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ICTP 40th Anniversary

**SMR.1572 - 26**

**Workshop on Novel States and Phase Transitions in Highly Correlated Matter**

**12 - 23 July 2004**

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# Magnetic excitations in cuprates

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**GERMANY**

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# Magnetic excitations in cuprates

B. Keimer
MPI for Solid State Research

Open experimental questions:

1. generic & materials specific aspects
2. systematics with layer sequence, doping ($\rightarrow$ overdoped regime)
3. incommensurate spin dynamics: 1D or 2D?
4. origin & bulk nature of superstructures

New approach:

neutron and x-ray scattering from small, perfect crystals

# Collaborators

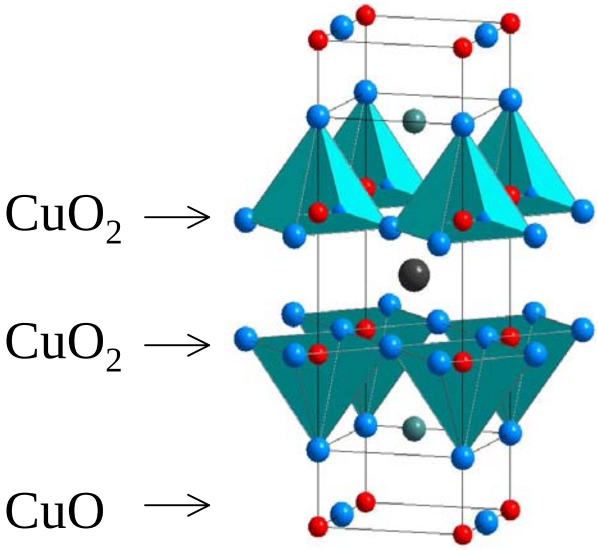
**MPI Stuttgart**
S. Bayrakci, C. Bernhard, **V. Hinkov**,
A. Kulakov, B. Liang, C.T. Lin, A. Maljuk,
J. Strempfer, C. Ulrich, I. Zegkinoglou

**CEA Saclay**
P. Bourges, **S. Pailhes**, Y. Sidis

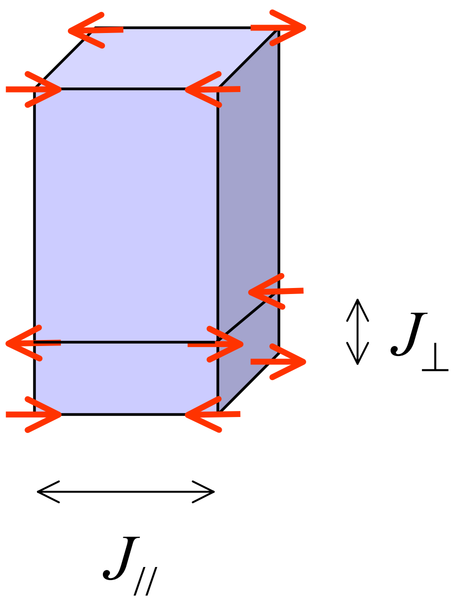
**CEA Grenoble**
L.P. Regnault

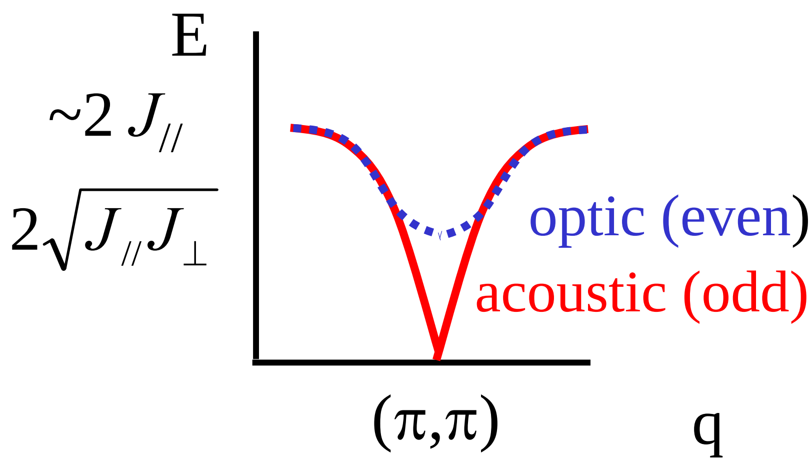
**DESY Hamburg**
M. v. Zimmermann

# $YBa_2Cu_3O_{6+x}$




## Antiferromagnetic $YBa_2Cu_3O_6$

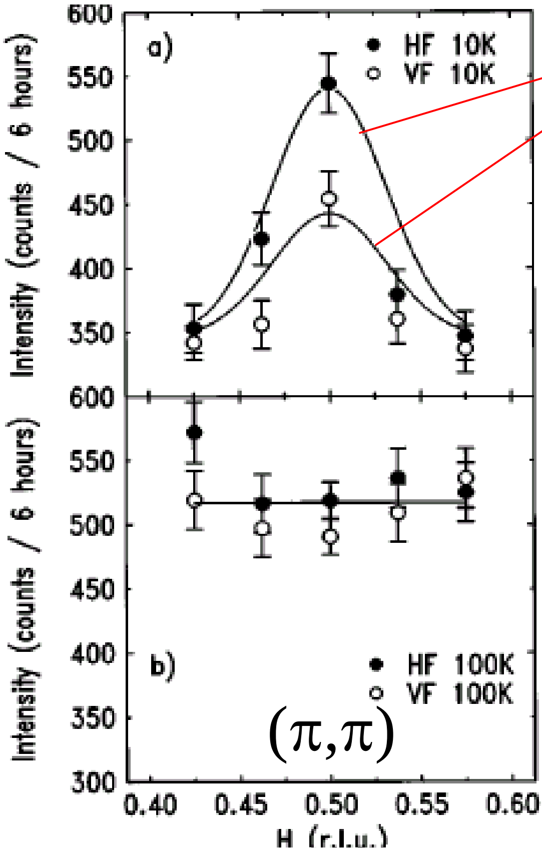


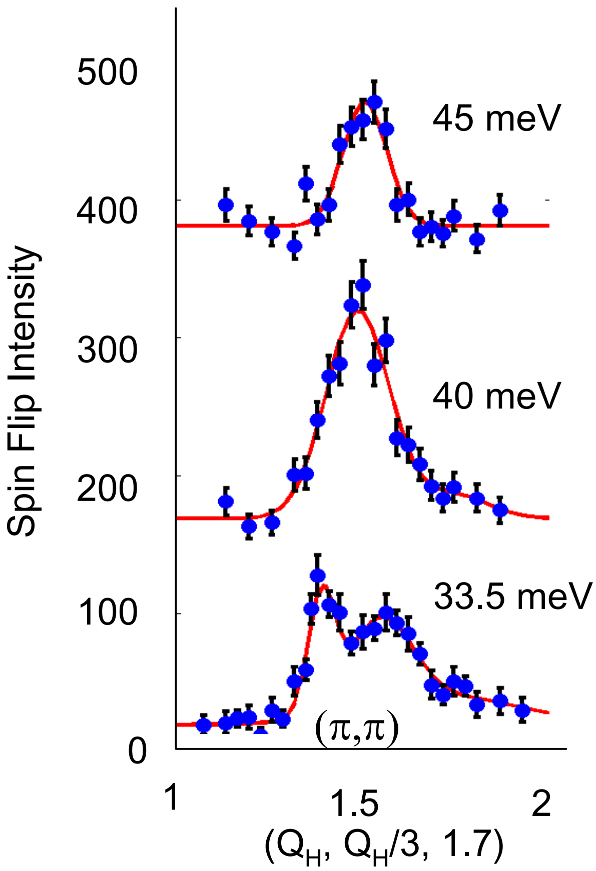

| | | |
|---|---|---|
| $2J_{//} \sim 200$ meV<br>$2\sqrt{J_{//}J_{\perp}} \sim 70$ meV | ➡ | $J_{//} \sim 100$ meV<br>$J_{\perp} \sim 10$ meV |

# Resonant Mode in $YBa_2Cu_3O_7$

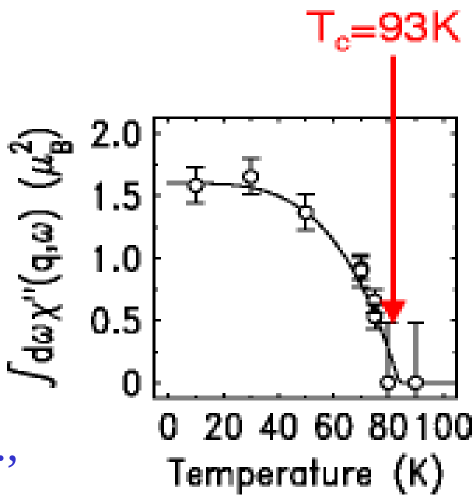
$YBa_2Cu_3O_7$, 40 meV spin-flip scattering




difference yields
Im χ(q,ω) free of
background effects



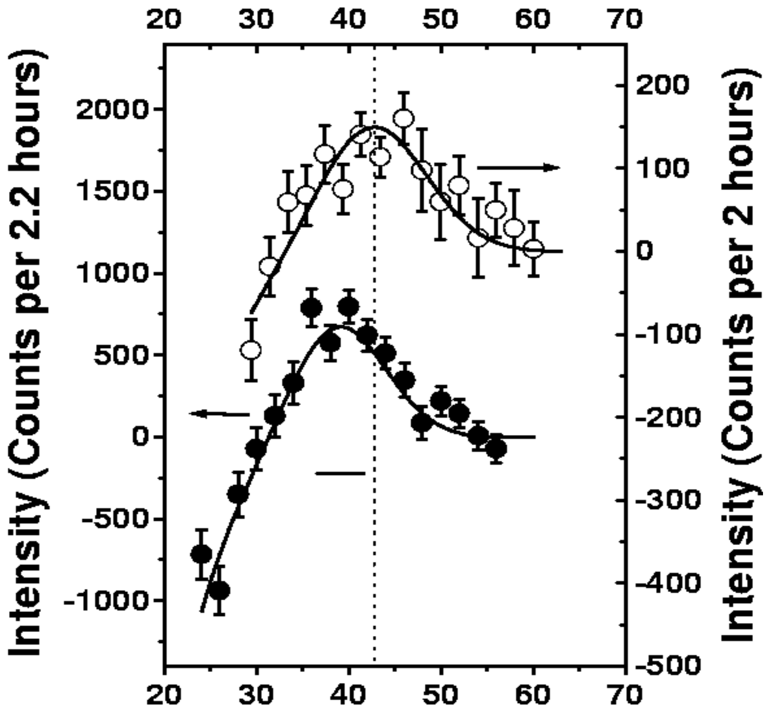

Bourges et al., Science 2000




Fong et al.,
PRB 1996

spectral weight near q=(π,π) comparable to antiferrromagnetic magnons in $YBa_2Cu_3O_6$

# Resonant Mode in $Bi_2Sr_2CaCu_2O_{8+x}$




○ optimally doped ($T_c$=91K)

● overdoped ($T_c$=83K)

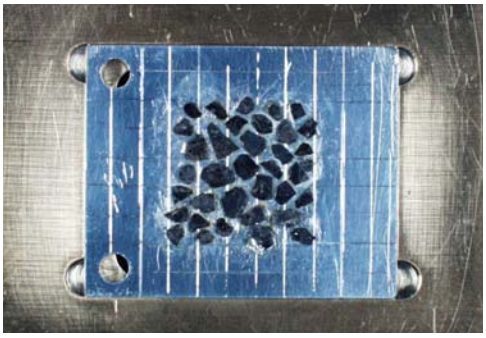
- resonant mode present in $Bi_2Sr_2CaCu_2O_{8+x}$
  → quantitative comparison with ARPES, tunneling
- broadened due to disorder
- mode energy decreases in overdoped state

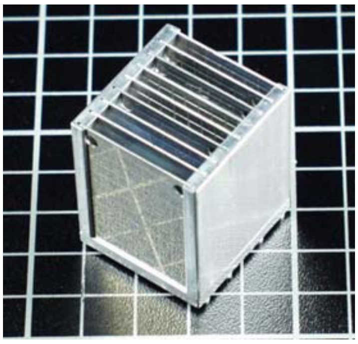
H.F. Fong et al., Nature 1999

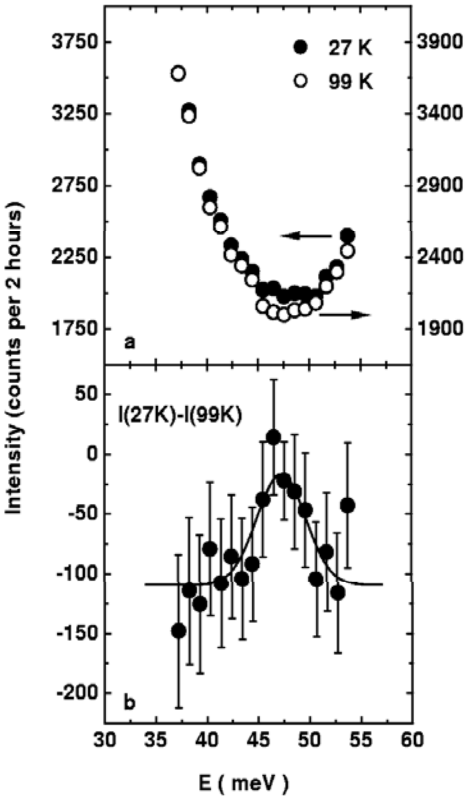
H. He et al., Phys. Rev. Lett 2000

# Resonant Mode in Single-Layer Cuprate

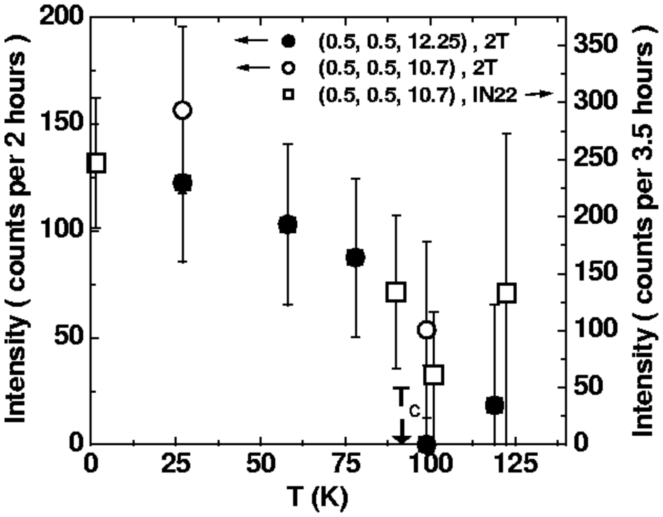
co-align ~350 small crystals to within ~ 1.5°
→ sufficient volume for inelastic neutron scattering








**$Tl_2Ba_2CuO_6$**
**$q = (\pi,\pi)$**

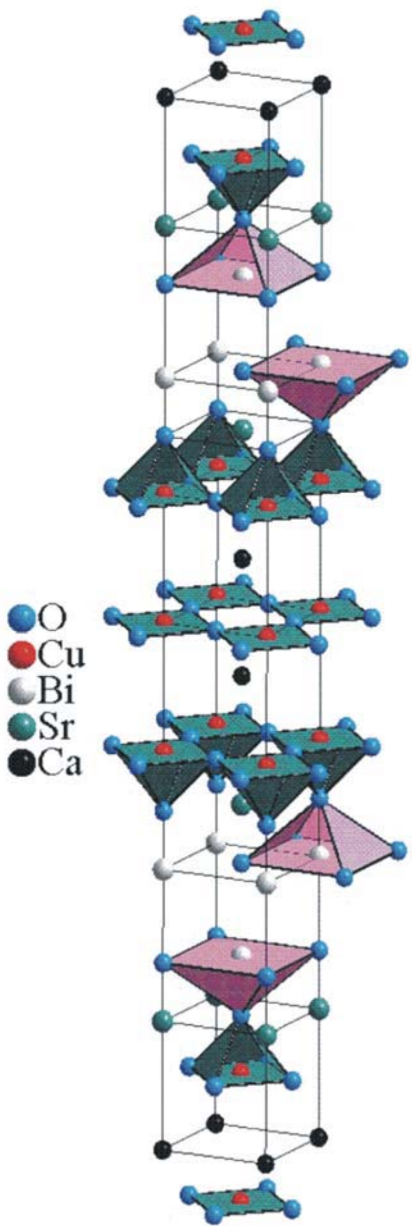


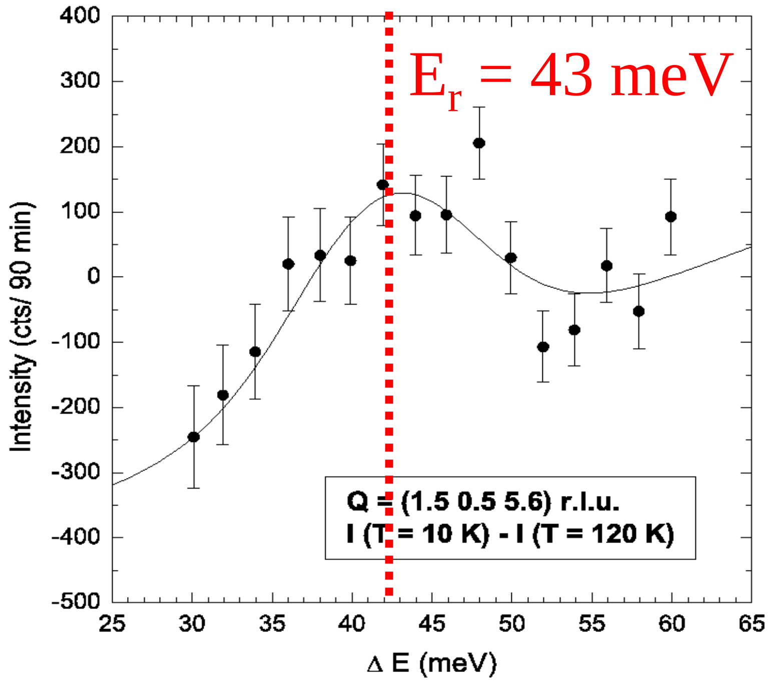

H. He et al., Science 2002

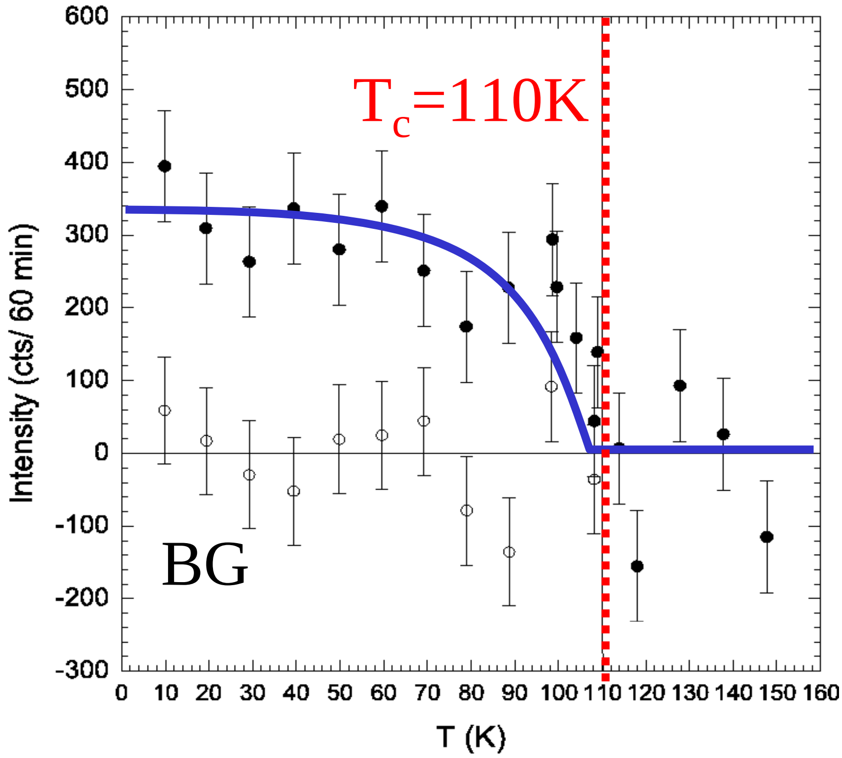
→ resonant mode generic to
- single $CuO_2$ layer
- copper oxides with intrinsically high $T_c$

# Resonant Mode in Trilayer Cuprate

$Bi_2Sr_2Ca_2Cu_3O_{10+x}$

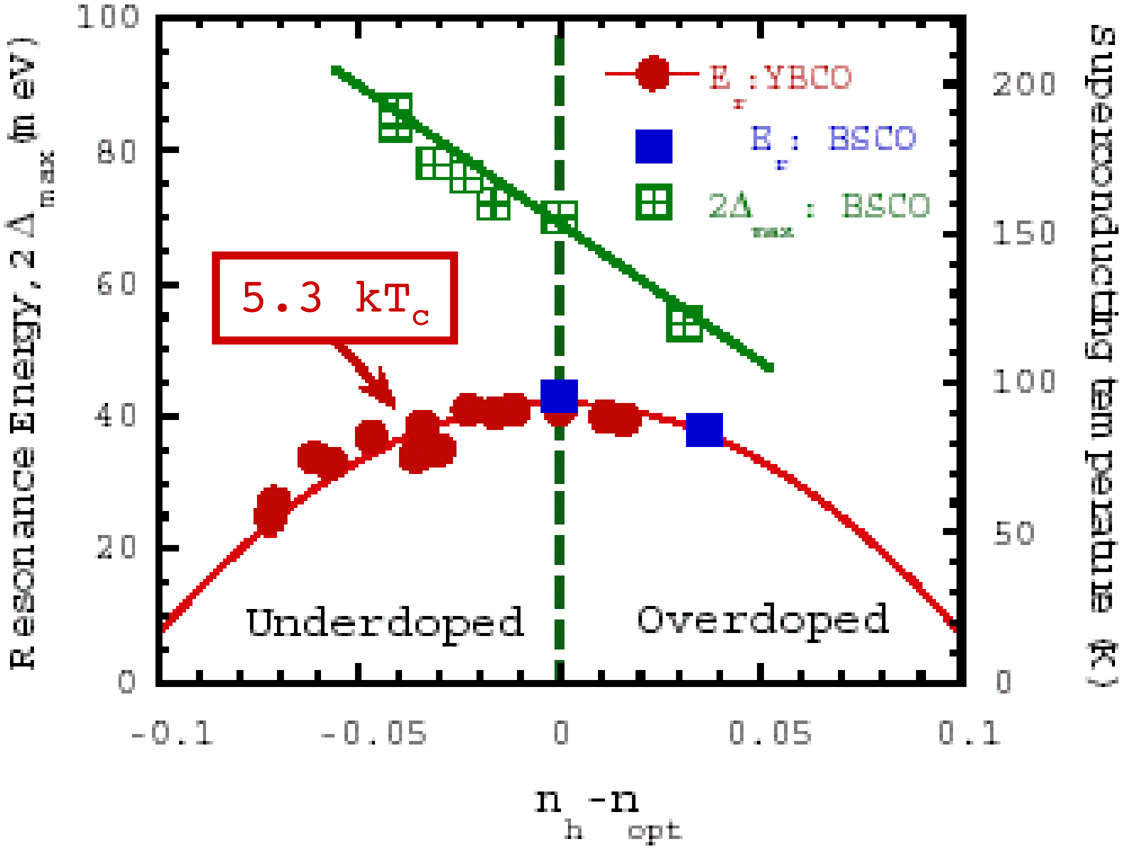



S. Bayrakci

# Doping Dependence



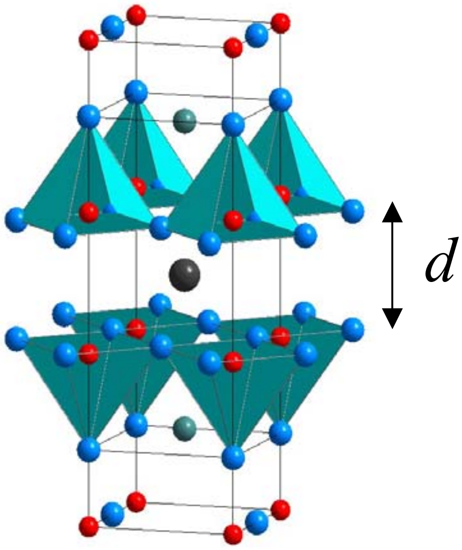

# Dependence on Layer Sequence

| # of layers in unit cell | $E_{res} / k_B T_c$ at optimum doping | |
|---|---|---|
| 1 | 5.9 | Tl2201 |
| 2 | 5.2 | Y123, Bi2212 |
| 3 | 4.4 | Bi2223 |

# Mean Field Theory: Bilayer Superconductor

$$\chi_0^{ij}(q,\omega) = \tfrac{1}{4}\sum_k \left(1 - \frac{\varepsilon_k \varepsilon_{k+q} + \Delta_k^i \Delta_{k+q}^j}{E_k^i E_{k+q}^j}\right) \frac{1}{\omega - (E_k^i + E_{k+q}^j) + i\delta}$$

$$i,j = \begin{cases} \text{antibonding } (a) \\ \text{bonding } (b) \end{cases}$$




$$\chi_0^{even}(q,\omega) = \chi_0^{aa}(q,\omega) + \chi_0^{bb}(q,\omega)$$

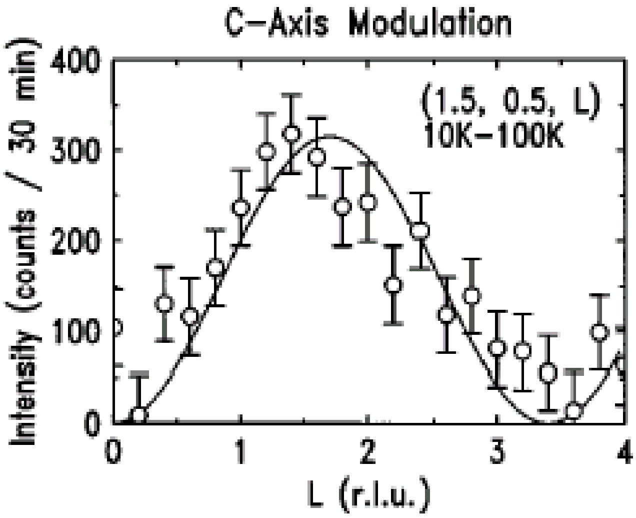
$$\chi_0^{odd}(q,\omega) = \chi_0^{ab}(q,\omega) + \chi_0^{ba}(q,\omega)$$

$$\chi^{even}(q,\omega) = \frac{\chi_0^{even}(q,\omega)}{1 + (J(q) + J_\perp)\chi_0^{even}(q,\omega)}$$

$$\chi^{odd}(q,\omega) = \frac{\chi_0^{odd}(q,\omega)}{1 + (J(q) - J_\perp)\chi_0^{odd}(q,\omega)}$$

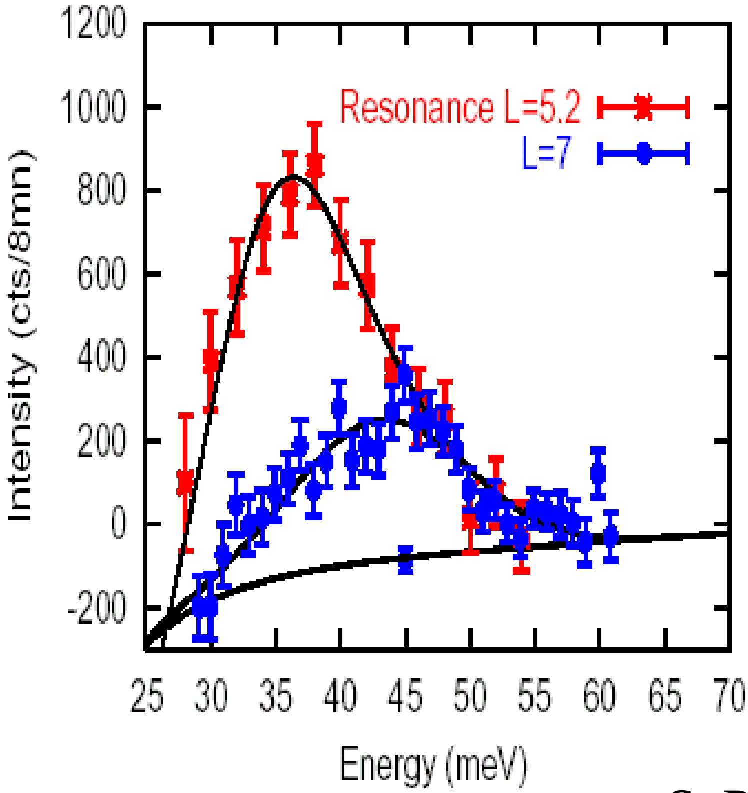
$J_\perp = 0.1J$ from optical magnon gap in insulator

$$\chi(q,q_z,\omega) = \chi^{odd}(q,\omega)\sin^2(\tfrac{q_z d}{2}) + \chi^{even}(q,\omega)\cos^2(\tfrac{q_z d}{2})$$




only odd resonant mode originally observed in optimally doped $YBa_2Cu_3O_{6+x}$ and $Bi_2Sr_2CaCu_2O_{8+x}$

# Overdoped $Y_{0.9}Ca_{0.1}Ba_2Cu_3O_7$




odd

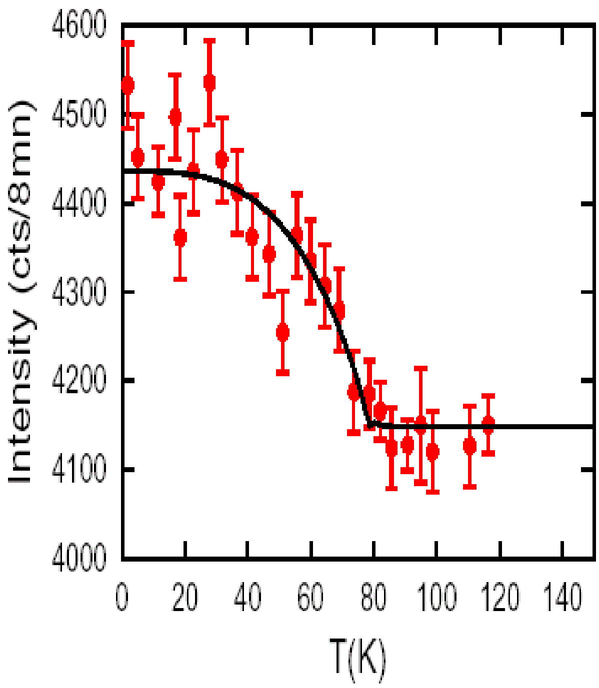
even

N.B.: integrated spectral weight similar to optimum doping

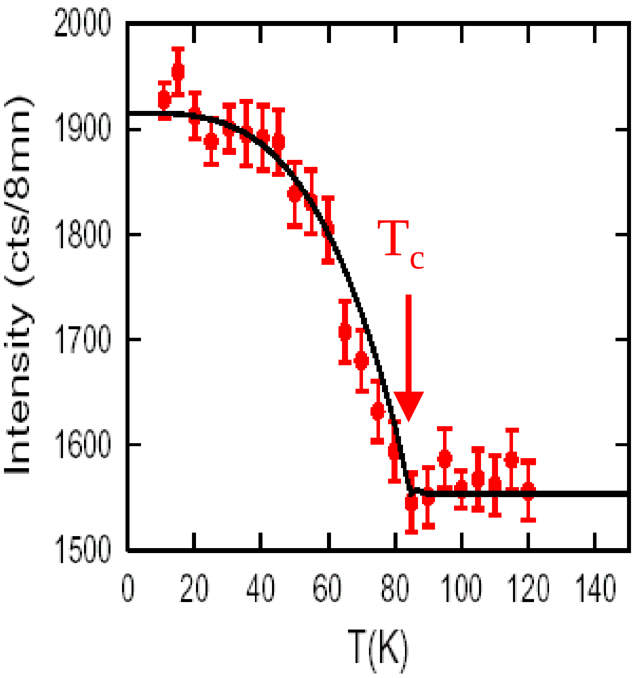
S. Pailhes et al, PRL 2003

T-dependence

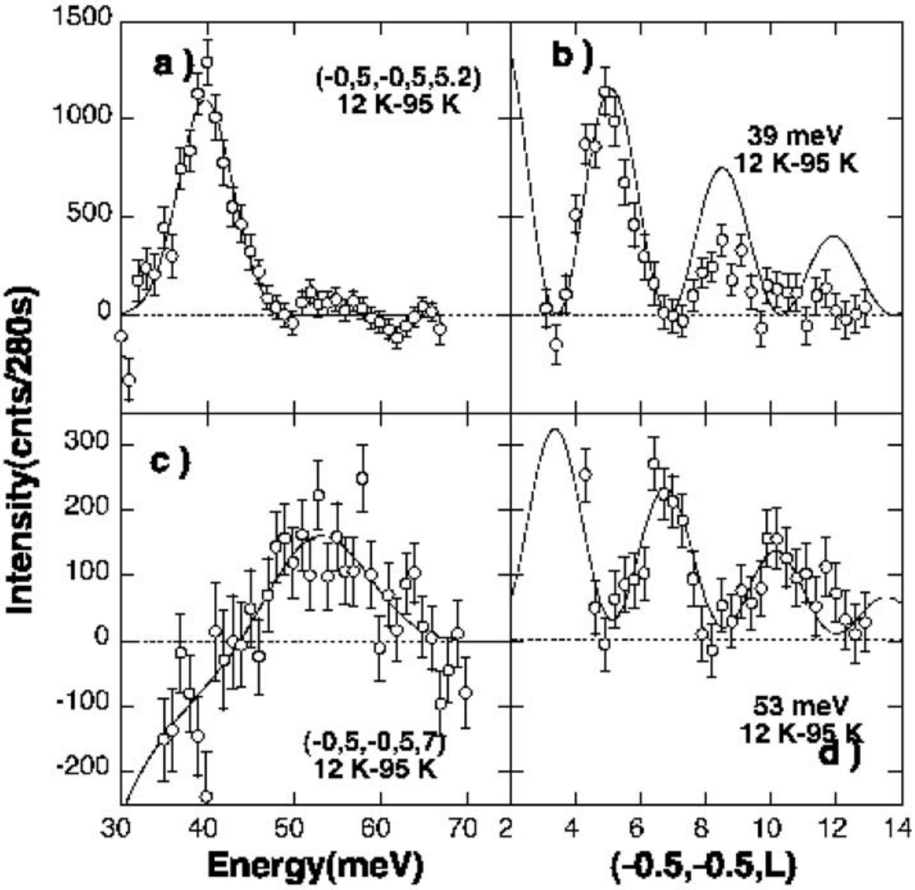
E = 43 meV, even




E = 35 meV, odd

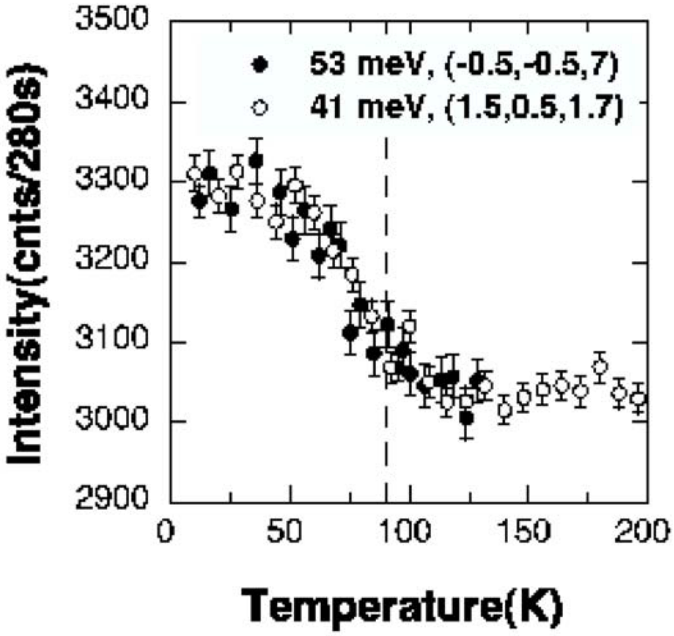


# Optimally doped $YBa_2Cu_3O_{6.85}$




odd

even

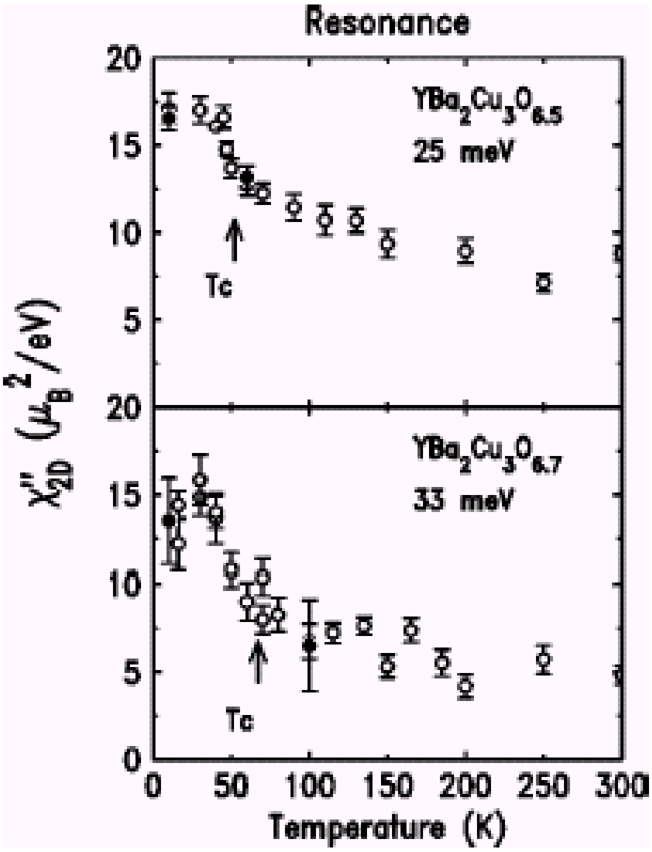


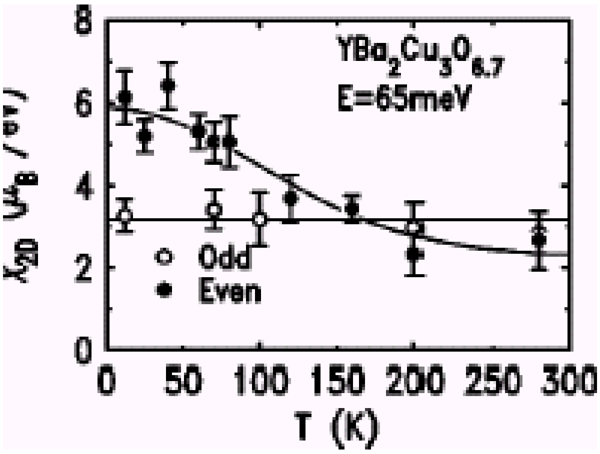

Pailhes et al., cond-mat/0403609

# Underdoped YBCO

• normal state intensity decreases rapidly with increasing doping

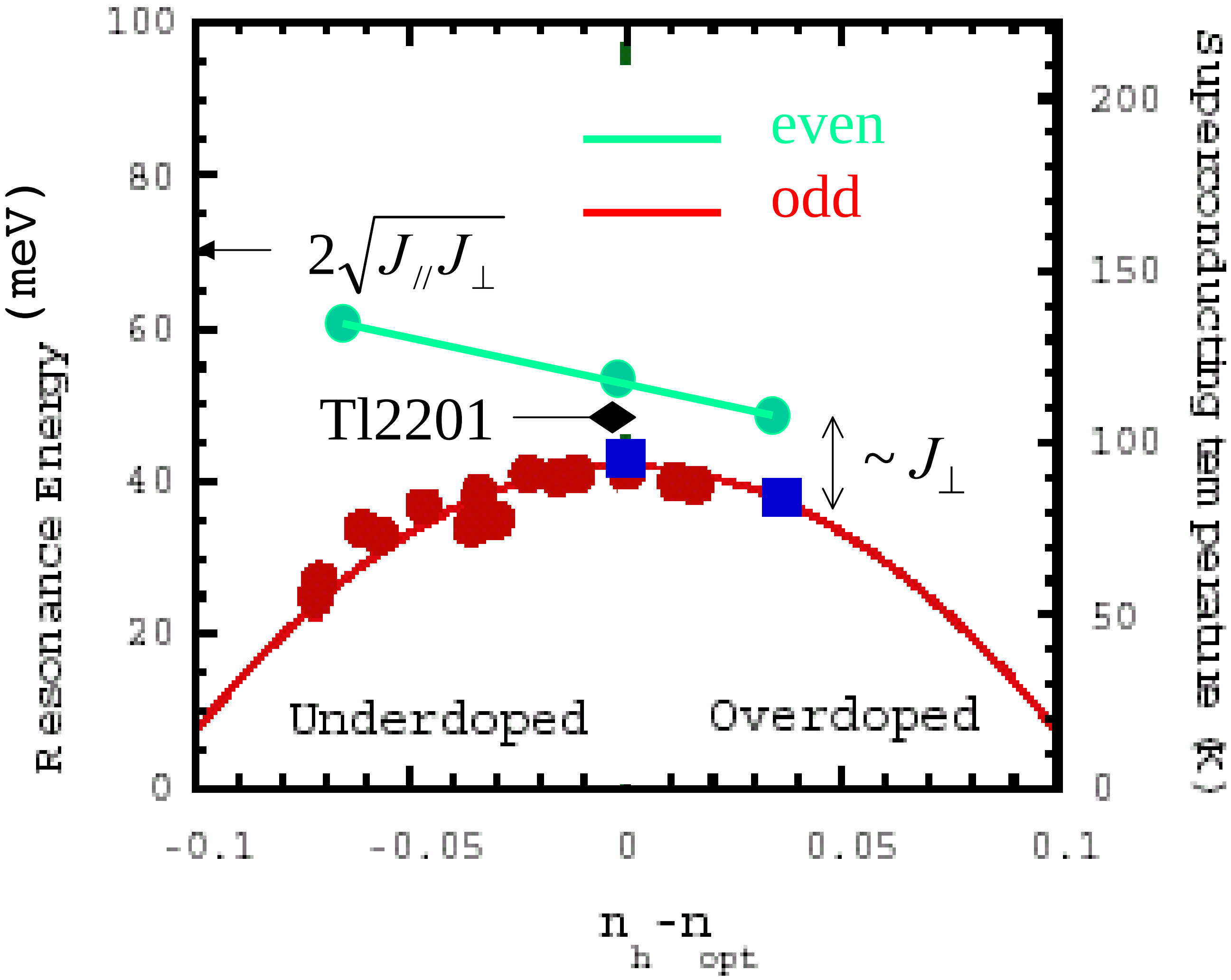
• onset of spectral weight anomaly
at $T_c$ for $n > n_{opt}$
at higher temperature for $n < n_{opt}$




Fong et al., PRB 2000

# Summary: Even/Odd Modes




Energies of even/odd modes

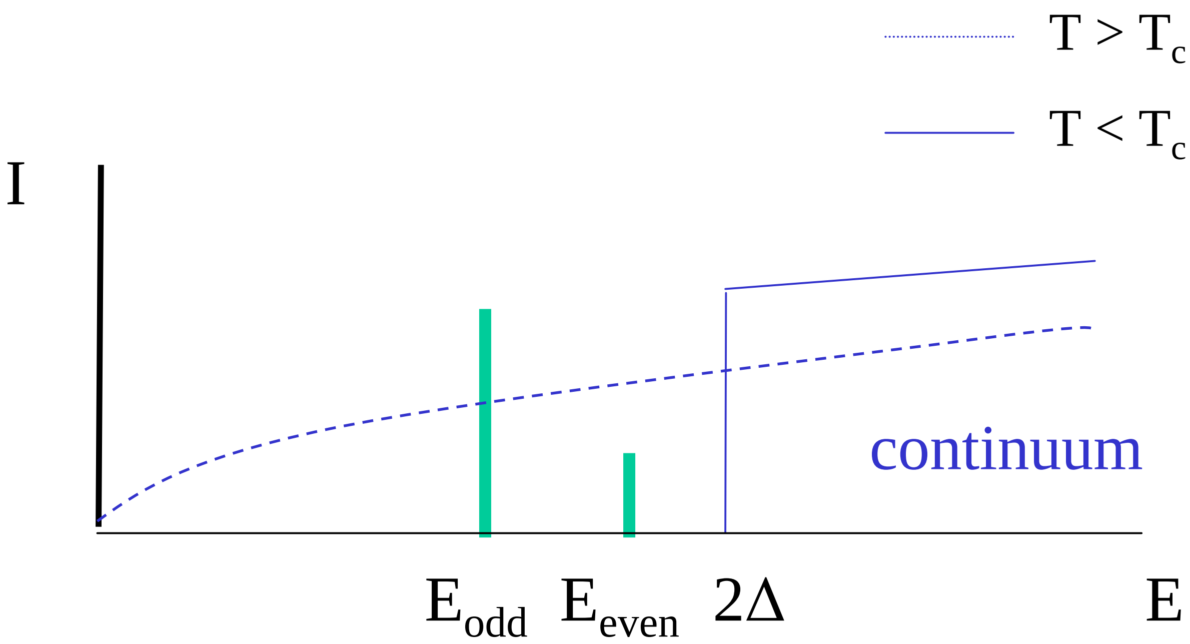
• split by bare $J_\perp$ in overdoped regime
higher binding energy for multilayer materials

• with decreasing doping, extrapolate to
optical/acoustic magnons in AF insulator

# Spectral Weights of Even & Odd Modes at (π,π)

renormalization of $\chi_0(q,\omega)$ by interactions:

Stoner model: $$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - J(q)\,\chi_0(q,\omega)}$$



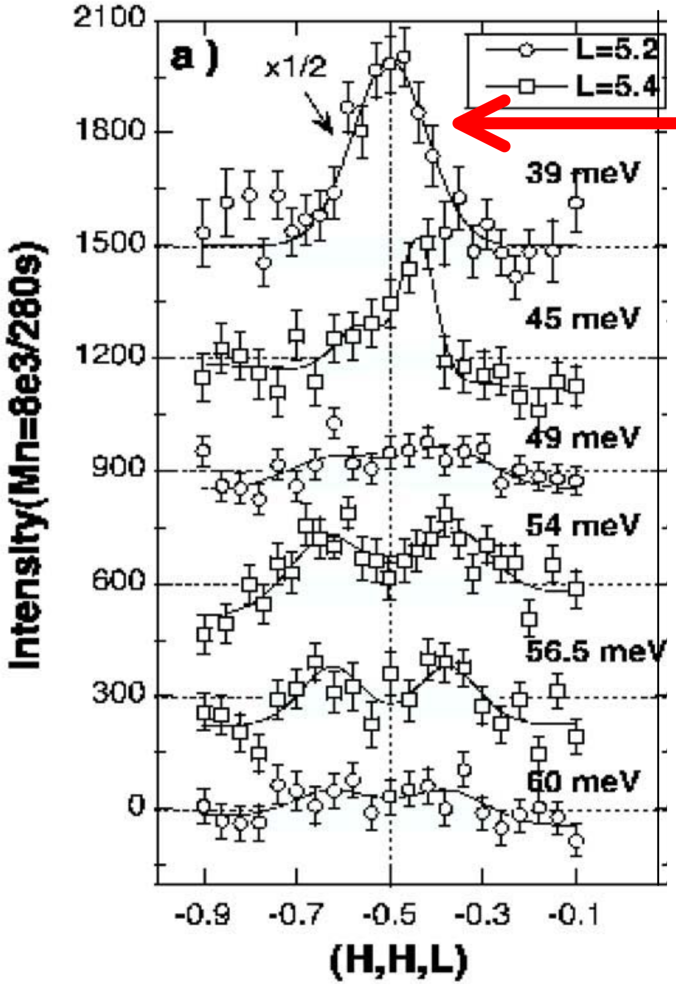

$$\frac{I_{even}}{I_{odd}} \cong \frac{2\Delta - E_{even}}{2\Delta - E_{odd}}$$

Millis & Monien, PRB 96

$\Rightarrow 2\Delta \sim 49$ meV overdoped YBCO

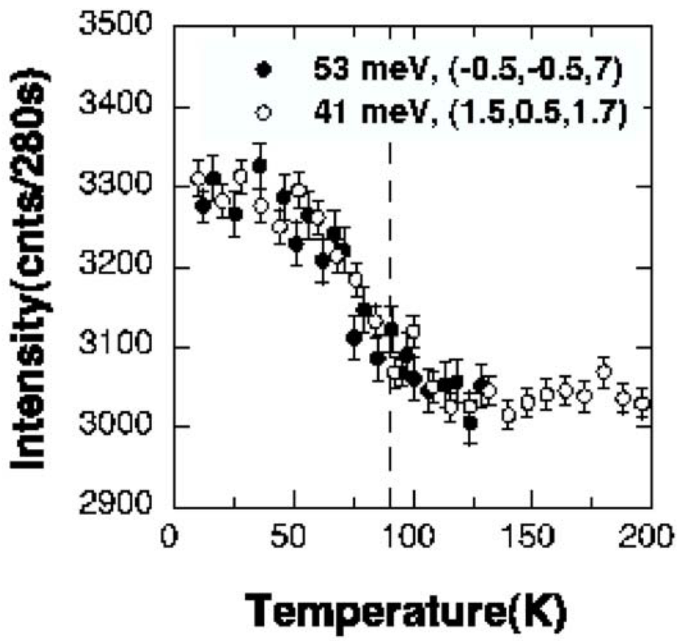
$\sim 60$ meV optimally doped YBCO

# New Look at Optimally doped $YBa_2Cu_3O_{6.85}$




resonant mode

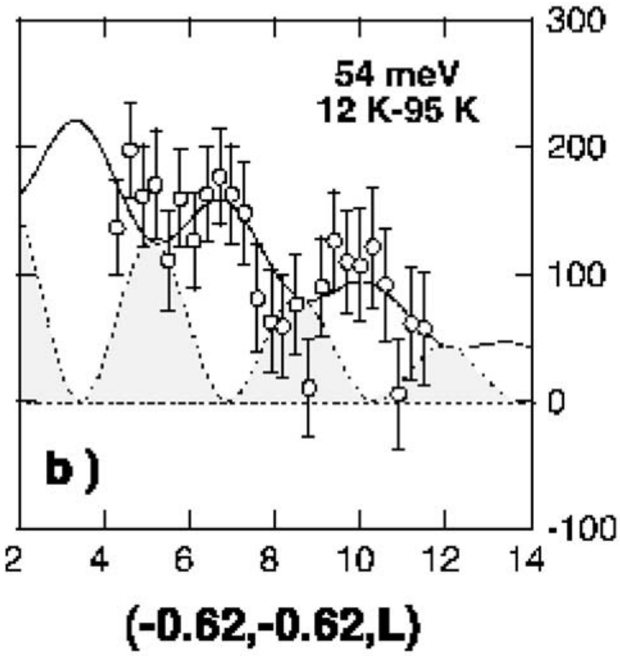
weak
incommensurate
excitations in
narrow band




same temperature
dependence as
resonant mode

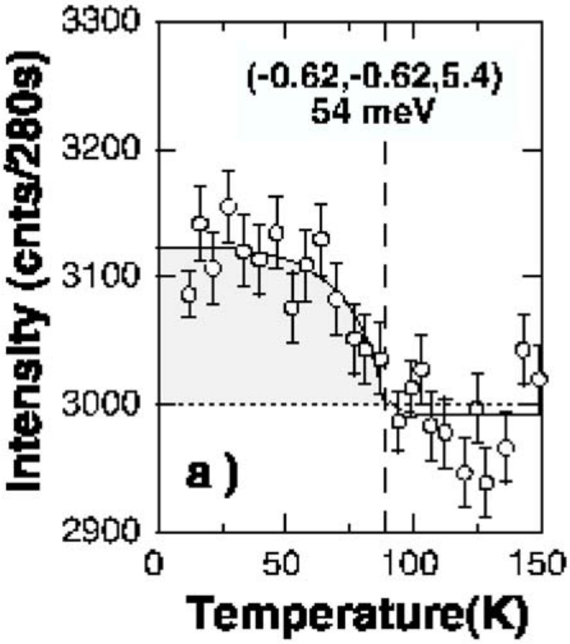
Pailhes et al.,
cond-mat/0403609

# Optimally doped $YBa_2Cu_3O_{6.85}$




- intensity follows magnetic form factor (rules out phonons)

- predominantly odd character

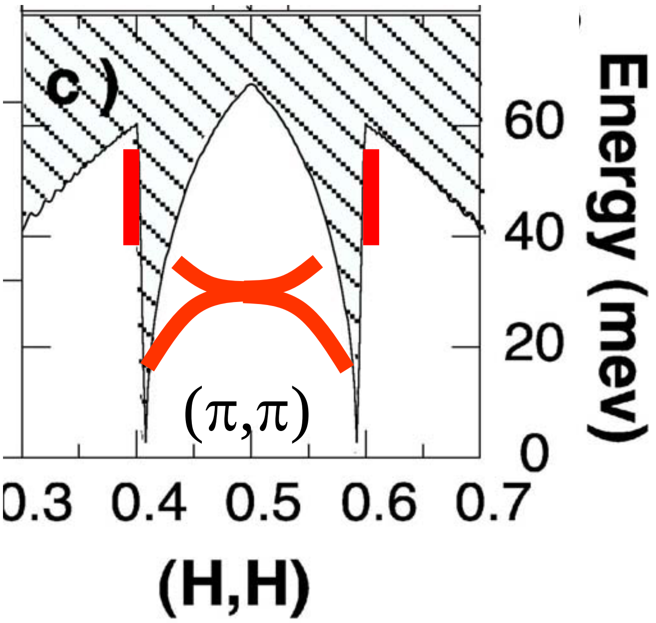



same temperature dependence as resonant mode

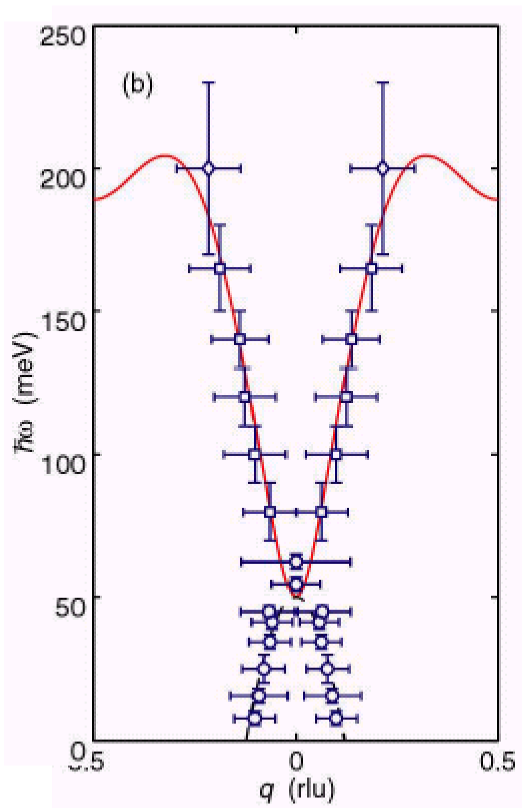
# Summary

• Locus of magnetic excitations in

$YBa_2Cu_3O_{6+x}$ $La_{1.875}Ba_{0.125}CuO_4$



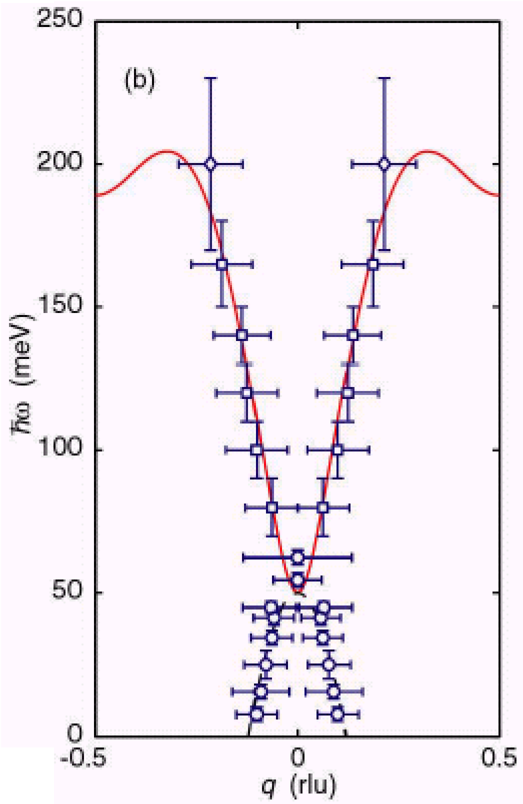

Pailhes et al., cond-mat/0403609

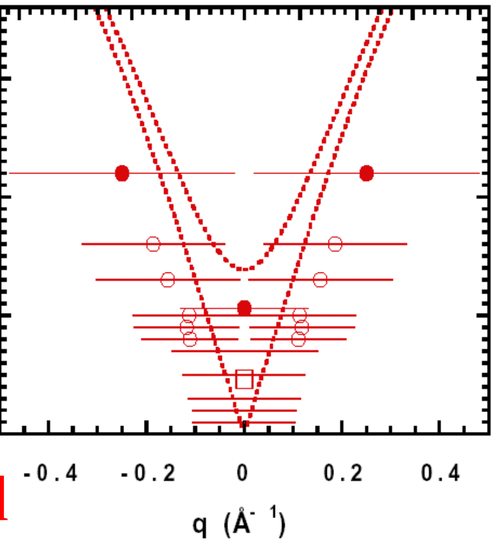



Tranquada et al., Nature 2004

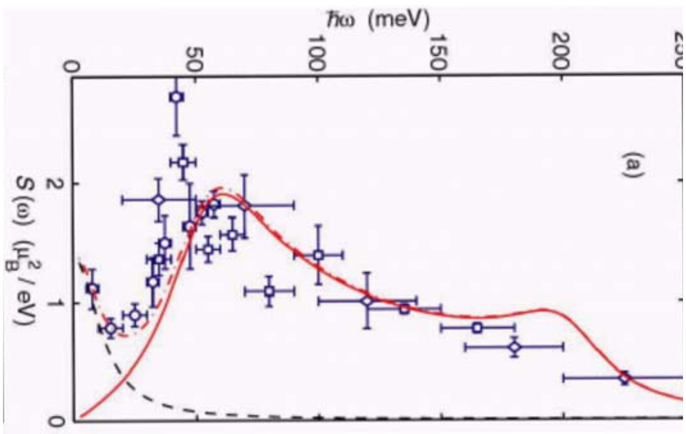
**→ "universal" magnetic response of copper oxides?**

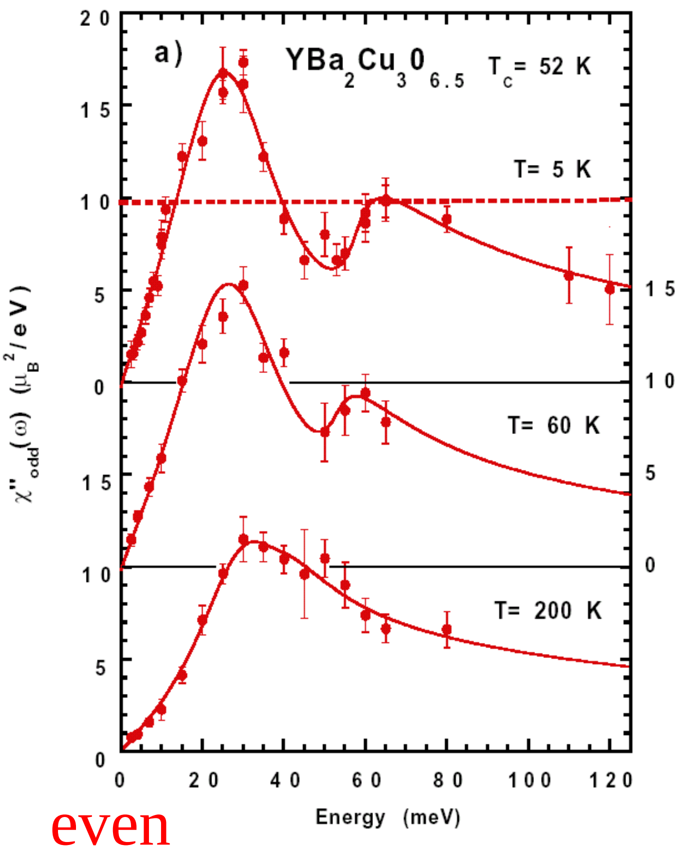
$La_{1.875}Ba_{0.125}CuO_4$ $YBa_2Cu_3O_{6.5}$



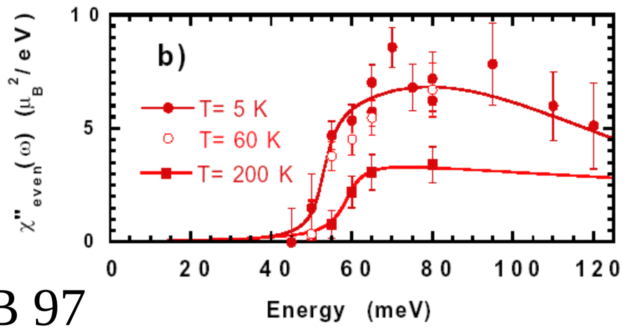




odd




even

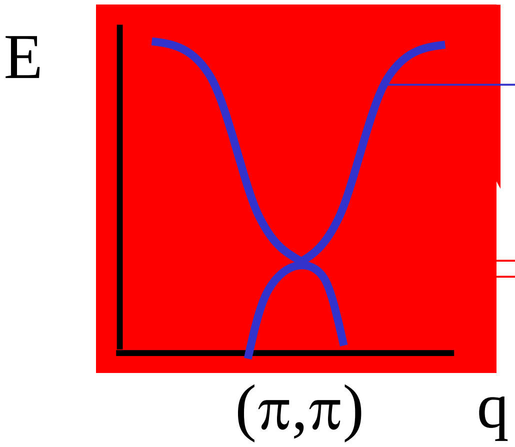



Tranquada et al.,
Nature 2004

Bourges et al., PRB 97

# Magnetic Response of High-$T_c$ Superconductors

$YBa_2Cu_3O_{6.85}$

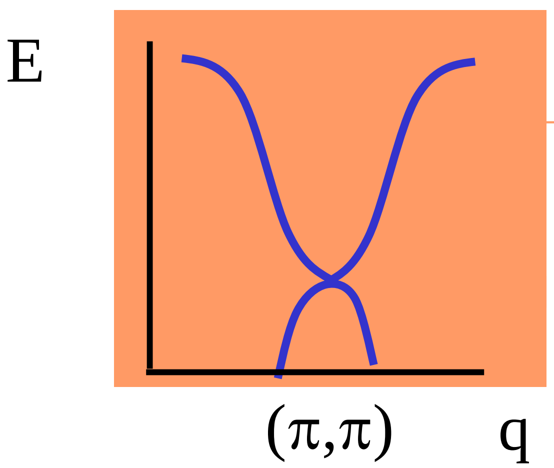



"universal" response

strong damping by quasiparticles

$T \gtrsim T_c$

$La_{1.85}Sr_{0.15}CuO_4$




weak damping by quasiparticles

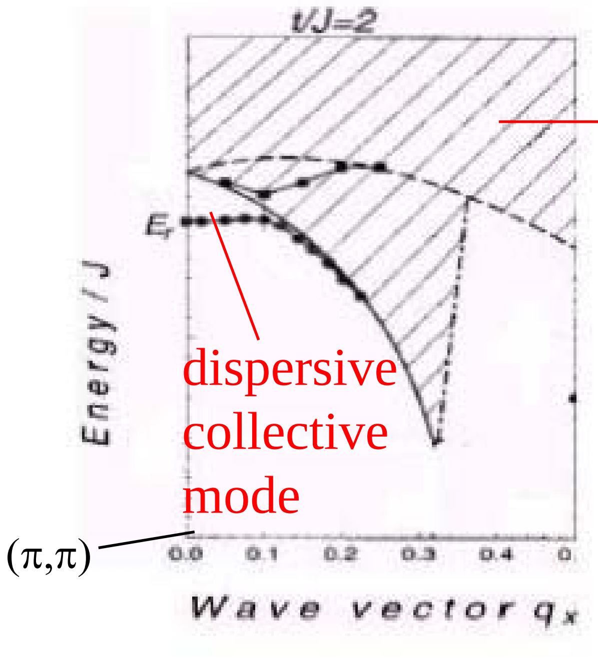
$T \lesssim T_c$

→ Morr & Pines, PRL 1998

# Mean Field Theory

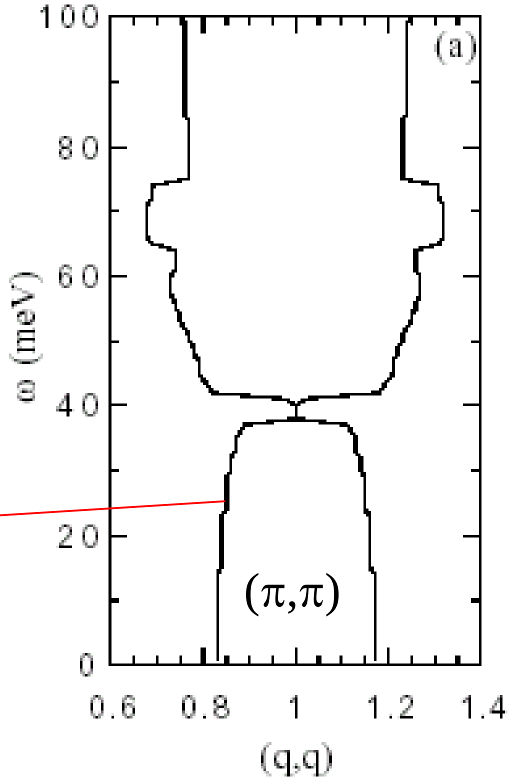
renormalization of $\chi_0(q,\omega)$ by interactions:

Stoner model: $$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - J(q)\ \chi_0(q,\omega)}$$




particle-hole
spin flip continuum

Onufrieva & Pfeuty, PRB 2002

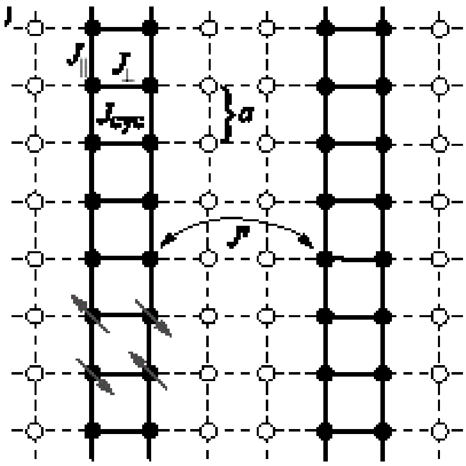


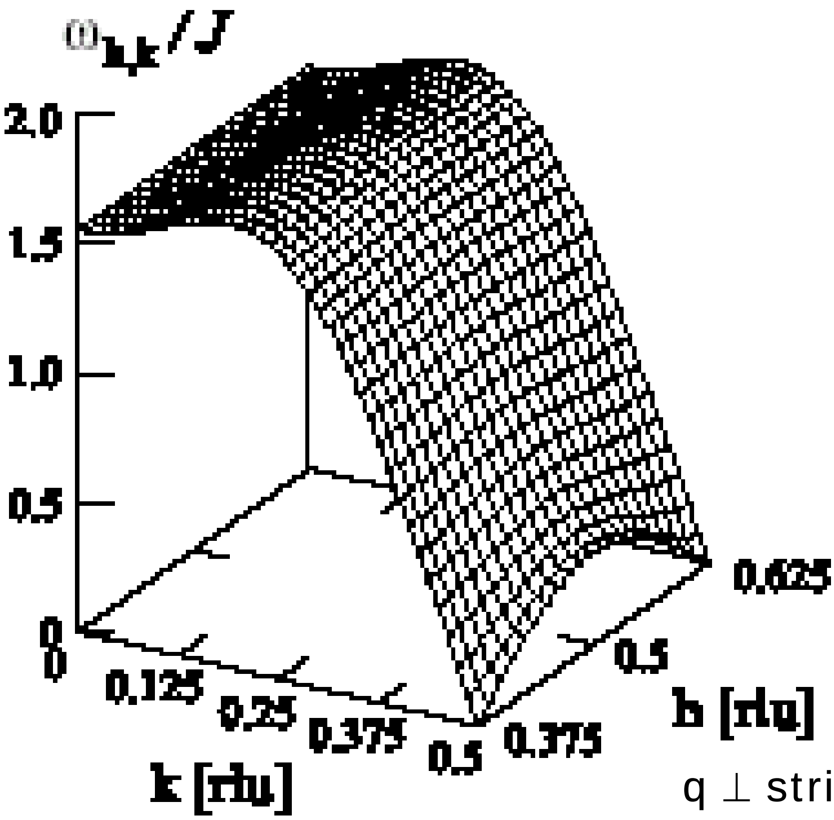

maximum of Imχ

M. Norman, PRB 2000

- superconducting gap required for true collective mode
- can weakly damped collective mode exist in „pseudogap"?

# Spin Excitations of Coupled Stripes




q ⊥ stripe

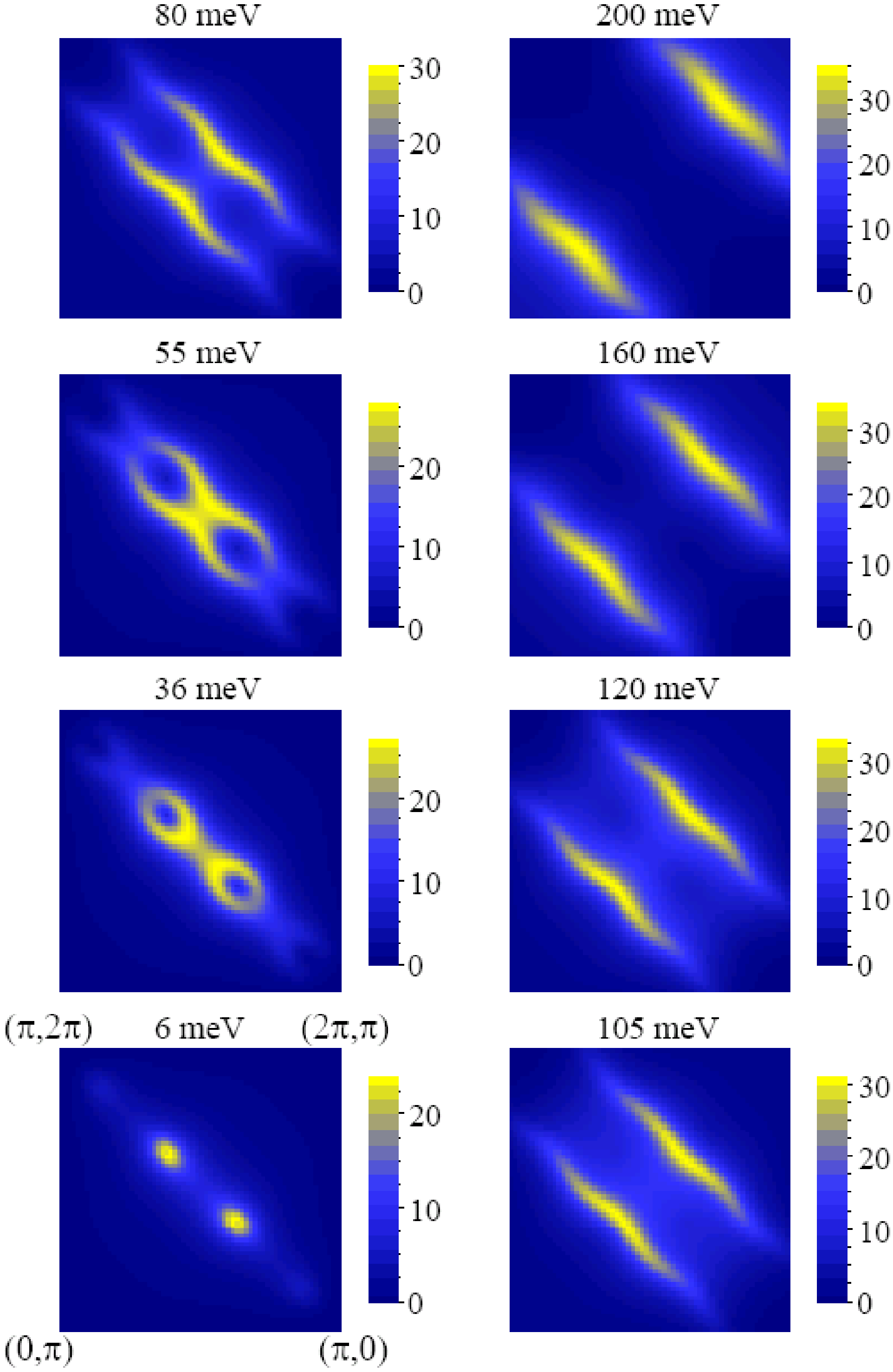
q | | stripe

G. Uhrig et al., cond-mat/0402659

M. Vojta and T. Ulbricht, cond-mat/0402377

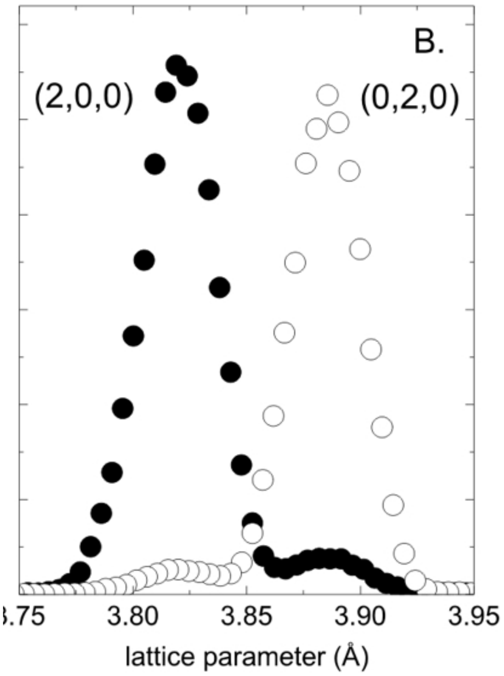
# Spin Excitations of Coupled Stripes

## constant-energy cuts

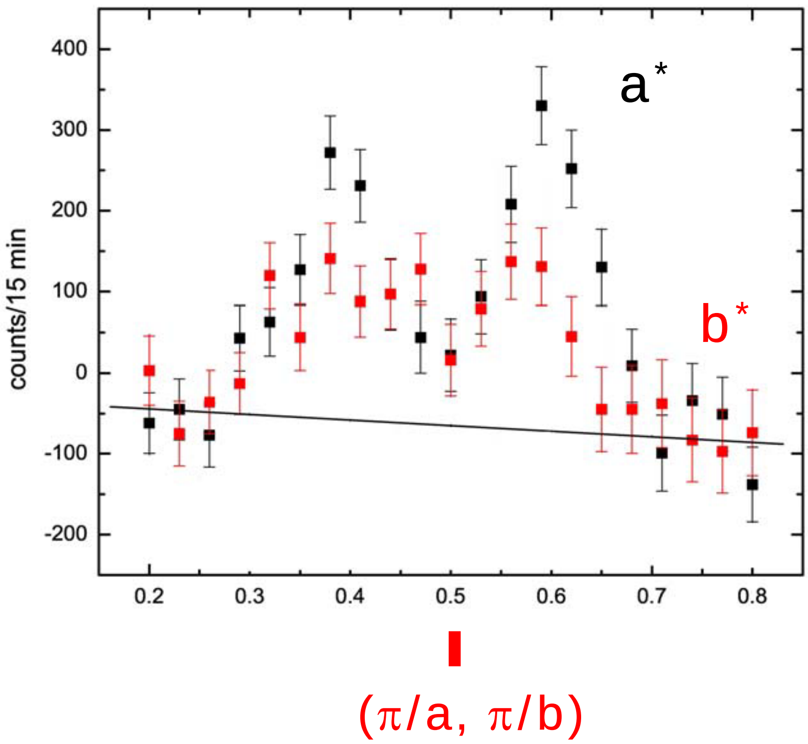


# Incommensurate Spin Excitations: 1D or 2D?

~95% detwinned mosaic of $YBa_2Cu_3O_{6.85}$ ($T_c$=90K)



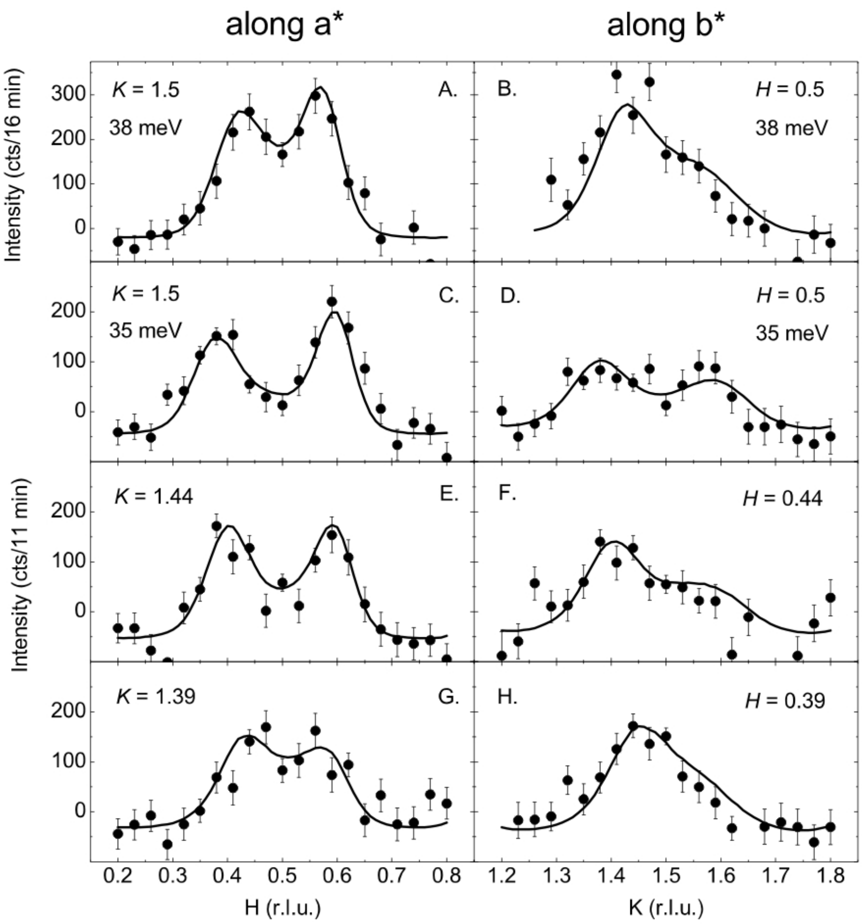

crystallographic
Bragg reflections



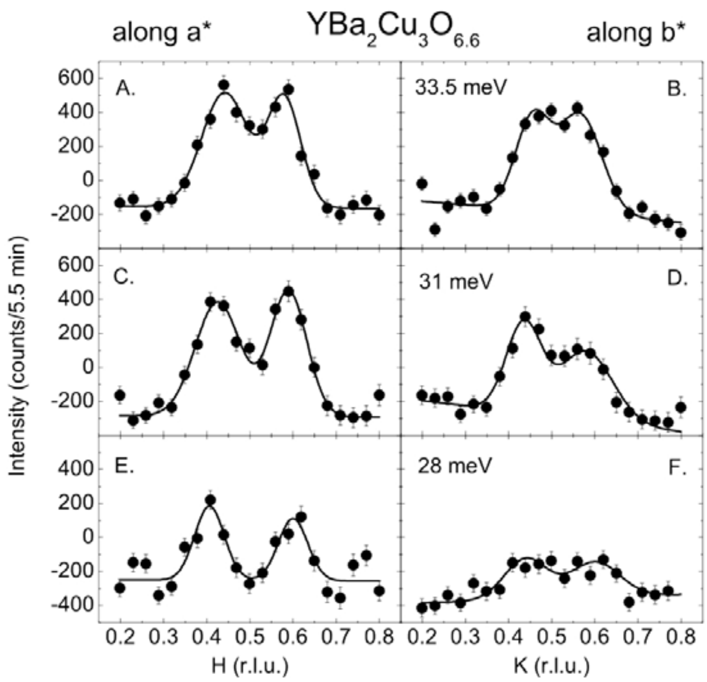

magnetic excitations
E=35meV < $E_{res}$ = 40 meV

V. Hinkov et al.
Nature, in press

# Map of Magnetic Spectral Weight



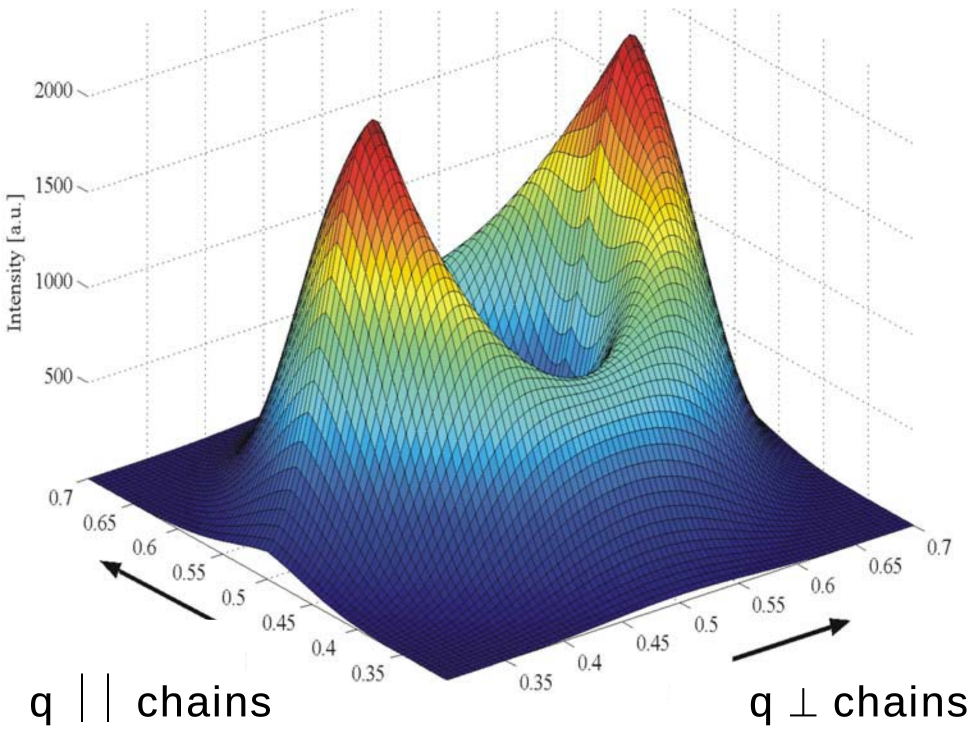

$YBa_2Cu_3O_{6.85}$
($T_c$=90K)



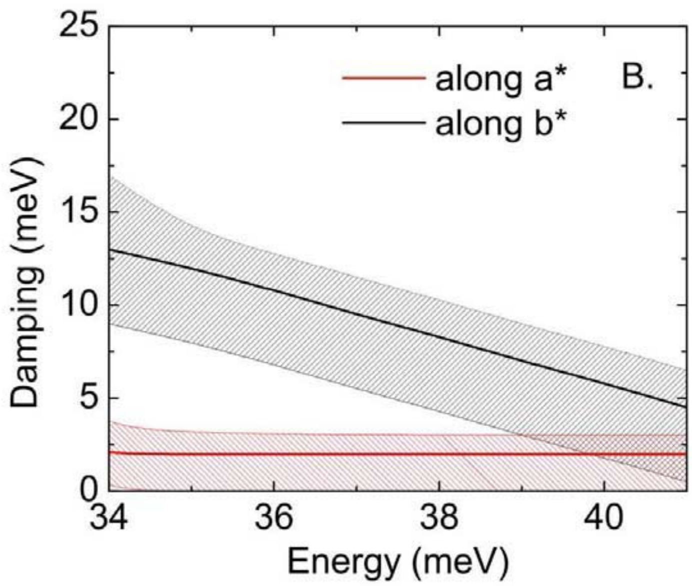

$YBa_2Cu_3O_{6.6}$
($T_c$=60K)

# Map of Magnetic Spectral Weight

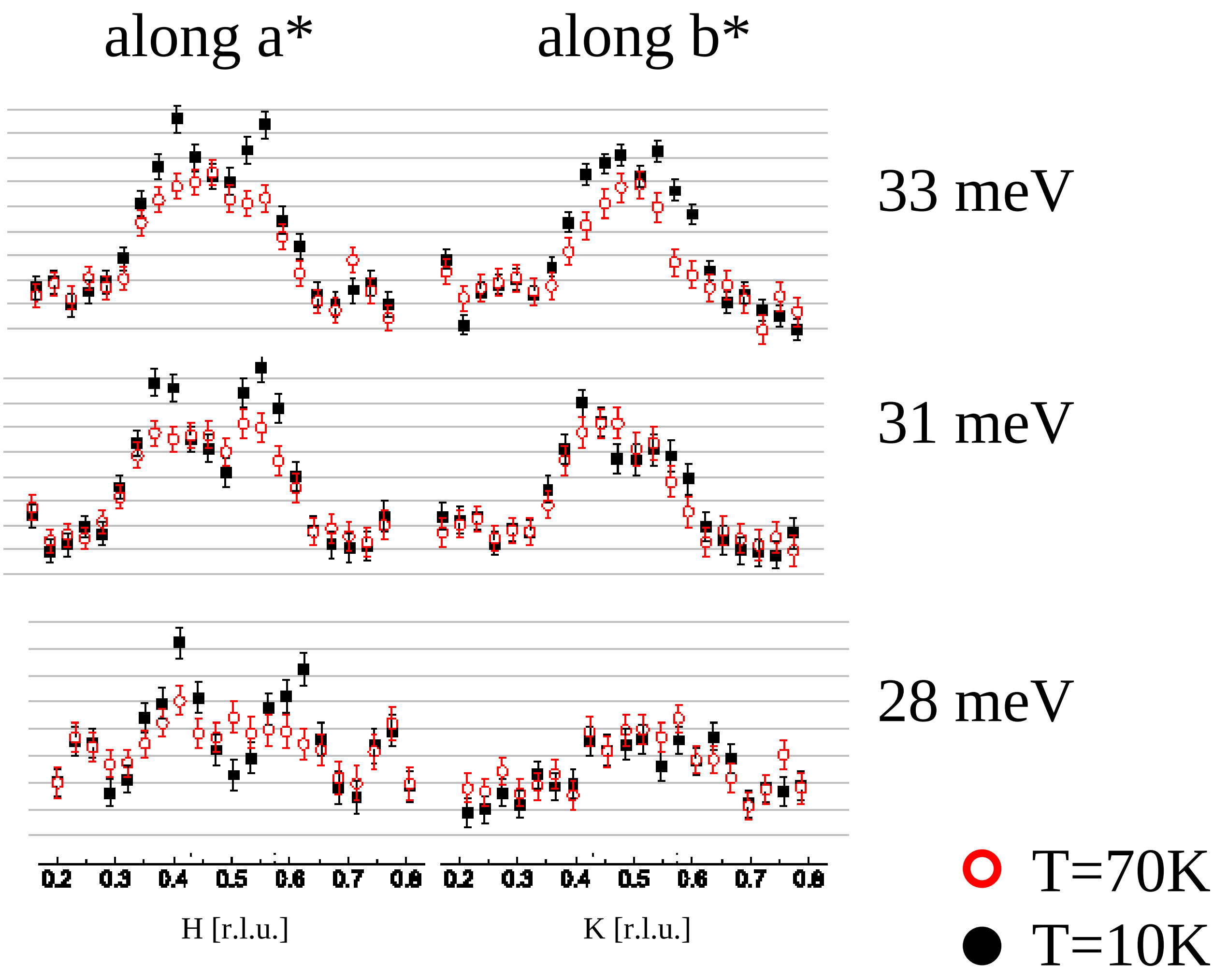
|Q|-integrated intensity almost isotropic




anisotropic damping



# Underdoped $YBa_2Cu_3O_{6.6}$




Incommensurability **reduced** in normal state

# Summary: Untwinned $YBa_2Cu_3O_{6+x}$

Anisotropic **two-dimensional** spin excitations inconsistent with static arrrray of stripes

Origin of in-plane anisotropy of intensity/damping?

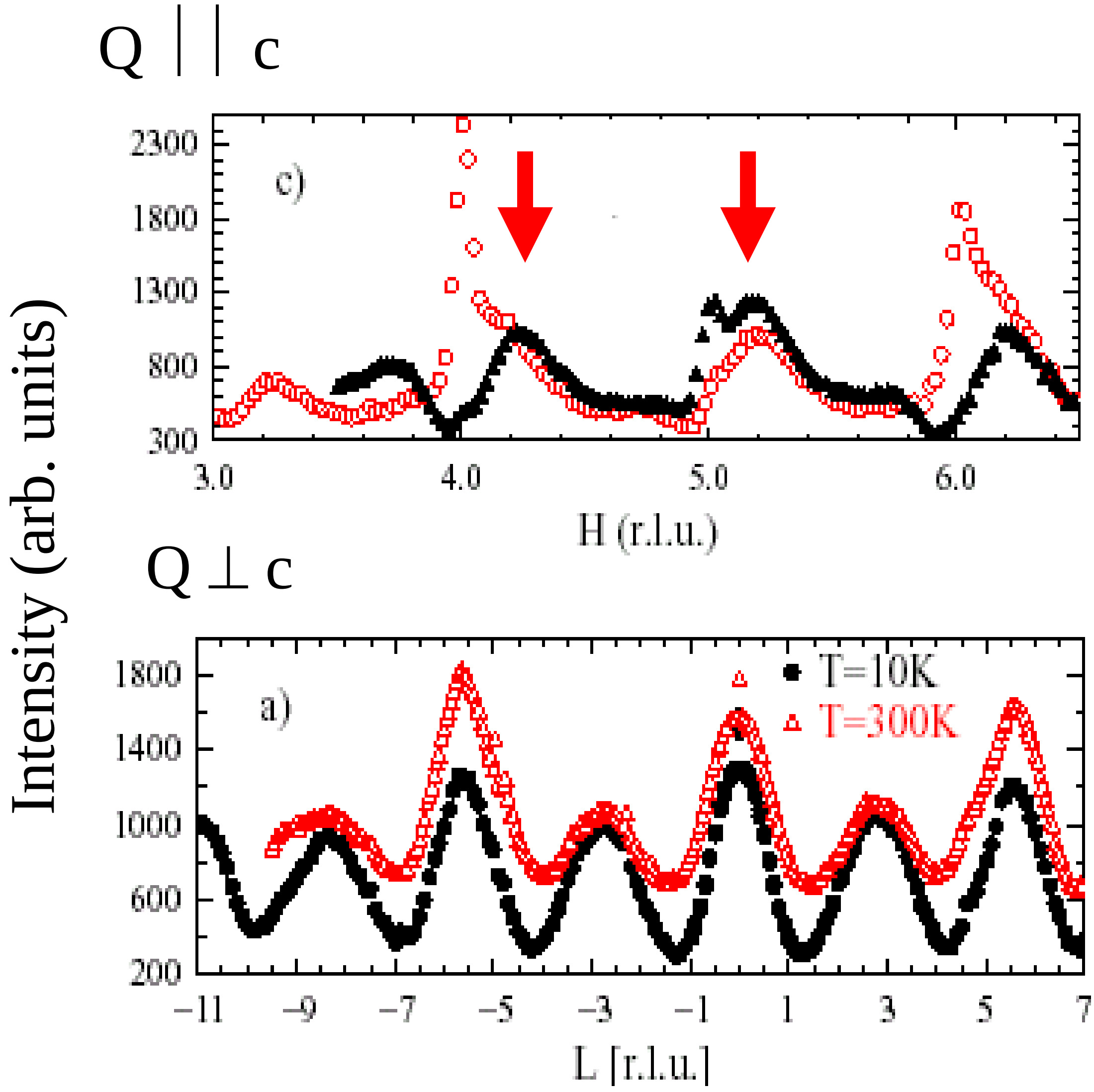
- $cos^2(q_z d/2)$ intensity modulation rules out direct contribution from CuO chains
- in-plane Fermi surface anisotropy?
- quantum nematic phase?
- relationship to checkerboard charge order?

Possible complications:

- charge/orbital order on chains
- oxygen ordering

# X-ray diffuse scattering in $YBa_2Cu_3O_{6+x}$

optimally doped $YBa_2Cu_3O_{6.92}$ ($T_c$=92.3 K)

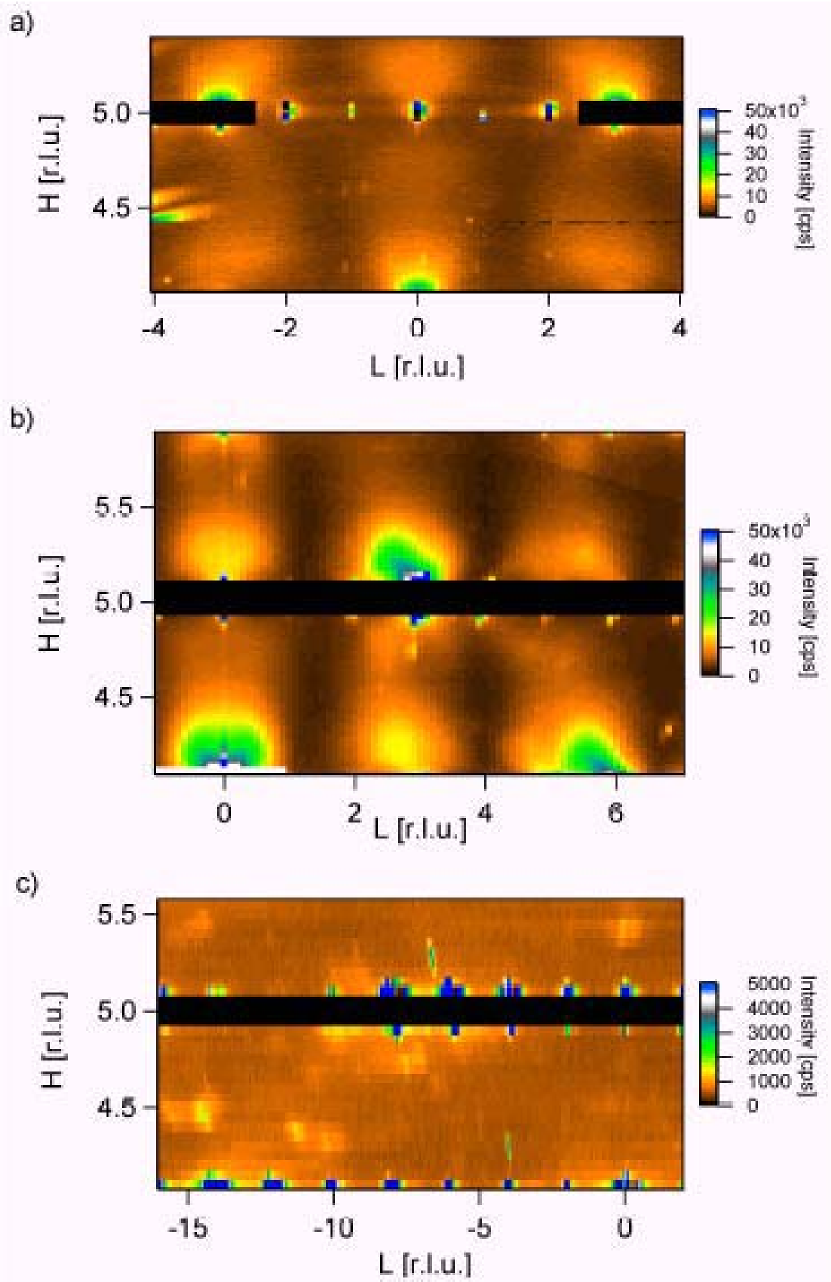



- superstructure with four-unit-cell periodicity

- displacements of atoms in entire unit cell

Strempfer et al., PRL in press

# Doping and material dependence



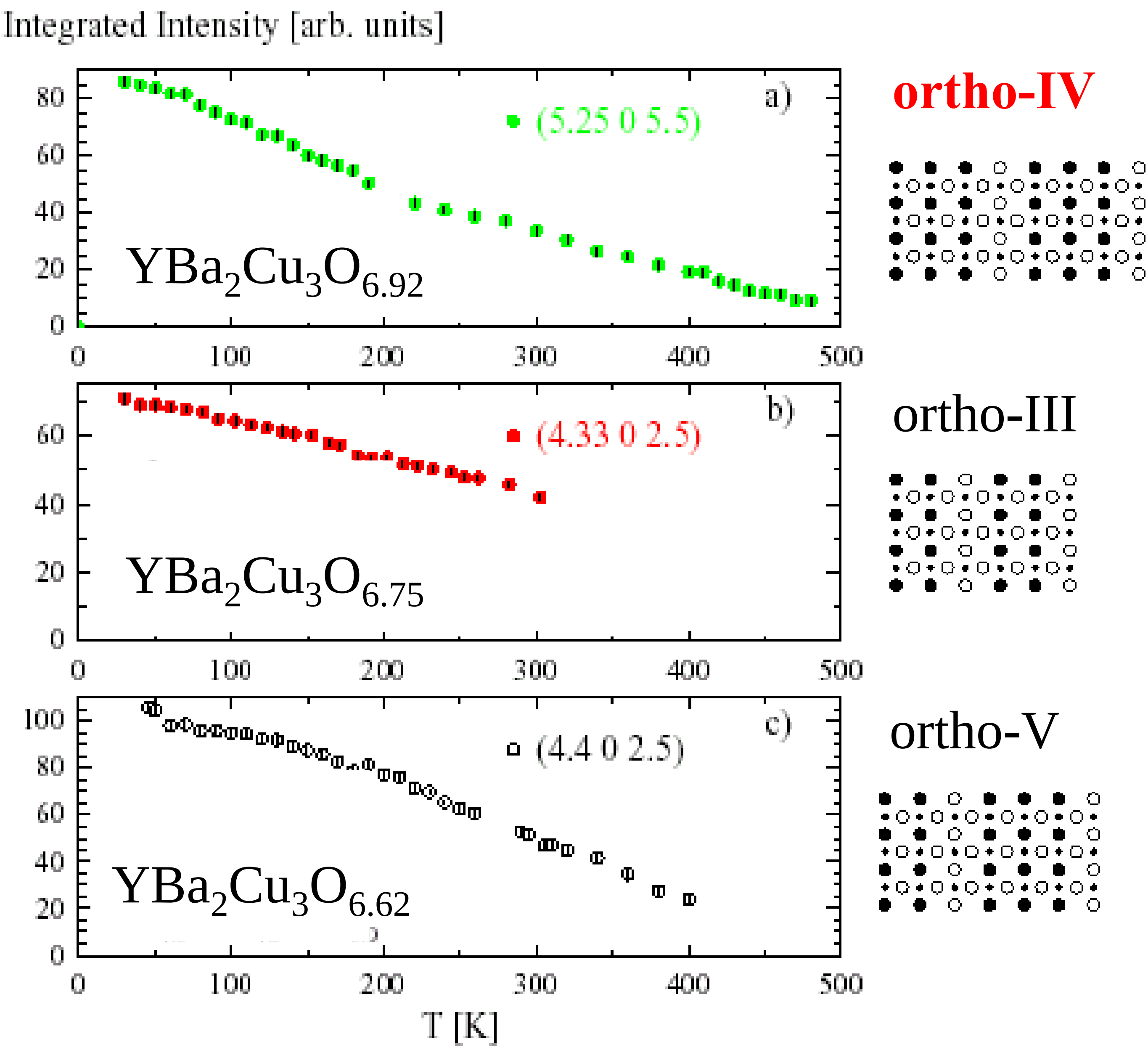

$YBa_2Cu_3O_{6.92}$
($T_c$=92.3 K)

$Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{6.92}$
($T_c$=73 K)

$YBa_2Cu_4O_8$
($T_c$=81 K)

- superstructure depends on **oxygen content**, not on doping level
- not observed in materials without oxygen defects

# Temperature dependence




**no pronounced anomalies at $T_c$ or $T^*$**

# Conclusions: X-ray diffuse scattering

• oxygen superstructures are material-specific aspect of real lattice structure of YBCO at all doping levels

• reported anomalies at $T^*$ not confirmed (Islam et al., PRB 2002)

• oxygen ordering has to be taken into account when interpreting phonon anomalies

→ correlations between oxygen vacancies in other high-$T_c$ cuprates?