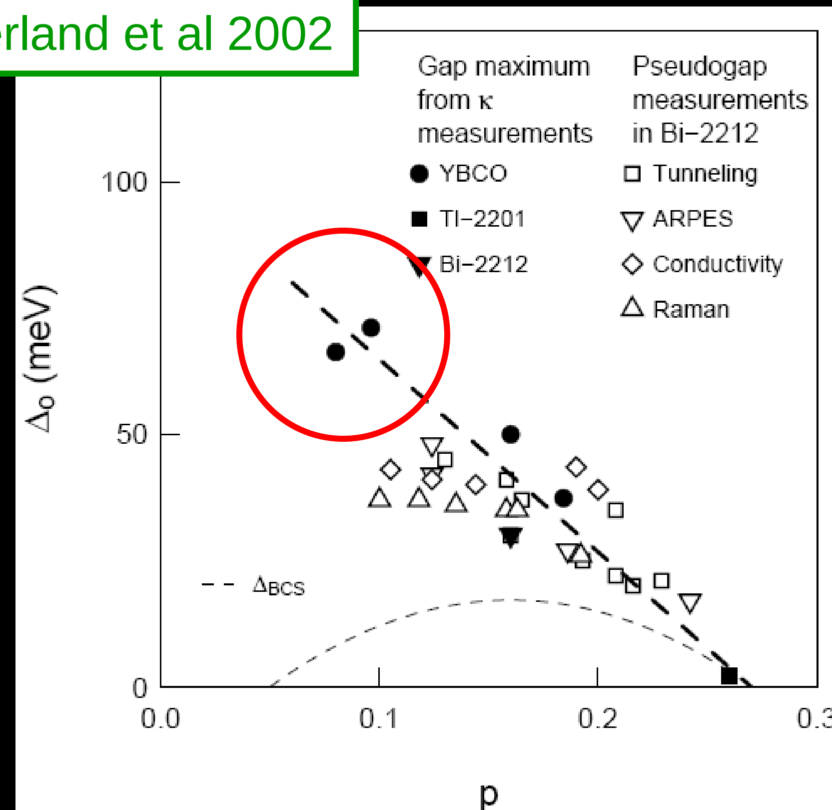


Importance for “2-gap” question

Tanaka et al 2006



Sutherland et al 2002



If κ isn’t universal, you can’t use it to extract gap velocity v_2!

How does disordered magnetism influence quasiparticles?

e.g, transport:

Bogoliubov-de Gennes eqns:

$$\mathcal{H} = \sum_{ij} \Phi_i^\dagger \begin{bmatrix} t_{ij} & \Delta_{ij} \\ \Delta_{ij}^\dagger & -t_{ij}^* \end{bmatrix} \Phi_j \, ,$$

Thermal conductivity

$$\kappa(T) = \frac{1}{2\pi\hbar T} \int dx \, x^2 \left(-\frac{\partial f}{\partial x} \right) \langle S_T(x) \rangle \, ,$$

Kernel

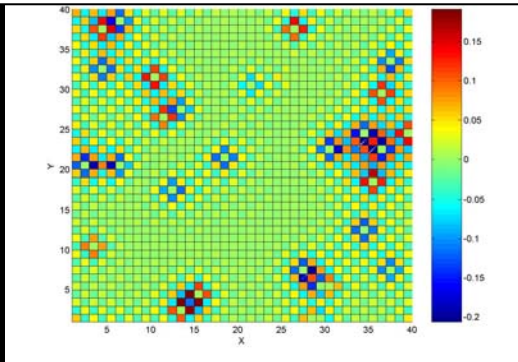
$$S_T(x) = \frac{2\pi^2\hbar^2}{N} \sum_{n,n'} |\langle \hat{v}_g \rangle_{nn'}|^2 \delta(x - E_n) \delta(E_n - E_{n'})$$

BdG mat. elts. of group velocity

BdG eigenvalues

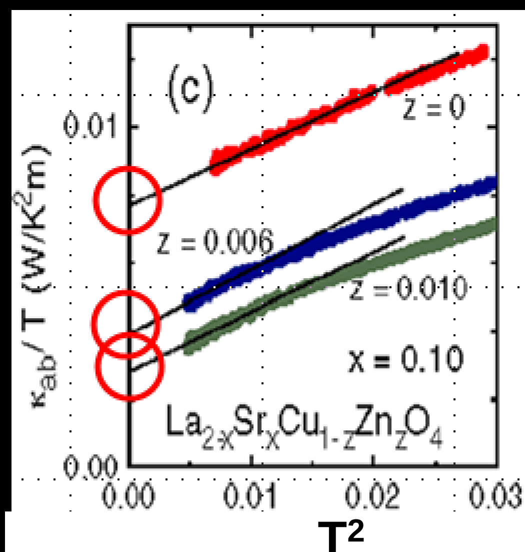
Thermal conductivity—why does κ_0 decrease as one underdopes?

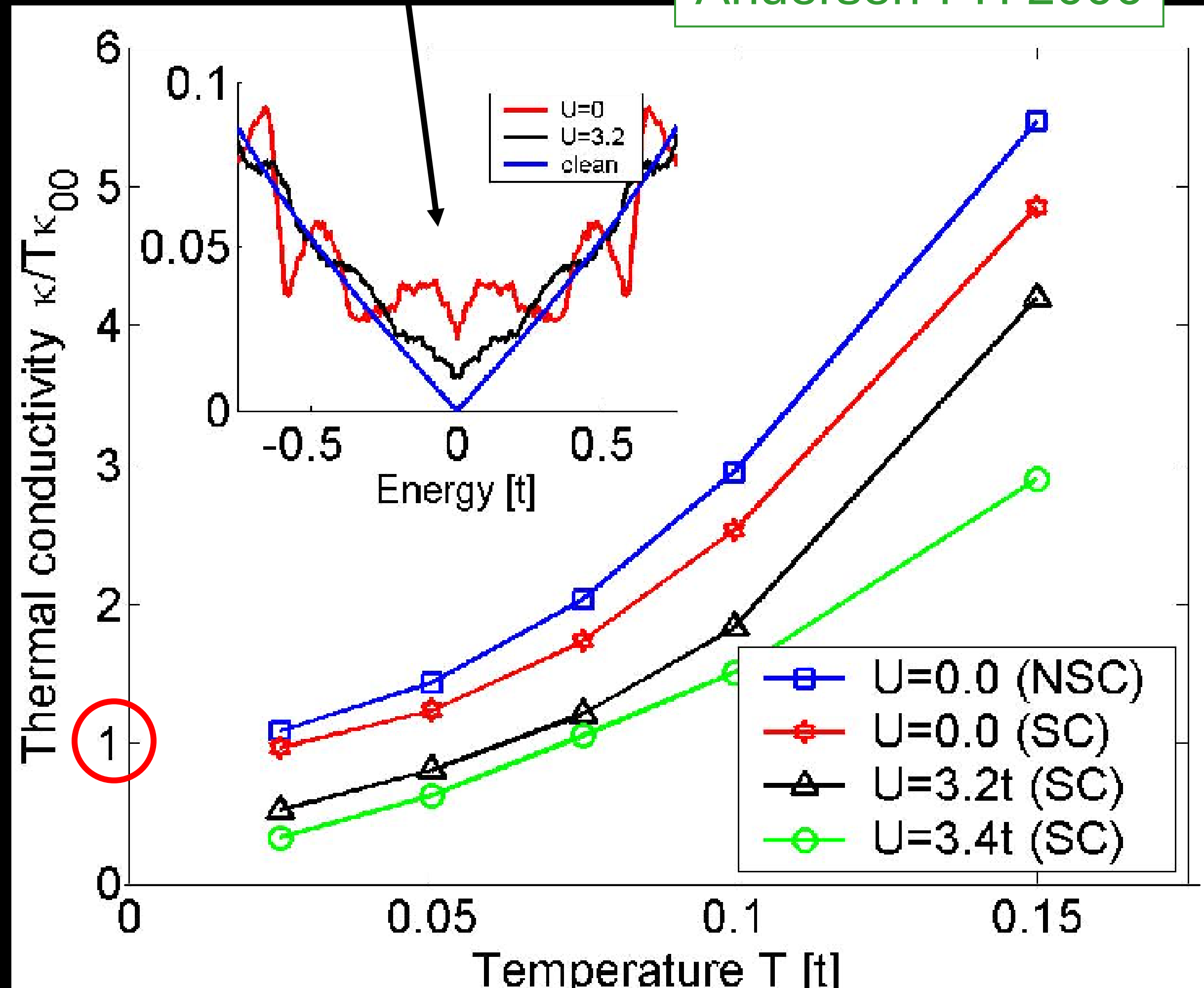
Magnetization: 2% disorder, U=3t



see also Garg et al 2008

Andersen-PH 2006





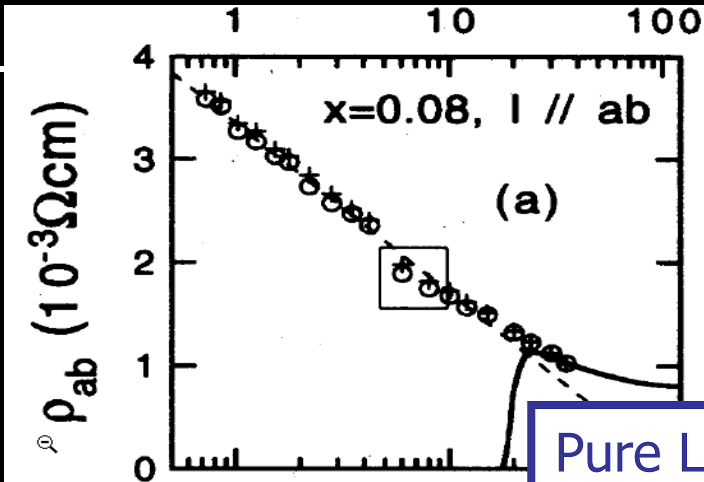
Sun et al 2006

low T suppression of κ(T)/T compared to universal value reproduced within present scenario. The origin is a reduced DOS at low energy.

Resistivity upturns:

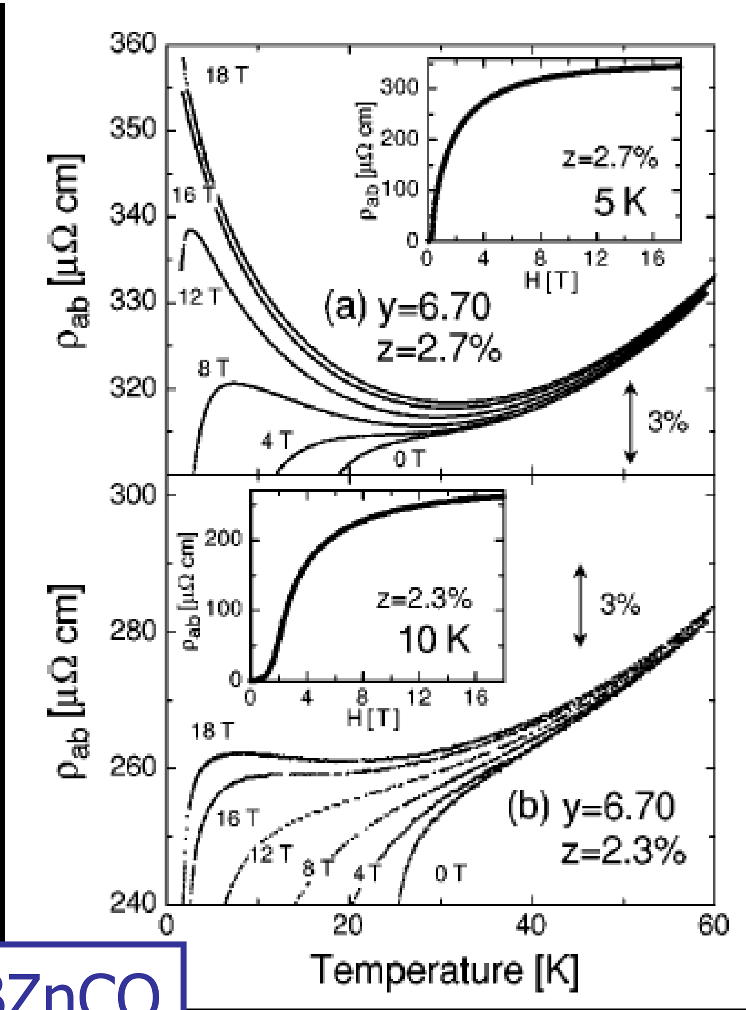
W. Chen, B. Andersen and PH, arXiv:0905.1449

Ando et al 1995

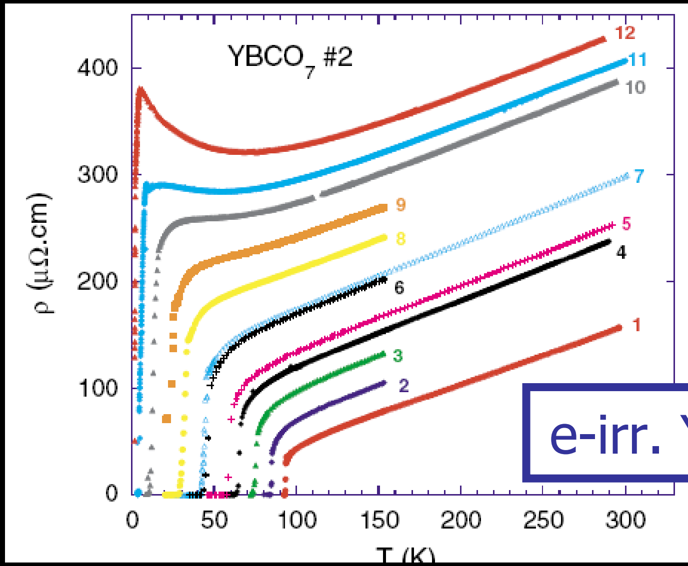


Pure LSCO

Segawa et al 1999



YBZnCO



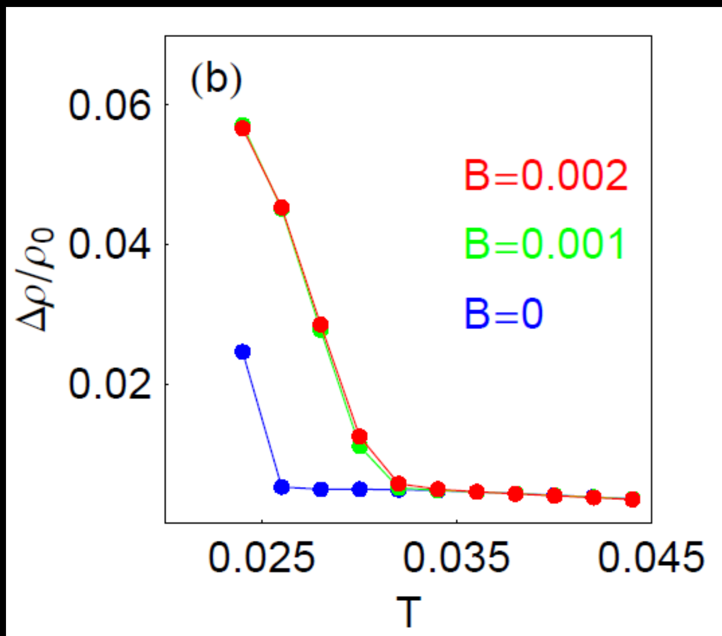
e-irr. YBCO

Rullier-Albenque et al 2003

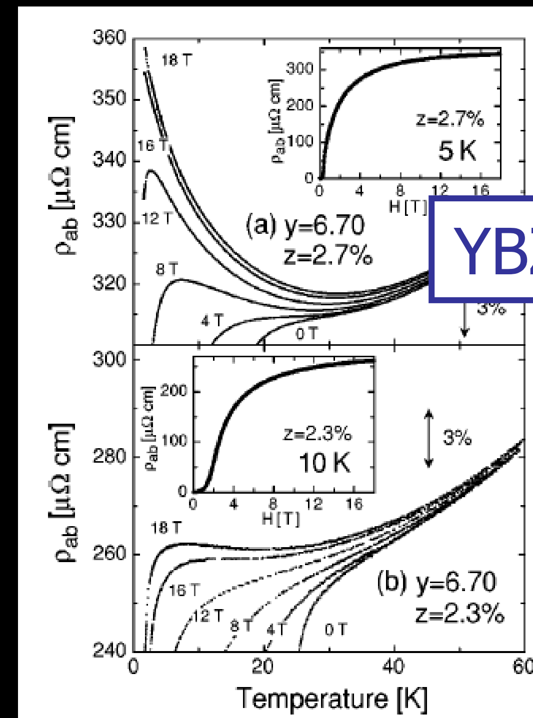
Resistivity upturns

W.Chen, B Andersen & PH 2009

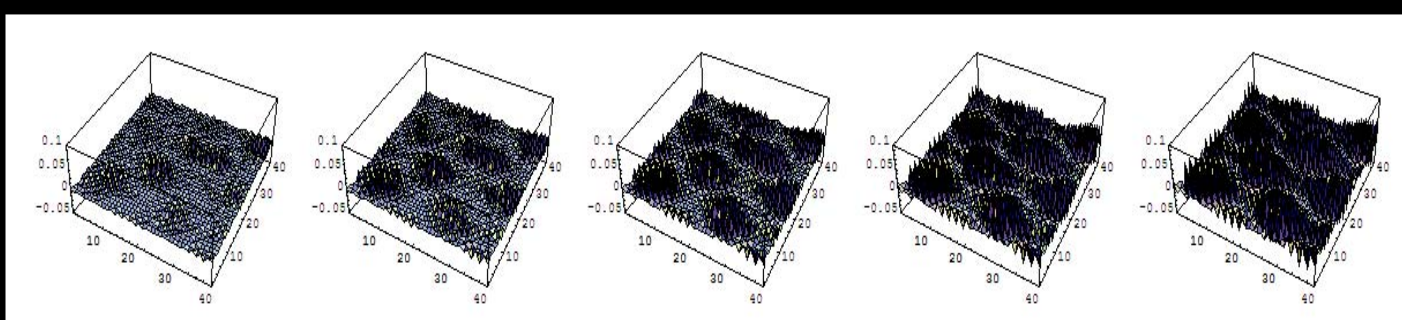
See also Kontani and Ohno 2006

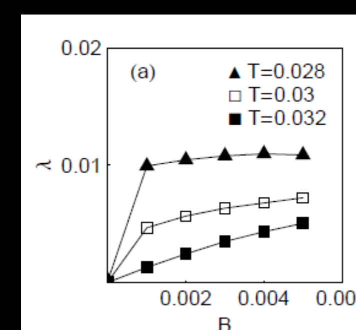


Segawa et al 1999



YBZnCO

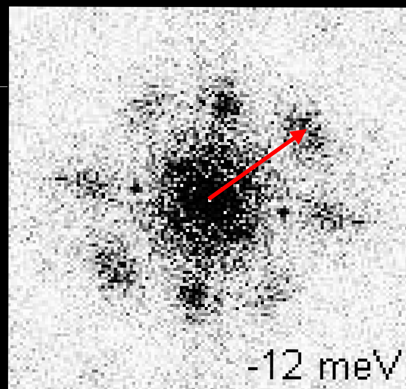


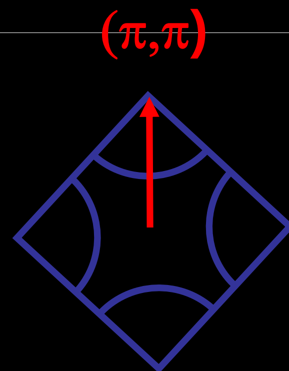


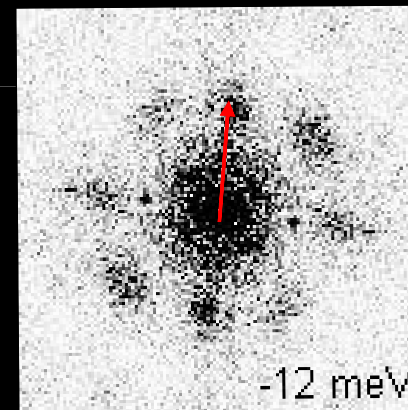
increasing B

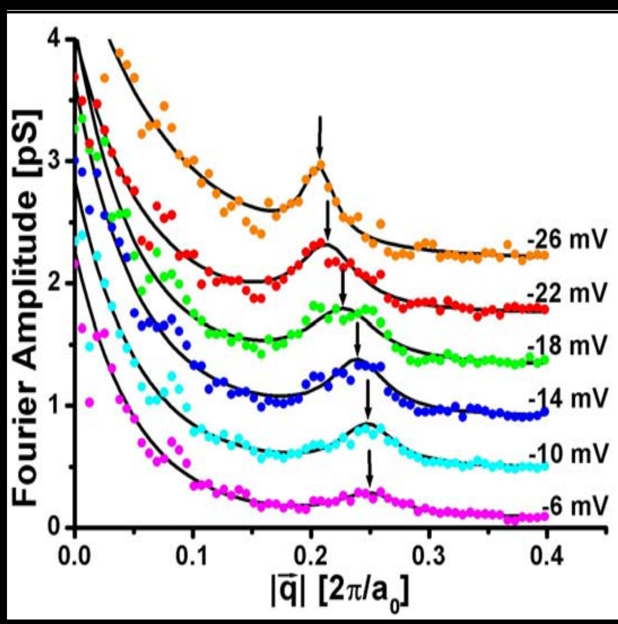
STS FT-LDOS on BSCCO-2212 surfaces

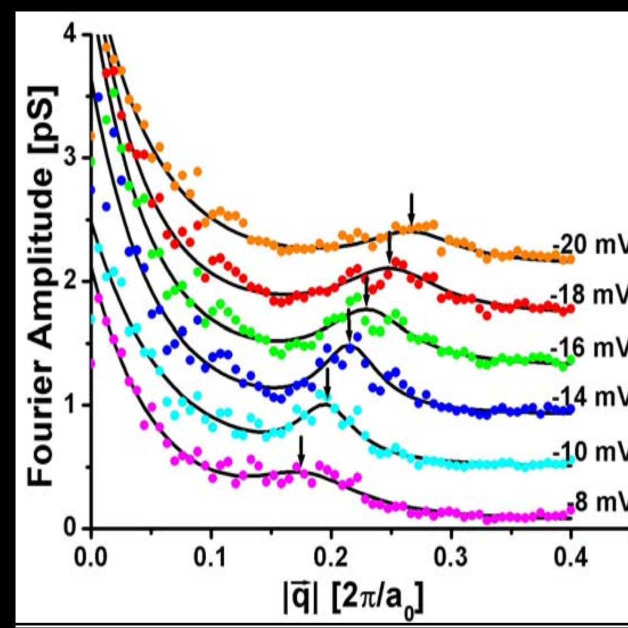
$$\rho(\vec{q},\omega)=\int\frac{d^2r}{(2\pi)^2}e^{i\vec{q}\cdot\vec{r}}\rho(\vec{r},\omega)$$











Hoffmann *et al.* (2002)

"Octet model": d-wave SC

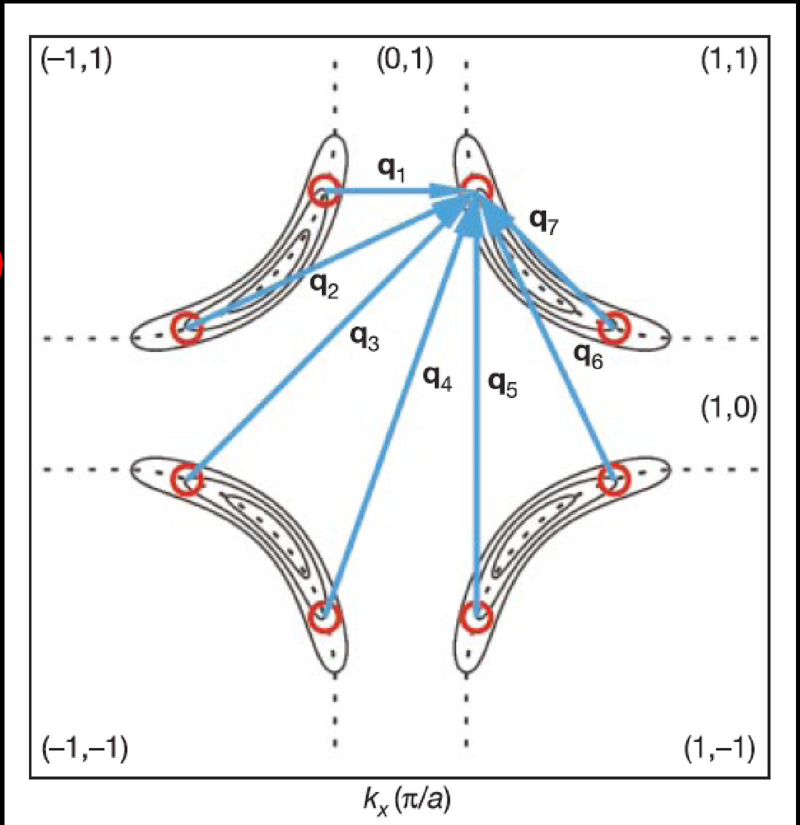
$$\rho(\vec{q},\omega)=\int\frac{d^2r}{(2\pi)^2}e^{i\vec{q}\cdot\vec{r}}\rho(\vec{r},\omega)$$

Quasiparticle dispersion in superconductor

$$E_\pm(\vec{k})=\pm\sqrt{\varepsilon(\vec{k})^2+\Delta(\vec{k})^2}$$

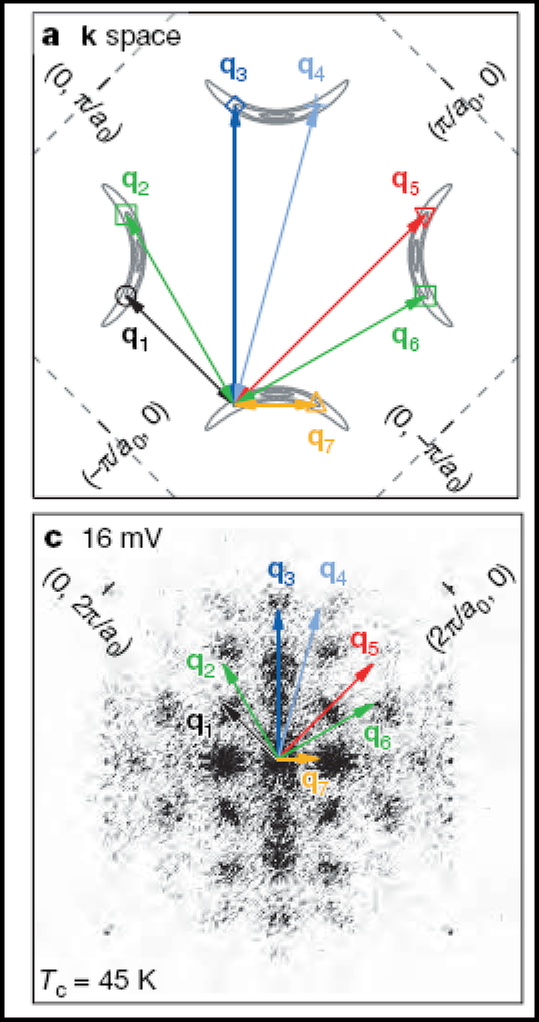
→ For d-wave superconductor LDOS largest at tip of bananas (octet-model) (er…not true)

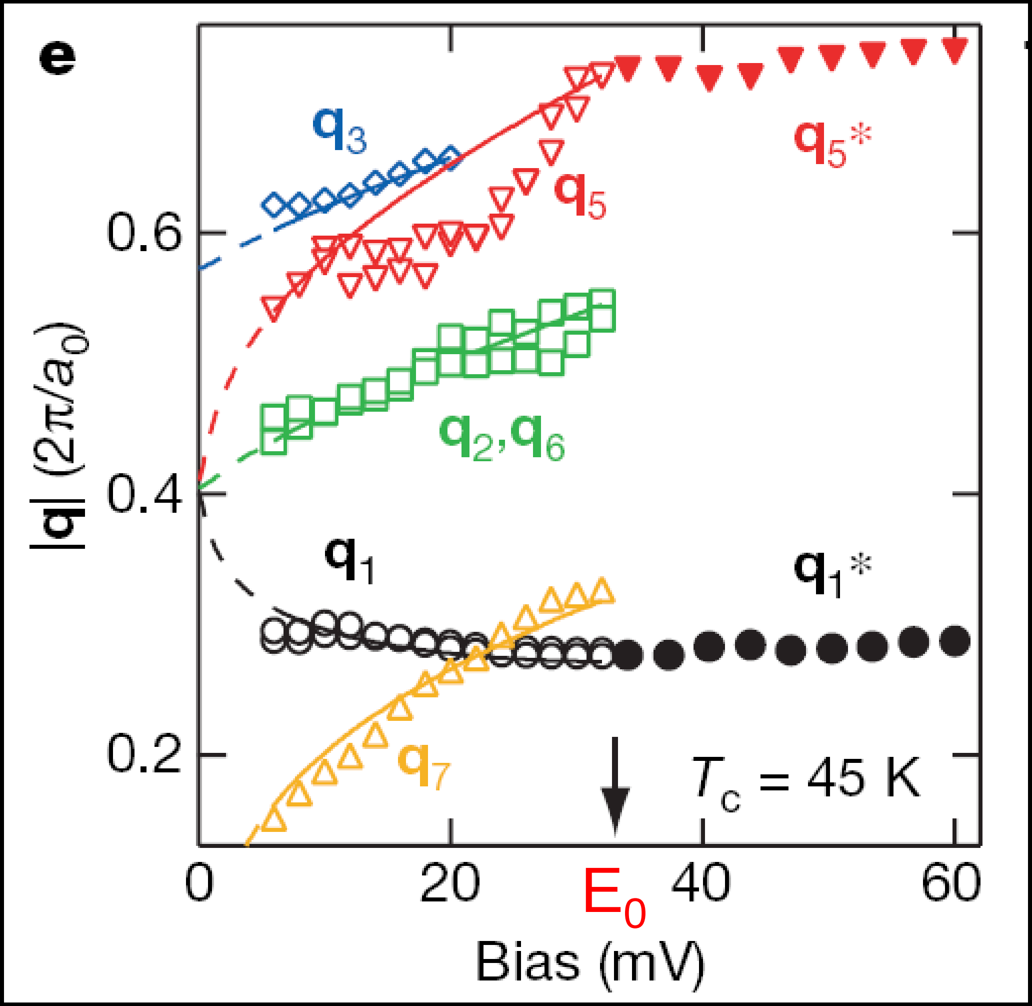
→ Expect peaks in FT-LDOS at wavevectors connecting banana tips (yes)



Extinction of QPI peaks at critical energy E_0 in underdoped samples

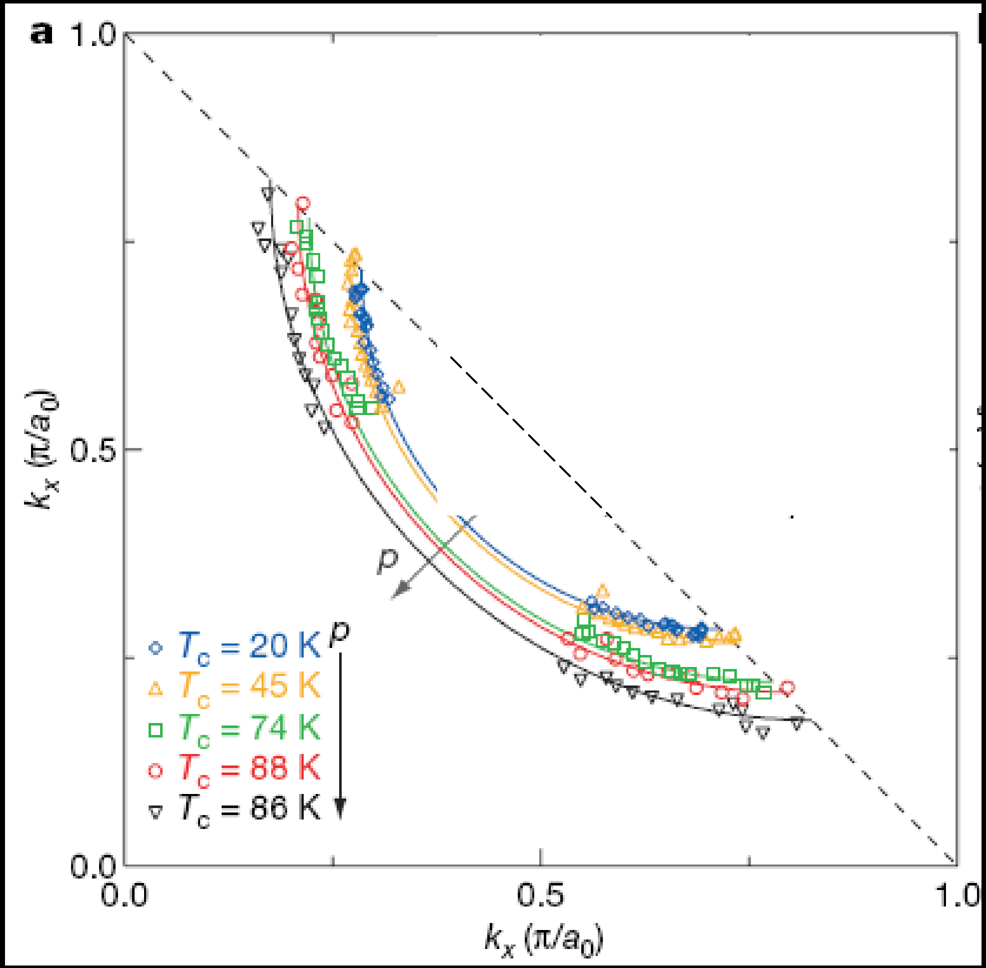
Details of Kohsaka et al 2008: QPI on underdoped Bi-2212





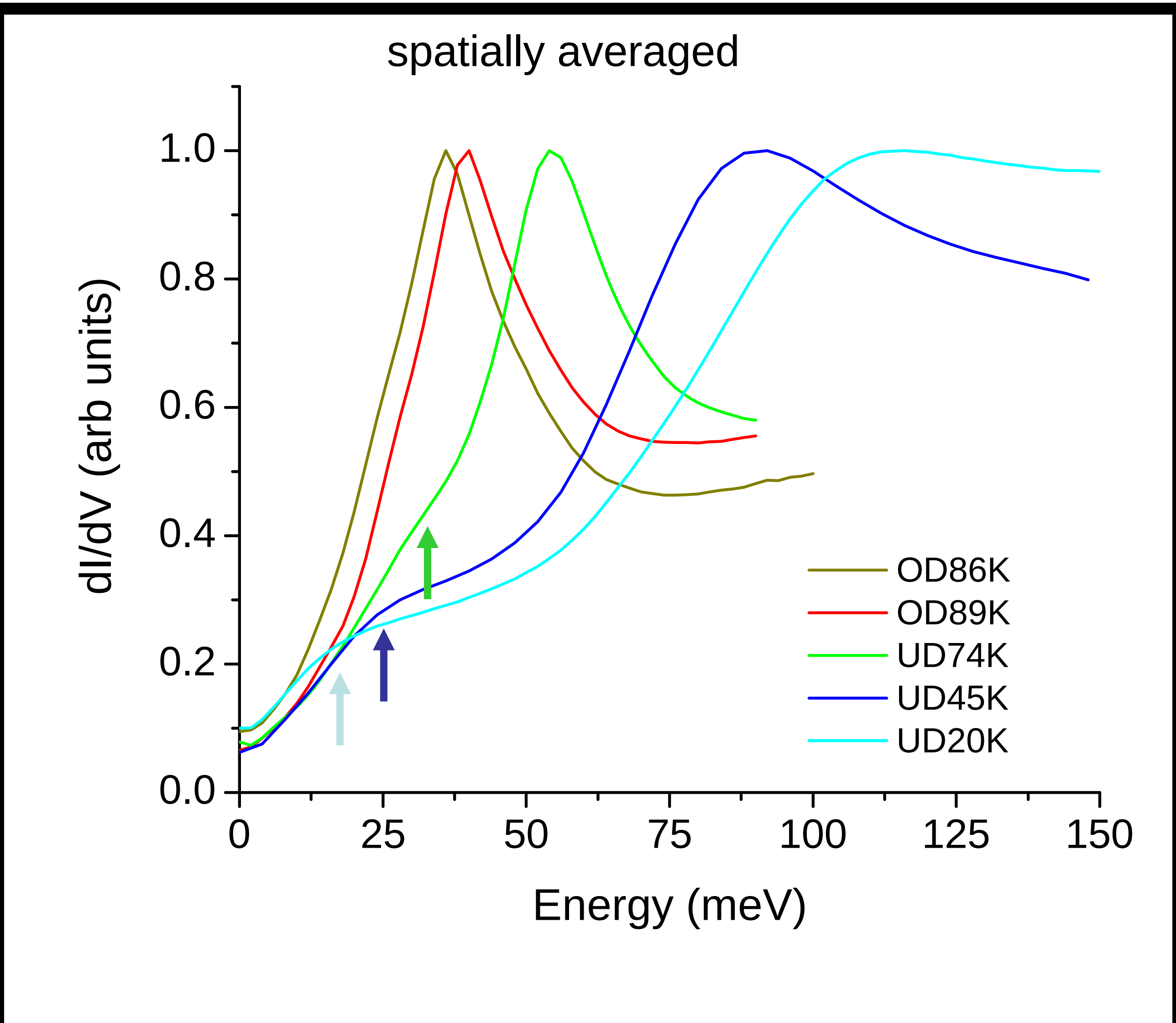
QPI and AF order

Kohsaka et al: intense scattering near antinode?



But:weak disorder scattering or AF spin fluct scattering not sufficient:
Graser et al 2008

“STS kink energy”



Model: coexisting AF+dSC

B.M. Andersen and PH 2008

$$H = \sum_{\mathbf{k}\sigma} [\epsilon(k) - \mu]\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{k} \left[\sum_{\sigma} \sigma M c^\dagger_{\mathbf{k}+\mathbf{Q}\sigma} c_{\mathbf{k}\sigma} + \Delta(k) c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \right] + \mathrm{H.c.},$$

$$= \sum_{k} \psi^\dagger_{\mathbf{k}} A(k) \psi_{\mathbf{k}}$$

$$A(k) = \begin{pmatrix} \epsilon_1(k) + \epsilon_2(k) - \mu & M & \Delta(k) & 0 \\ M & -\epsilon_1(k) + \epsilon_2(k) - \mu & 0 & -\Delta(k) \\ \Delta^*(k) & 0 & -\epsilon_1(k) - \epsilon_2(k) + \mu & M \\ 0 & -\Delta^*(k) & M & \epsilon_1(k) - \epsilon_2(k) + \mu \end{pmatrix}$$

eigenenergies

$$E_{1,2}(k) = \sqrt{\left([\epsilon_2(k) - \mu] \pm \sqrt{\epsilon_1^2(k) + M^2} \right)^2 + \Delta^2(k)},$$

$$\epsilon_1(k) = 2t\,(\cos k_x + \cos k_y)\,,$$
$$\epsilon_2(k) = 4t' \cos k_x \cos k_y + 2t'' (\cos 2k_x + \cos 2k_y)$$

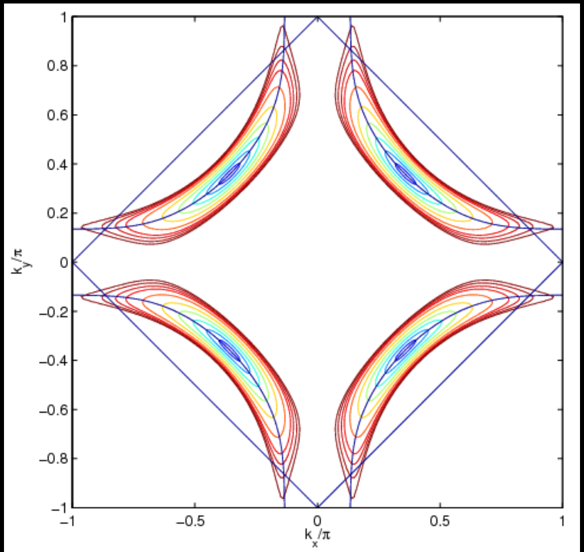
add impurities:

$$H_{imp} = \sum_{\mathbf{k},\mathbf{k}' \in RBZ} \psi^\dagger_{\mathbf{k}} V(k,k') \psi_{\mathbf{k}'}$$

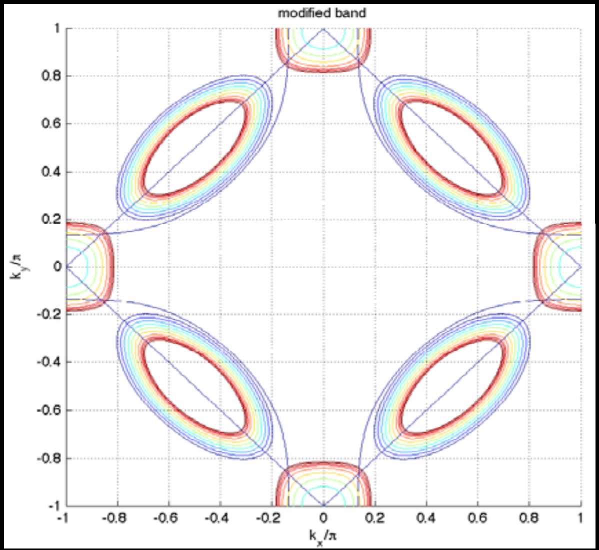
$$V(k,k') = V \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & -1 & -1 \end{pmatrix}$$

FT-STS from dsC vs. dSC+AF

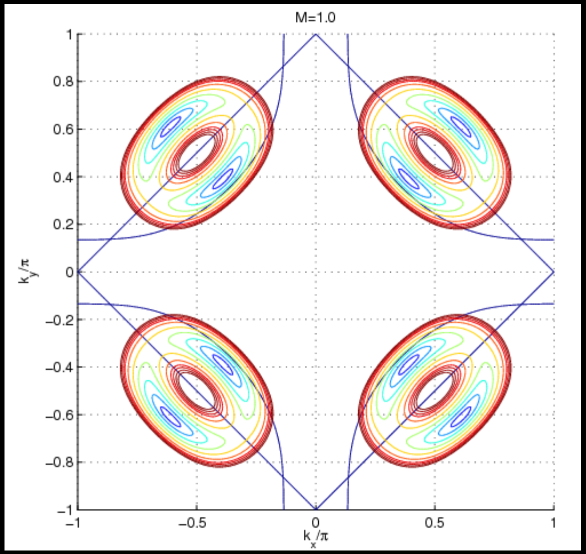
I. Contours of constant energy (CCE)



dSC



AF



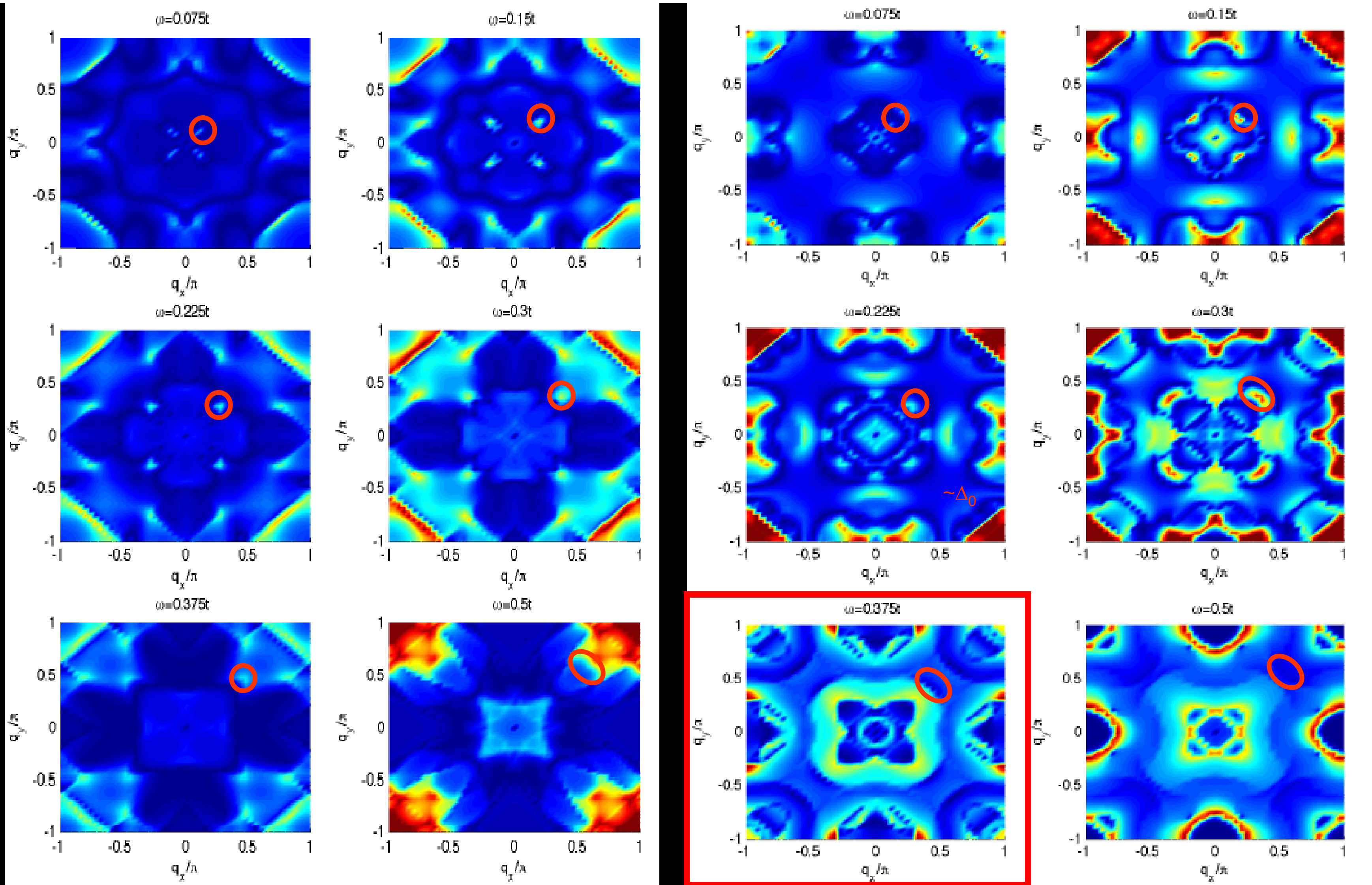
dSC+AF

In mixed case, CCE's "remember" dSC state until critical energy E_0

FT-STS from dSC vs. dSC+AF

III. Destruction of localized q-spots by AF order
due to different coherence factors in AF state

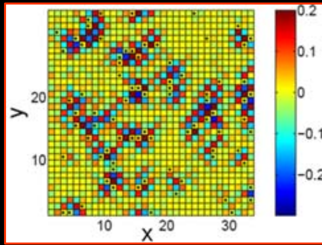
Δ=0.6t M=0

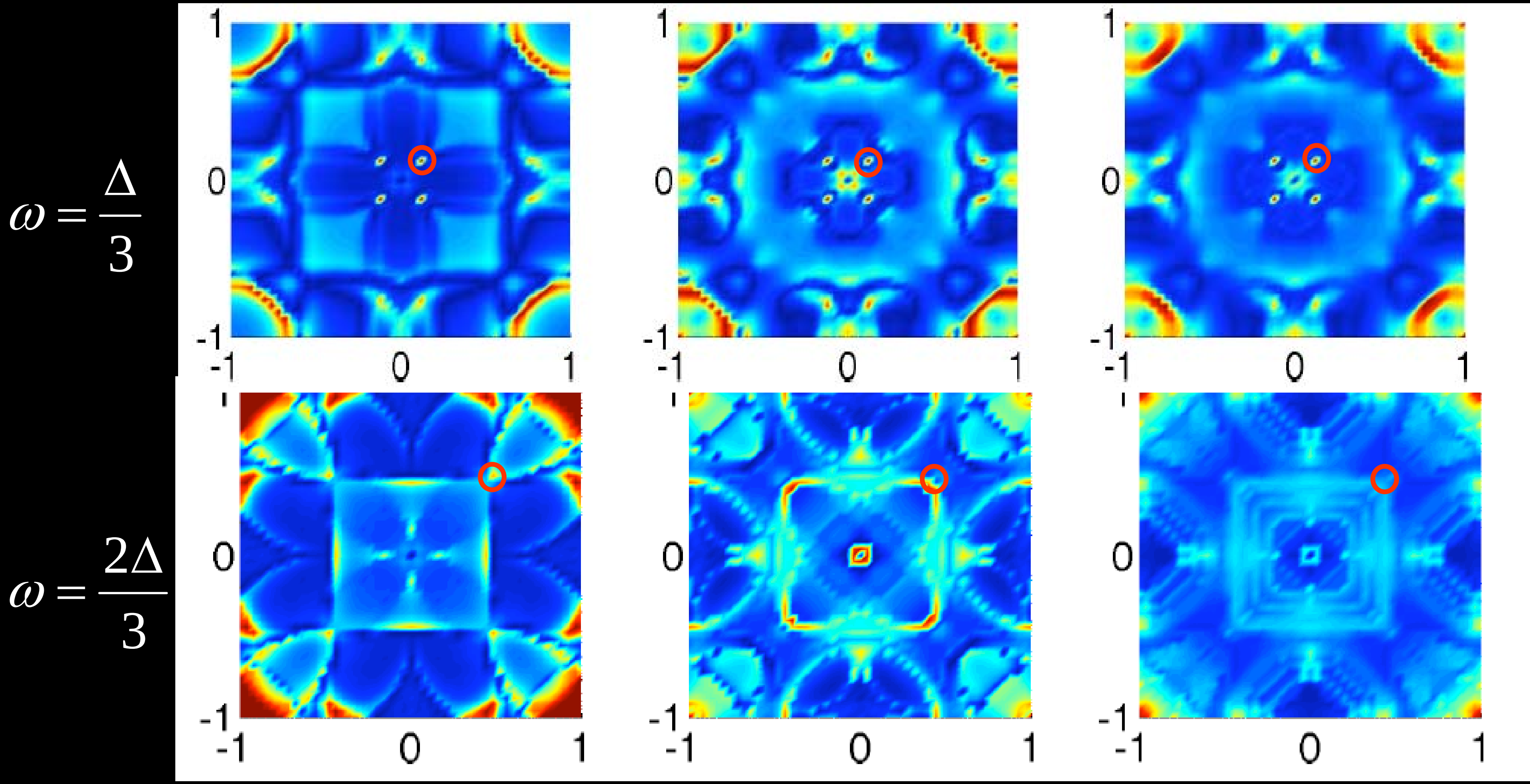


Δ=0.6t M=1t

FT-STS from dsC vs. dSC+AF

IV simulate effect of short range nature of AF state





dwSC

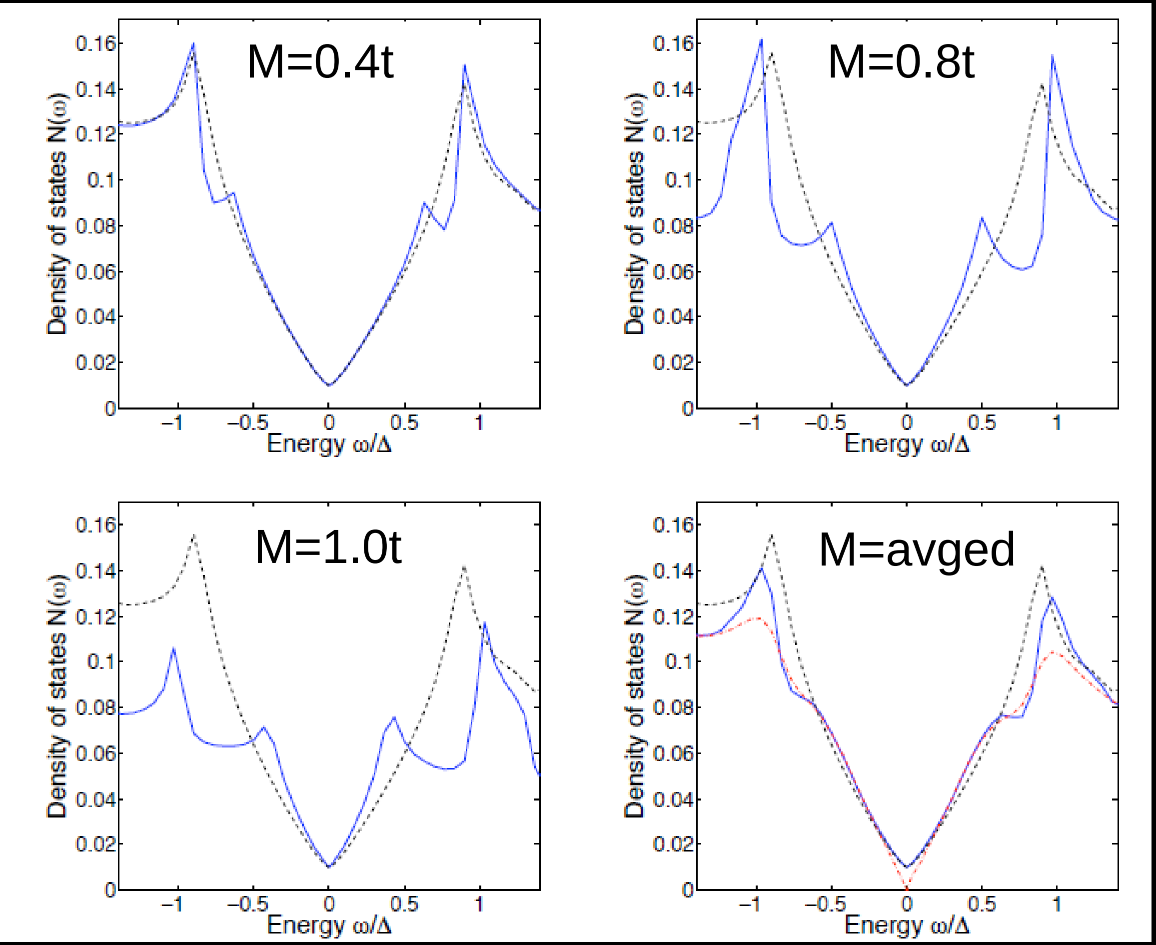
dwSC + AF

dwSC + AF averaged

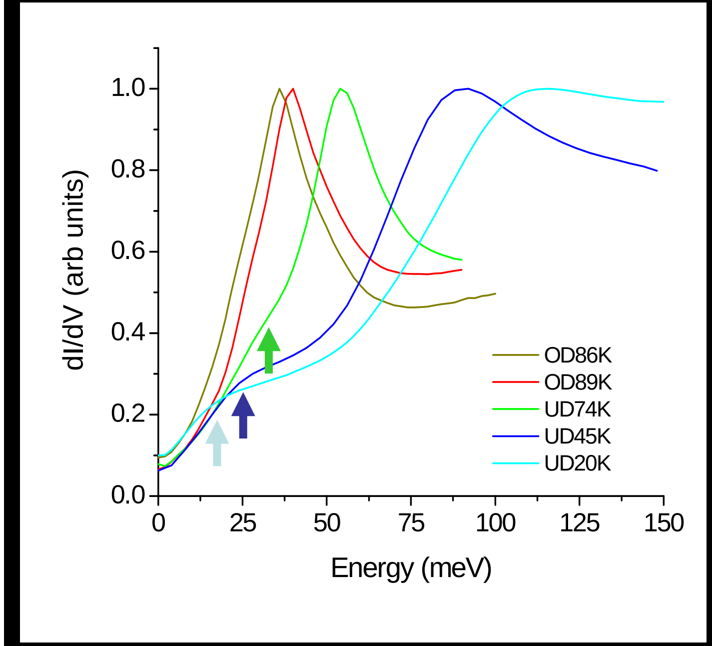
More realistic simulations of disorder-induced magnetic landscape needed

Effect on LDOS

- What happens when E=critical E_0?



Alldredge et al STS kink



Conclusions

- “Intrinsically disordered” cuprates exhibit spin glassy behavior coexisting with d-wave state $\Rightarrow$ scattering from disordered magnetic droplets explains many expts.:

  -- Broadening of NMR lines in YBCO by Zn, Li

  -- Effect of disorder on static magnetism, dynamic neutron response

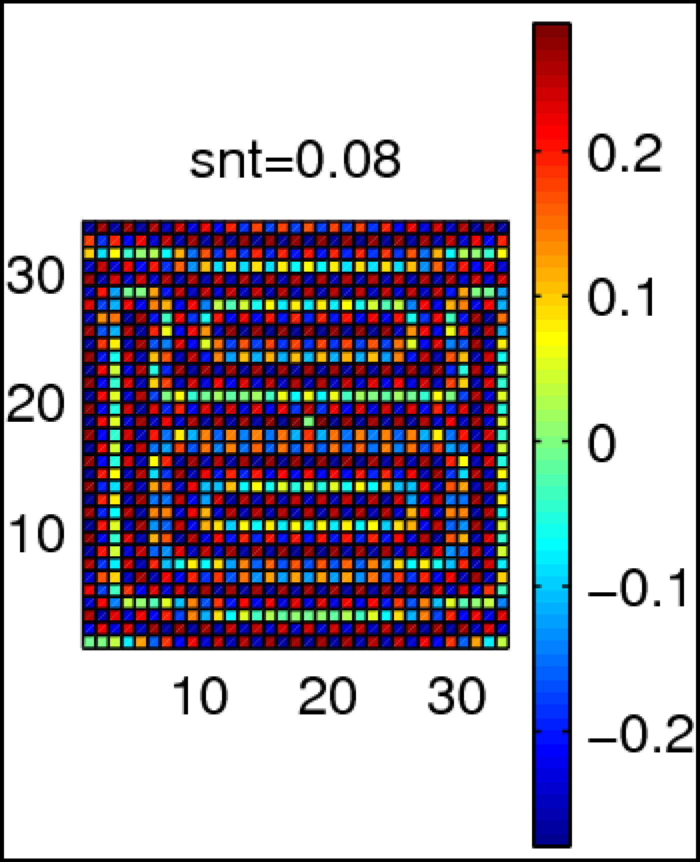
  -- Resistivity upturns in metallic samples

  -- Nonuniversal suppression of thermal conductivity in underdoped samples

  -- Disappearance of QPI and appearance of DOS kink feature appears in DOS when CCE’s touch zone face

- Questions:
  - relation to stripes
  - does charge order follow or lead?

Stripes?



This model: disordered stripes are stabilized for large U

Possible: crossover from droplets to disordered stripes with underdoping