Spin dynamics in high-Tc superconductors using neutron scattering technique

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Collaborators:

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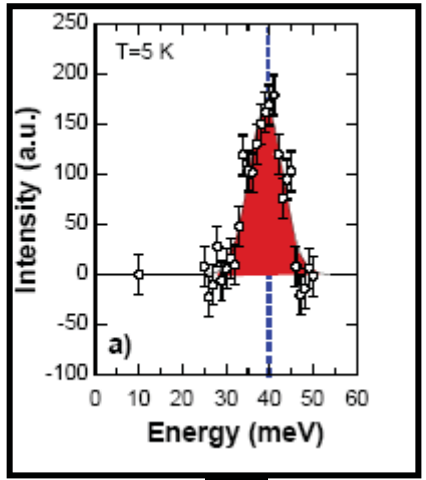
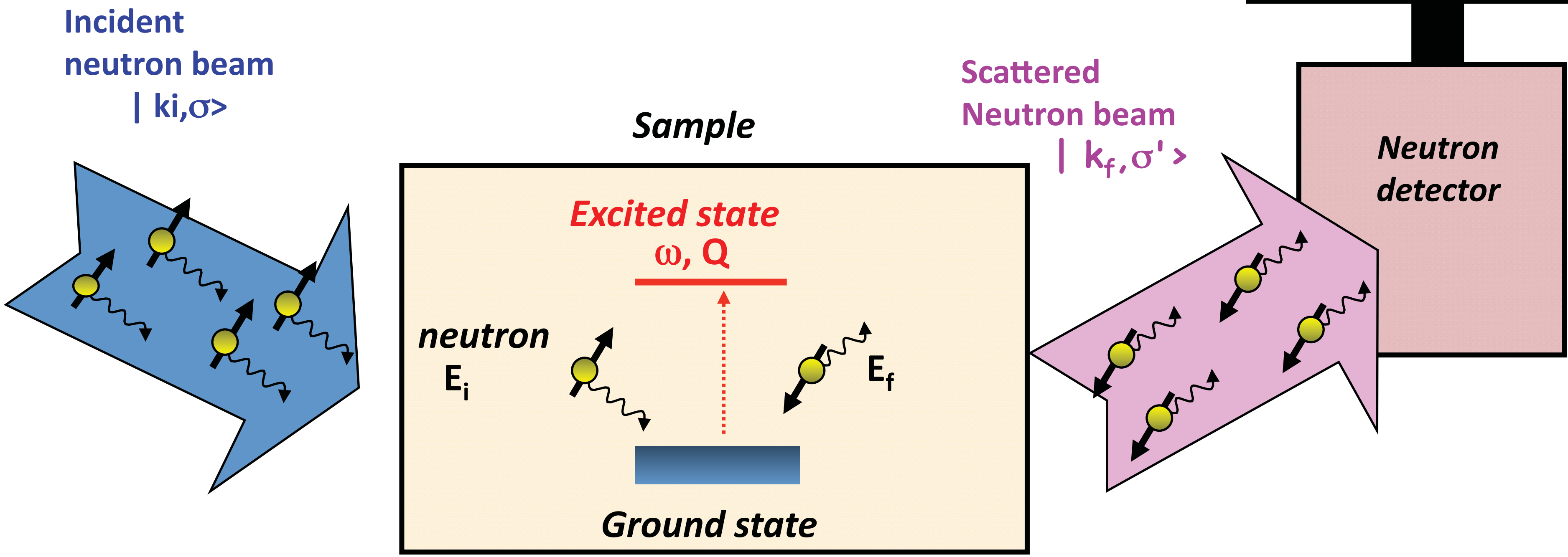
- CENG: *L. P. Regnault*
- ILL: *A. Ivanov, L. Capogna*
- CRETA: *X. Chaud*
- LEMA: *I. Laffez, F. Giovanelli, S. de Almeida*

Neutron scattering technique





Neutron scattering technique can probe what spins do as a function of space and time

Neutron scattering technique: *Magnetic scattering from unpaired electrons*

Kinematic constraints

$$\begin{cases} \vec{k}_i - \vec{k}_f = \vec{Q} \\ Ei - Ef = \hbar\omega \end{cases}$$

Magnetic scattering: partial differential cross-section

$$\frac{d^2\sigma}{d\Omega d\omega} = r_0^2 \frac{k_f}{k_i} |f(\vec{Q})|^2 \exp(-2W(\vec{Q})) \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \frac{Q^\alpha Q^\beta}{Q^2}) S^{\alpha\beta}(\vec{Q}, \omega)$$

Orientation factor
only magnetic components perpendicular to Q contribute

Magnetic form factor

Debye-Waller factor

Magnetic structure factor= S(Q,ω) = FT. of the spin-spin correlation function

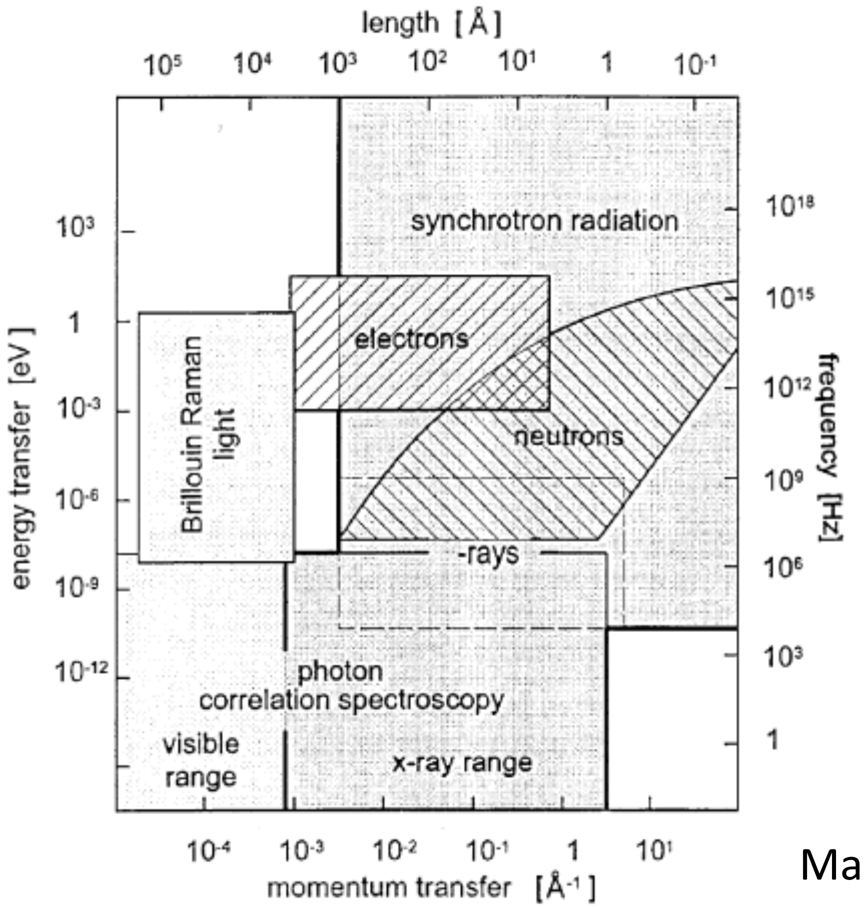
$$S^{\alpha\beta}(\vec{Q}, \omega) = \frac{1}{2\pi} \sum_{i,j} \exp(-i\vec{Q}.(\vec{R}_i - \vec{R}_j)) \int dt < S_i^\alpha(0) S_j^\beta(t) > \exp(i\omega t)$$

Fluctuation dissipation theorem

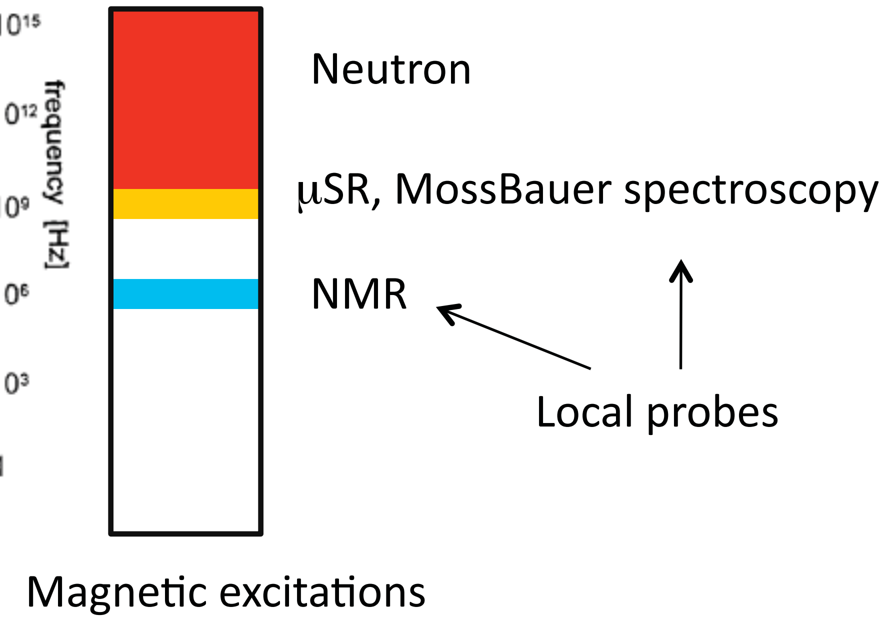
$$S^{\alpha\beta}(\vec{Q}, \omega) = \frac{1 + n(\omega, T)}{\pi} \frac{\chi''_{\alpha,\beta}(\vec{q}, \omega)}{(g\mu_B)^2}$$

Neutron energy and wave length

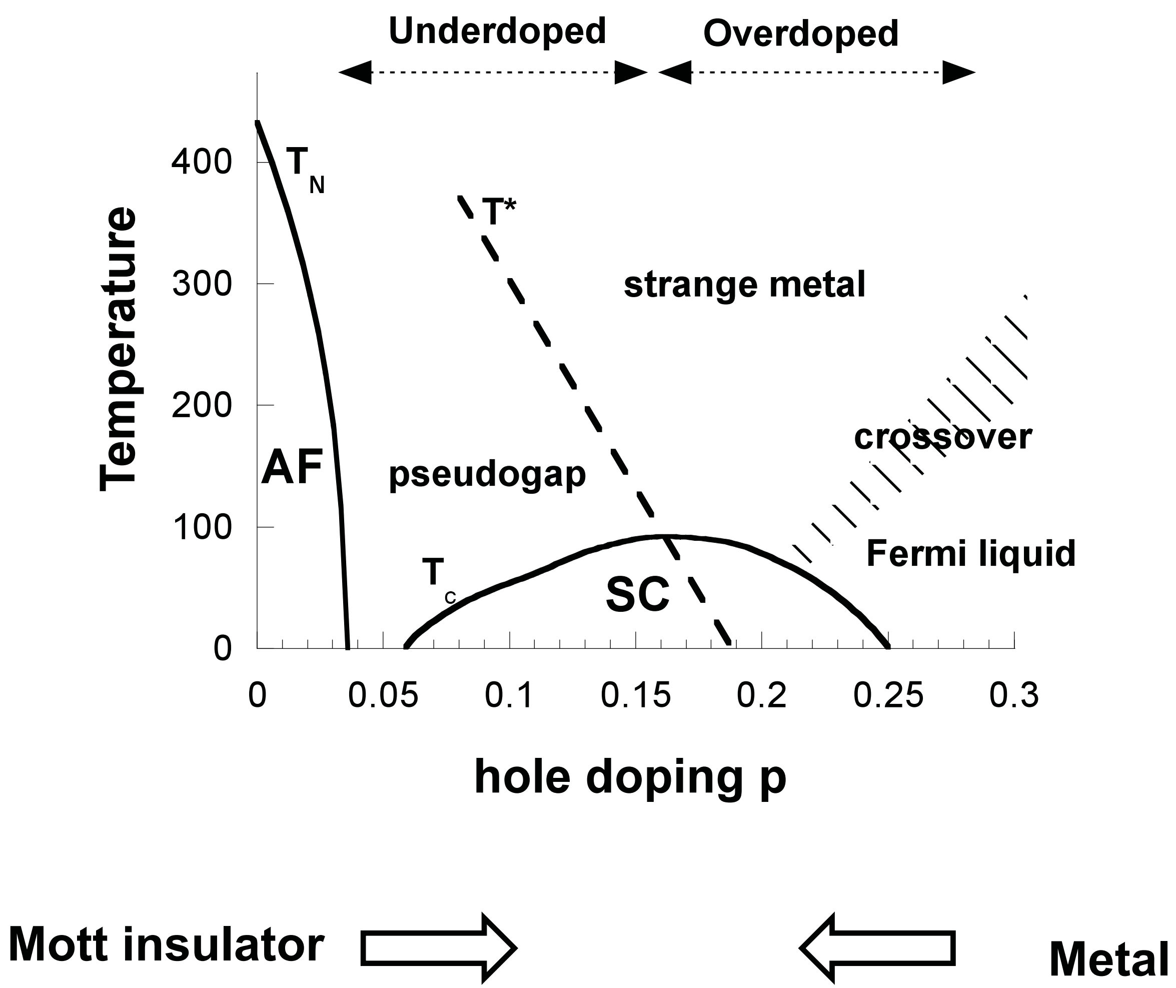
Neutron spectroscopy can be used to probe the nuclear and magnetic structures of a sample and the related nuclear and magnetic excitations. This is a <u>bulk</u> and <u>non destructive</u> measurement.



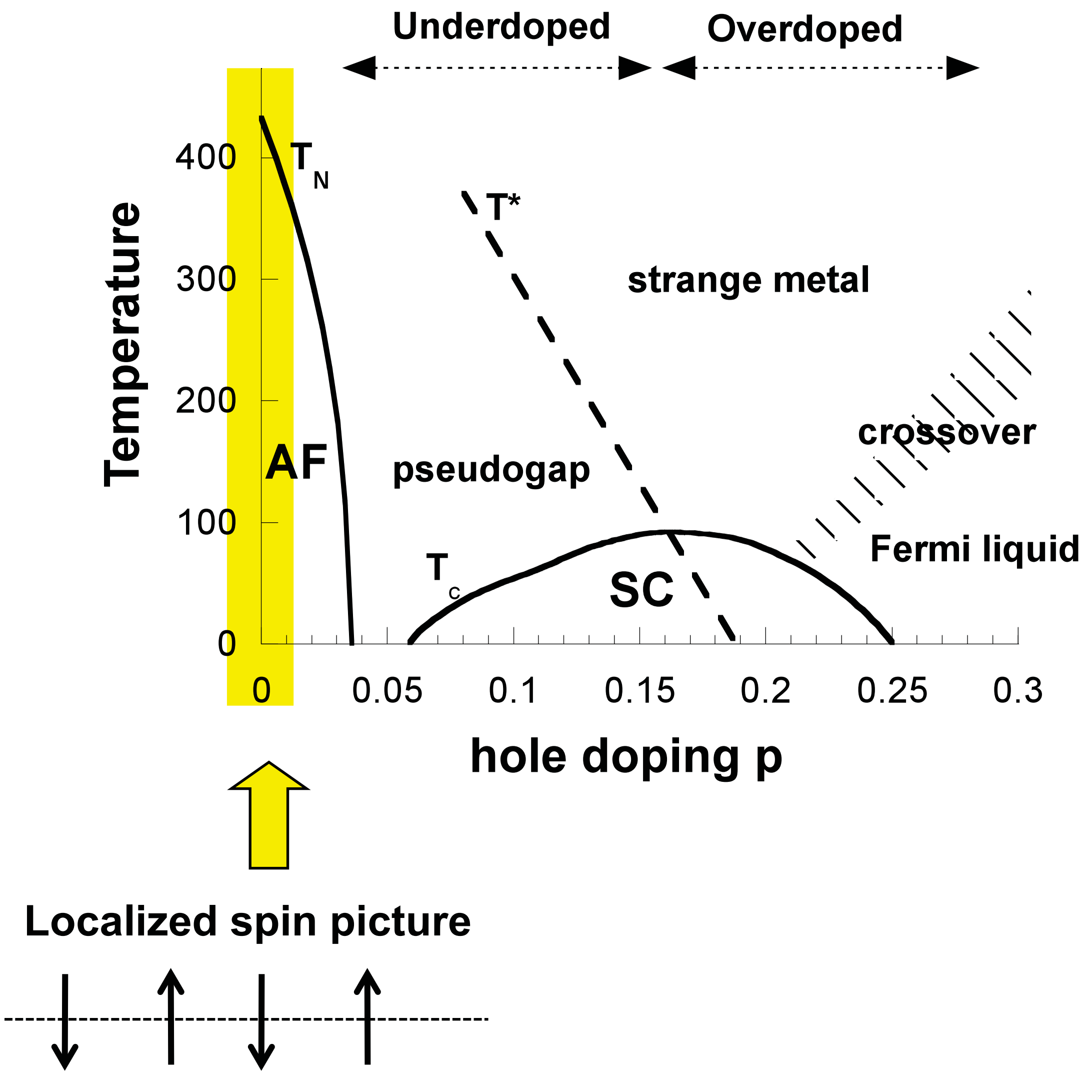
Neutron scatering vs. Other inelastic probes



High-Tc superconducting cuprates generic phase diagram

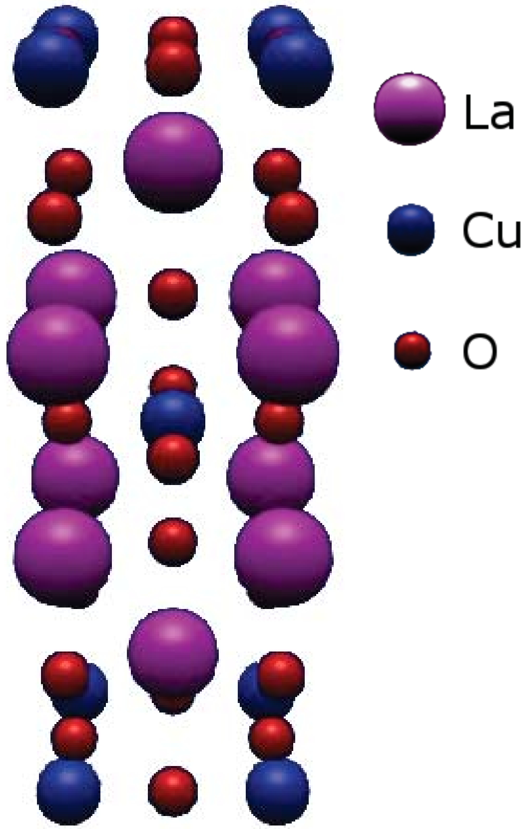


Mott insulating state: Spin waves

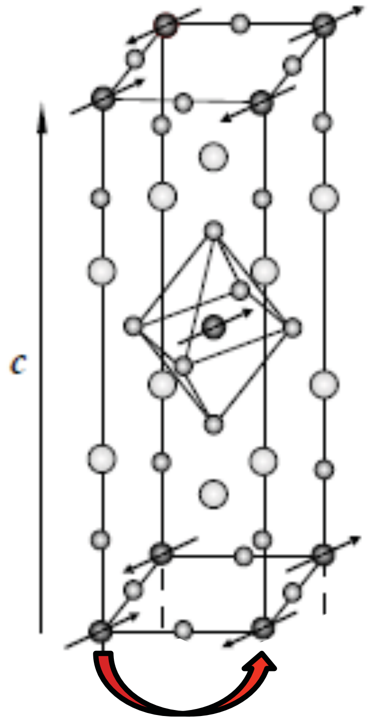


Mono-layer system

$La_{2-x}Sr_xCuO_4$



$La_{2-x}Sr_xCuO_4$



J : super-exchange

Heisenberg Hamiltonian

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

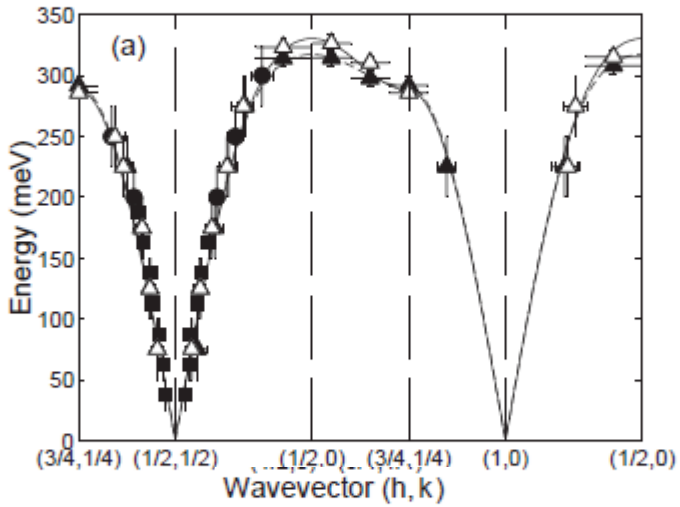
Linear spin wave theory

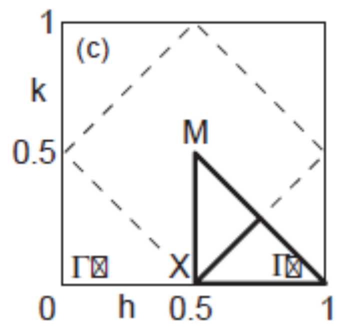
at low energy

ω= c q

$$c = \sqrt{8} S Z_c J a / \hbar$$

$$Z_c \approx 1.18$$





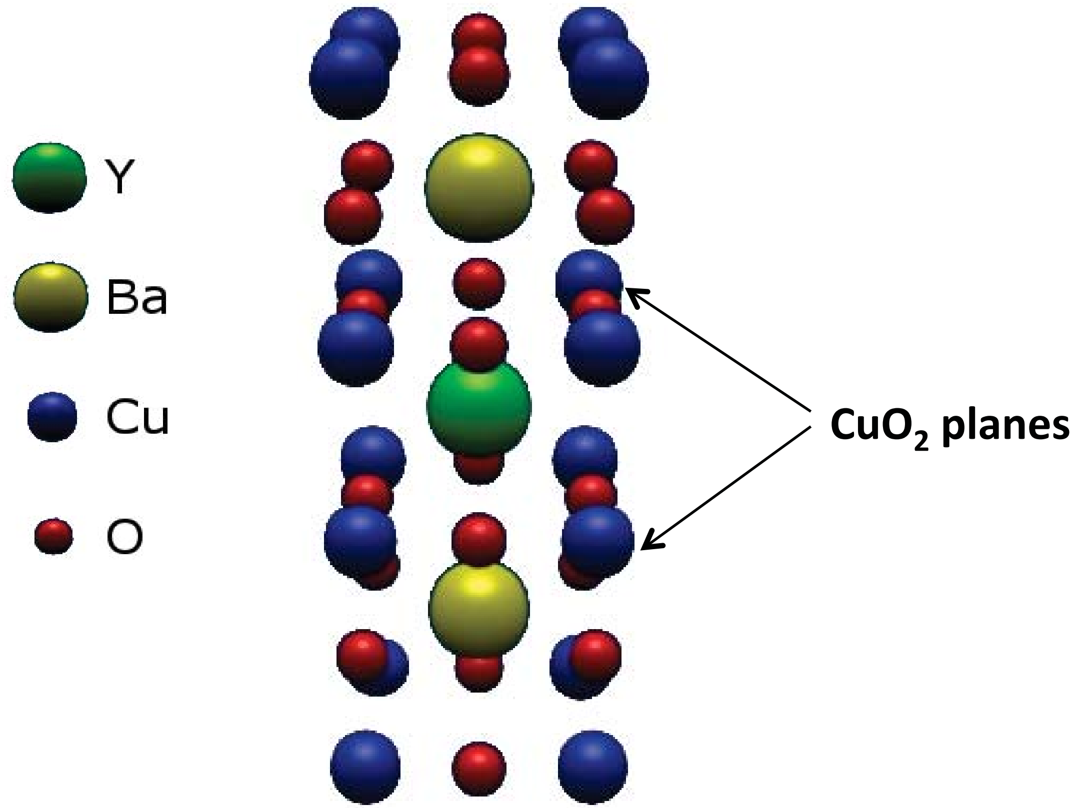
R. Coldea, PRL (2001).

Super-exchange interaction

Compound	T_N (K)	m_{Cu} (μ_B)	J (meV)	Crystal Symmetry	Layers per cell	Refs.
La_2CuO_4	325(2)	0.60(5)	146(4)	O	1	[65, 64, 68]
$Sr_2CuO_2Cl_2$	256(2)	0.34(4)	125(6)	T	1	[69, 70, 71]
$Ca_2CuO_2Cl_2$	247(5)	0.25(10)		T	1	[72]
Nd_2CuO_4	276(1)	0.46(5)	155(3)	T	1	[73, 74, 75, 76]
Pr_2CuO_4	284(1)	0.40(2)	130(13)	T	1	[77, 73]
$YBa_2Cu_3O_{6.1}$	410(1)	0.55(3)	106(7)	T	2	[78, 32]
$TlBa_2YCu_2O_7$	> 350	0.52(8)		T	2	[79]
$Ca_{0.85}Sr_{0.15}CuO_2$	537(5)	0.51(5)		T	∞	[80]

Bi-layer system

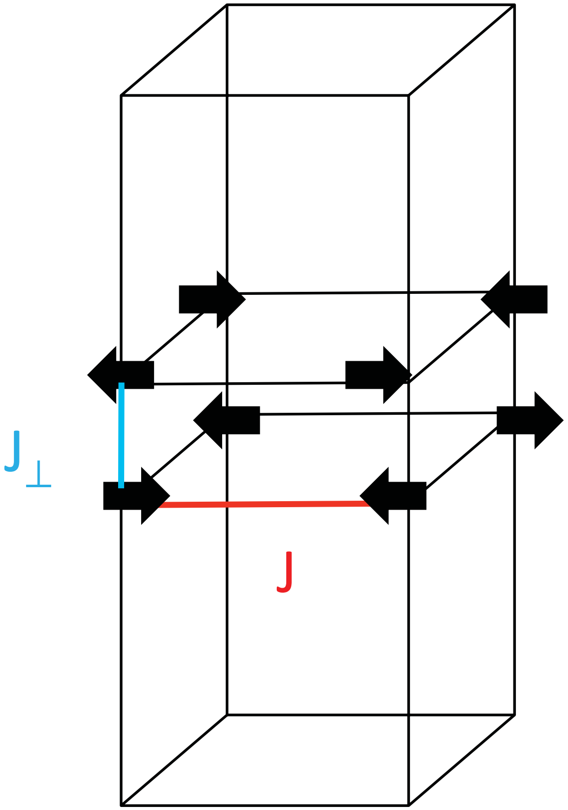
$YBa_2Cu_3O_{6+x}$

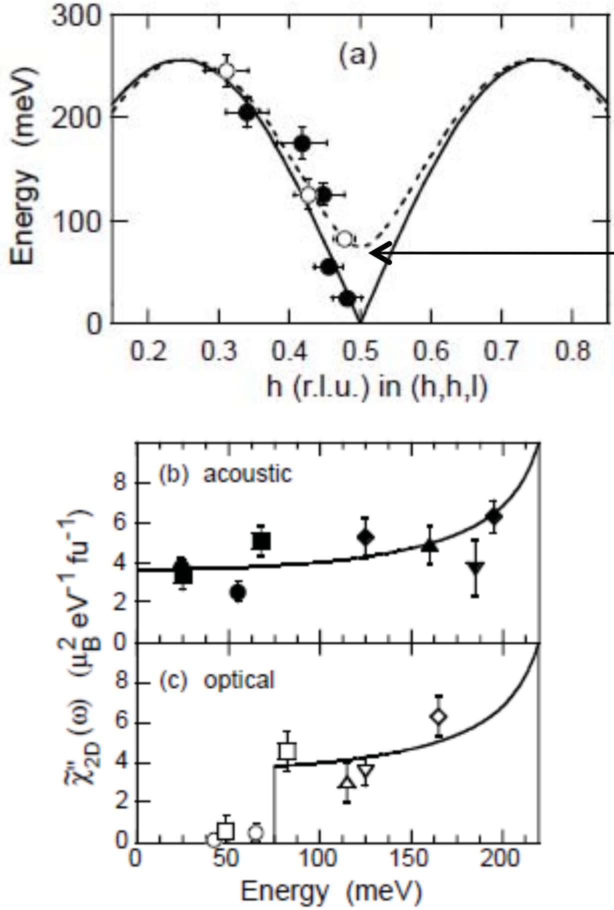


Linear spin wave theory

2 modes: acoustic + optical

$YBa_2Cu_3O_{6+x}$





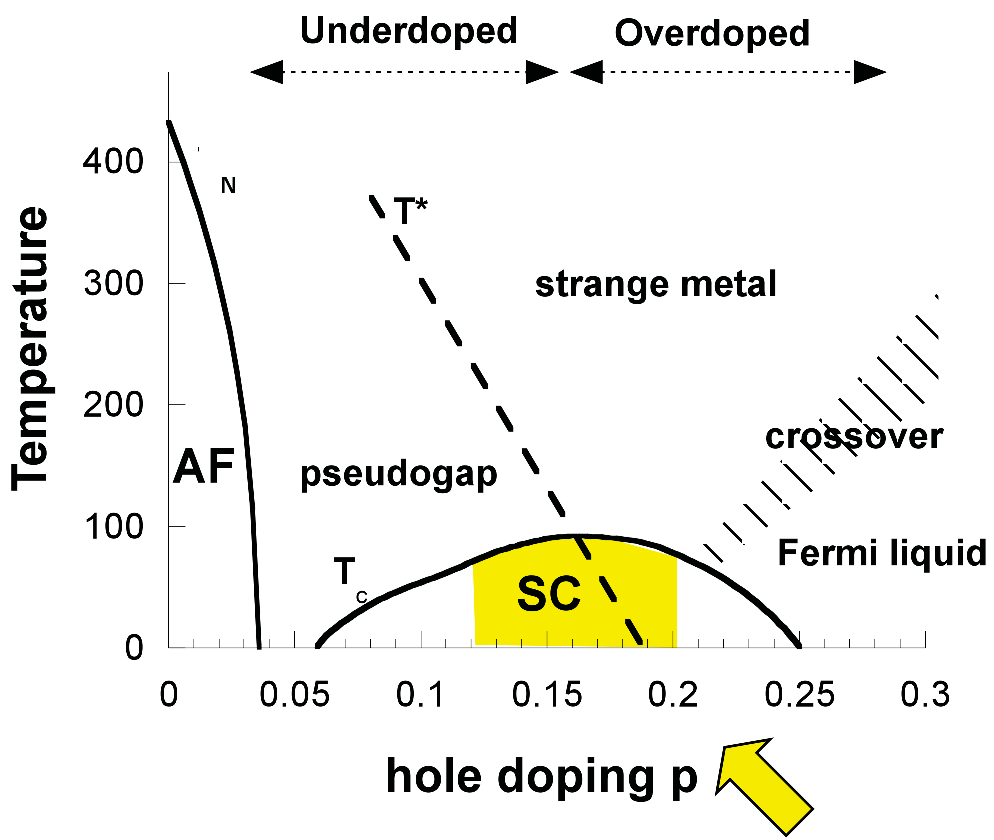
$$\omega_{opt} = 2\sqrt{J_\perp J}$$

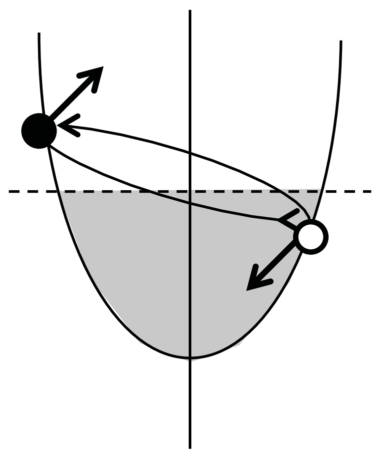
$$\omega_{opt} = 67 \pm 5 \text{ meV}$$

$$J_\perp = 9.6 \text{ meV}$$

Reznik, PRB (1996)
Hayden, PRB (1996).

Superconducting state (close at optimal doping): Magnetic resonance peak



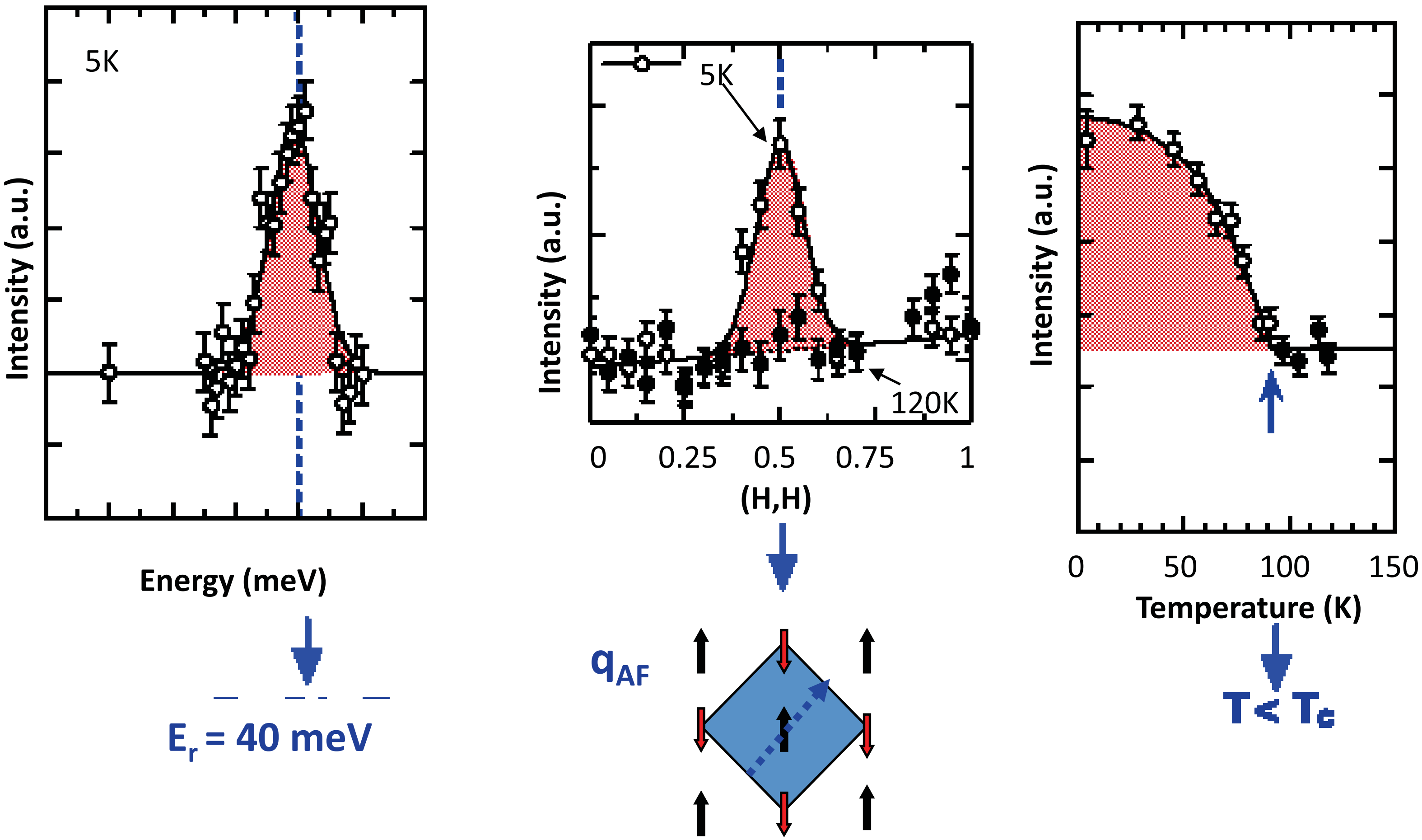


Itinerant spin picture

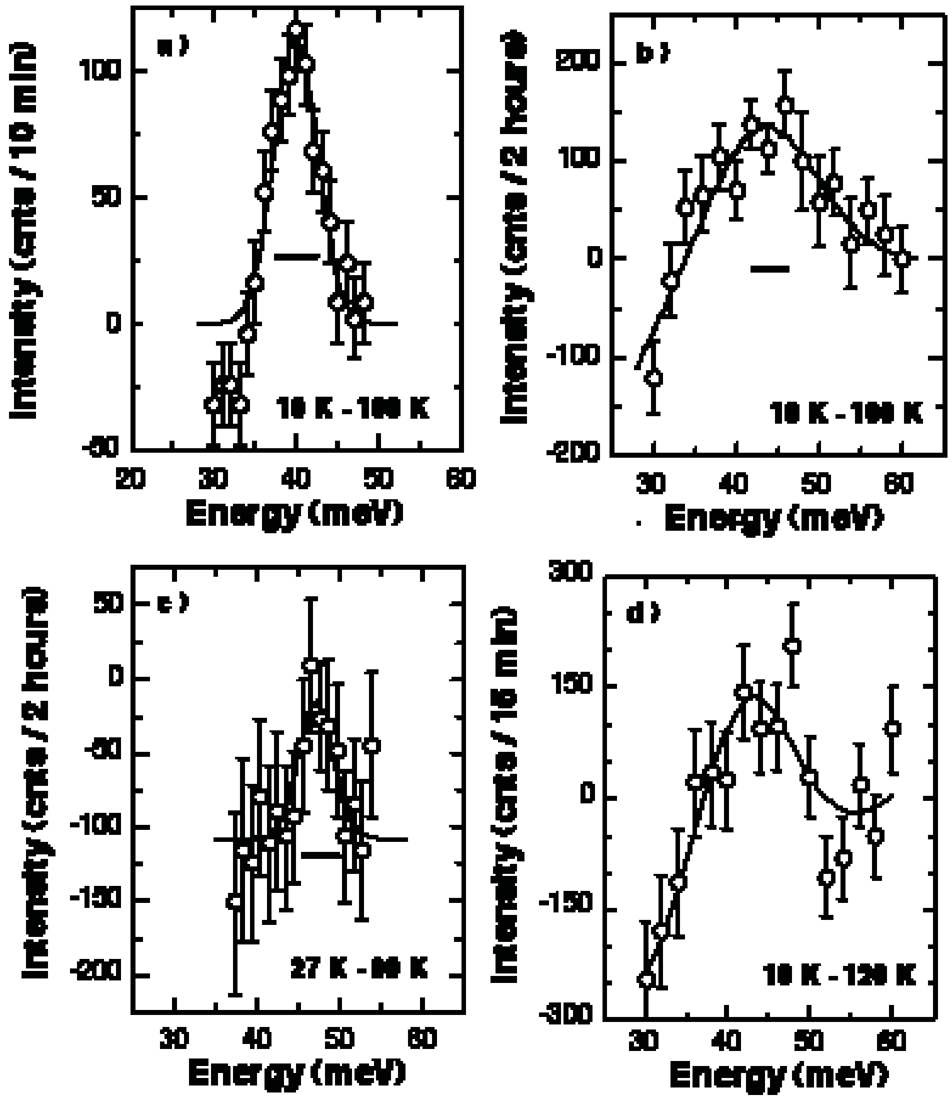
Inelastic neutron scattering measurements brought to light
a new magnetic excitation that does not exist
in the superconducting state of conventional superconductors
The so-called « magnetic resonance peak»

J. Rossat Mignot et al., Physica C 185-189, 86 (1991)

P. Bourges et al., PRB (1996)



A generic excitation in the SC state



a) Y123 (T_c=93 K) Bi-layer

H.F. Fong *et al.*, Phys. Rev. B 54, 6708 (1996).

d) Bi2212 (T_c=91 K) Bi-layer

H.F. Fong *et al.*, Nature 398, 588 (1999).

c) Tl2201 (T_c=90 K) Mono-layer

H. He *et al.*, Science 295, 1045 (2002).

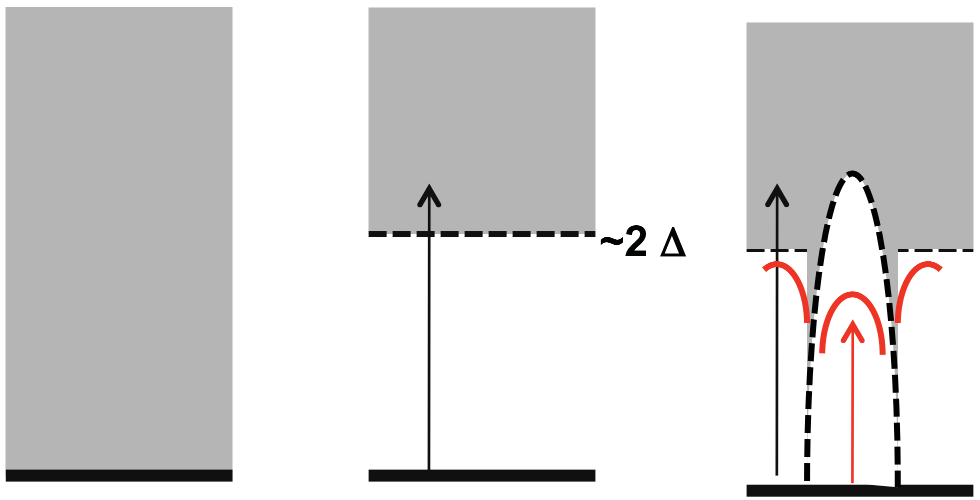
d) Bi2223(T_c=110 K) Tri-layer

S. Bayrakci *et al.* (2003)

S=1 collective mode in the SC state: the spin exciton scenario

Normal state | **SC state** s-wave | **SC state** d-wave

Stoner continuum



RPA spin susceptibility

$$\chi(\mathbf{q},\omega) = \frac{\chi_0(\mathbf{q},\omega)}{1 - \frac{2I(q)}{(g\mu_B)^2}\chi_0(\mathbf{q},\omega)}$$

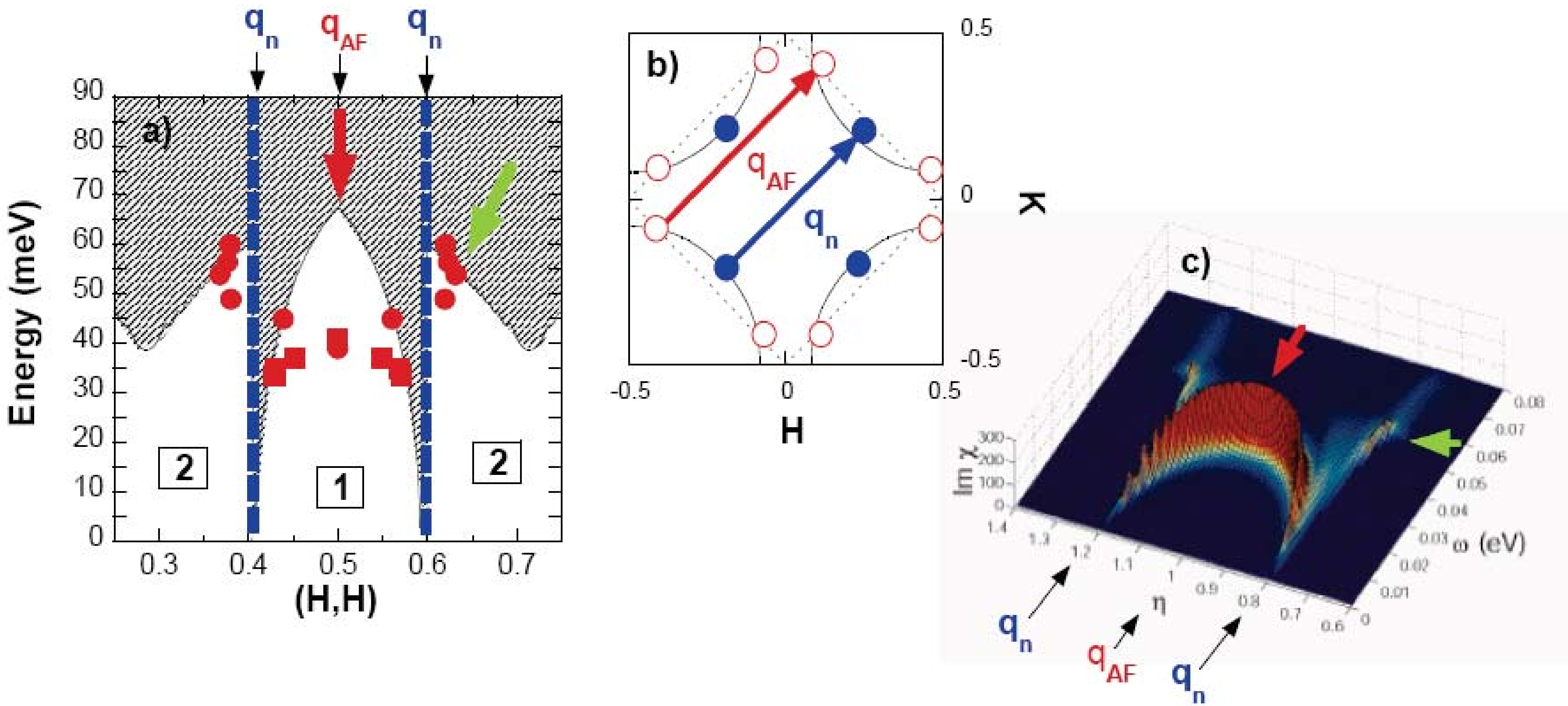
2D systems
$\Delta_k \Delta_{k+Q} < 0$

S=1 bound state below the gapped Stoner continuum

See for instance:

Onufrieva et al., PRB (2002)
Eremin et al., PRL (2005)

S=1 collective mode in the SC state: the spin exciton scenario



INS $YBa_2Cu_3O_{6.85}$ (UD-T_c=89 K)

Bourges et al., Science (2000)
Pailhès et al., PRL (2004)
Reznik et al., PRL (2004)

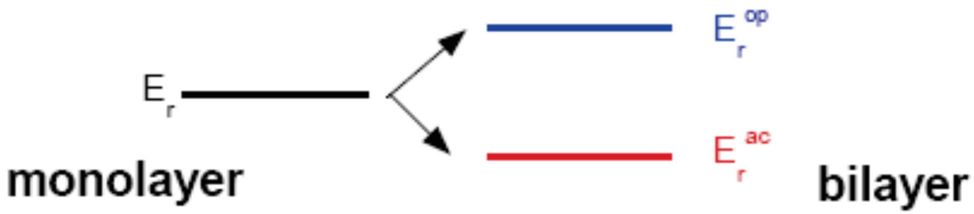
Theory

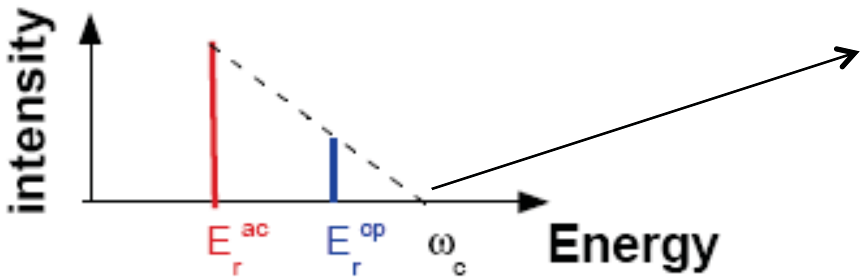
Onufrieva et al., PRB (2002)
Eremin et al., PRL (2005)

What can we learn from a Bi-layer system ?

$$Im\chi(\mathbf{q},\omega>0) = \pi\frac{1}{(\frac{2I(q)}{g\mu_B})^2}(\frac{dRe\chi_0(\mathbf{q},\omega)}{d\omega}|_{\omega\to-\Omega_r(\mathbf{q})}]^{-1}\delta(\omega-\Omega_r(\mathbf{q}))$$

$$Im\chi(\mathbf{q},\omega>0) \simeq \pi\frac{1}{(\frac{2I(q)}{g\mu_B})^2}\frac{1}{\beta}\frac{\omega_c(\mathbf{q})-\omega}{\omega_c(\mathbf{q})}\delta(\omega-\Omega_r(\mathbf{q}))$$

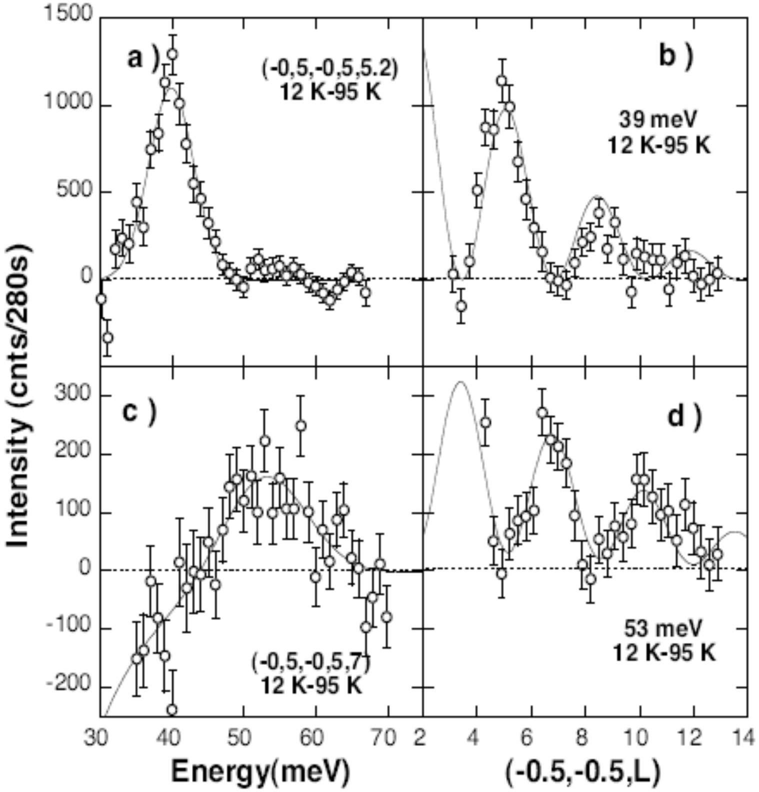




One should be able to determine
ω_c the threshold of the continuum
from neutron scattering

By-layer systems: odd and even resonance modes

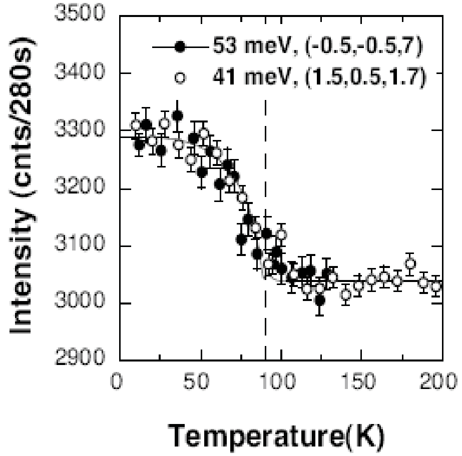
$YBa_2Cu_3O_{6.85}$ (UD-T_c=89 K)



Bi-layer modulation

$$\frac{\partial^2\sigma(\mathbf{Q},\omega)}{\partial\Omega\partial\omega} \propto f^2(Q)\Big[\sin^2(\pi z L) Im[\chi_o(\mathbf{Q},\omega)] + \cos^2(\pi z L) Im[\chi_e(\mathbf{Q},\omega)]\Big],$$

Characteristic T-dependence



Mono-layer vs. Bi-layer

$Tl_2Ba_2CuO_{6+x}$ — $YBa_2Cu_3O_{6+x}$

47 meV → even 53 meV

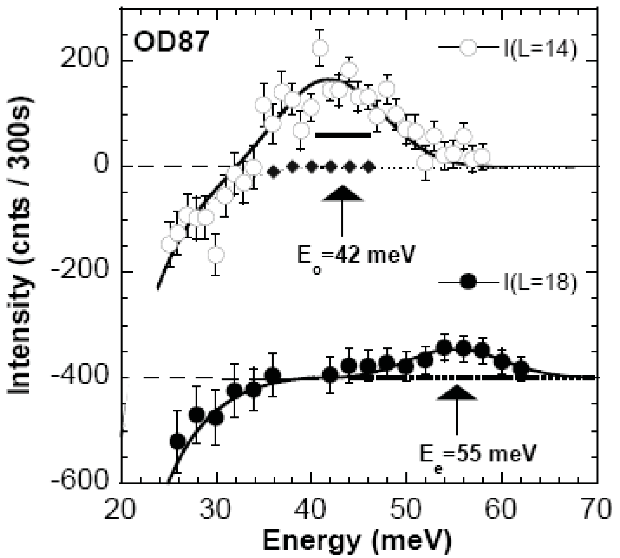
47 meV → odd 41 meV

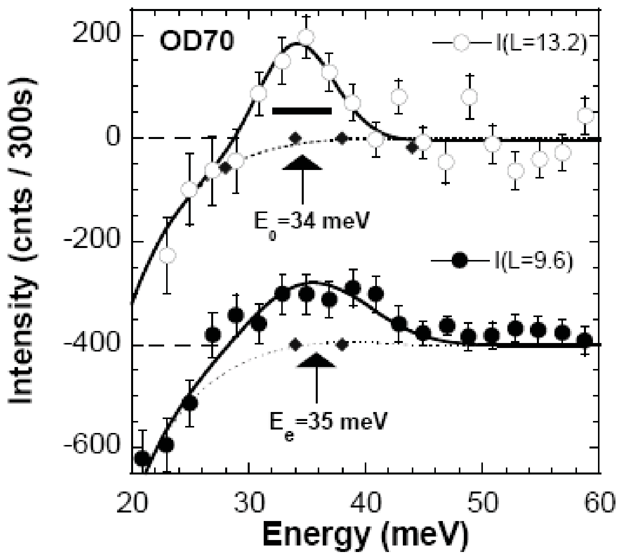
+/-6meV ~$J_\perp$

INS

Pailhès et al., PRL (2003)
Pailhès et al., PRL (2004)
Pailhès et al., PRL (2005)

$Bi_2Sr_2CaCu_2O_8$

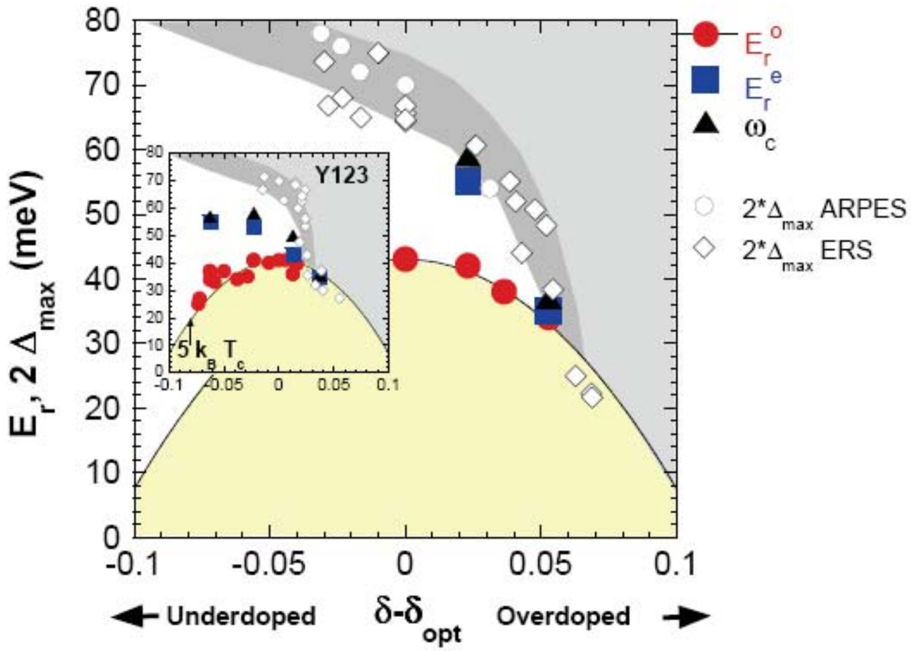




INS

Capogna et al. , PRB (2008)

Bi-layer systems: odd and even resonance modes



<u>Two regimes</u>

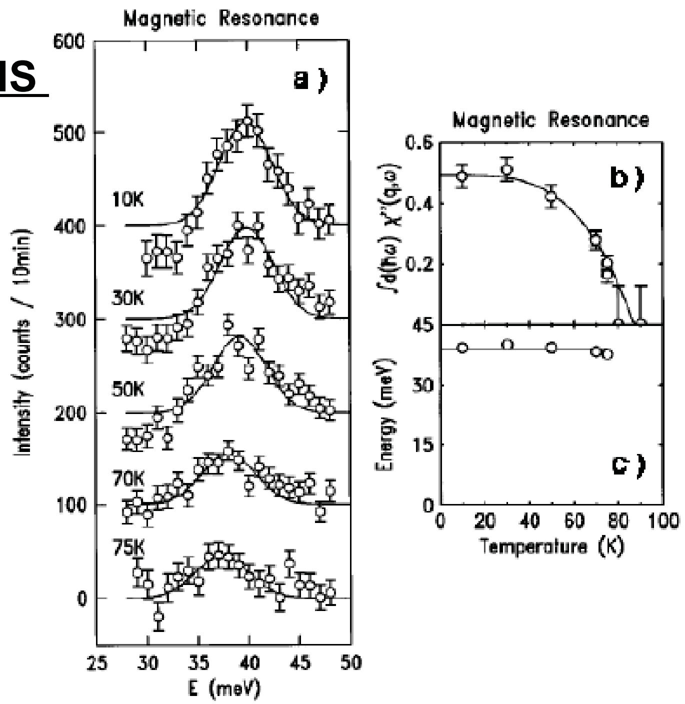
I : $5k_BT_c \sim E_r^o < E_r^e < 2\Delta_{max}$

δ_c ~ 0.2 ~ *end point of the pseudo-gap state*

II : $5k_BT_c \sim E_r^o \simeq E_r^e \simeq 2\Delta_{max}$

Spin-fermion coupling: The feedback effect

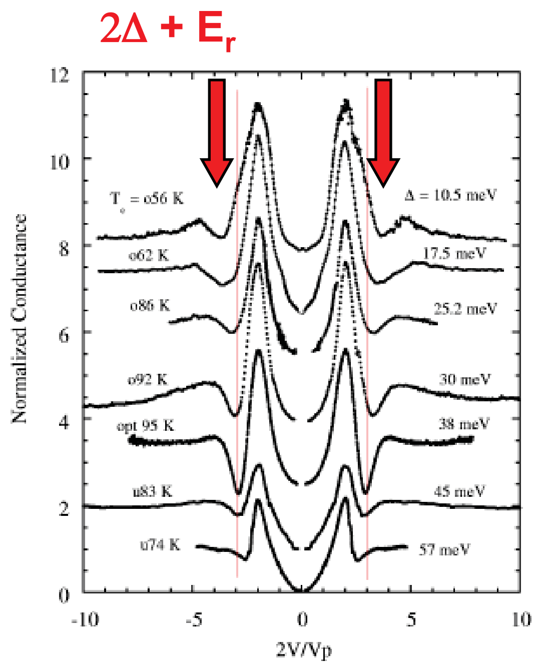
INS



$YBa_2Cu_3O_7$ (T_c=92.7 K)

Fong et al, PRL (1995)

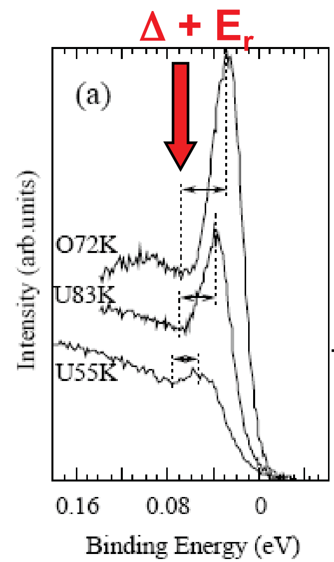
Theory
See for instance
Onufrieva et al, PRL (2009)



$Bi_2Sr_2CaCu_2O_8$

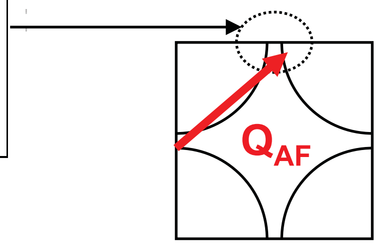
STM
(SIS junction)

Zasadsinski et al., PRL (2001)



ARPES

Campuzano et al, PRL (1999)

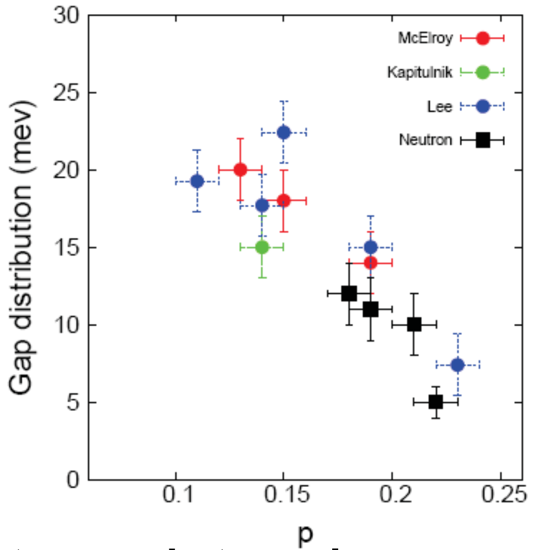


SC gap distribution and magnetic resonance peak broadening in $Bi_2Sr_2CaCu_2O_8$

INS *Fauqué et al. , PRB (2008)*

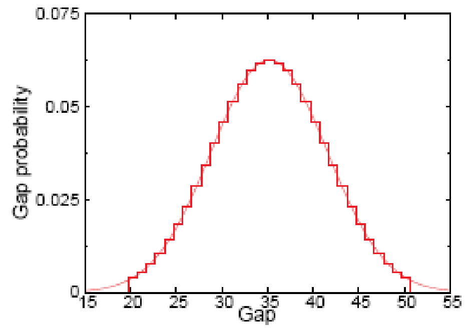
E-broadening of the magnetic resonance peak in Bi2212

Refs.	T_c(K)	E_r(meV)	σ_r(meV)	σ(meV)
Fong *et al*[10]	91	43	13 ± 2	12 ± 2
Present study	87	42	13 ± 2	11 ± 2
He *et al*[11]	83	38	12 ± 2	10 ± 2
Capogna *et al*[48]	70	34	8 ± 1	5 ± 1

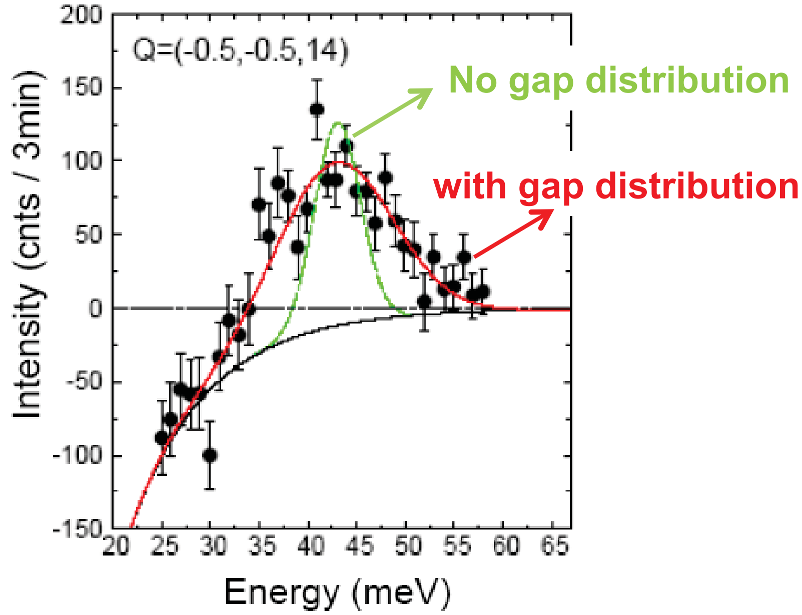


Spectroscopie tunnel

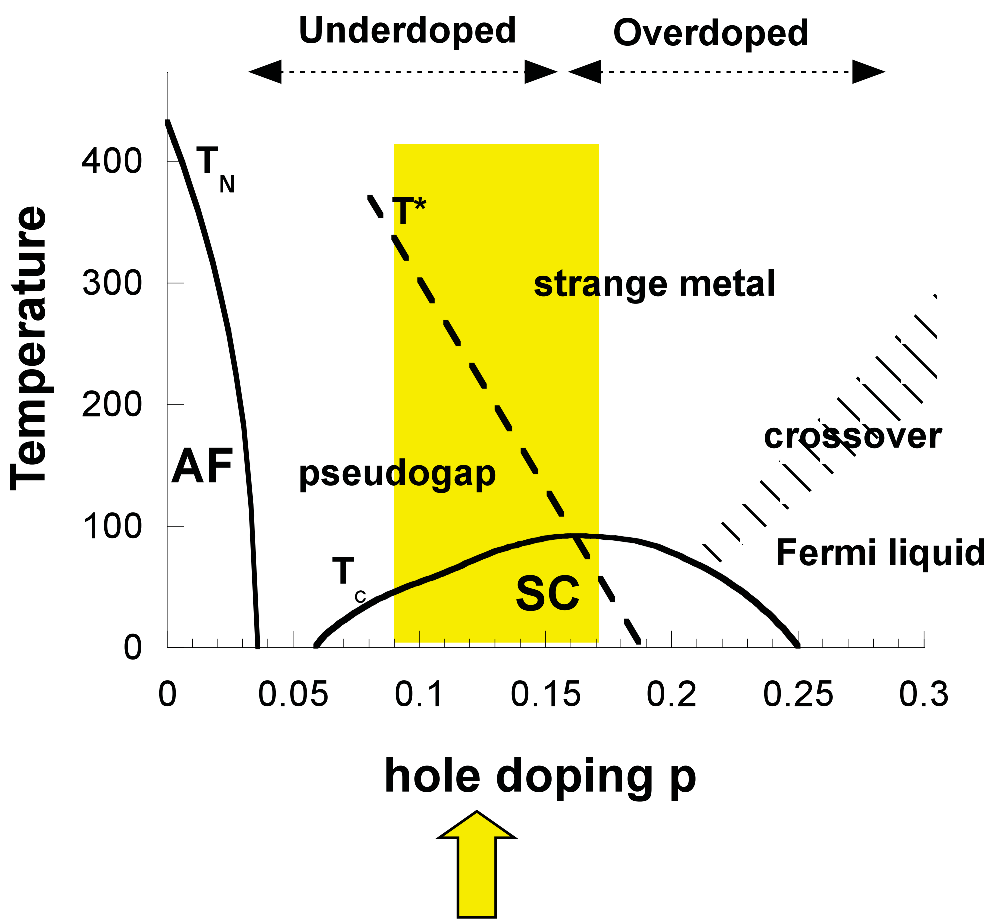
Howald et al., PRB(2001).
McElroy et al., PRL(2005).
Lee et al.,Nature (2006).
Fischer et al., Rev. Mod. Phys. (2007).



$$\chi(\mathbf{q},\omega) = \int \chi(\mathbf{q},\omega,\Delta)\exp(-4\ln 2\frac{(\Delta-\Delta_m)^2}{\sigma_\Delta^2})d\Delta$$



Spin dynamics in the underdoped regime beyond the itinerant picture



Localized or Itinerant spin picture ?

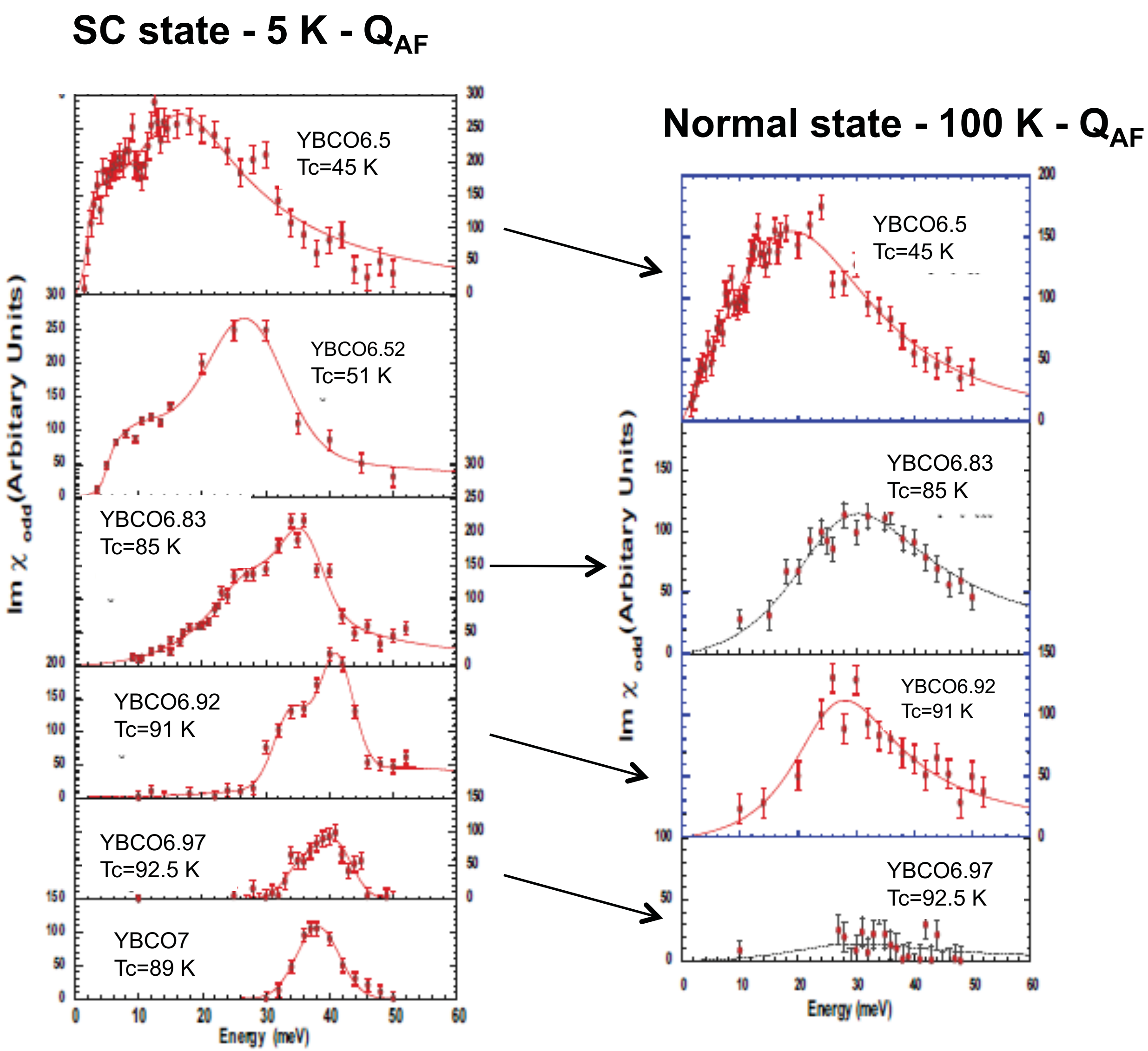
Underdoped regime

- ***The magnetic resonance does not dominate the spin excitation spectrum anymore***
- ***Strong enhancement of the normal state spin excitation spectrum***
- ***shift of the spectral weight towards low energy up on underdoping***

Weakly overdoped regime

- ***The magnetic resonance dominates the spin excitation spectrum in the SC state***
- ***The spin excitation spectrum is weak and featureless in the normal state***

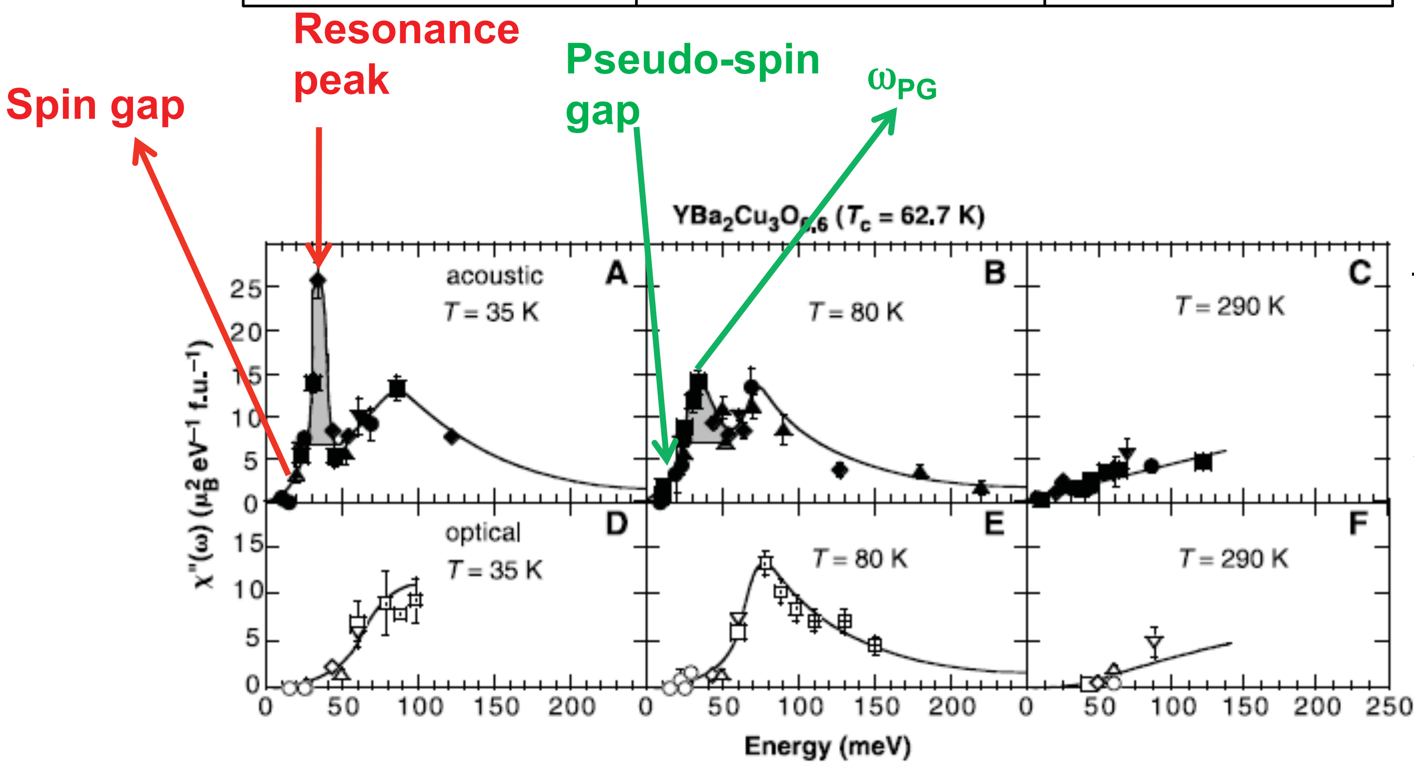
100 cnts = 300 μ_B/eV



P. Bourges, The gap Symmetry and Fluctuations in High Temperature Superconductors Ed. by J. Bok, G, 349-371 (Vol. 371 in NATO ASI series, Physics) - ArXiv:9901333

Spin dynamics in the underdoped regime
Density of AF spin fluctuations

SC state $T < T_c$	Pseudo-gap state $T_c < T < T^*$	$T^* < T$

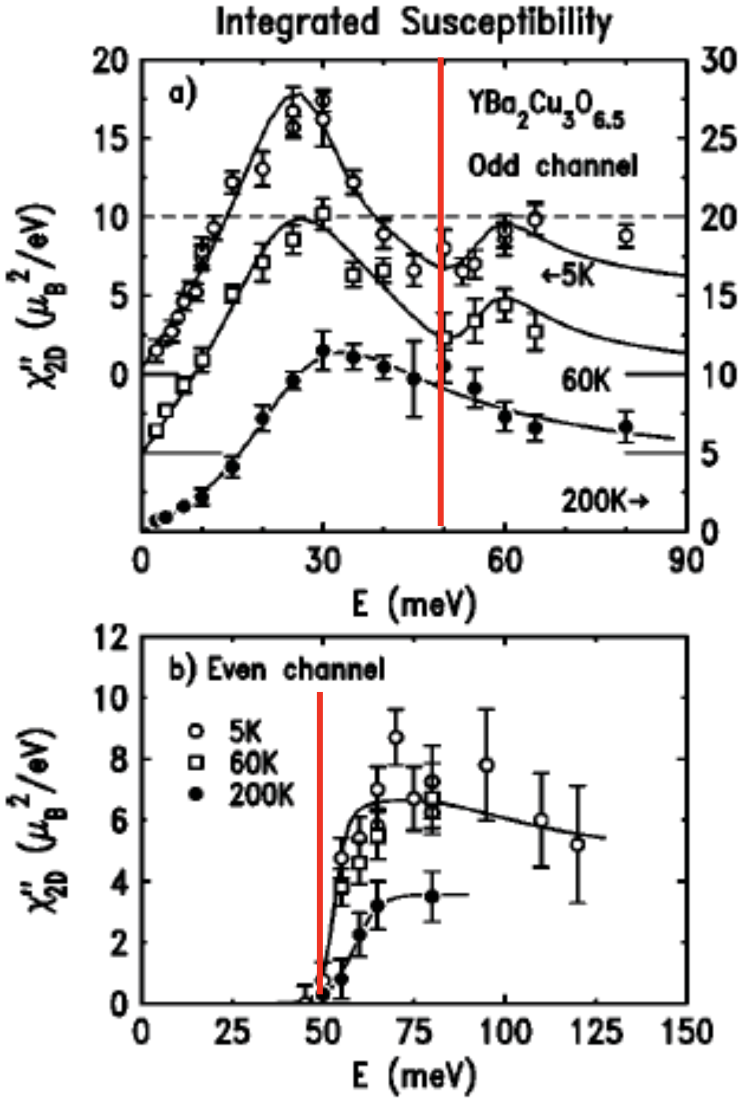


INS

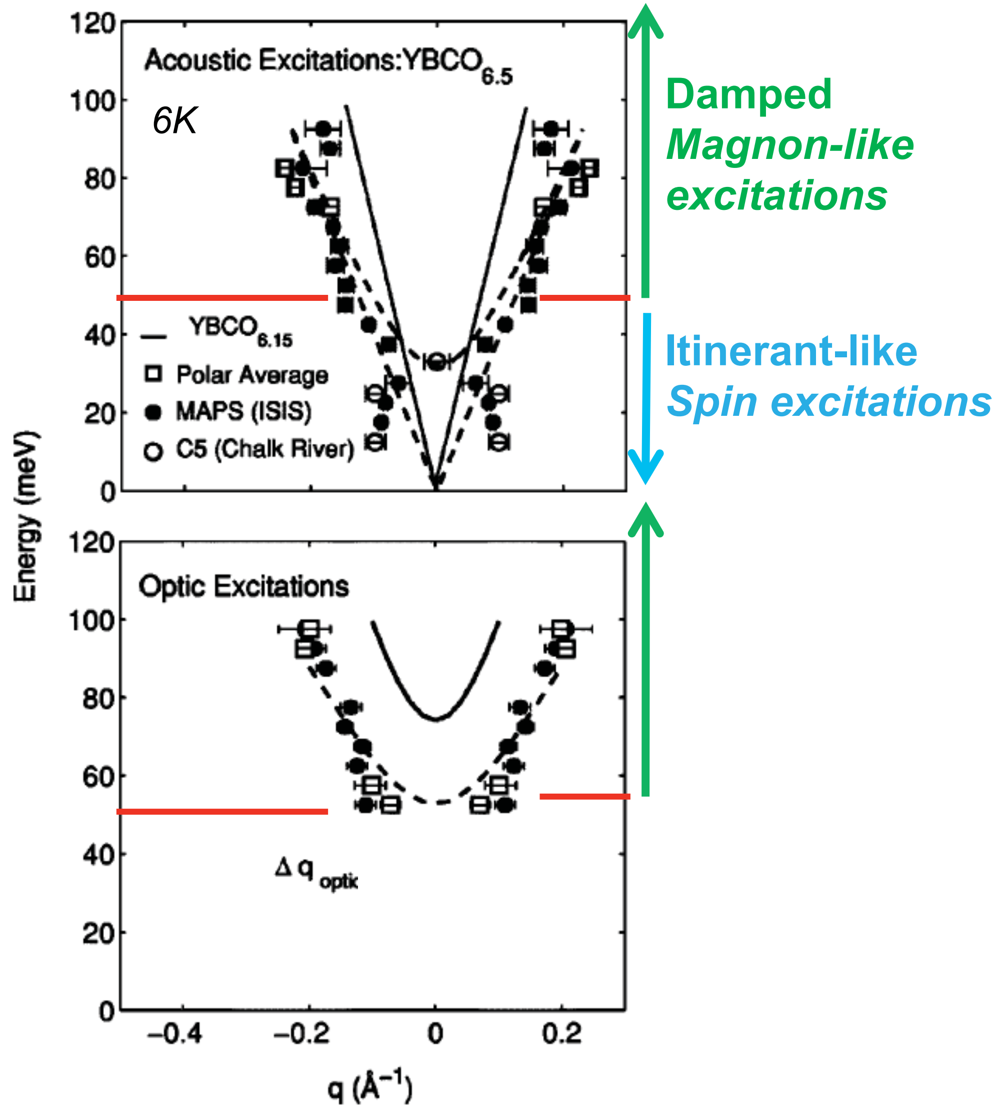
Dai et al, Science (1999)

Fong et al., PRB (2000)

Spin dynamics in the underdoped regime
Two- Energy scales ?



Fong et al., PRB (2000)

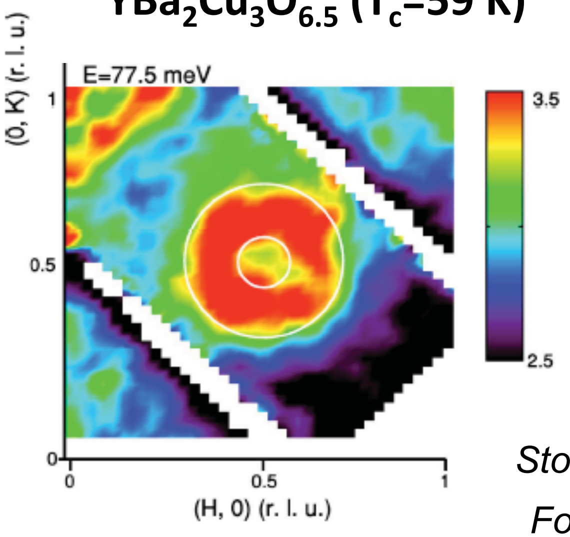


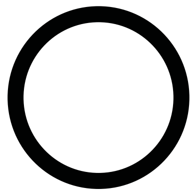
Stock et al., PRB (2005)

Spin dynamics in the underdoped regime
Damped spin wave-like excitations at high energy?

$YBa_2Cu_3O_{6.5}$ (T_c=59 K)

77.5 meV





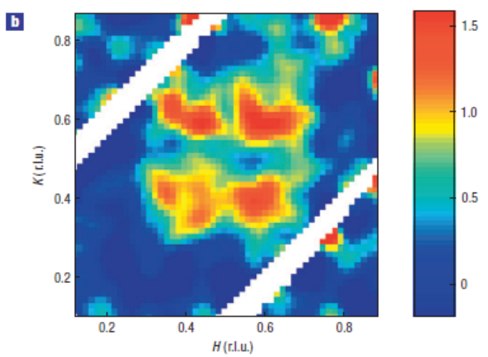
spin wave -like

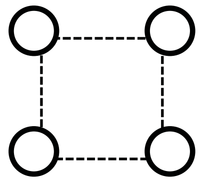
Stock et al., PRB (2005)

Fong et al., PRB (2000)

$YBa_2Cu_3O_{6.6}$ (T_c=63 K)

63 meV

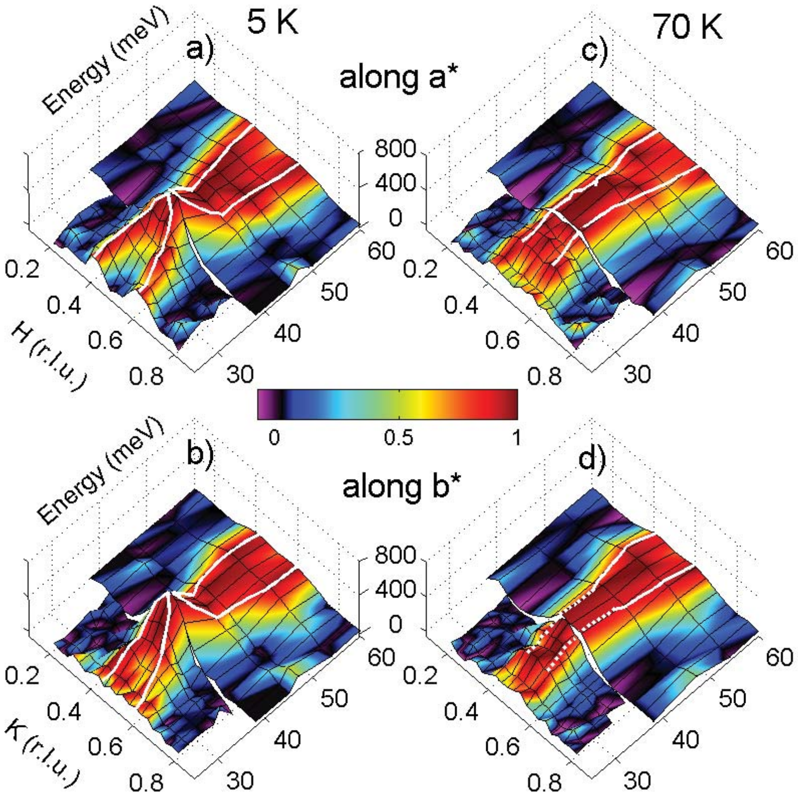


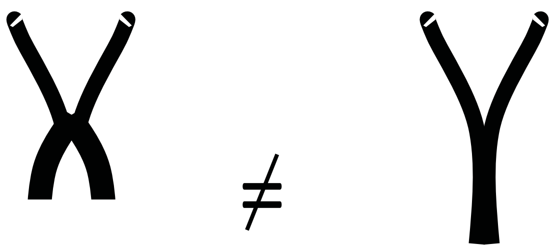


not spin wave -like

Hinkov et al., Nat. Phys. (2007)
Hayden et al. Nature (2004)

X – Y "*Magnetic chromosomes*"





$T < T_c$ $T > T_c$

$YBa_2Cu_3O_{6.6}$
(UD-T_c=63 K)
p ~0.12

Spectrum above T_c qualitatively different:

- No hour-glass dispersion
- No resonance anomaly
- „Y“-shaped dispersion

<u>INS</u>

Hinkov et al.,
Nature Phys. (2007)

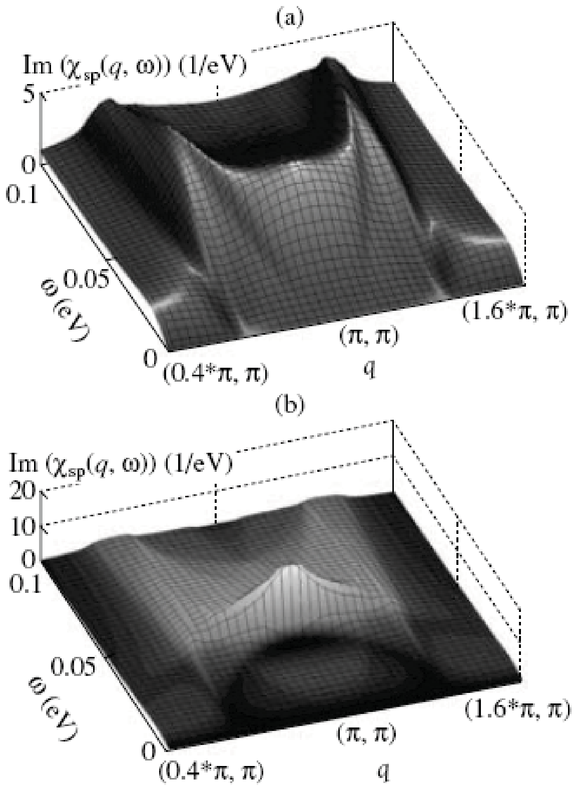
Itinerant-localized duality

Theory

Eremin et al, JETP Lett. (2006)

See also: Onufrieva et al., PRB (1995)

Normal state



SC state

RPA spin susceptibility

$$\chi(\mathbf{q},\omega) = \frac{\chi_0(\mathbf{q},\omega)}{1 - \frac{2I(q)}{(g\mu_B)^2}\chi_0(\mathbf{q},\omega)}$$

t-t'-J model + Hubbard operators

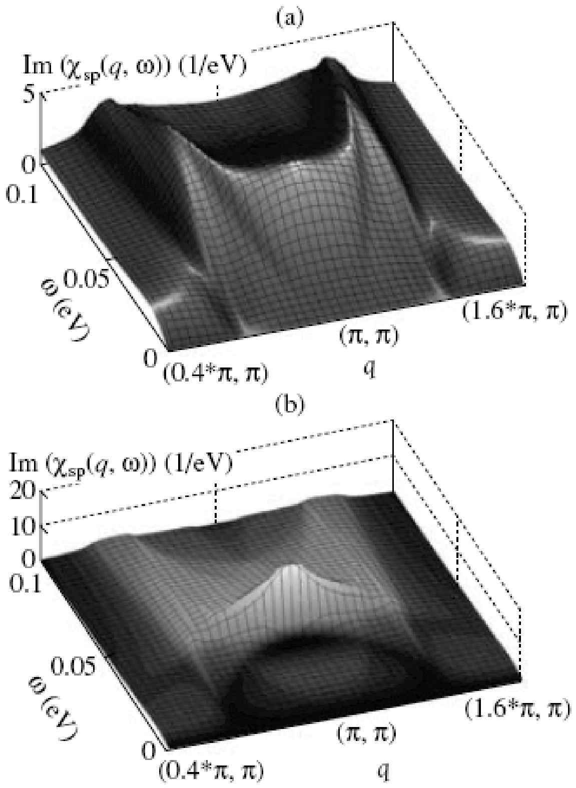
$\chi_0 \sim \chi_{localized} + \chi_{itinerant}$

Itinerant-localized duality

Theory
Eremin et al, JETP Lett. (2006)

See also: Onufrieva et al., PRB (1995)

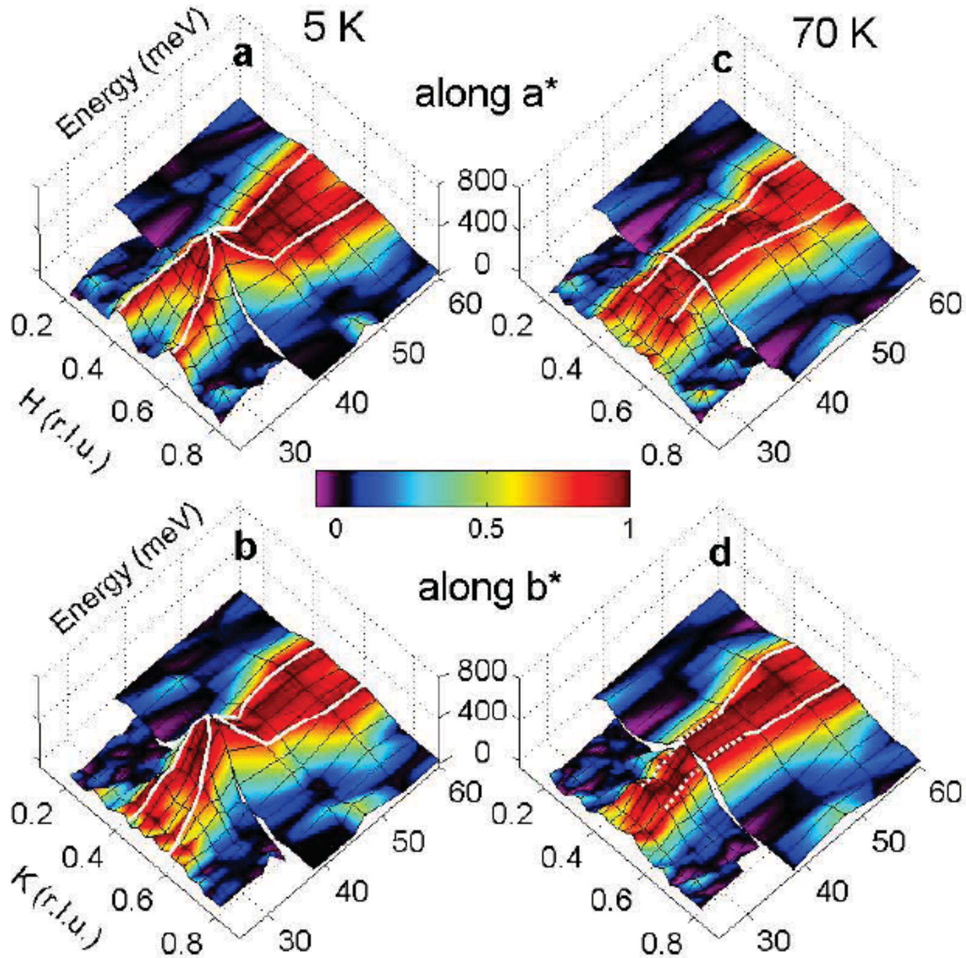
Normal state



SC state

INS
Hinkov et al. , Nature Phys. (2004)

$YBa_2Cu_3O_{6.6}$ (UD-T_c=63 K)

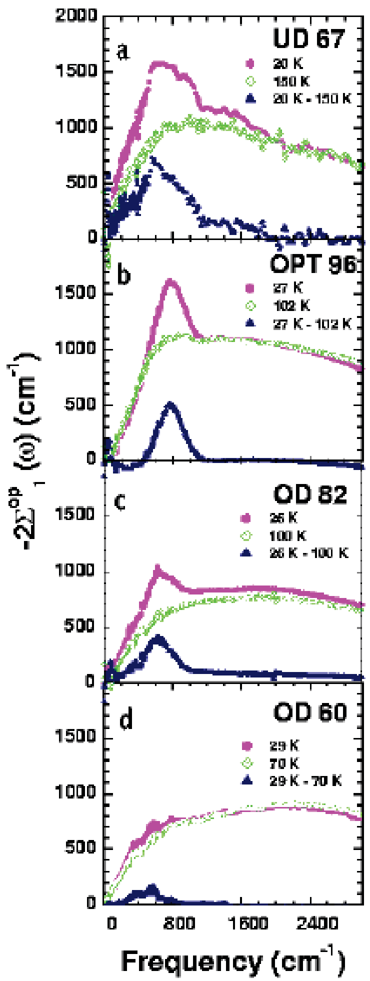


Quasiparticle self-energy versus spin excitation spectrum

$Bi_2Sr_2CaCu_2O_8$

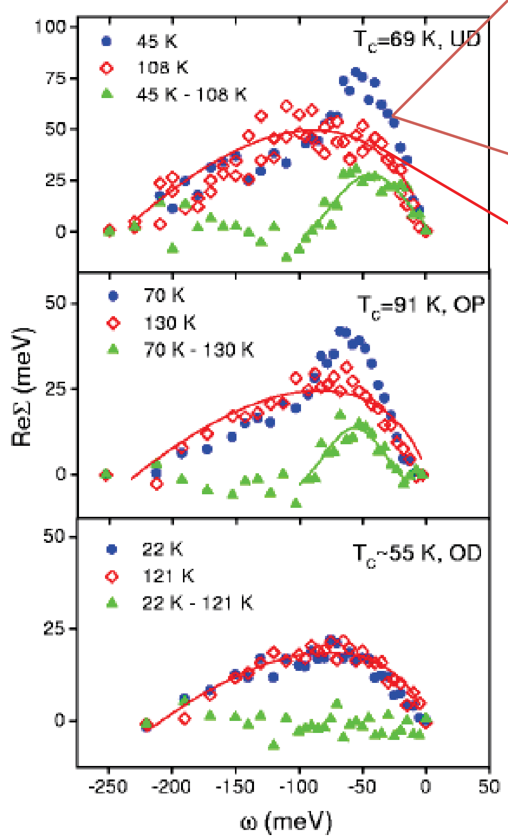
Conductivité optique

Hwang et al., Nature(2004)

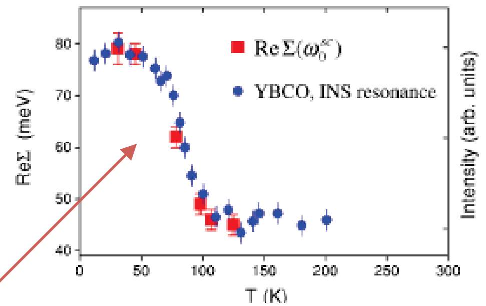


ARPES

Johnson et al.,PRL(2001)



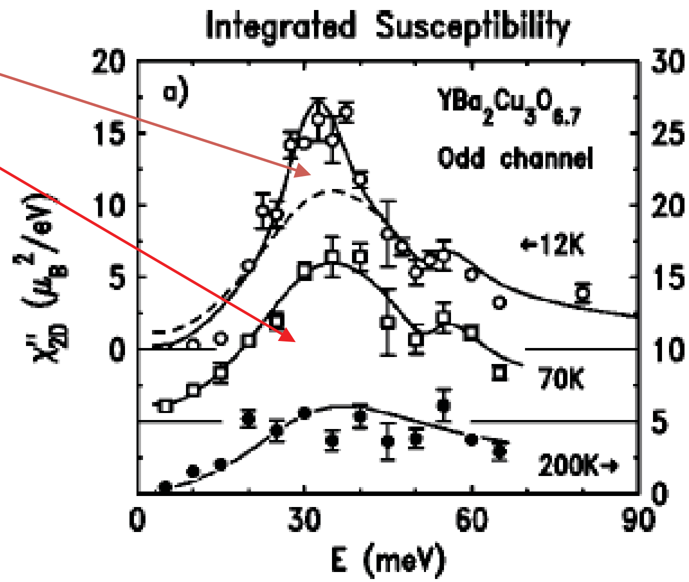
$YBa_2Cu_3O_{6.6}$ (UD-T_c=62.7 K)



INS

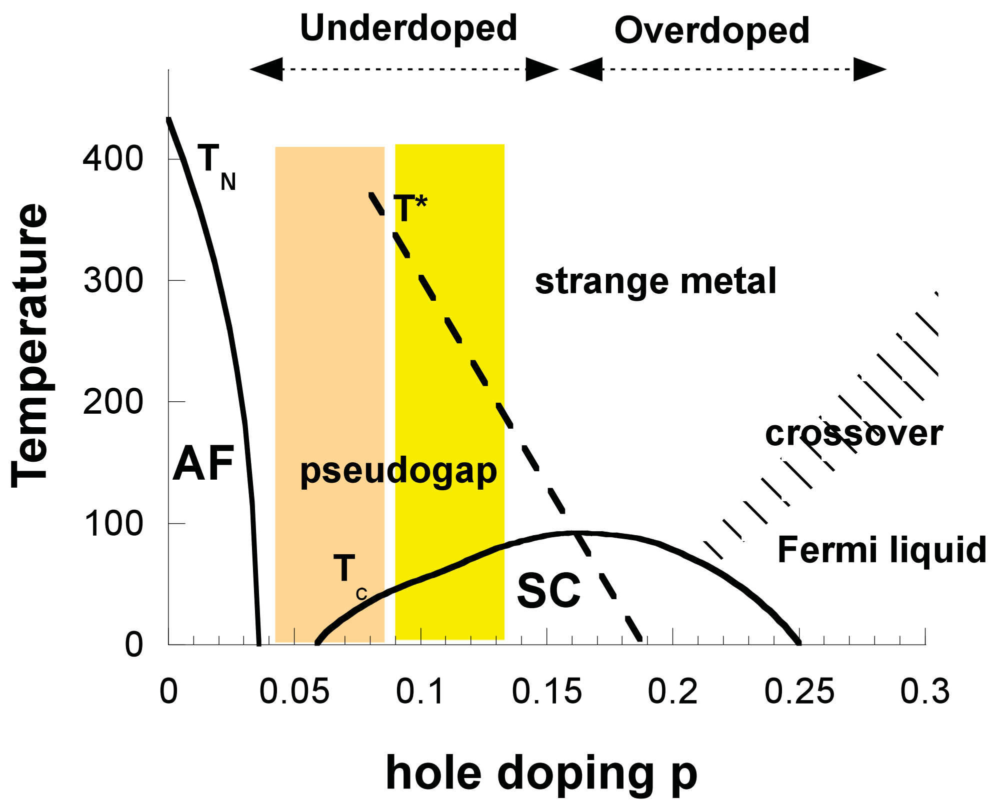
Dai et al., Science (1999)

$YBa_2Cu_3O_{6.7}$ (UD-T_c=67 K)



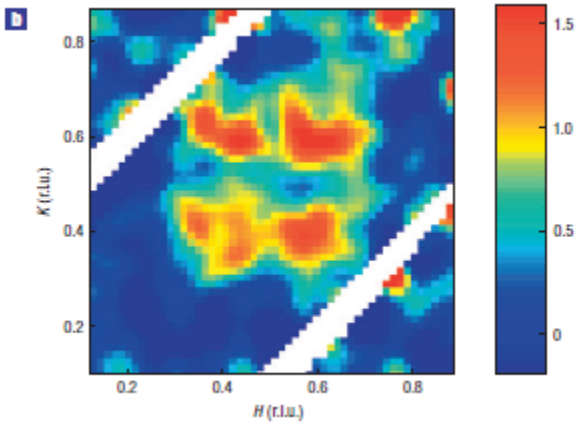
INS *Fong et al., PRB (2000)*

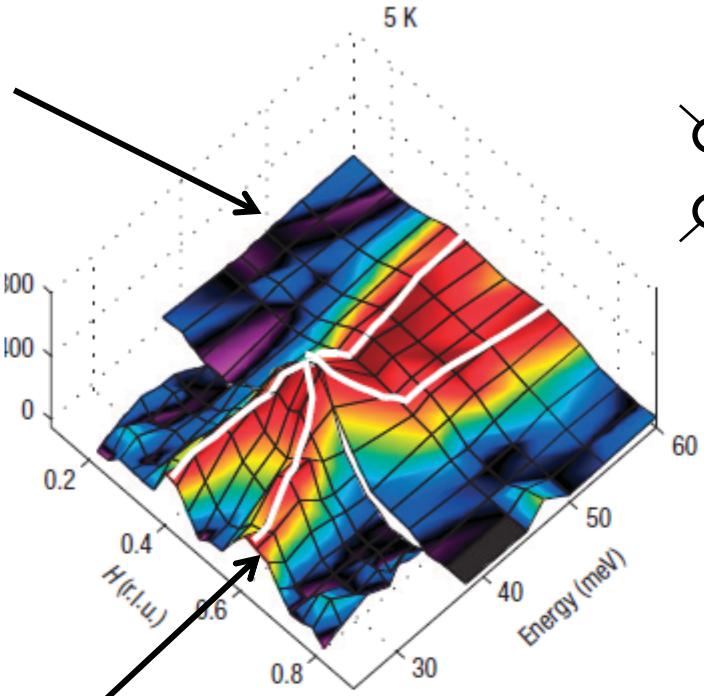
Spin dynamics in the underdoped regime
a-b anisotropy

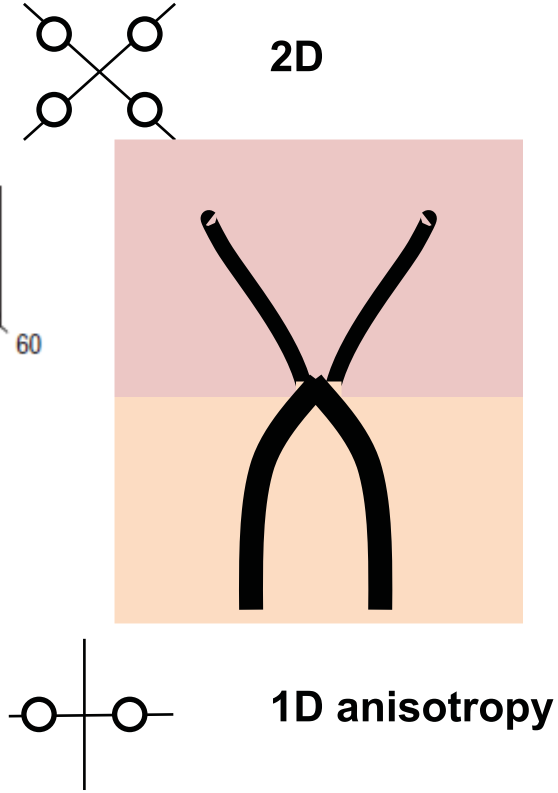


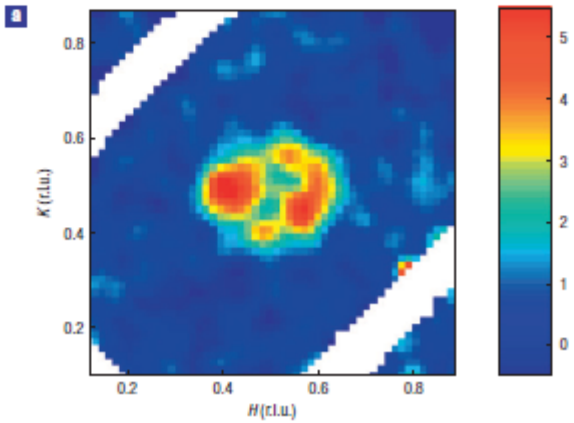
a-b anisotropy

$YBa_2Cu_3O_{6.6}$
(UD-T_c=63 K)
p ~0.12







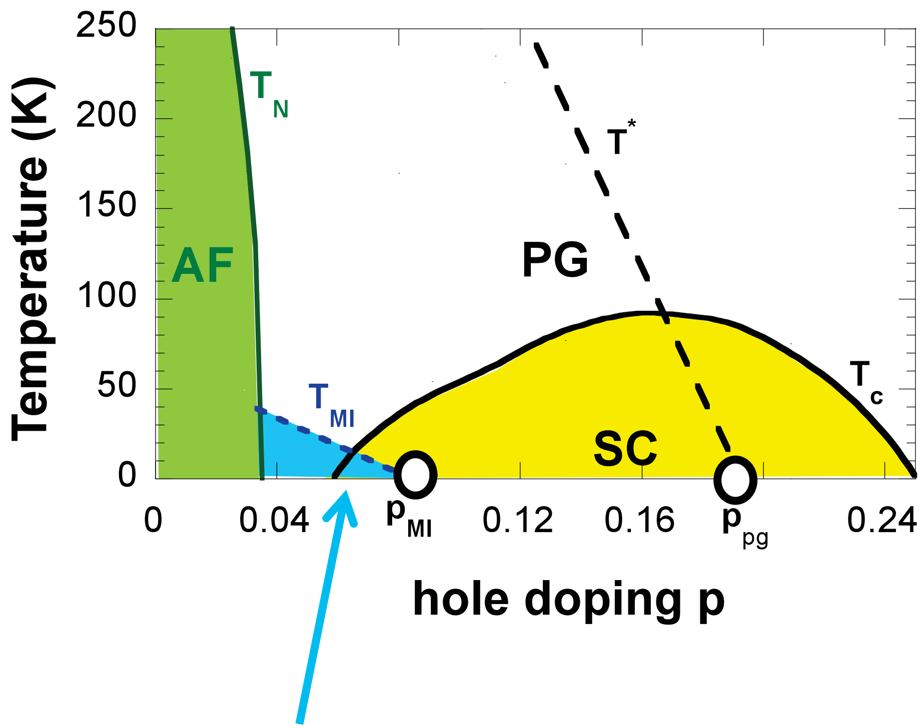


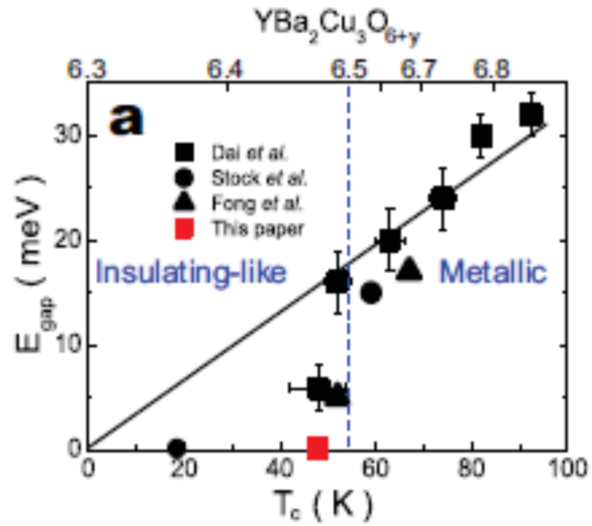
<u>**INS**</u>

Hinkov et al., Nature Phys. (2007)

<u>WARNING:</u> the a-b anisotropy increases above Tc

Change of the spin dynamics through Metal-insulator crossover in $YBa_2Cu_3O_{6+x}$





Upturn of the resistivity at low T

$$d\rho / dt < 0 \quad below \sim T_{MI}$$

Or when superconductivity is supressed under magnetic field

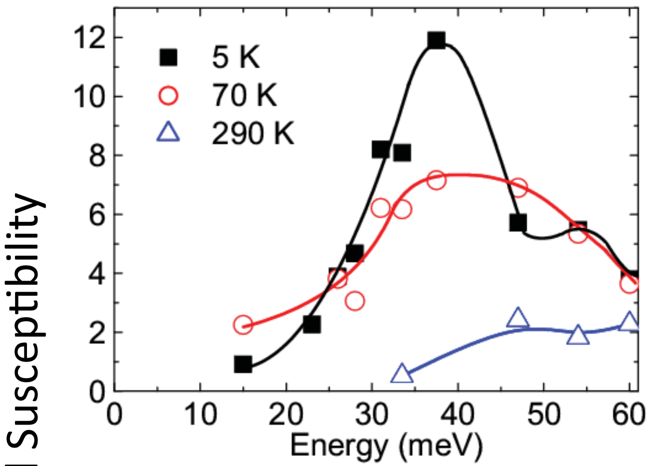
The spin gap becomes vanishingly small for $p < p_{MI}$

Rossat-Mignot et al., *Physica B* (1992

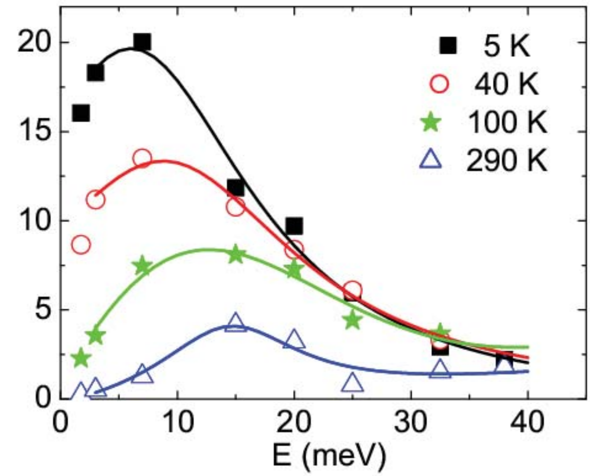
Li et al. , PRB (2008)

Dispersion and a-b anisotropy

$YBa_2Cu_3O_{6.6}$ $p>p_{MI}$

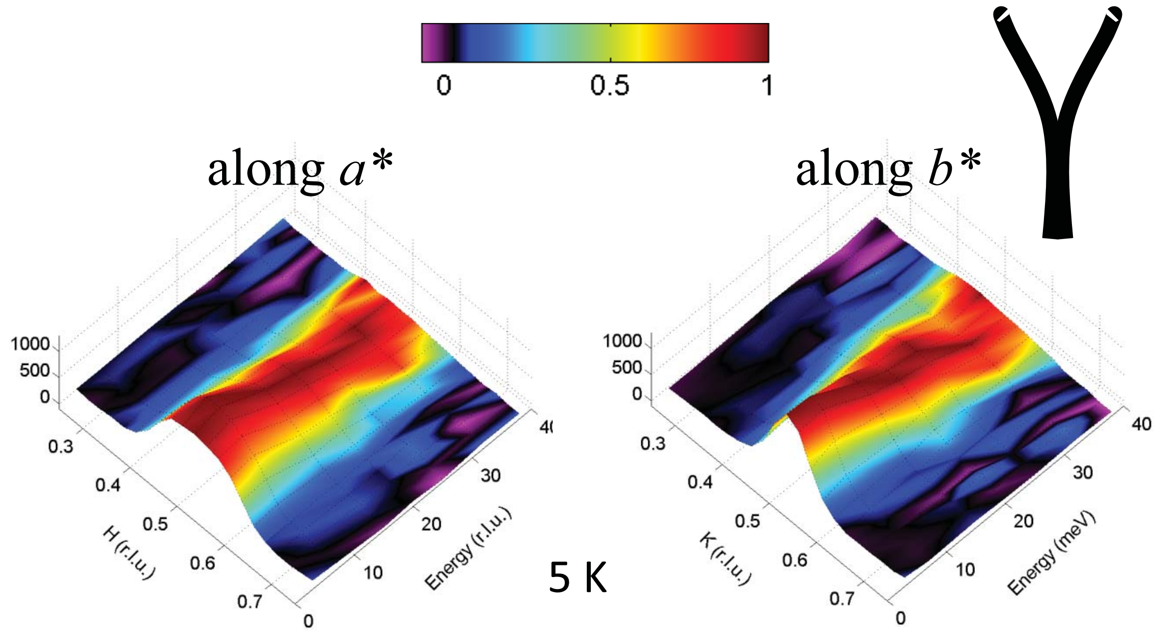


$YBa_2Cu_3O_{6.45}$ $p<p_{MI}$

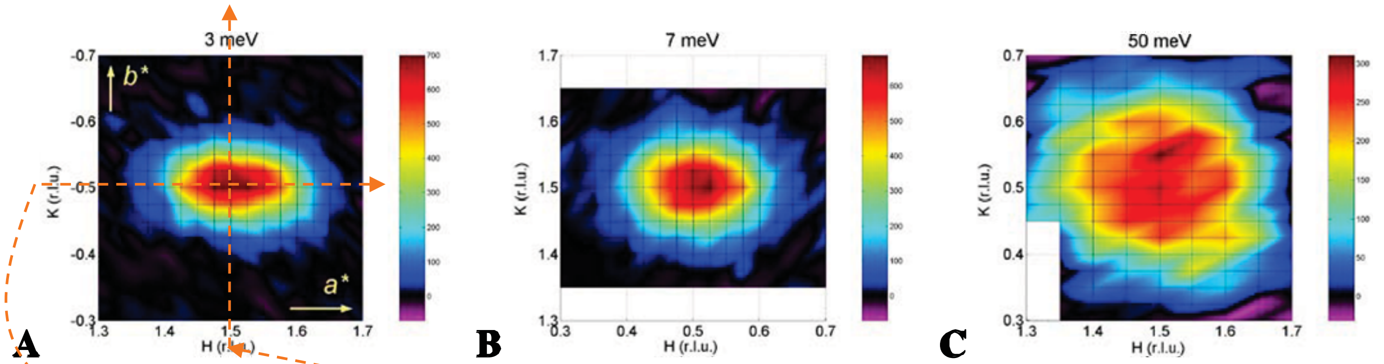


$YBa_2Cu_3O_{6.45}$ (T_c=35 K, p~0.08)

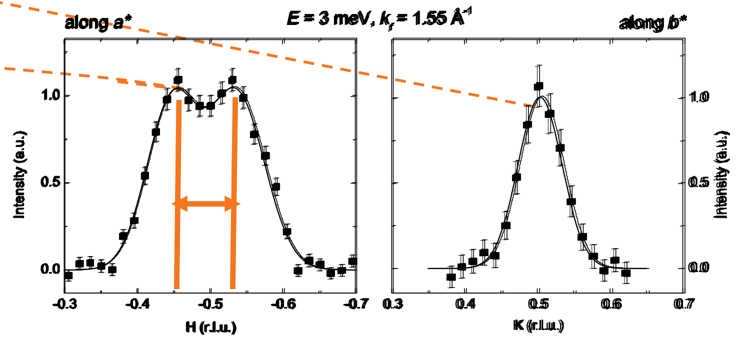
- Hardly any hour-glass dispersion
- Very weak resonance anomaly at best
- „Y"-shaped dispersion even below T_c – pure symmetry-broken phase showing up when superconductivity is weakened?



Spontaneous onset of a-b anisotropy

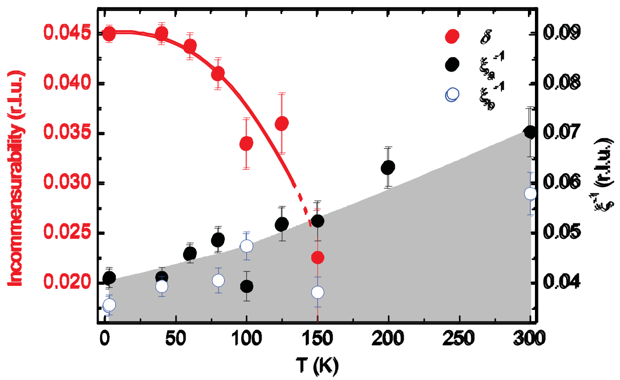


Hinkov et al., *Science* **319**, 597 (2008).



$YBa_2Cu_3O_{6.45}$ $p<p_{MI}$

Incommensurability

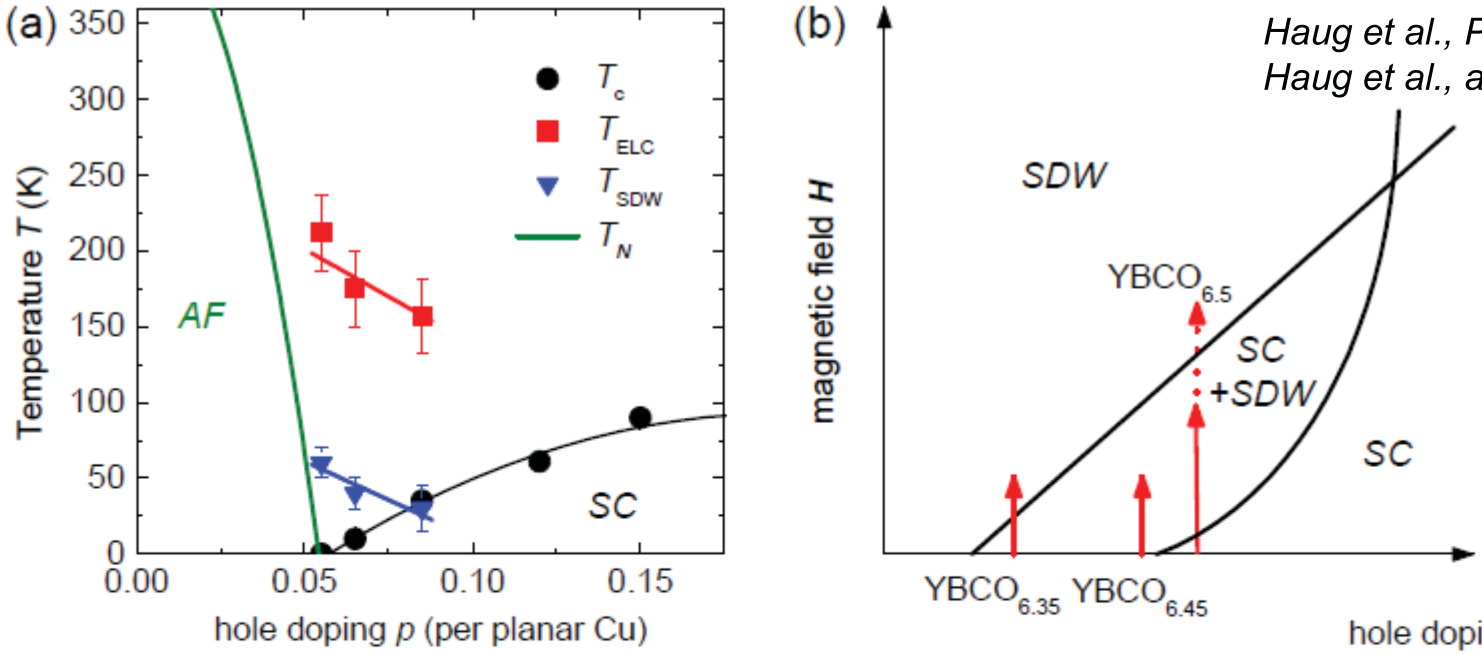


- Spontaneous onset of incommensurability at ~150 K

⇒Suggests underlying nematic electronic liquid crystal phase

.....the orthorhombic lattice distortion serves as weak orientational field

Evidence for "electronic liquid phases" In strongly underdoped $YBa_2Cu_3O_{6+x}$



Haug et al., PRL (2009)
Haug et al., arXiv :1008-4298

- T_{ELC} : breaking of C_4 rotation invariance

~ nematic electronic liquid crystal state

- T_{SDW} : breaking of the translation invariance

~ smectic electronic liquid crystal state

The SDW state is furter stabilized under magnetic field

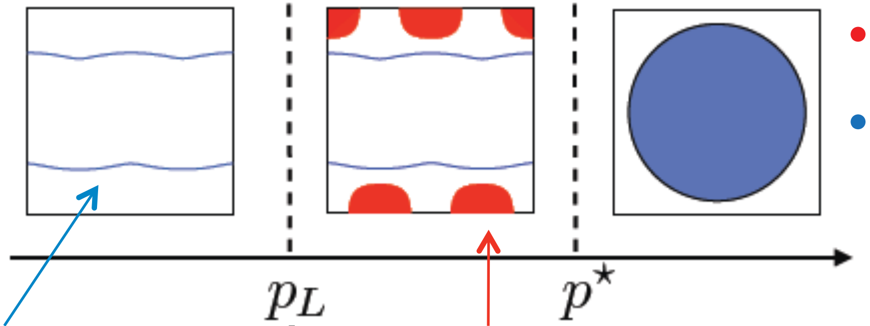
Possible connection with the folding of the Fermi surface inferred from quantum oscillation measurements

Doiron-Leyraud Nature (2007)

Incommensurate SDW in $YBa_2Cu_3O_{6+x}$
Quantum oscillations versus Neutron

Leboeuf et al., ArXiv:1009.2078

YBCO6.45 YBCO6.6



• Electron

• Hole

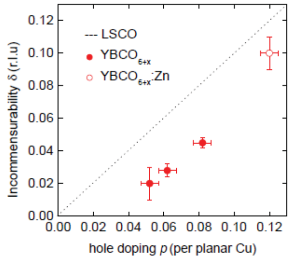
Quantum oscillations at large H consistent with a reconstruction of the Fermi surface

Quasi-1D

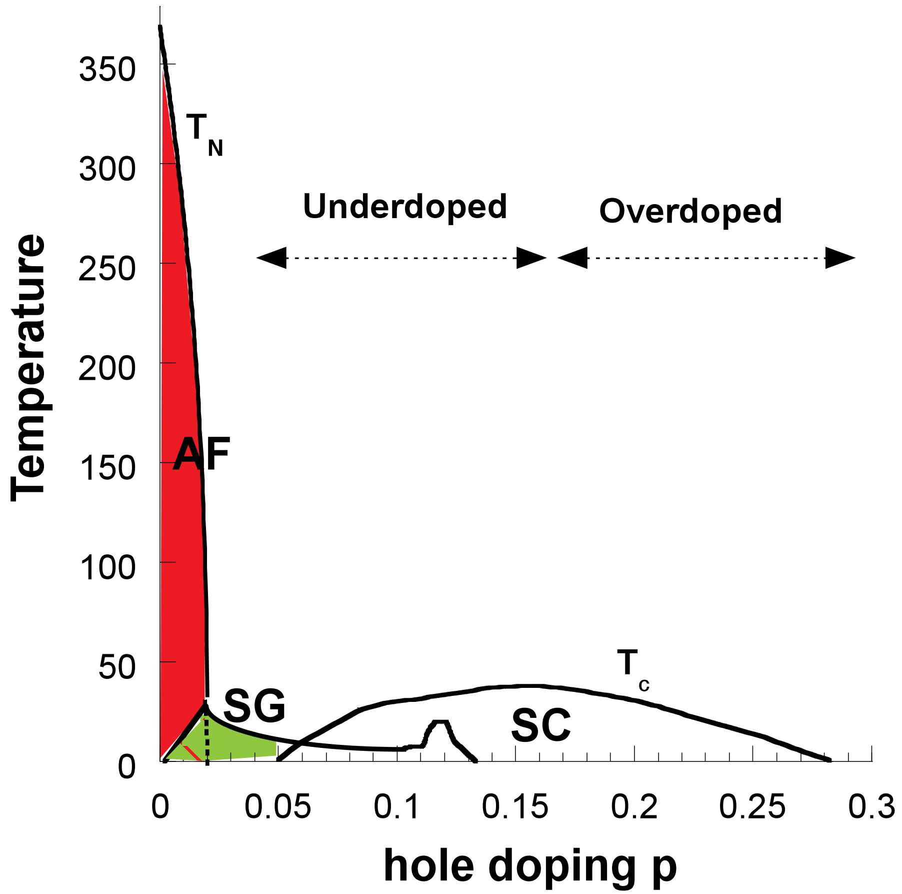
~ localization by disorder

High mobility

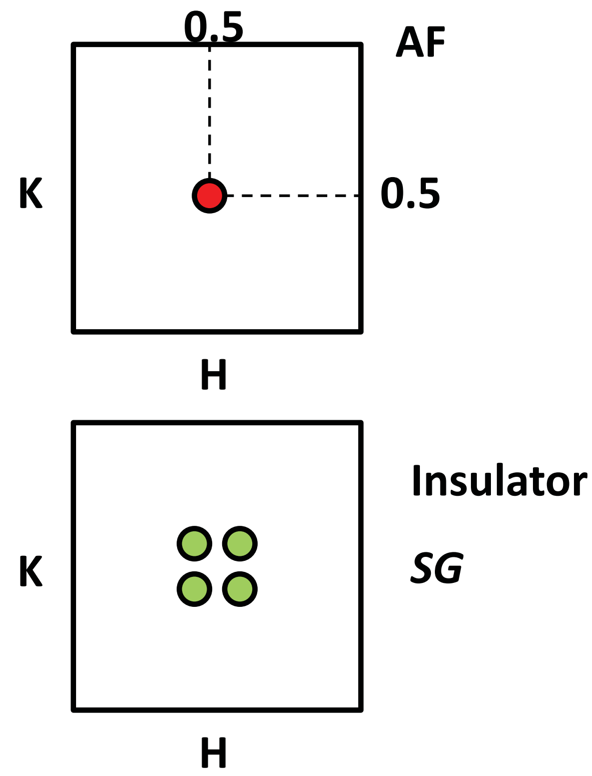
	No oscillation !	oscillations
Neutron scattering (H=0) Quasi-1D SDW	IC parameter δ~.045 Short ranged order !	IC parameter δ~.1 NO ORDER !!!!
Neutron + μSR	~Spiral SDW ~~stripe~~	Large spin (pseudo)-gap



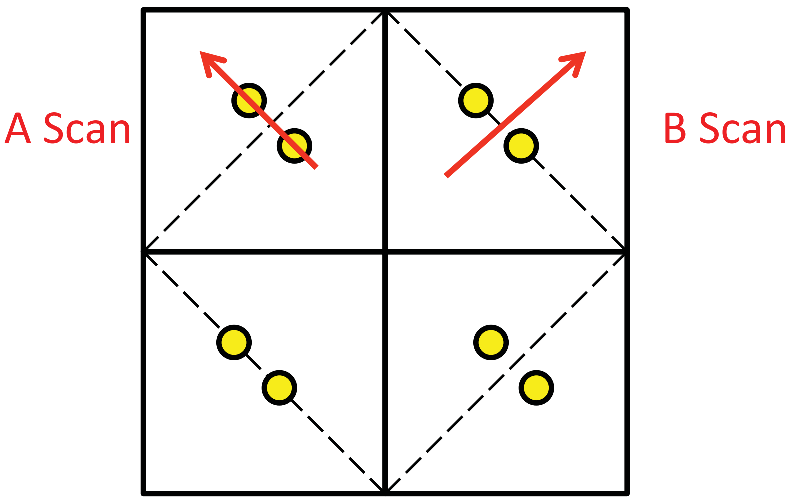
From commensurate to incommensurate spin correlations in $La_{2-x}Sr_xCuO_4$



Magnetic wave vectors



Lightly doped $La_{2-x}Sr_xCuO_4$
"diagonal" stripes or spin spiral ?

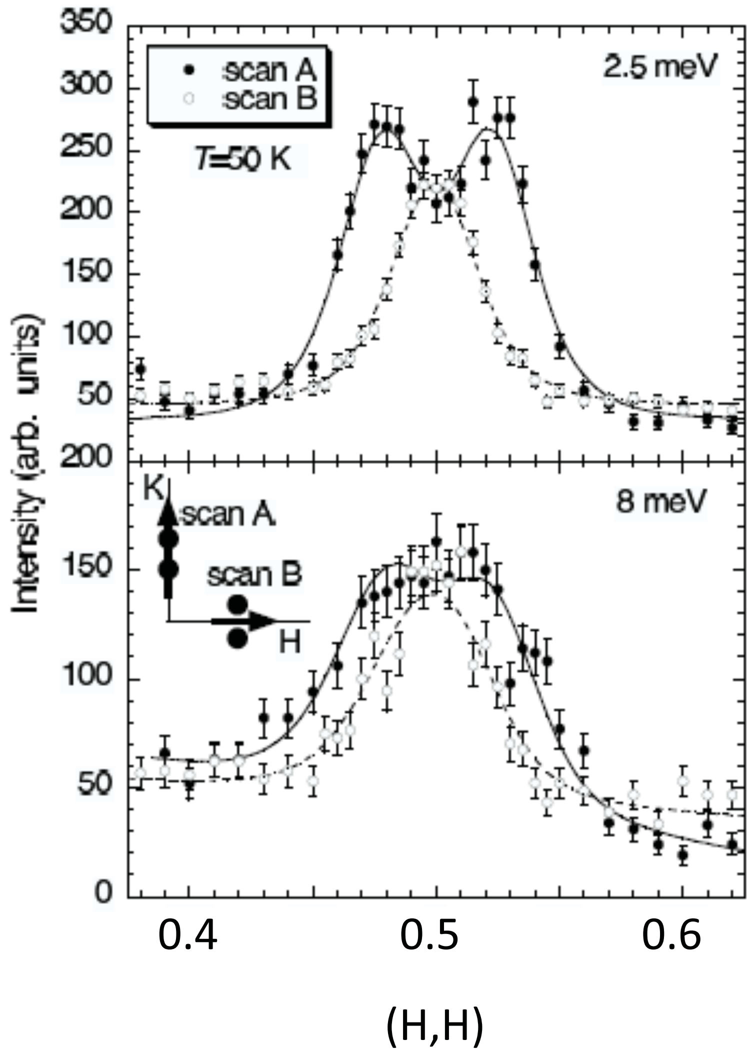


Tetragonal unit cell

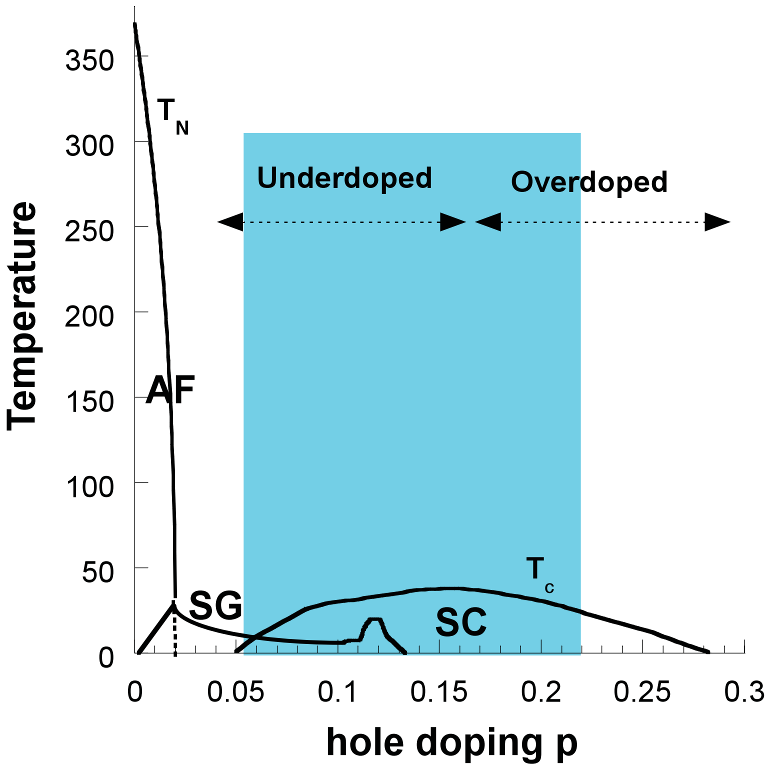
Orthorhombic unit cell

Insulating $La_{2-x}Sr_xCuO_4$
x=0.04 (p=0.04)
Twin free crystal

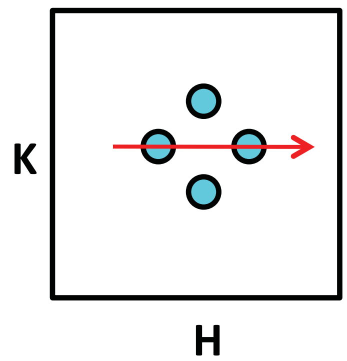
Matsuda et al., PRL (2009)



Incommensurate spin fluctuations In metallic $La_{2-x}Sr_xCuO_4$



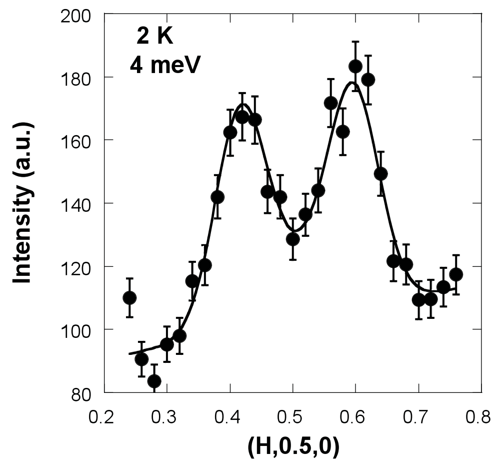
Magnetic wave vector



Metal

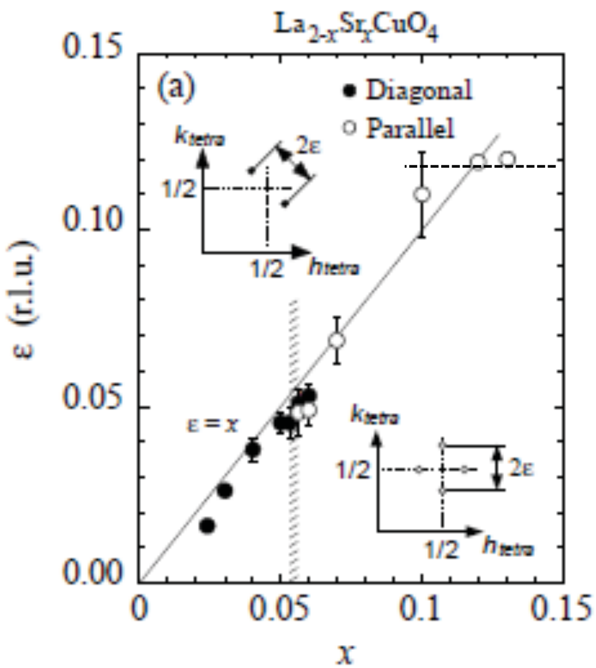
and

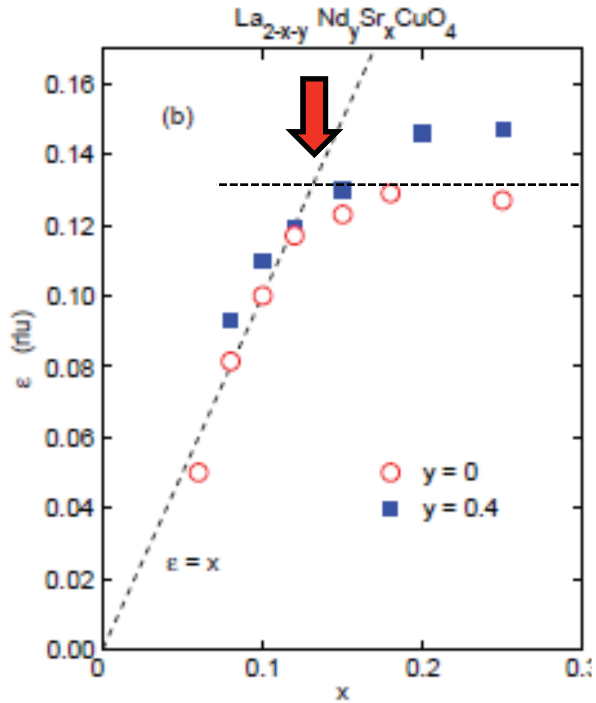
SC state

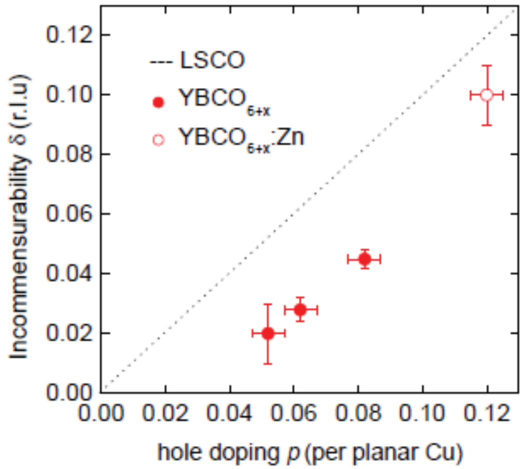


$La_{2-x}Sr_xCuO_4$
x=0.085 (p=0.085)
Twinned crystal

From "diagonal " to "parallel" Incommensurate *spin fluctuations*





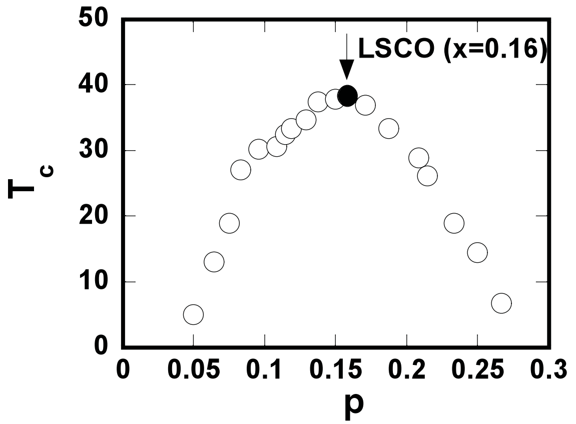


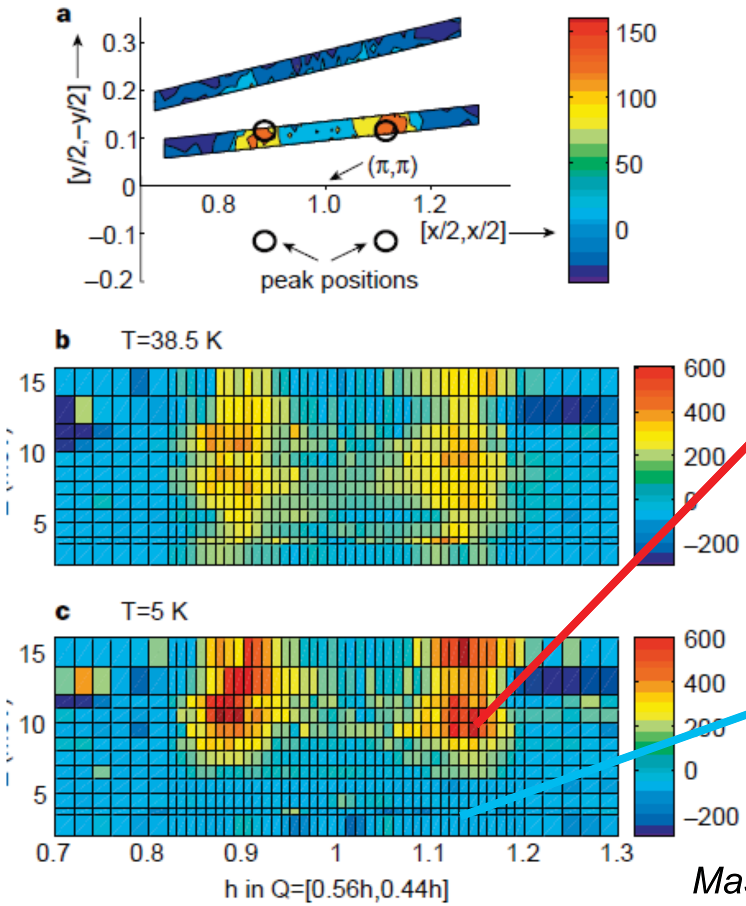
p=0.05 rotation of IC spin correlation at 45°

p>0.12 progressive saturation of the IC parameter

<u>Warning</u>: the incommensurability parameter is
~ twice smaller in strongly underdoped YBCO

Spin gap and coherence effect in superconducting $La_{2-x}Sr_xCuO_4$

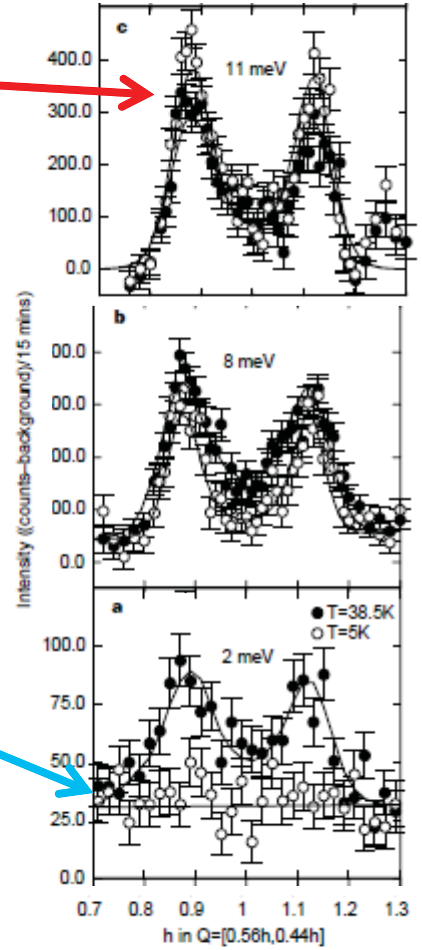




Coherence effect:

Narrowing & sharpening of IC excitations ($T<T_c$)

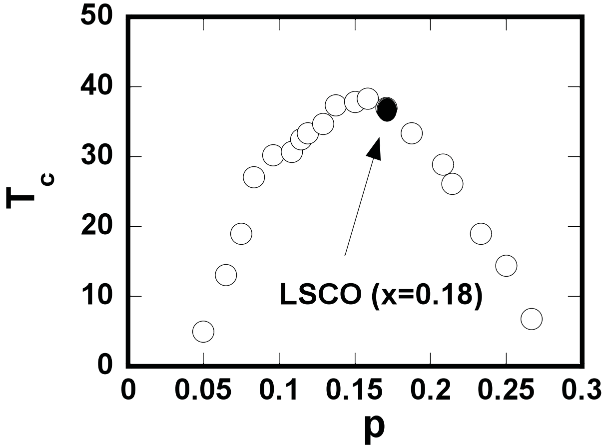
Opening of a spin gap in the SC state



Mason et al. , PRL (1996)

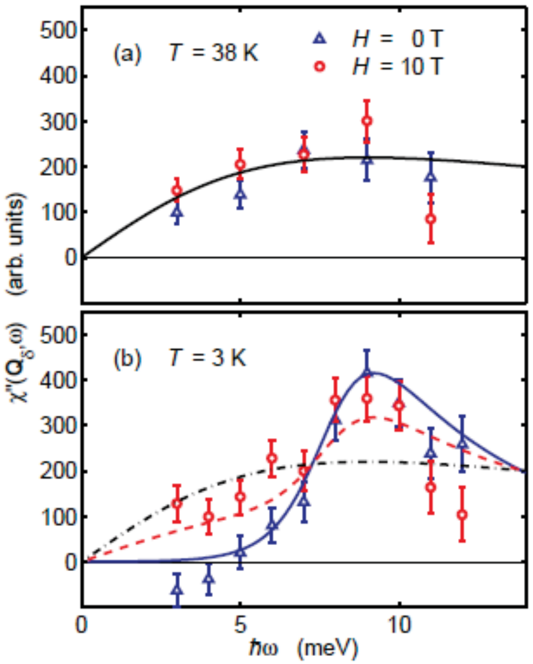
Lake et al., Nature (1999)

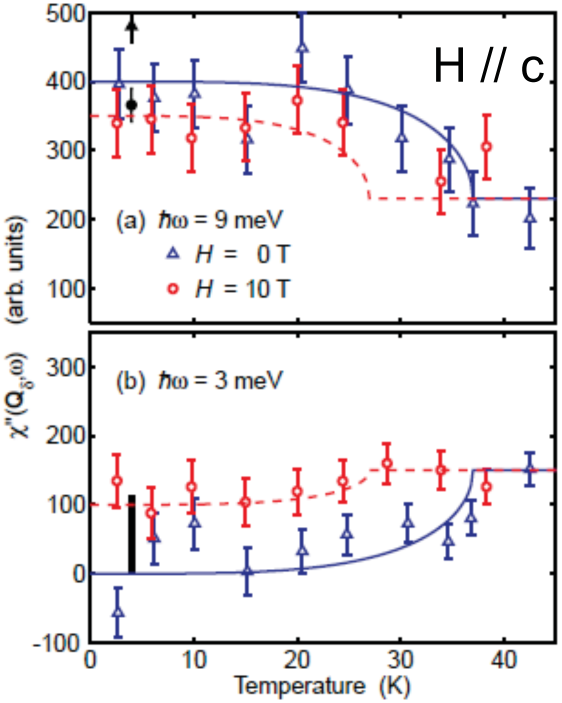
Magnetic field effect in overdoped $La_{2-x}Sr_xCuO_4$

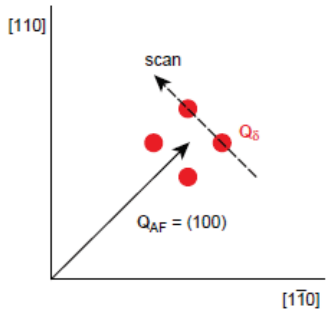


* broadening of IC excitation and progressive filling of the spin gap

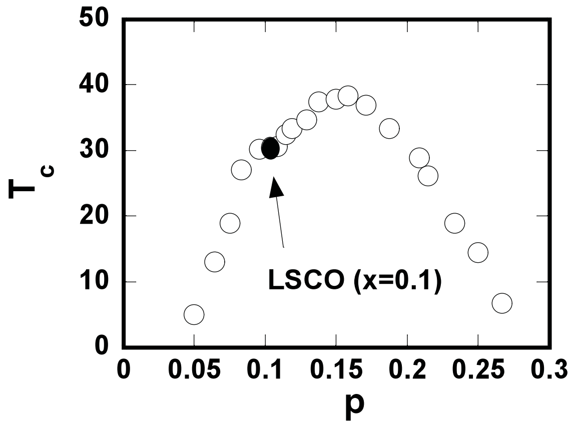
* H and non magnetic Zn impurities qualitatively give rise to similar effects





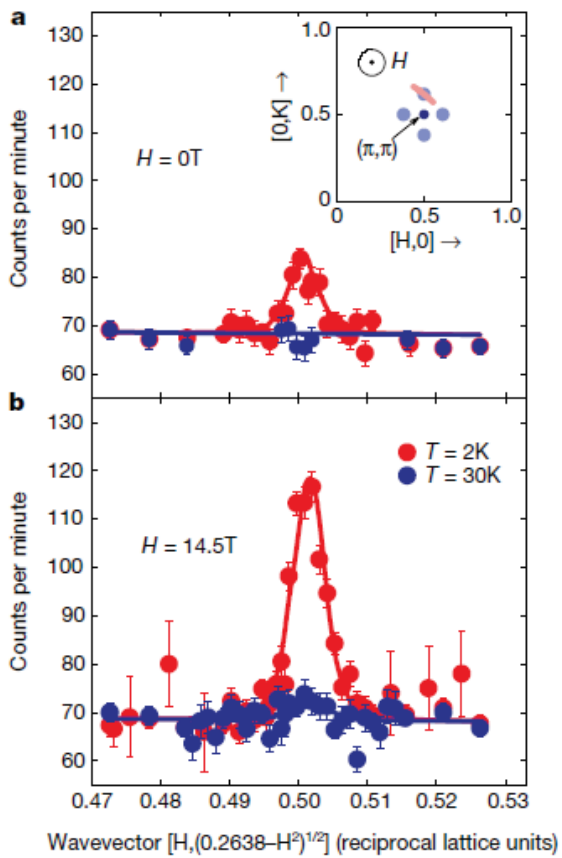


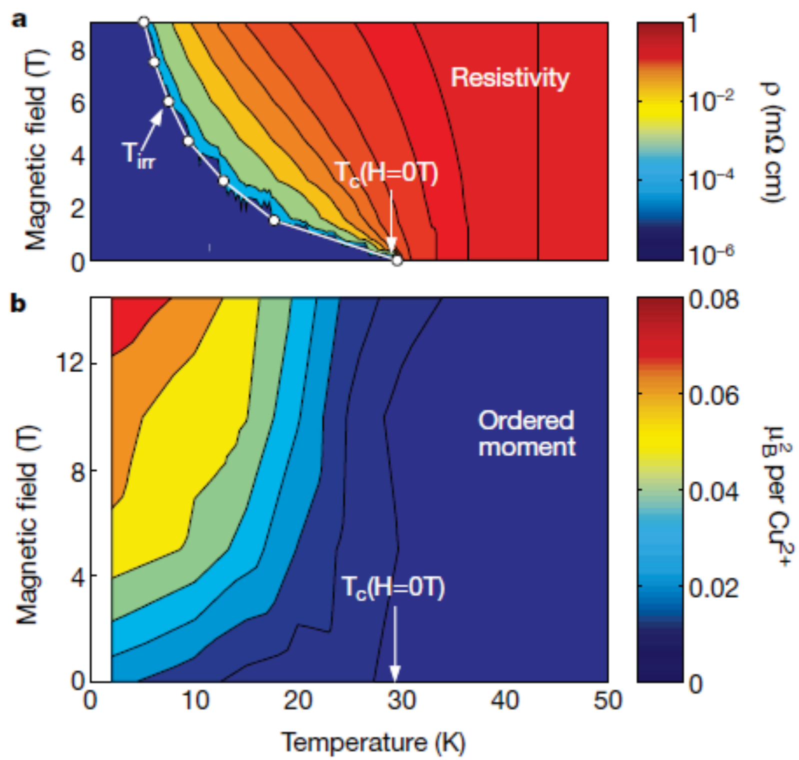
Tranquada et al. , PRB (2004)



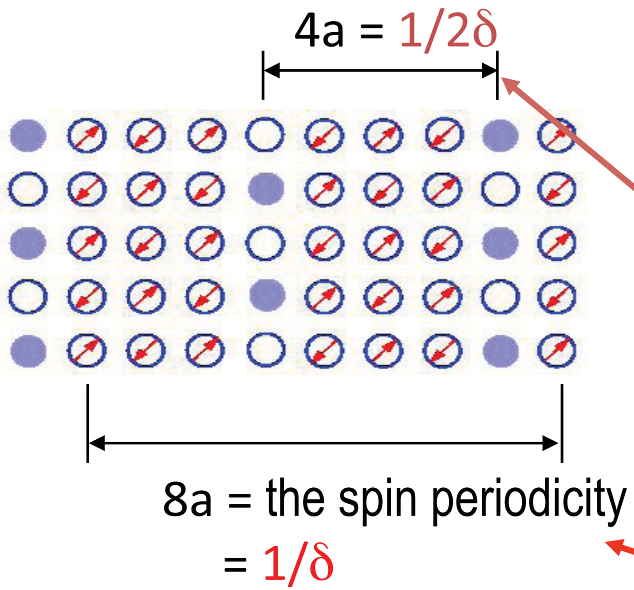
Incommensurate magnetic order induced by an applied magnetic field in underdoped $La_{2-x}Sr_xCuO_4$

Lake et al. , Nature (2002)
Lake et al. , Science (2001)
Katano et al., PRB (2000)



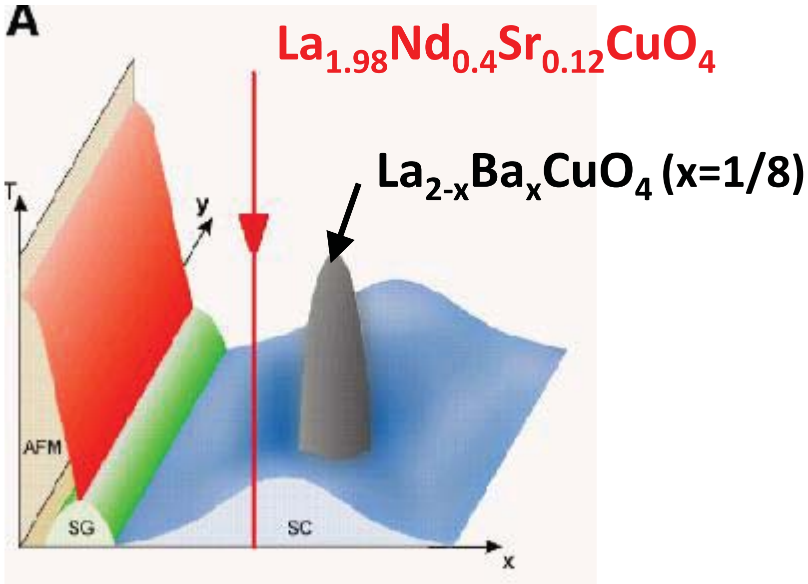


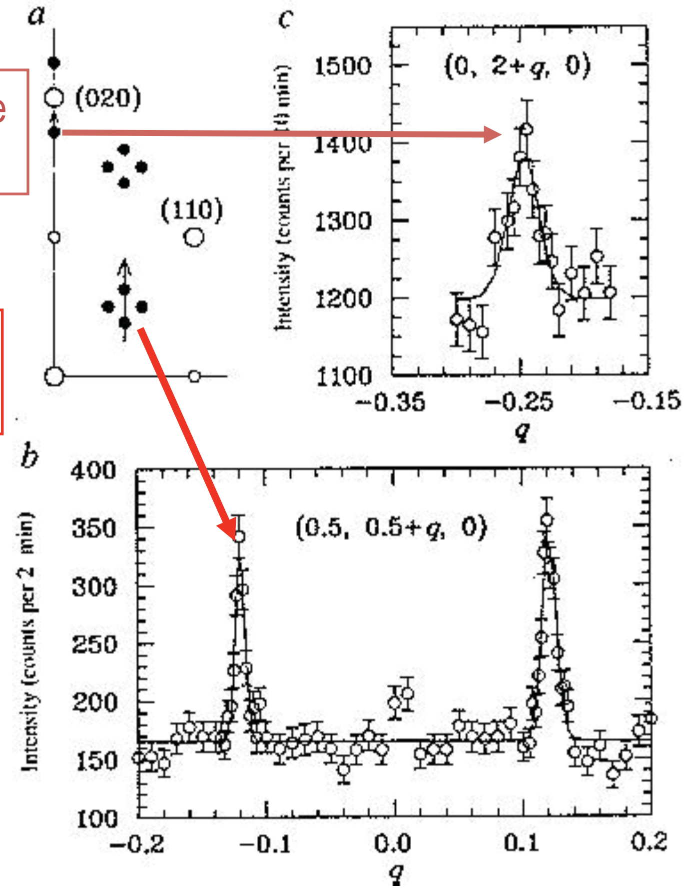
Self-organization of doped holes "parallel stripes "



Charge order

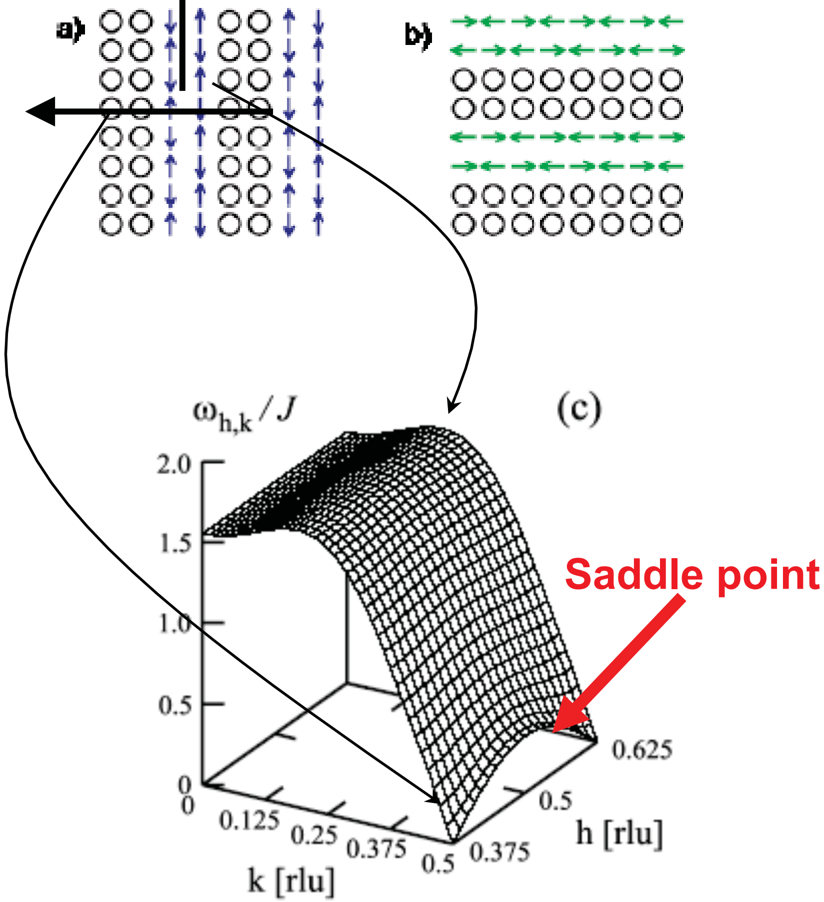
Spin order

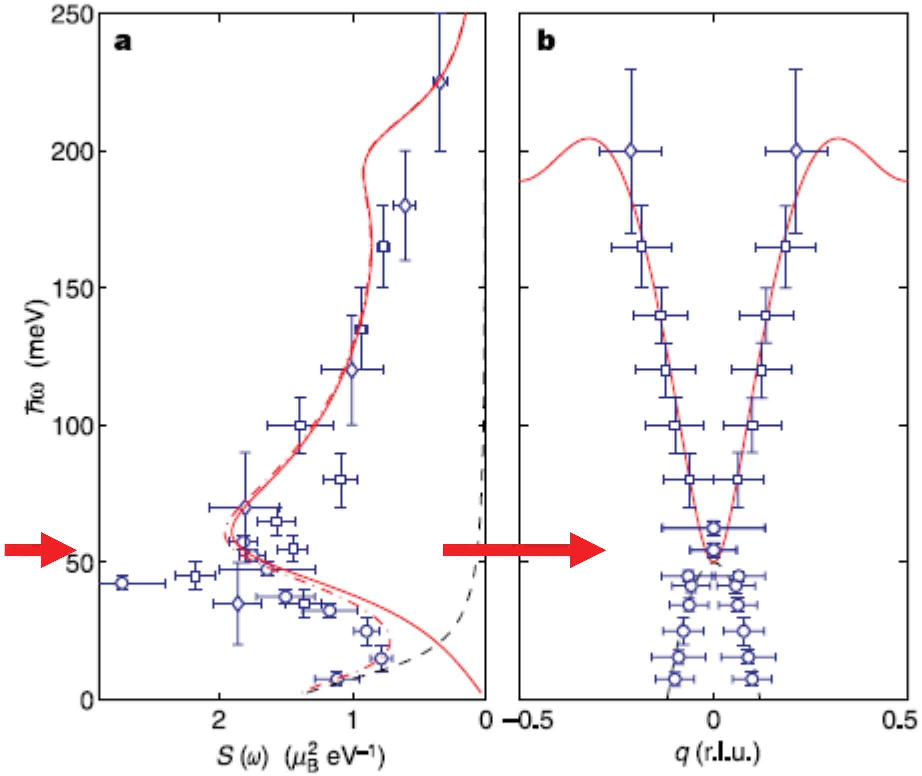




Tranquada et al. , Nature (1995)

Hourglass dispersion
In stripe ordered $La_{2-x}Ba_xCuO_4$ (x=1/8)





Theory

Vojta et al., PRL (2004)
Uhrig et al., PRL (2004)
Seibold et al., PRL (2005)
Vojta et al., PRL (2006)

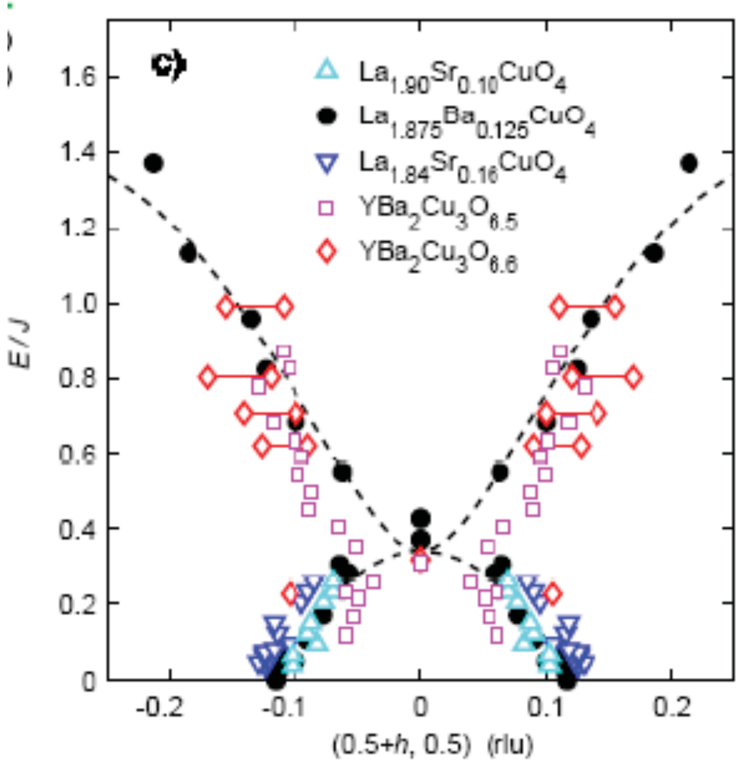
INS

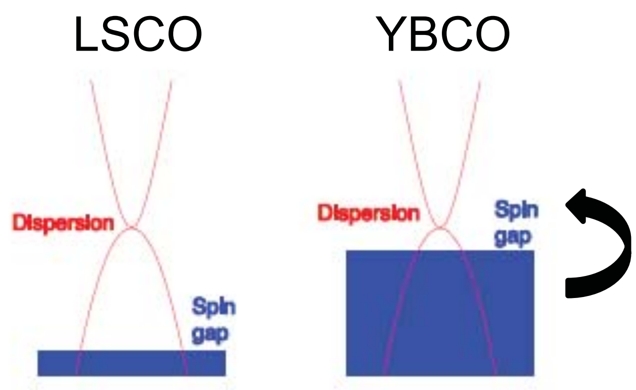
Tranquada et al. , Nature (2004)

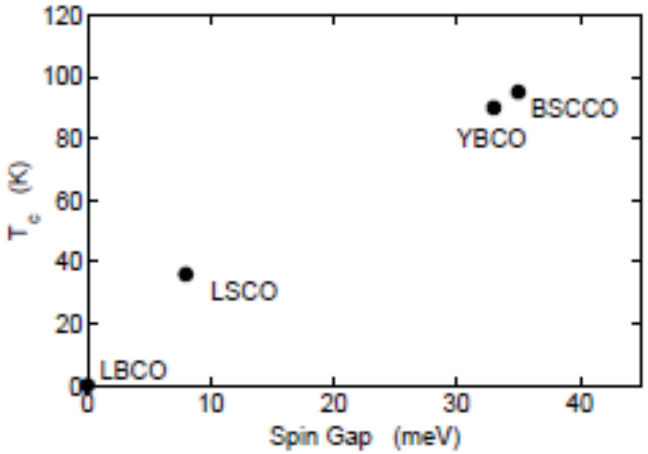
Hourglass dispersion
The "stripes" scenario

INS

Christensen et al., PRL (2004)
Tranquada et al., Nature (2004)
Hayden et al., Nature (2004)
Stock et al., PRB (2005)



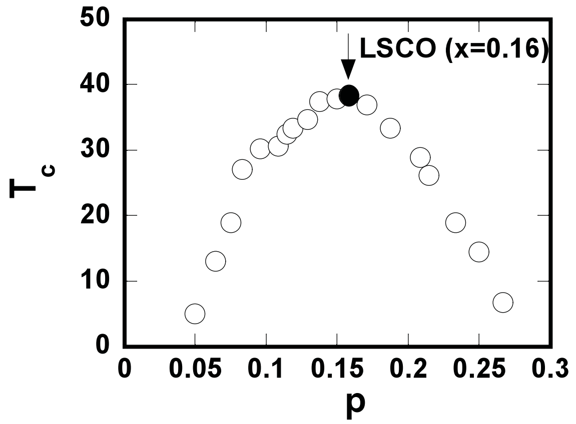




Transfer of spectral weight in the SC state and building up of resonant excitations

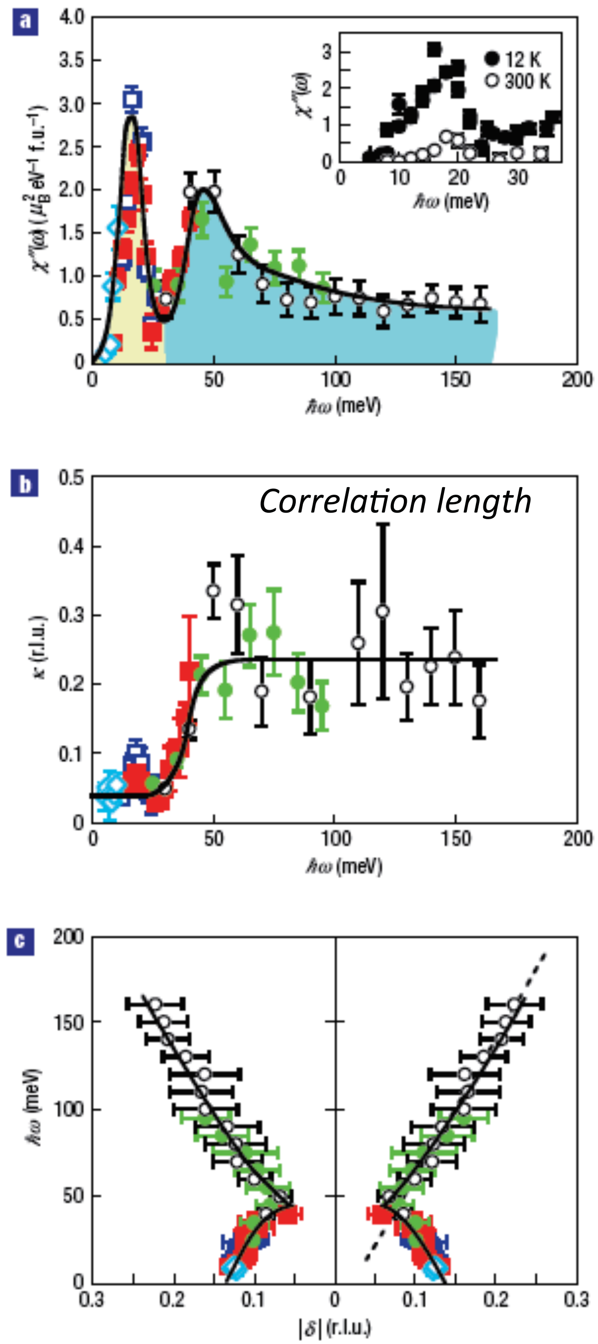
Two-energy scales *n optimally doped*
$La_{2-x}Sr_xCuO_4$ (x=0.16)

Back to itinerant-localized scenario ?

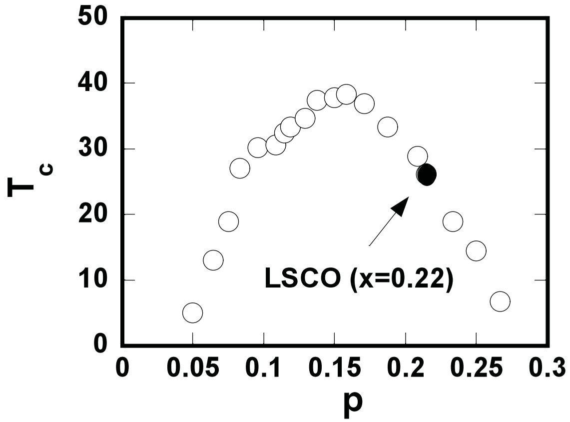


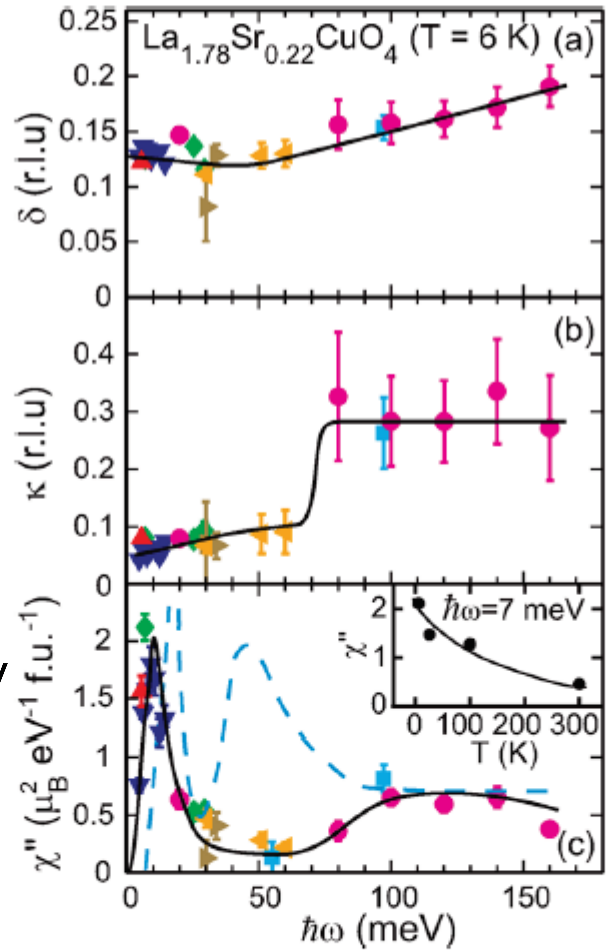
" Given the markedly different characteristics of the two components that make up the magnetic response in $La_{1.84}Sr_{0.16}CuO_4$, it is likely that they have different origins. One possible interpretation is that the lower-energy incommensurate structure is due to quasiparticle (electron–hole) pair creation, which might be calculated from an underlying band structure whereas the higher-energy structure is due to the residual antiferromagnetic interactions "

Vignolle et al., Nature (2007)



Redistribution of spectral weight *in overdoped* $La_{2-x}Sr_xCuO_4$ (x=0.22)



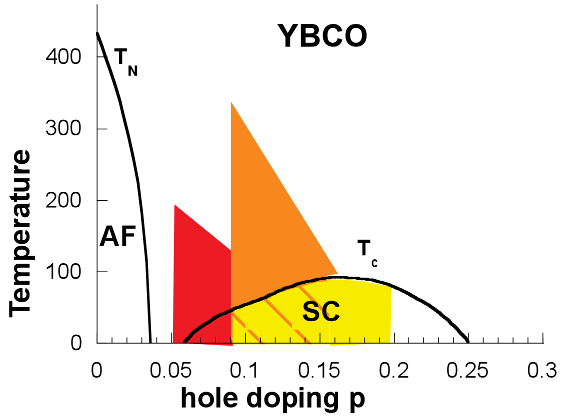


•persistence of High-E spin fluctuations

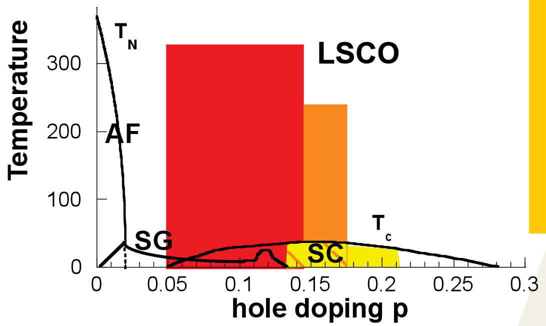
•Strong weakening of spin excitations near 50 meV (*absence of saddle point*)

Lipscombe et al., PRL (2007)

conclusion



In materials with T_c (opt)~ 90 K or larger
Spin gap + resonant S=1 excitations in the SC state
Itinerant picture
Indication of a strong spin fermion coupling



Underdoped regime
Mixte localized + itinerant picture ?.... 2 energy scales
When does the high E dispersion come from ?
What is the fingerprint of the pseudo-gap ?

When T_c is weak in underdoped materials
$p < p_{MI}$ (~0.85 in YBCO or ~0.16 in LSCO)
$d\rho/dt < 0$ as $T \rightarrow 0$
Indication of a quasi-1D IC-SDW as $T \rightarrow 0$ + related spin fluctuations
Spiral-SDW (YBCO) or stripes (LSCO)
Competing instability: NOT GOOD for superconductivity !!!!