



1957-12

Miniworkshop on Strong Correlations in Materials and Atom Traps

4 - 15 August 2008

Neutron and X-Ray scattering study on cuprate superconductors.

YAMADA Kazuyoshi
*Kyoto University
Institute For Chemical Research
Gokasho, Uji City
F-611 Kyoto
JAPAN*

Cuprate superconductivity and spin fluctuations

K. Yamada,

Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

M. Fujita, H. Hiraka

Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

M. Matsuda, S. Wakimoto

Japan Atomic Energy Agency, Ibaraki 319-1195, Japan

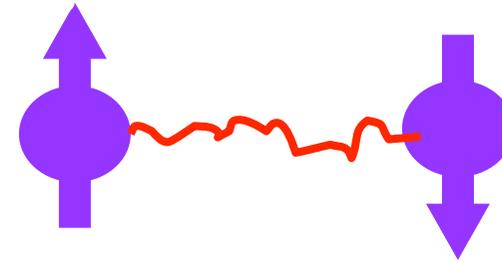
collaborators for neutron scattering

**C.H. Lee. (AIST), J.M. Tranquada (BNL), M. Kofu , S.H. Lee. (U. Virginia), B. Fak,
C. Frost (ISIS, RAL) ,M. Braden (U. Cologne), D. Reznik (LLB)**

collaborators for X-ray scattering

**A. Q. Baron (RIKEN) , J. Mizuki, T. Fukuda, K. Ikeuchi, K. Ishii(JAEA),
Y. Sakurai (JASRI) , Y. Murakami (Tohoku), D. Reznik (LLB)**

Is There Glue in Cuprate Superconductors?



Philip W. Anderson

Many theories about electron pairing in cuprate superconductors may be on the wrong track.

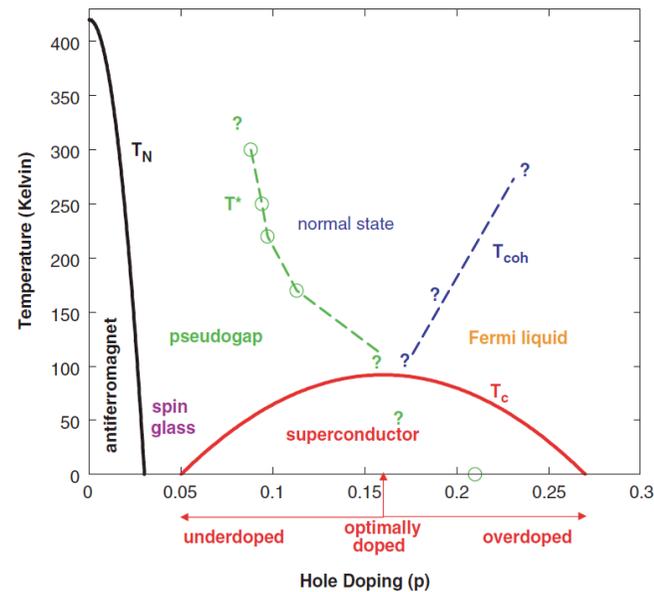


"We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?"

spin fluctuation ?
electron-phonon ?

High T_c cuprate superconductivity is still one the attractive field of material science

Figure 1 in M. Eschrig Adv. Phys. 55(2006)



many ?s in the phase diagram

Contents

- 1) Magnetic fluctuation of p-type cuprates (10min.)
- 2) Magnetic fluctuation of n-type cuprates (15min.)
- 3) "Magnetic" impurity-effect in p-type cuprates (15min.)

4) New pulsed neutron facility in J-PARC (3min.)

Advertisement

Magnetic scattering

$$S^{\alpha\beta}(\mathbf{Q}, \omega) = \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_r e^{i\mathbf{Q}\cdot\mathbf{r}} \langle S_0^\alpha(0) S_r^\beta(t) \rangle$$

Neutron sees spin-spin correlation (two-particle correlation)

Dynamical magnetic susceptibility

$$\chi''(\mathbf{Q}, \omega) = (1 - e^{-\hbar\omega/k_B T}) S(\mathbf{Q}, \omega)$$

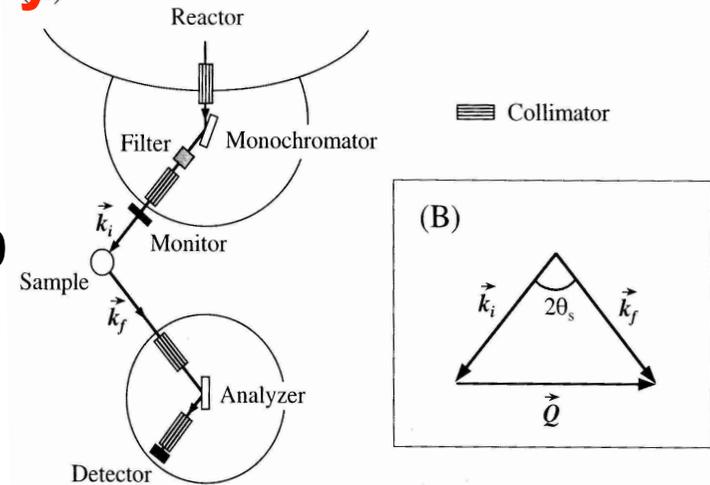
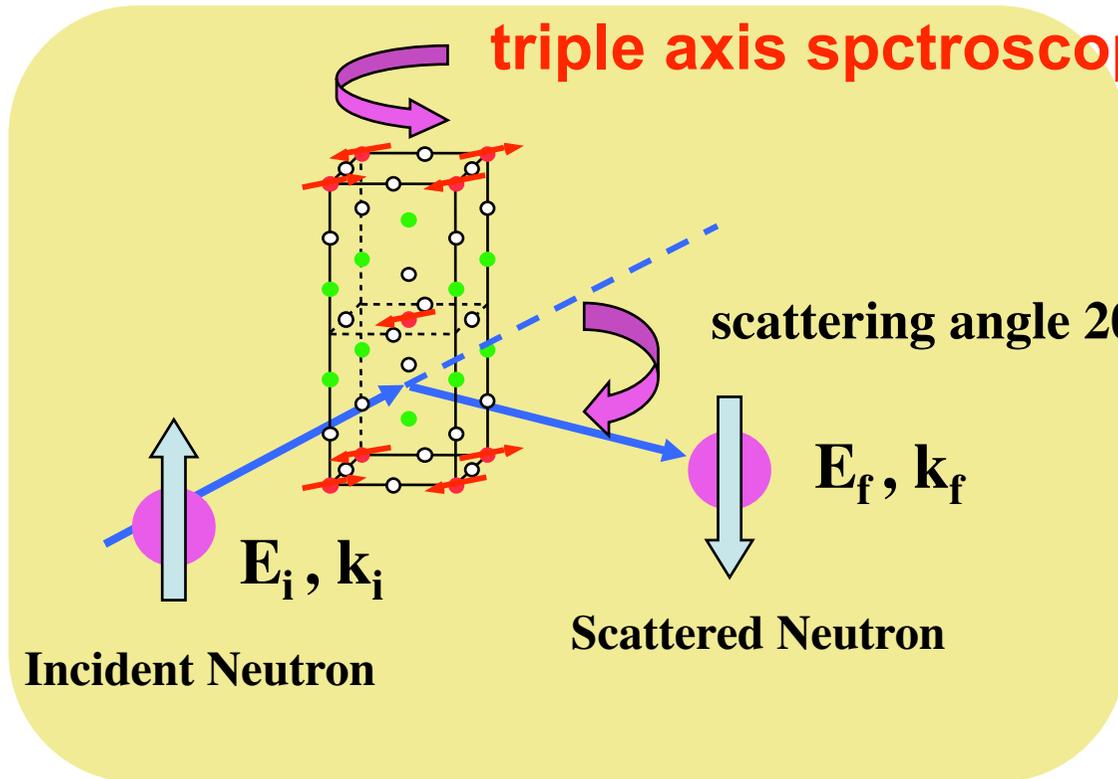
Local dynamical magnetic susceptibility

$$\chi''(\omega) = \int_{B.Z.} d\mathbf{Q} \chi''(\mathbf{Q}, \omega)$$

Instantaneous (t=0) spin correlation

$$\begin{aligned} S(\mathbf{Q}) &= \int_{-\infty}^{\infty} d\omega S(\mathbf{Q}, \omega)_{\mathbf{Q}:const.} \approx \int_{-Ei}^{\sim k_B T} d\omega S(\mathbf{Q}, \omega)_{\mathbf{Q}:const.} \\ &= \sum_r e^{i\mathbf{Q}\cdot\mathbf{r}} \langle S_0^\alpha(0) S_r^\beta(t) \rangle_{t=0} \end{aligned}$$

What is neutron scattering experiment?

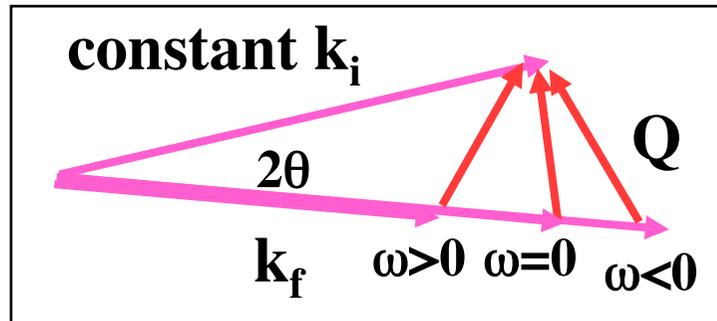


$$E_i = (\hbar k_i)^2 / 2m$$

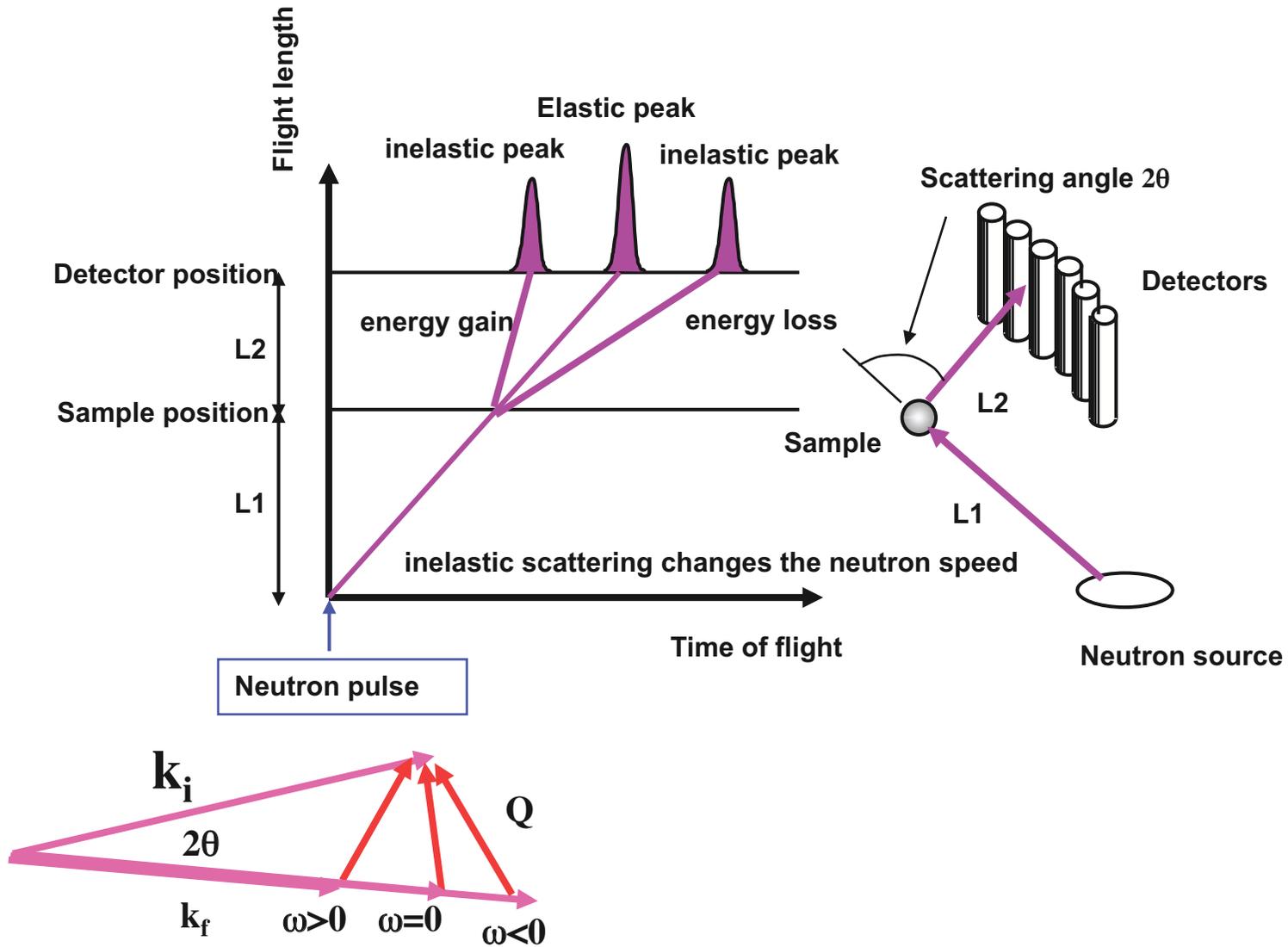
$$E_f = (\hbar k_f)^2 / 2m$$

$$Q = k_i - k_f$$

$$\hbar\omega = E_i - E_f$$



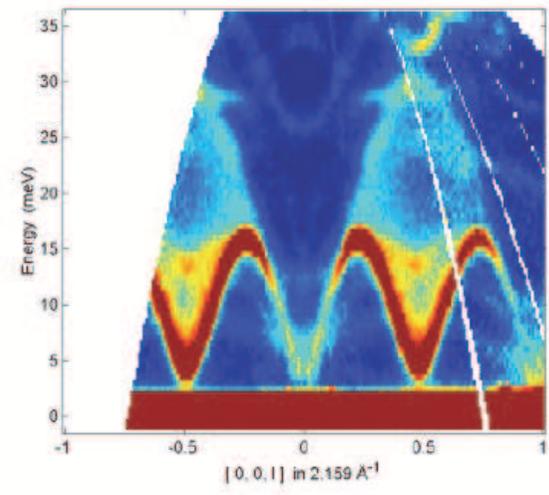
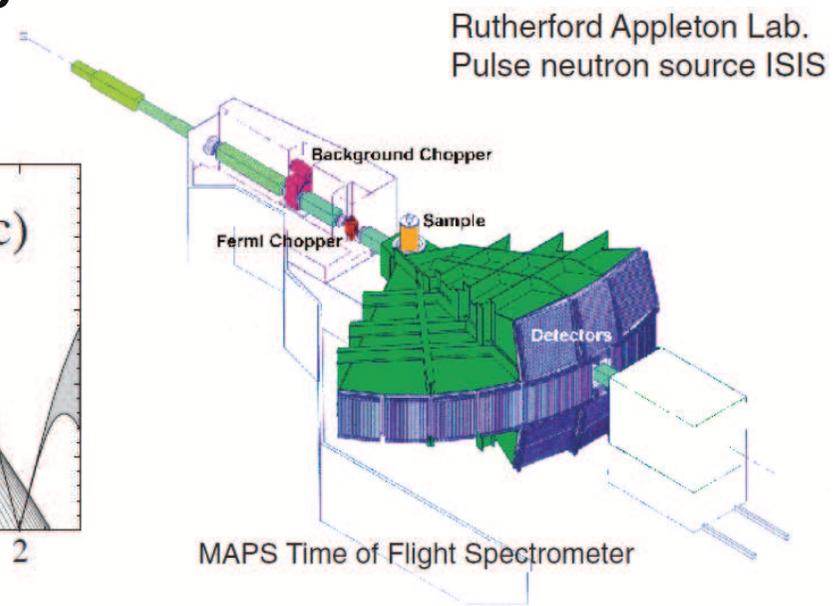
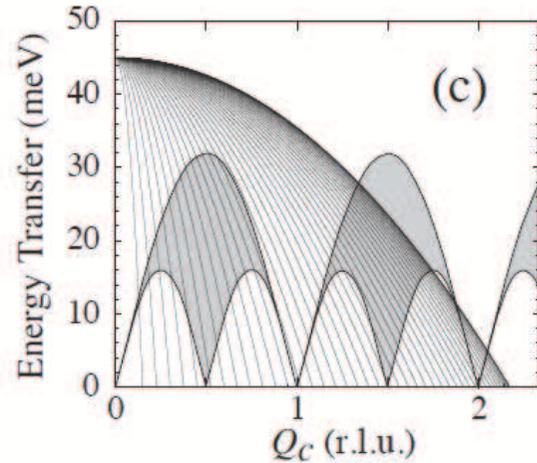
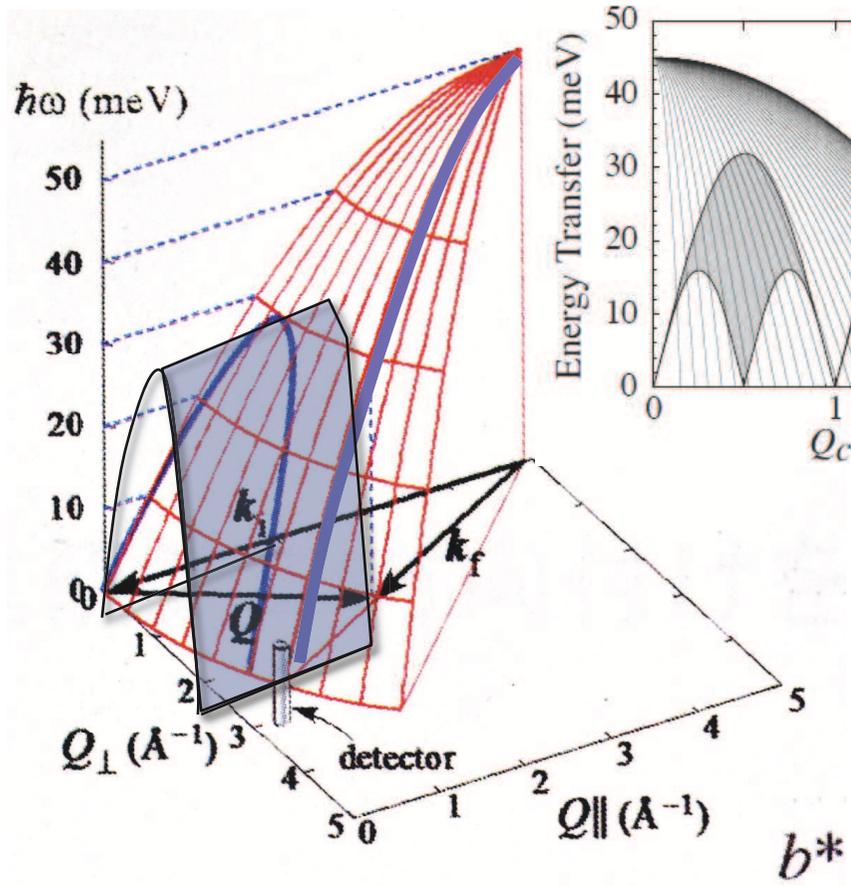
Inelastic scattering by monochromated beam



By using TOF method with monochromated beam inelastic signal can be obtained at fixed scattering angle

Scattered neutrons scan along a locus in a (Q, ω) space with a finite resolution

TOF-scan at a fixed scattering angle



Contents

1) Magnetic fluctuation of p-type cuprates (10min.)

interpretation of hour-glass type of magnetic excitation spectrum
-doping-induced two energy scales-

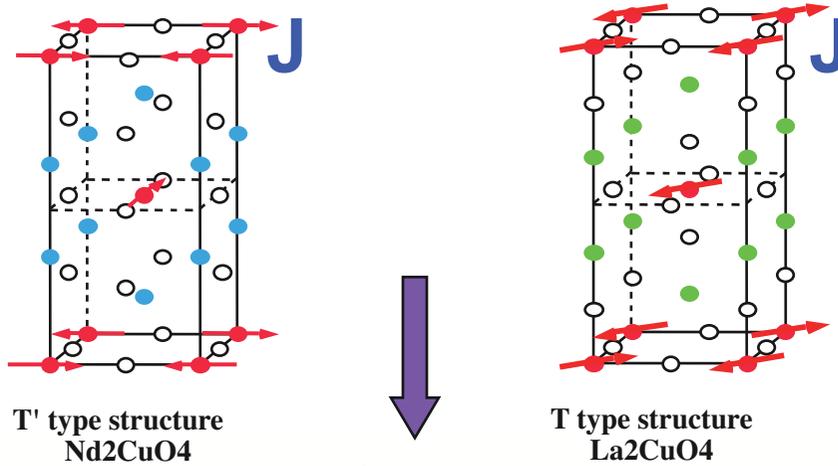
2) Magnetic fluctuation of n-type cuprates (15min.)

3) "Magnetic" impurity-effect in p-type cuprates (15min.)

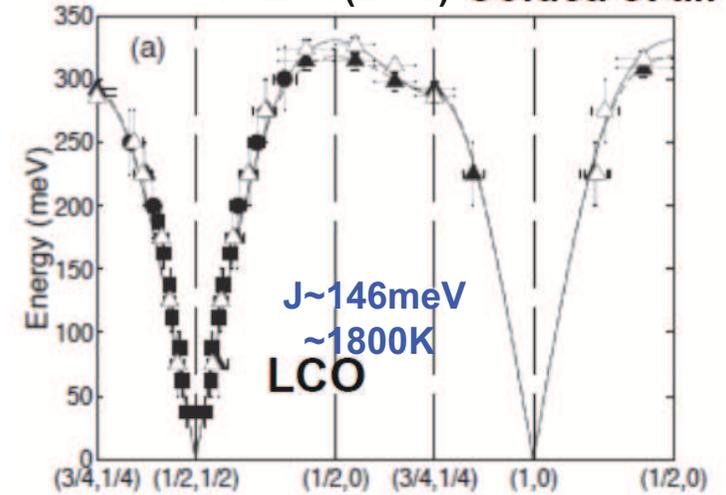
4) New pulsed neutron facility in J-PARC (5min.)

Advertisement

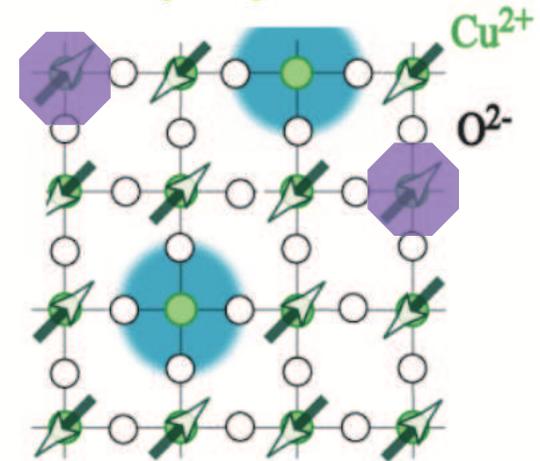
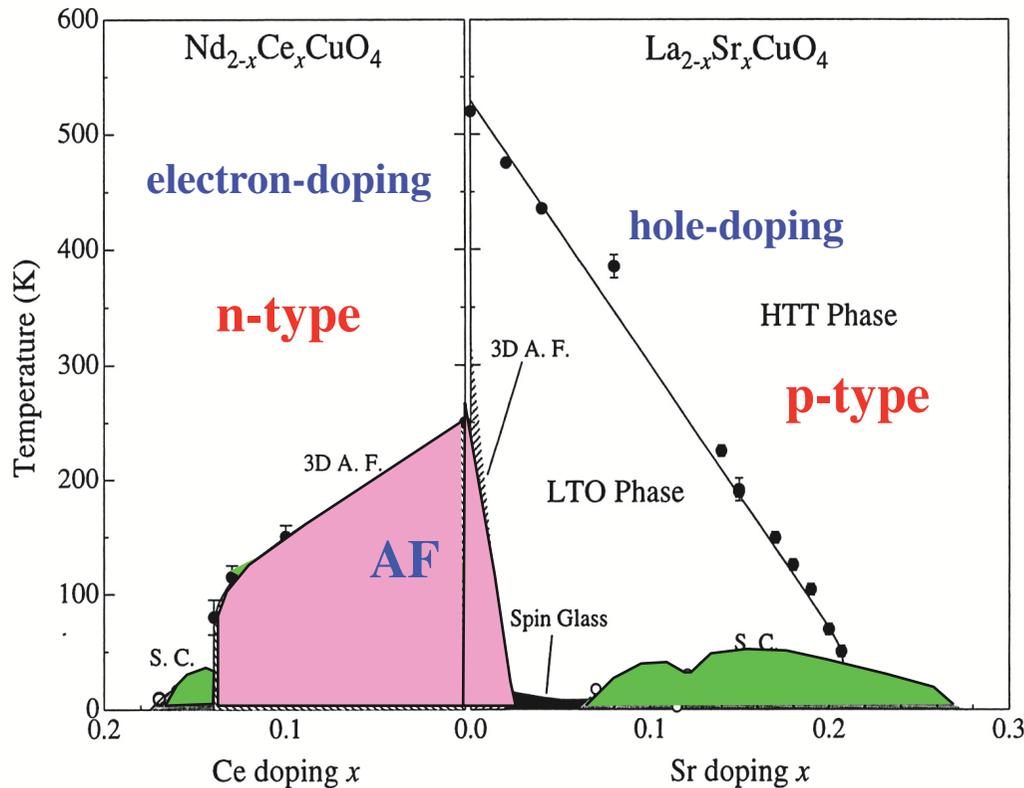
Carrier-doping into Mott insulators induces superconductor



PRL 86(2001) Coldea et al.



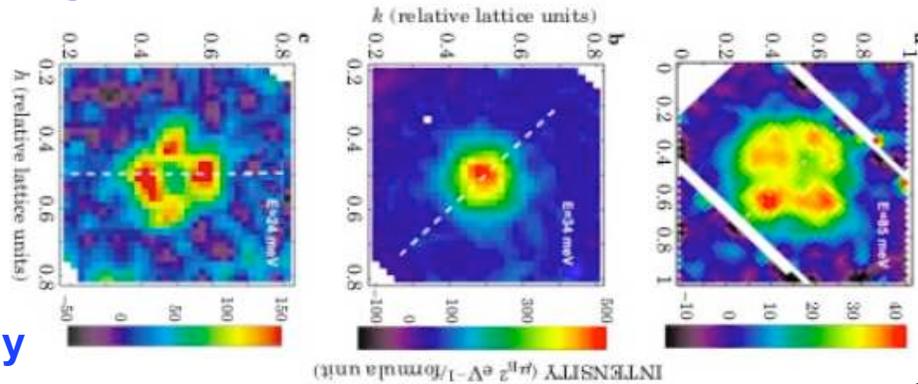
J is strong enough to make pairing



hole: ~O_{2p} orbital
electron: ~Cu_{3d} orbital
(two types of carriers ?)

Hourglass shape of magnetic excitation in superconducting phase

YBa₂Cu₃O_{6.6}
Superconducting state



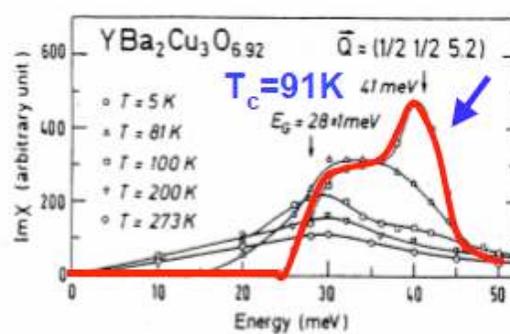
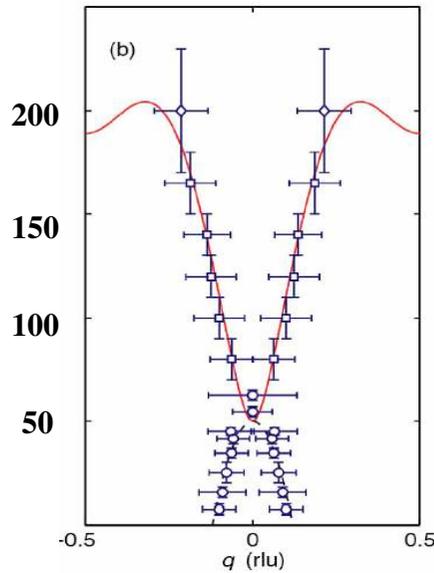
S. Hayden et al,
Nature 429 (2004)

low energy

high energy

La_{2-x}Ba_xCuO₄
x = 1/8
Normal state

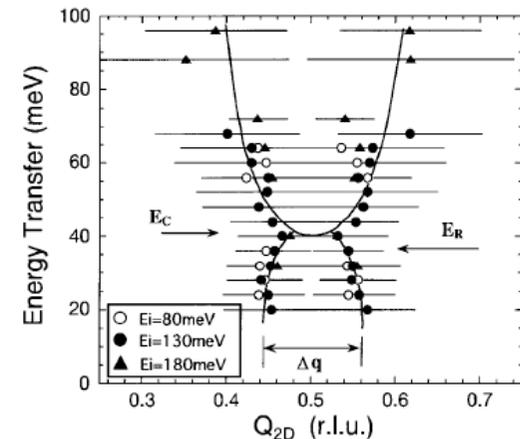
meV



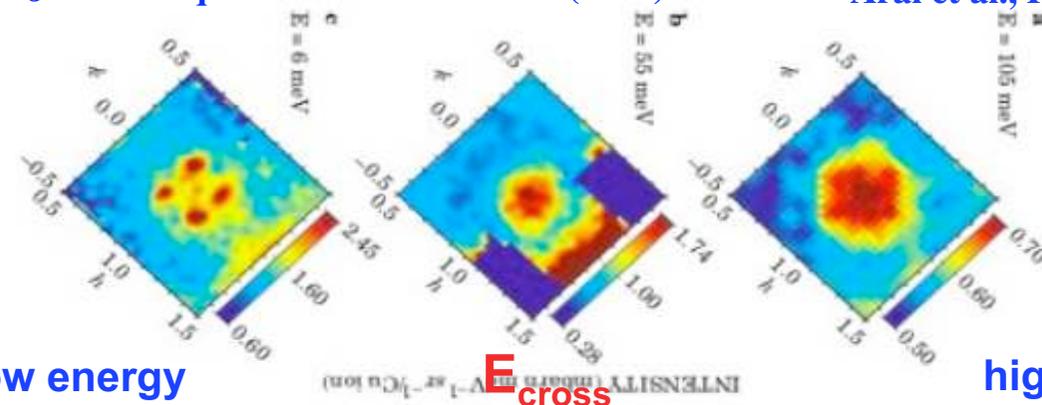
E_{res}/E_{cross}

J. Rossot-Mignod et al., Physica C ('91)

J.M. Tranquada et al. Nature 429 (2004)



Arai et al., PRL(1999)



low energy

high energy

E_{cross}

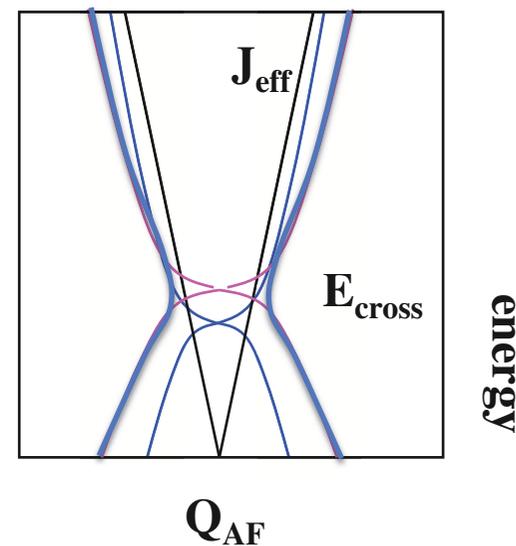
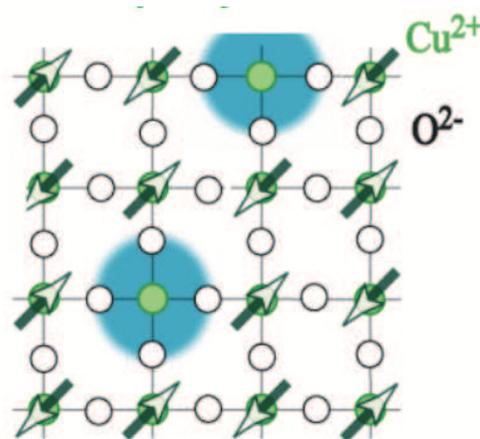
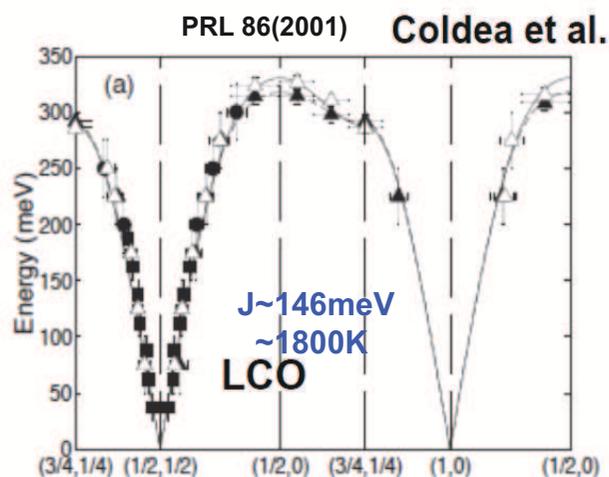
Our interpretation of hour glass type magnetic excitation

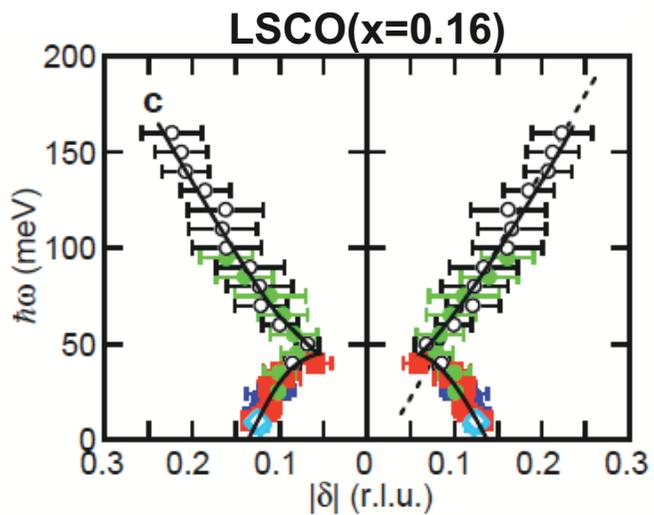
Two energy scales E_{cross} and J_{eff} can be defined

E_{cross} is the crossing energy between the downward and upward excitation. In YBCO, Bi2212, E_{cross} nearly corresponds to resonance peak energy.

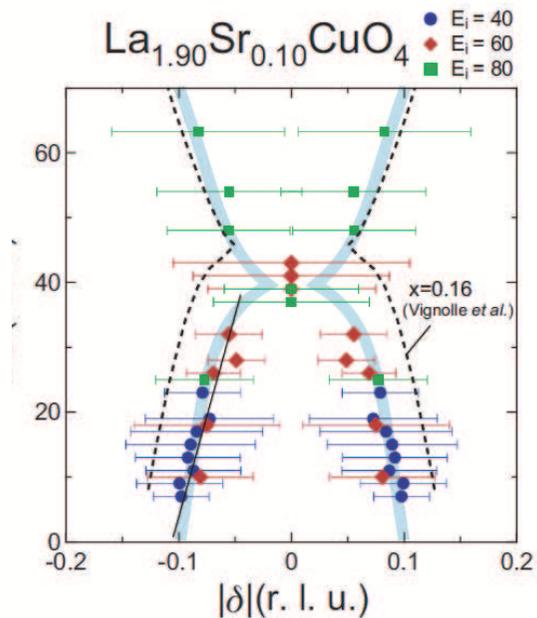
J_{eff} is defined from the upward excitation.

$E_{\text{cross}}(J_{\text{eff}})$ decreases (increases) with decreasing doping and is continuously connected to the spin excitation of undoped Mott insulator

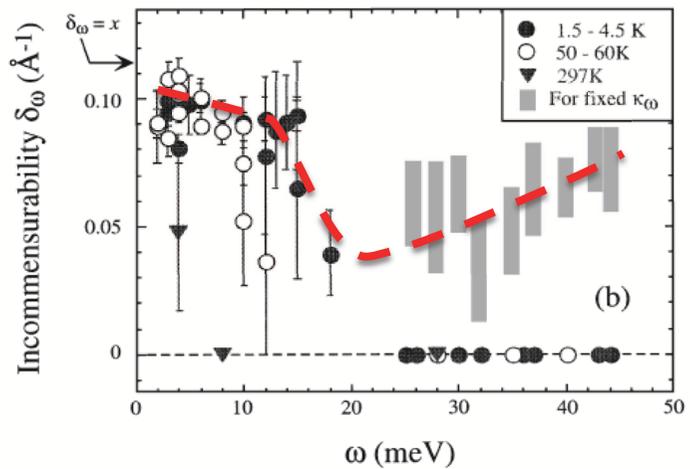
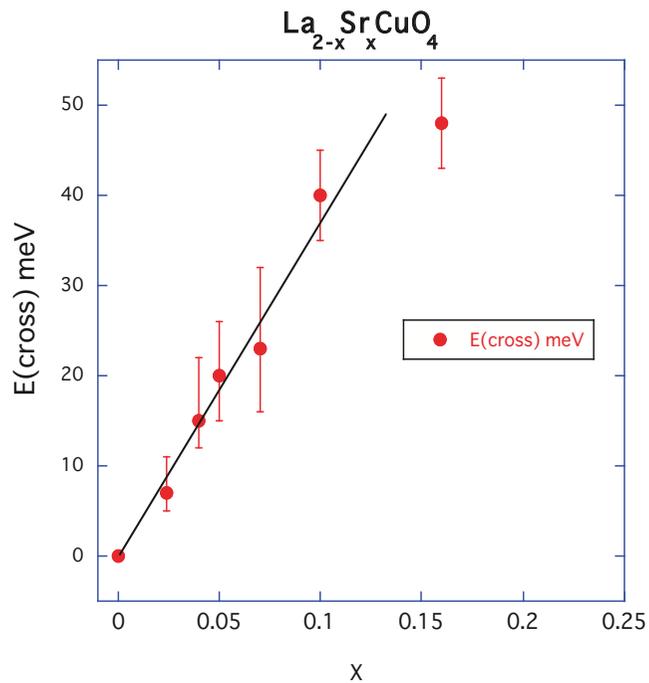




Vignolle et al.(2007)

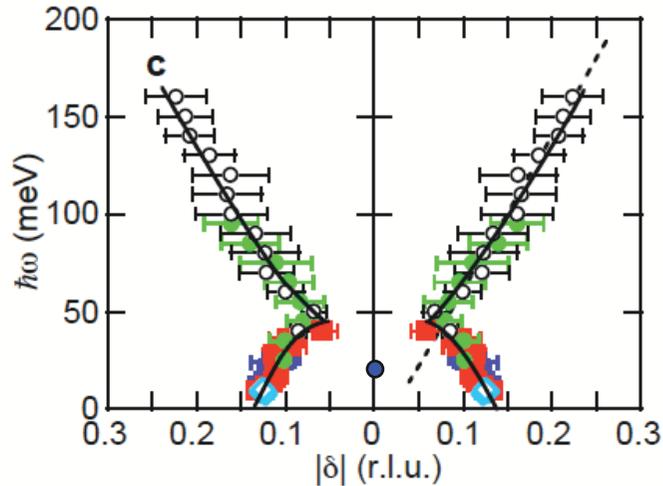


Kofu et al.

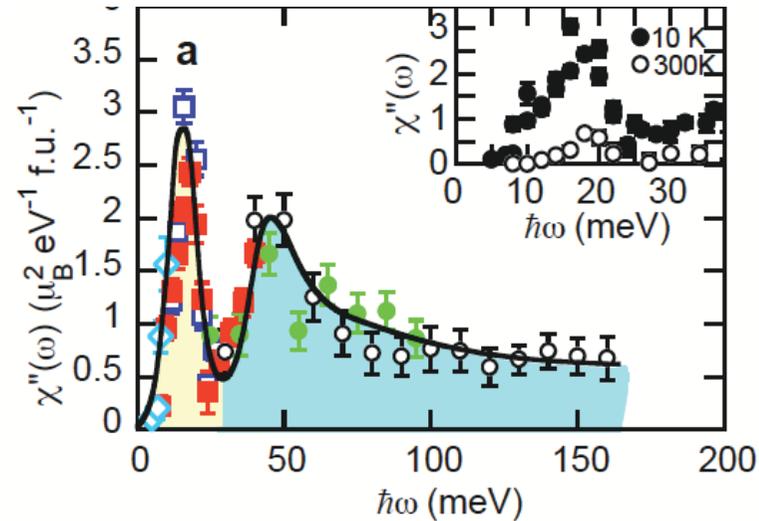


Similarity between LSCO (optimally doped) and YBCO (underdoped)

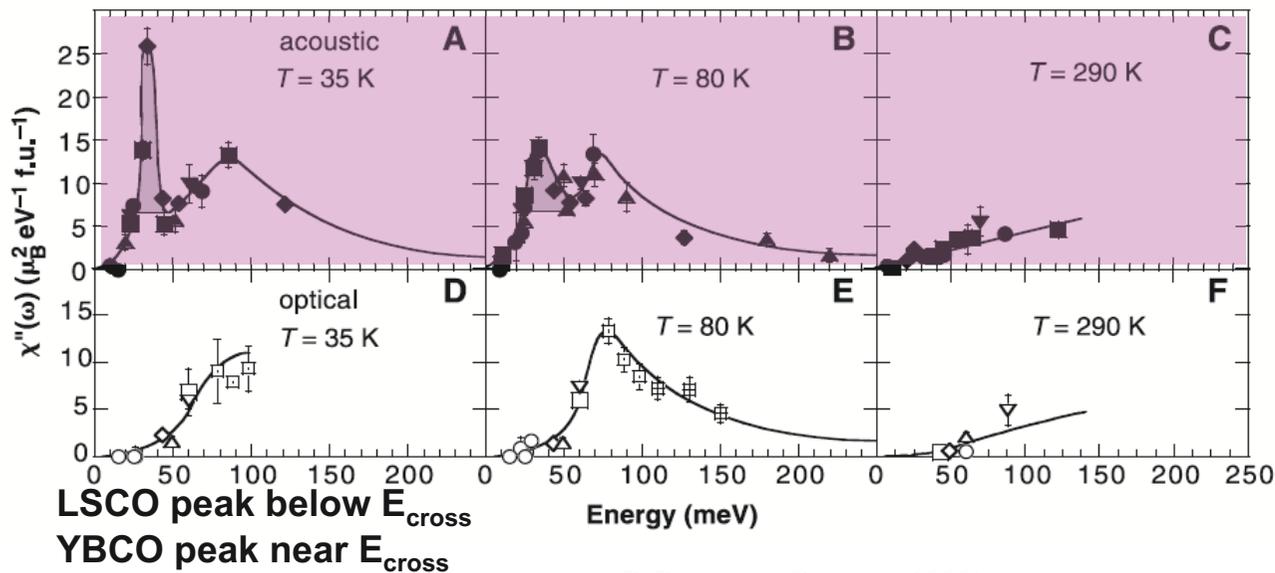
B. Vignolle et al., cond-mat/0701151



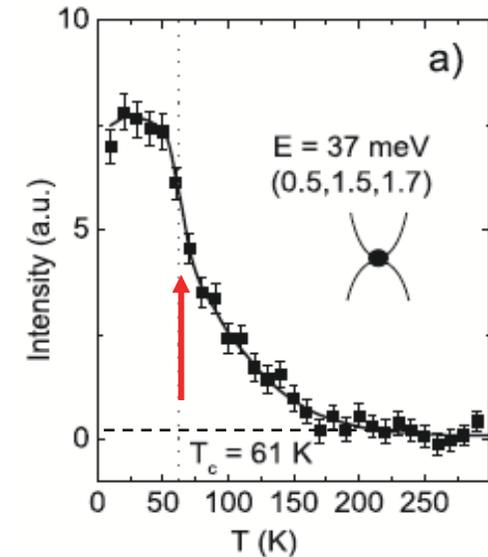
LSCO(x=0.16)



YBa₂Cu₃O_{6.6} ($T_c = 62.7$ K)

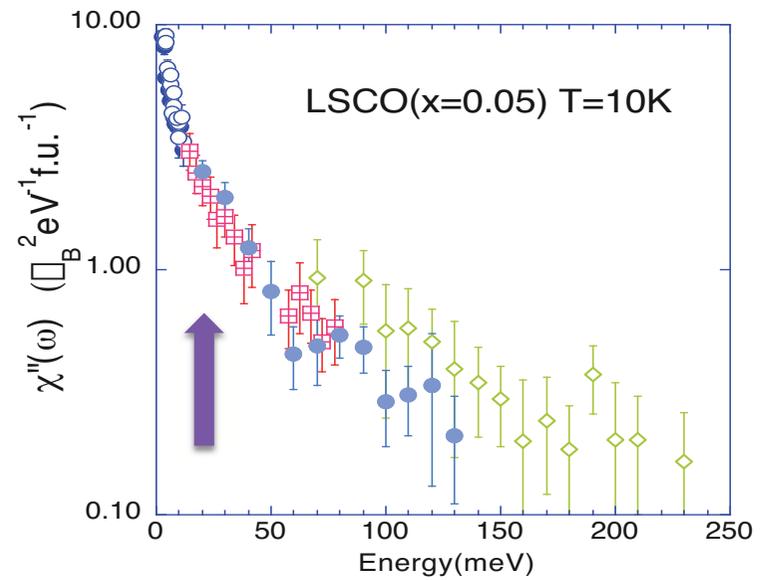
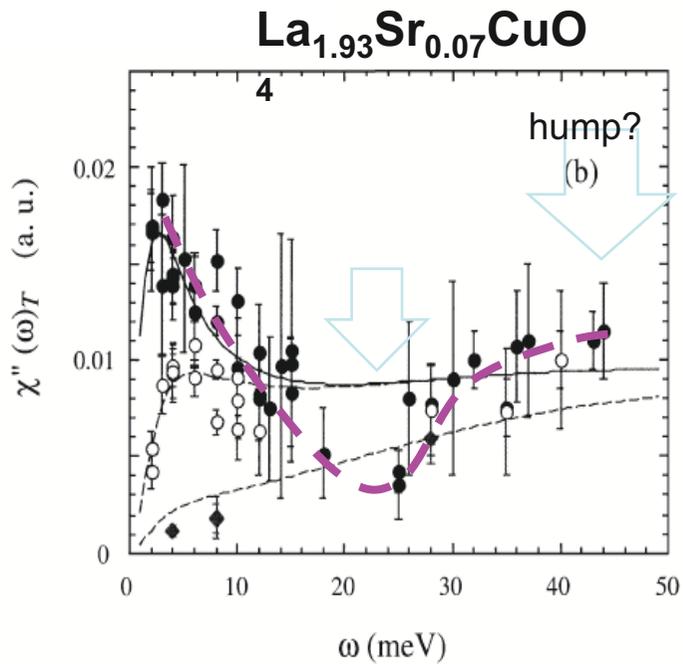
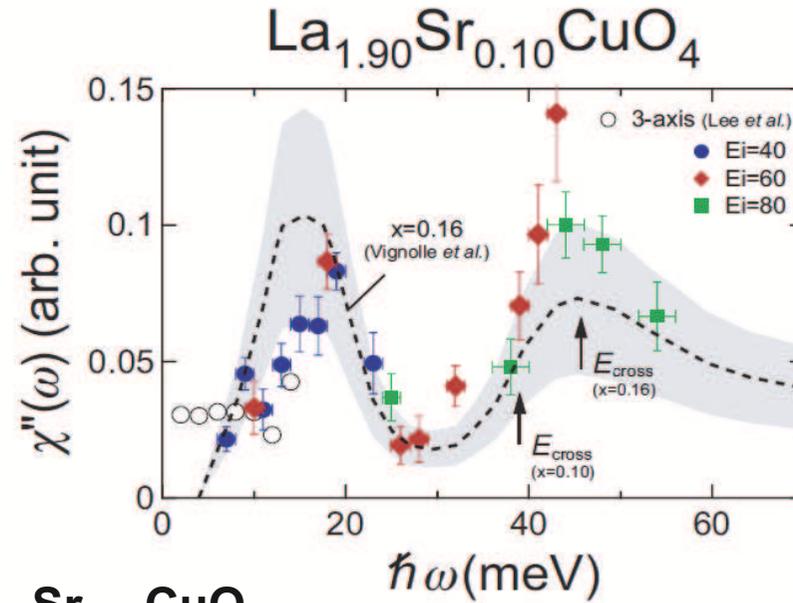


P. Dai et al., Science (1999)



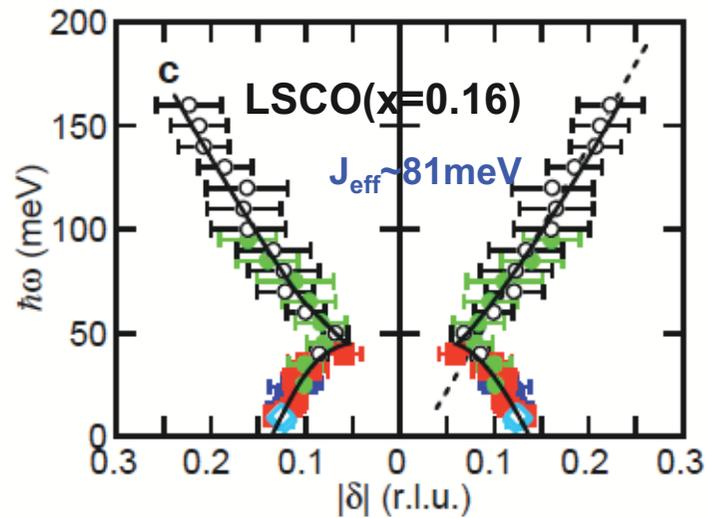
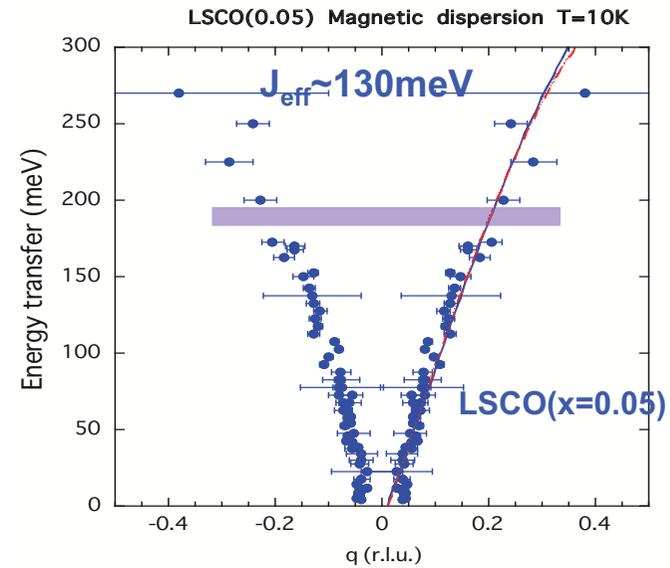
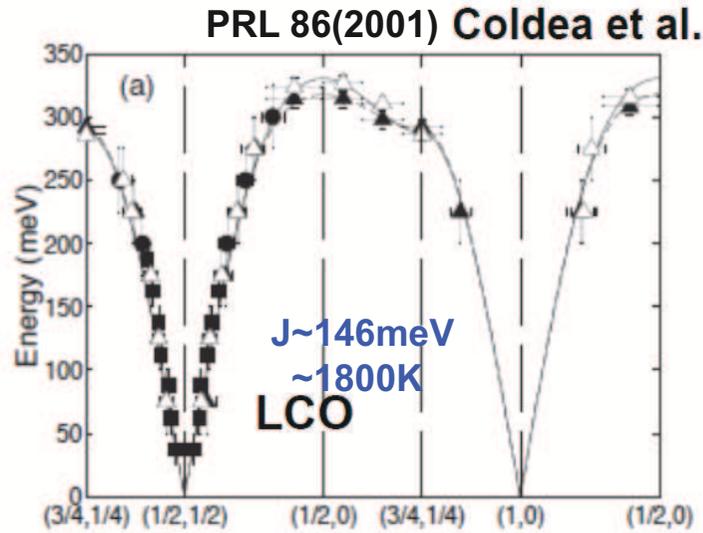
V. Hinkov et al., cond-mat/0601048

E_{cross} does not correspond to the hump energy in $\chi''(\omega)$

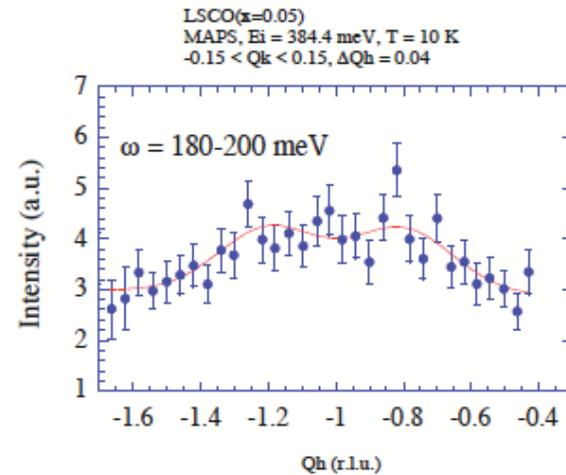


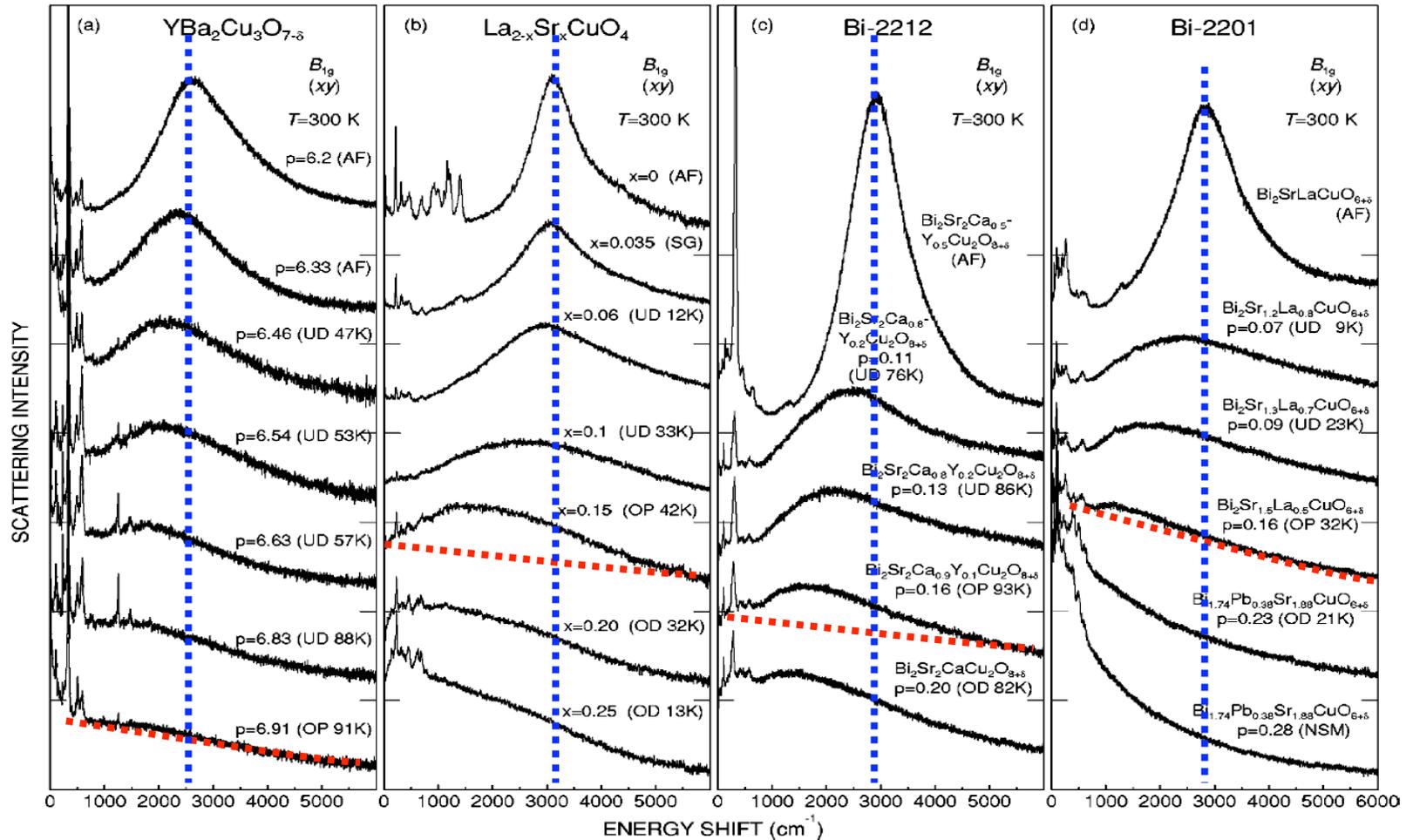
We can also define higher energy scale : renormalized J , J_{eff}

J_{eff} decreases with increasing doping



Vignolle et al.(2007)



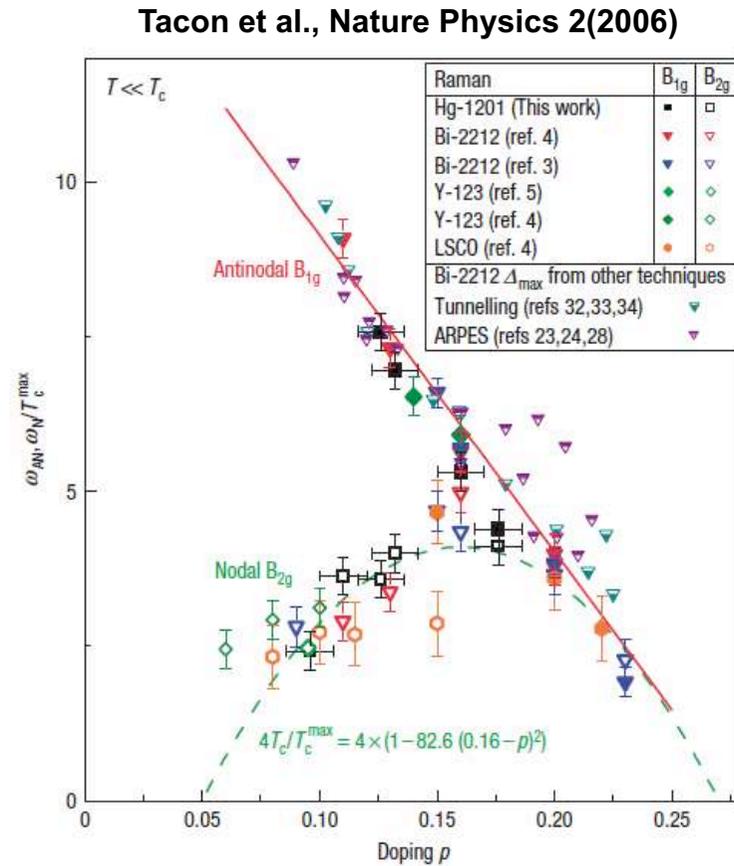
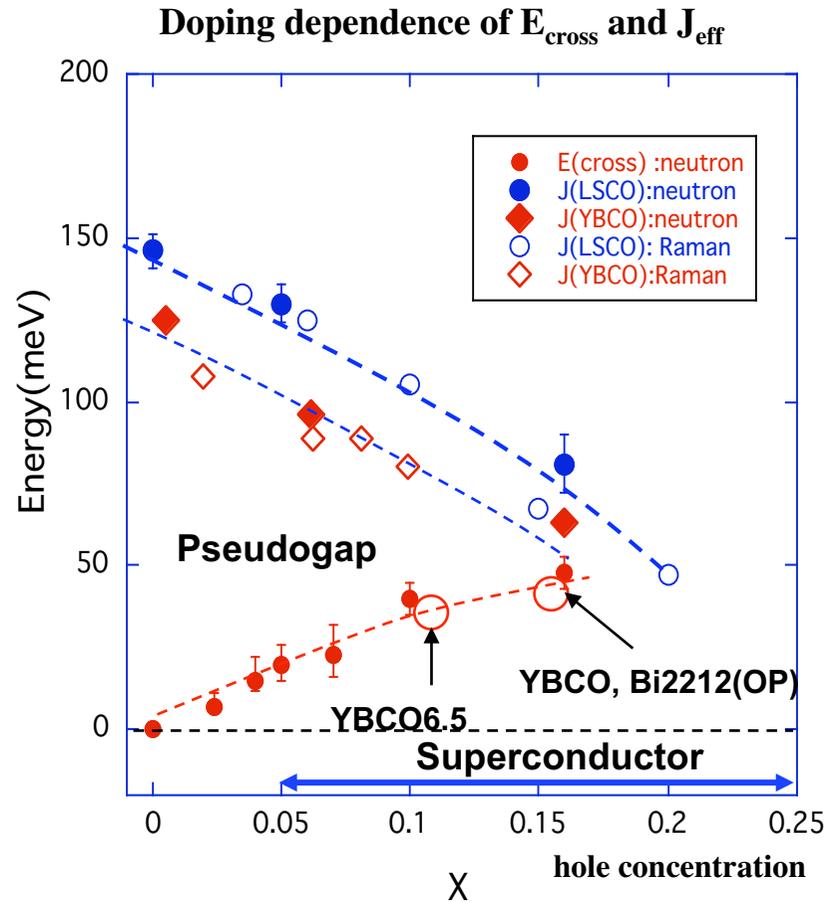


Sugai et al., PRB(2003)

Peak position of two-magnon scattering is proportional to renormalized $J(x)$
 ---> $J(x)$ well corresponds to J_{eff} by neutron scattering

Spin dynamics

Two energy scales in charge dynamics



Contents

1) Magnetic fluctuation of p-type cuprates (10min.)

2) Magnetic fluctuation of n-type cuprates (15min.)

doping dependence in the overdoped superconducting phase

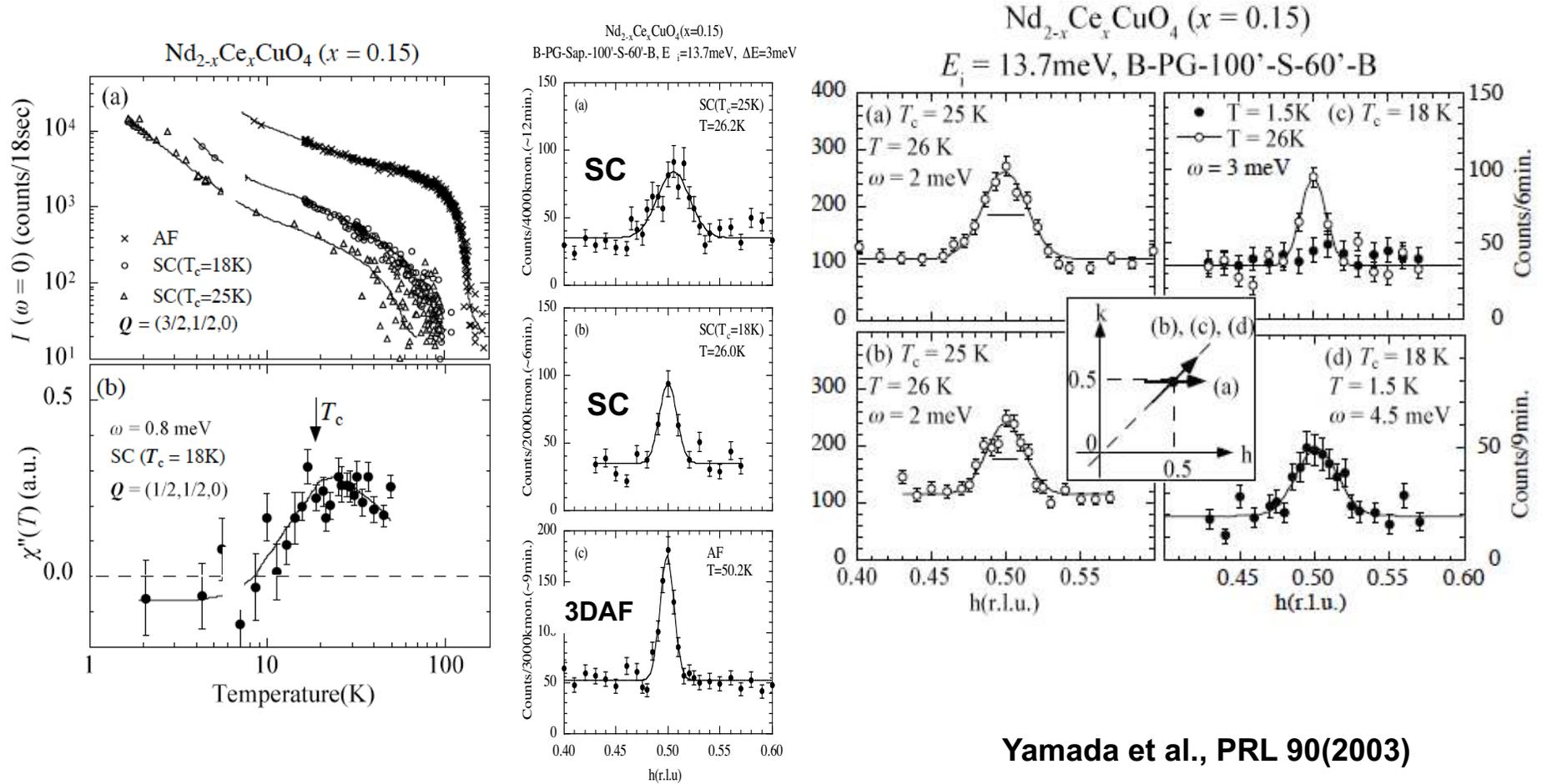
3) "Magnetic" impurity-effect in p-type cuprates (15min.)

4) New pulsed neutron facility in J-PARC (5min.)

Advertisement

n-type cuprates : SC and AF ordered phases are touched

commensurate spin correlation in both SC and AF phase

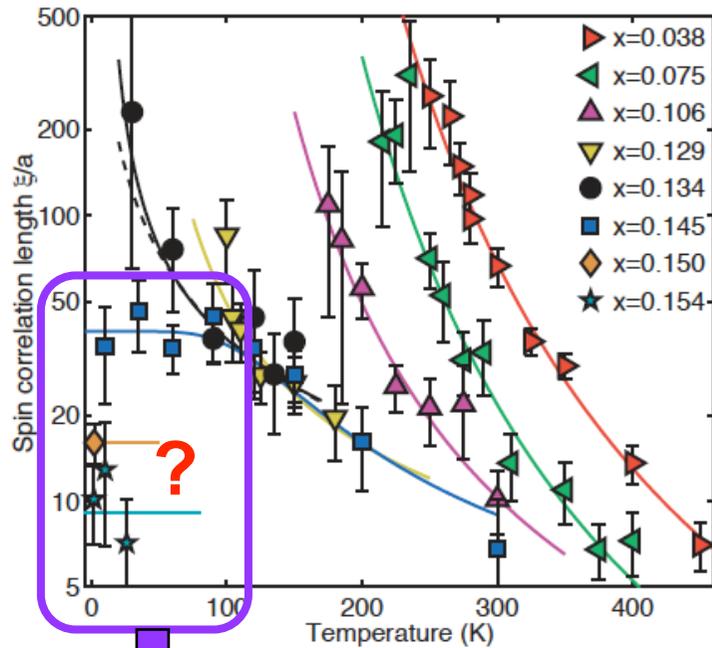


Two types of spin fluctuations in n-type cuprate NCCO

J_{eff} from instantaneous spin correlation length in paramagnetic state

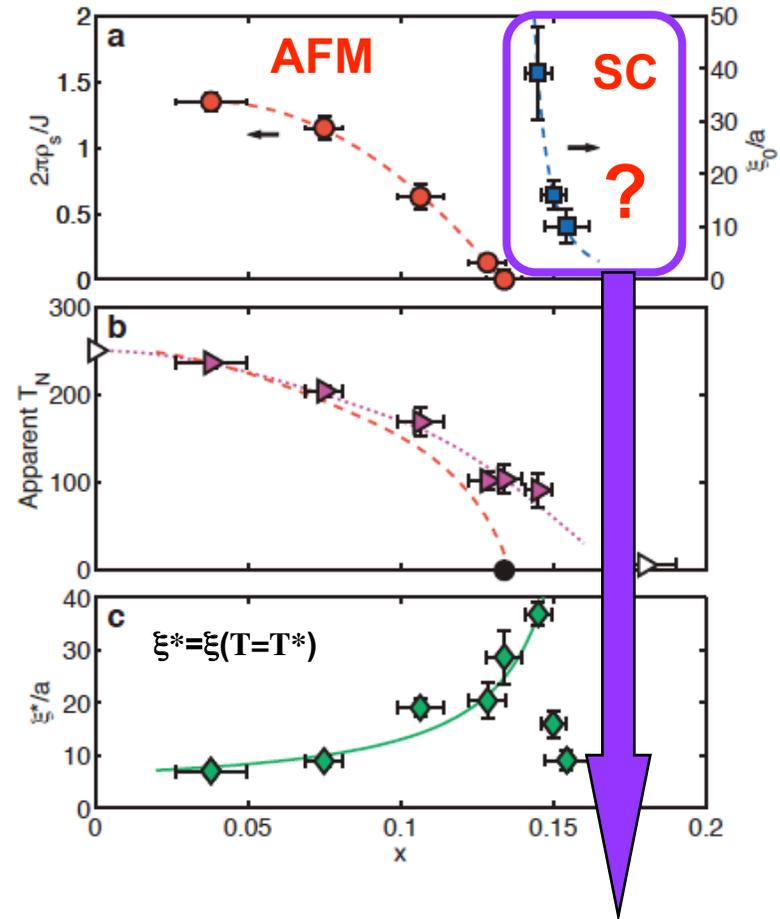
$$\xi(x, T) = A(x) \exp(2\pi\rho_s(x)/T)$$

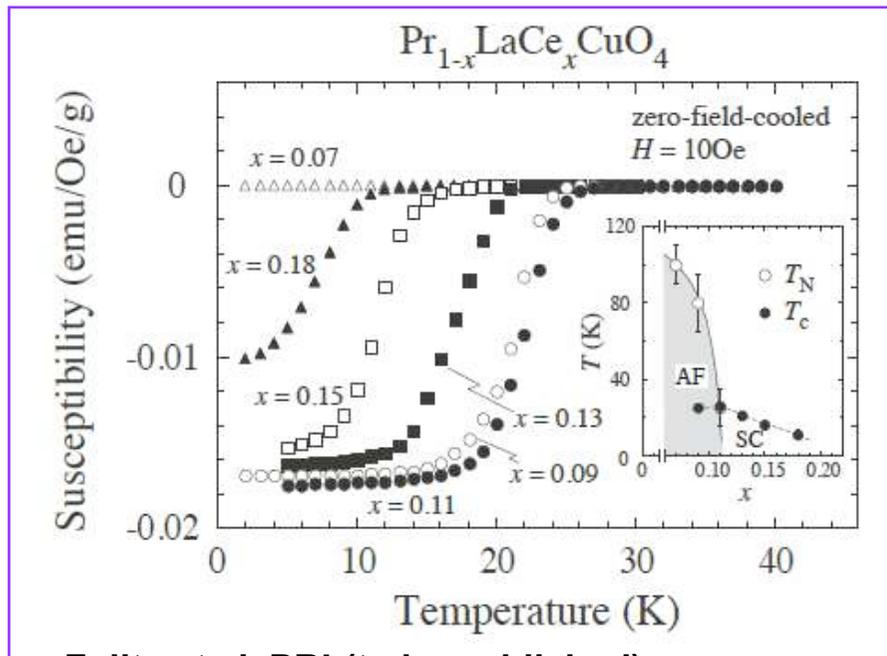
$\rho_s(x)$: spin stiffness $\propto J_{\text{eff}}$



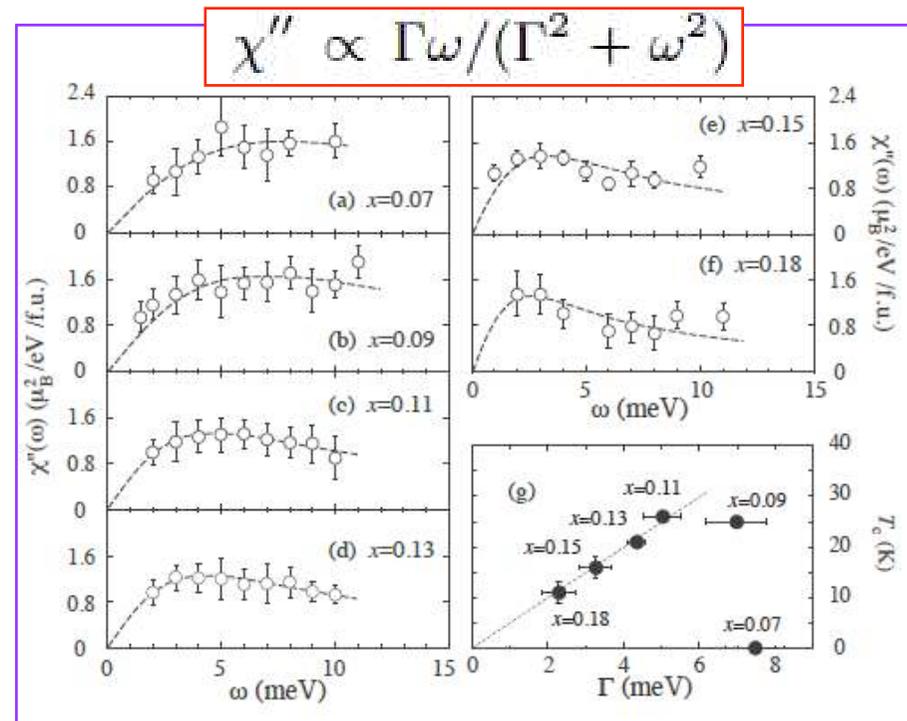
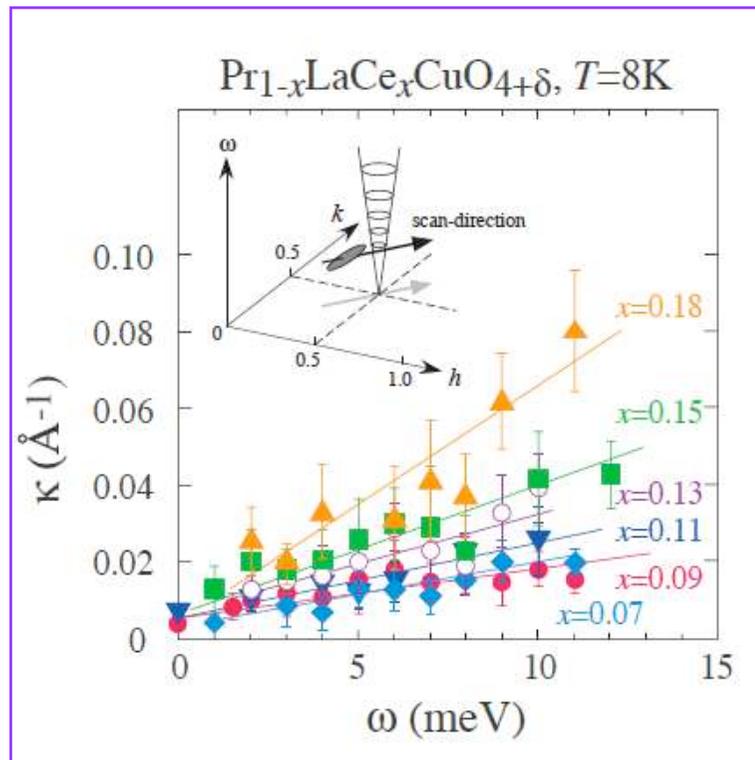
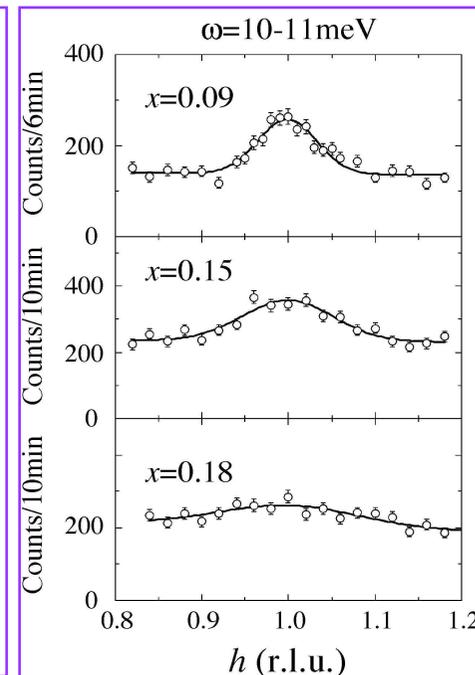
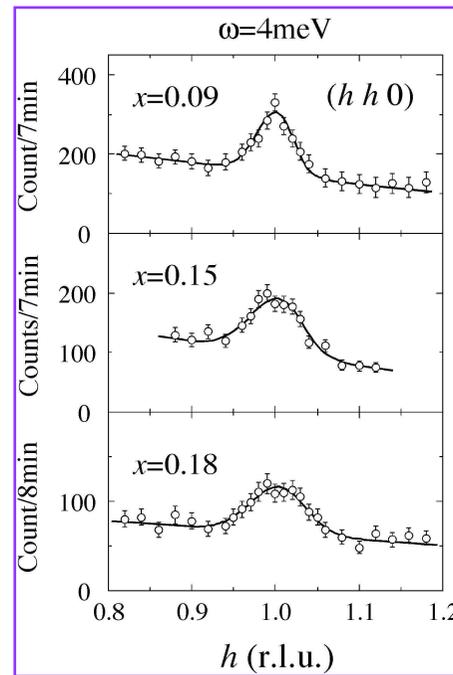
$\xi(T)$ saturates at low temperature in the SC phase

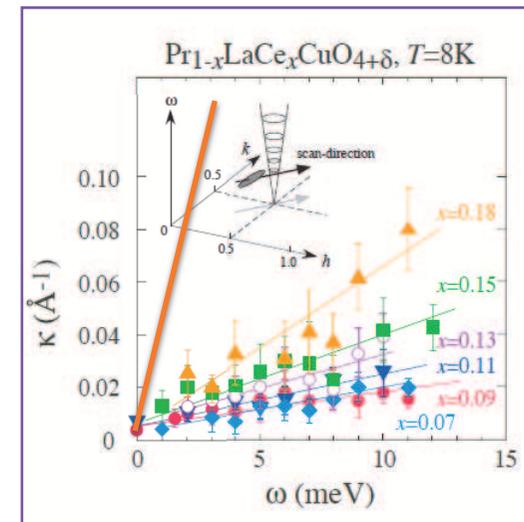
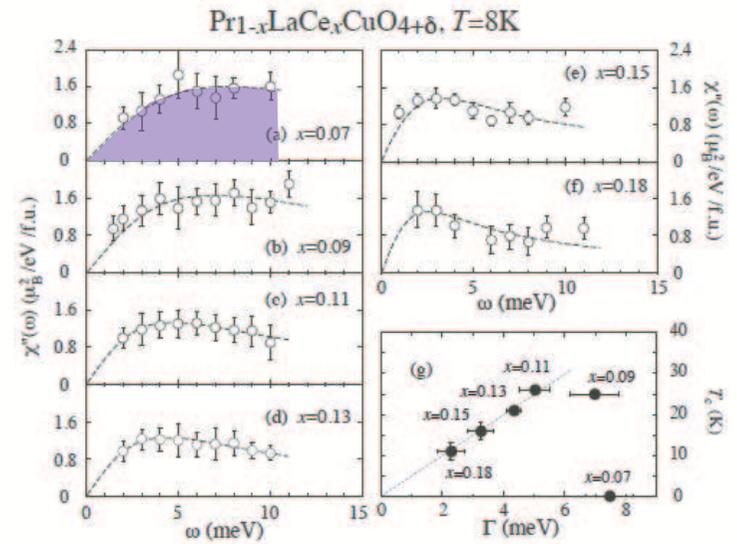
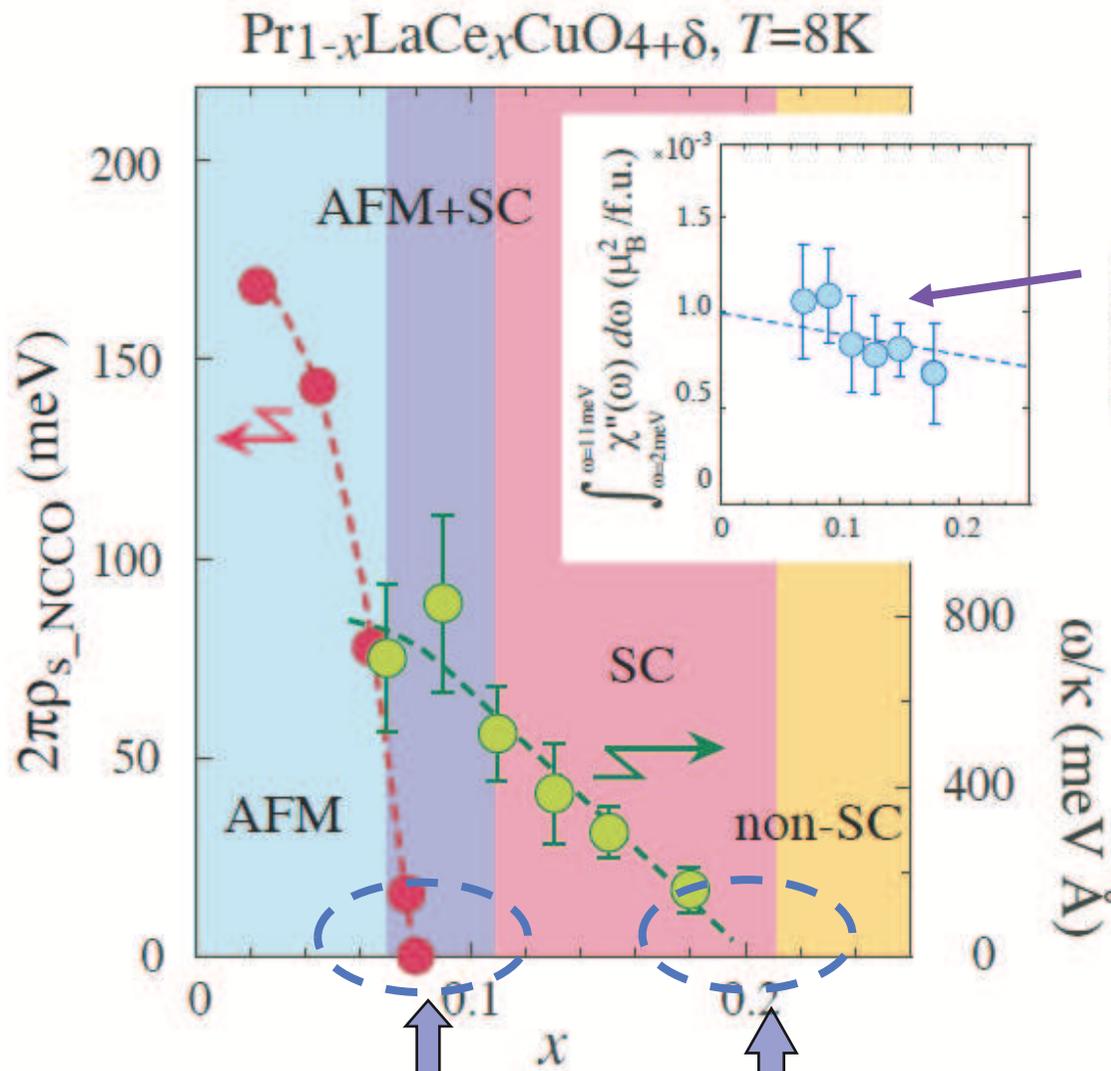
Motoyama et al., Nature 445(2007)





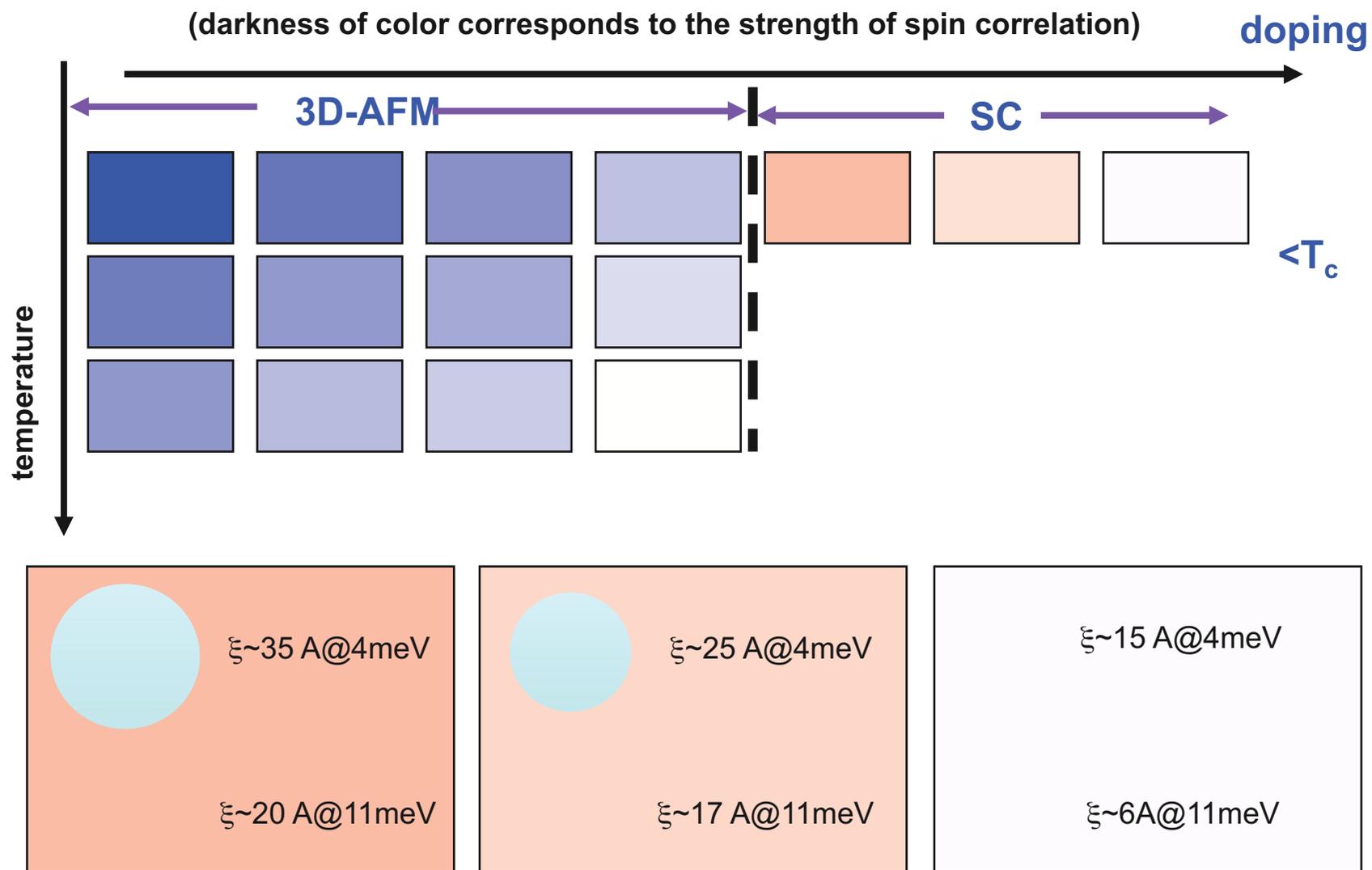
Fujita et al., PRL (to be published)



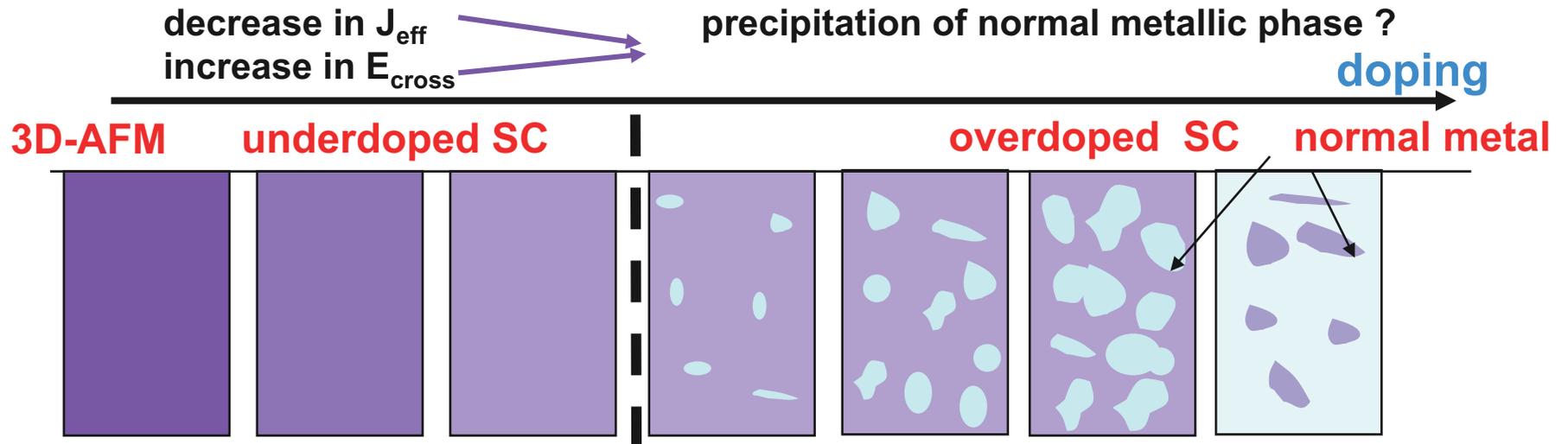


instantaneous spin stiffness disappears at AFM-SC boundary

low energy spin stiffness disappears at SC-metal(non-SC) boundary

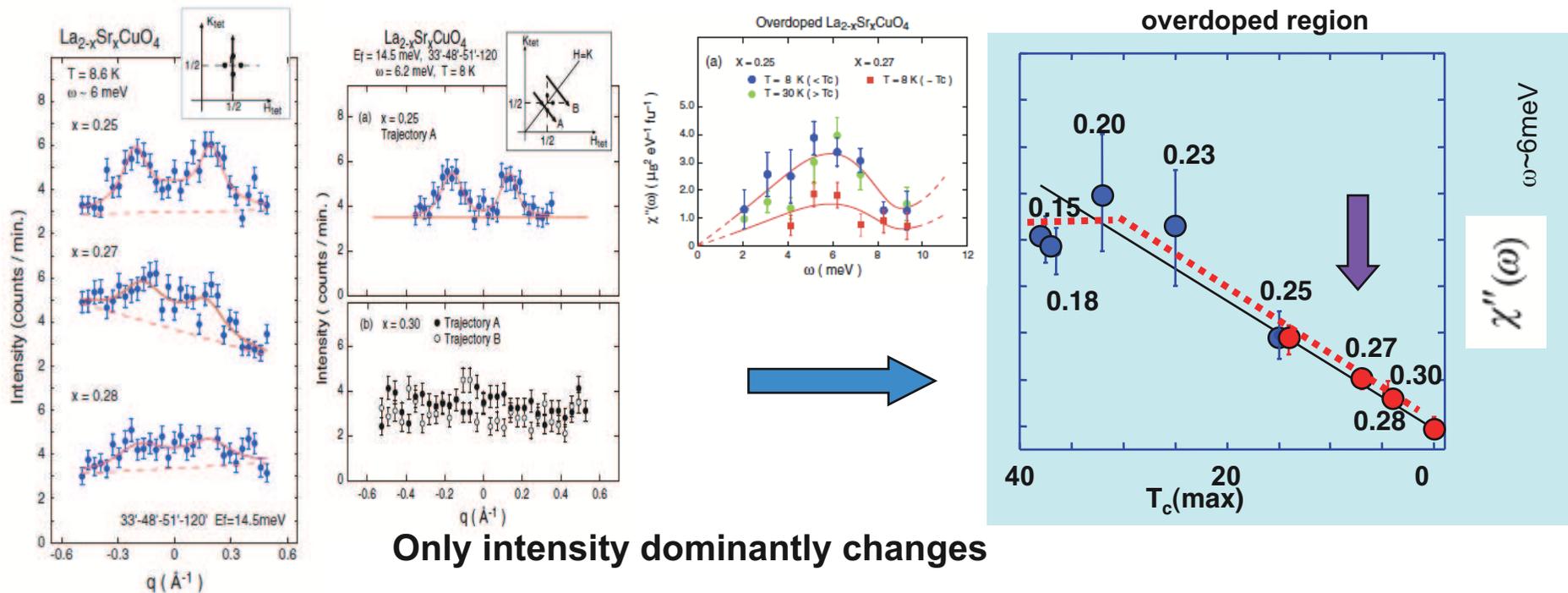


continuous reduction of spin stiffness upon doping



(darkness of color corresponds to the strength of spin correlation)

Wakimoto et al., PRL(2006)



N-type cuprates are normal ?

Magnetic fluctuations in n-type high- T_c superconductors reveal breakdown of fermiology

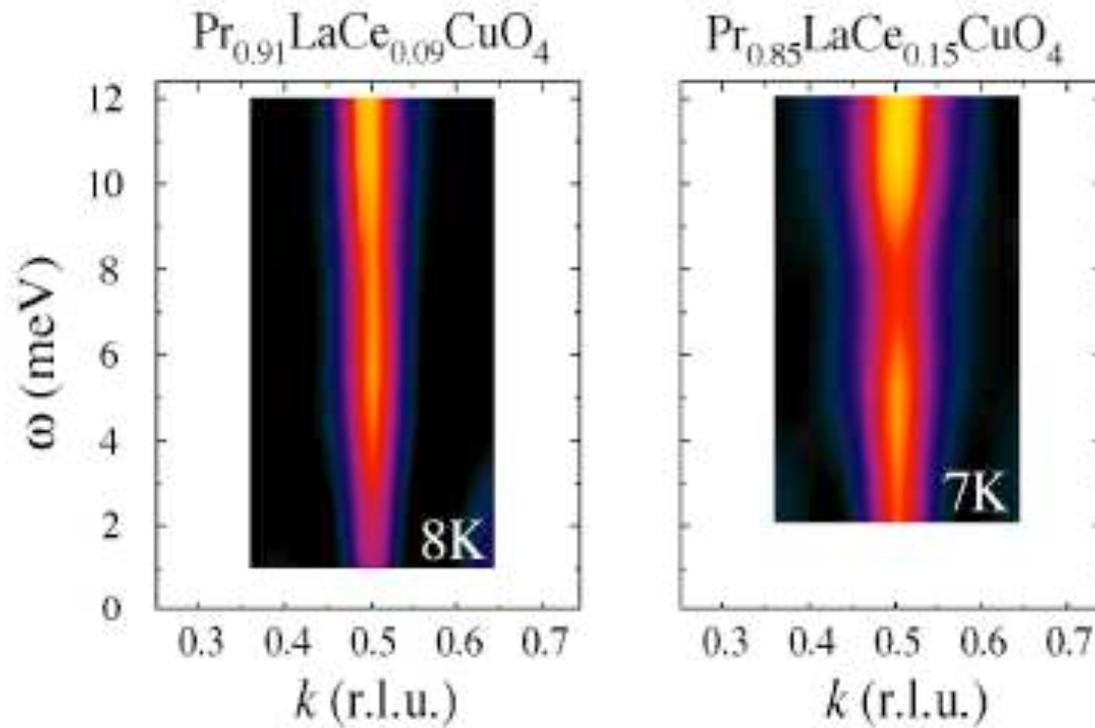
F. Krüger¹, S. D. Wilson², L. Shan³, S. Li², Y. Huang³, H.- H. Wen³, S.-C. Zhang⁴, Pengcheng Dai^{2,5}, J. Zaanen¹

cond-mat 07054424

Electron-doping

Fermi liquid model cannot reproduce commensurate low energy spin fluctuations in electron-doped cuprates

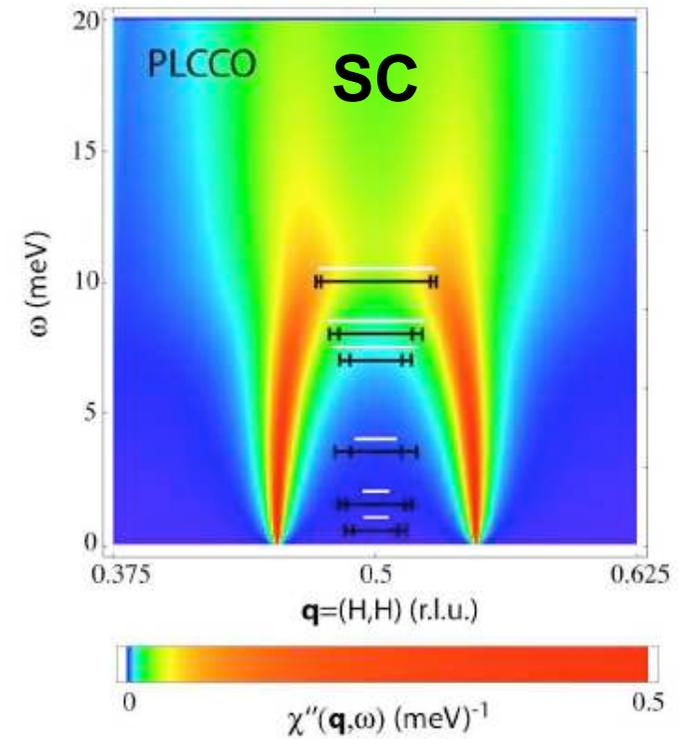
Experiment



AF

SC

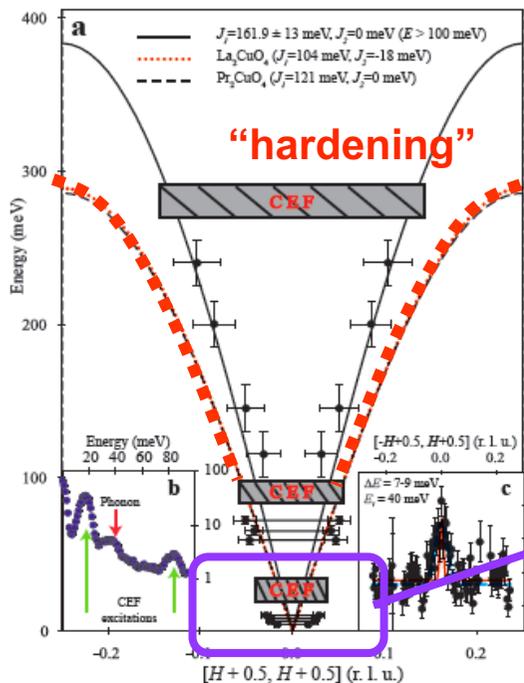
Fermi liquid model calculation



Krüger et al., cond-mat 07054424

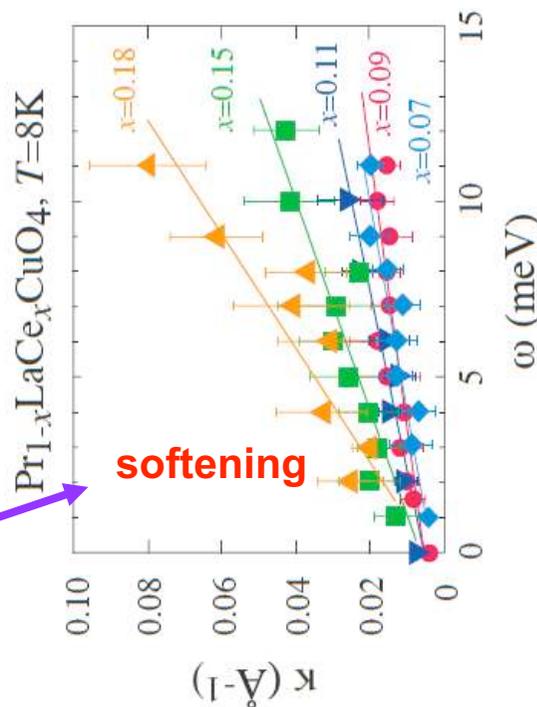
The high energy magnetic excitation is also anomalous

MAPS

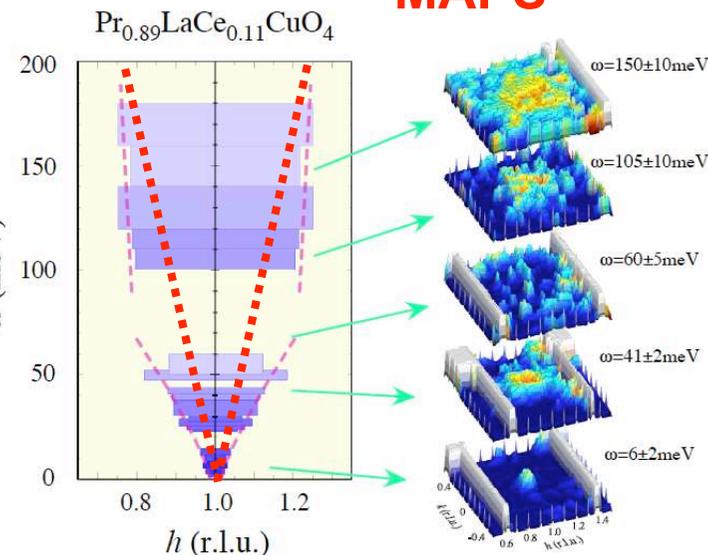


Wilson et al. PRL(2006)

“Hardening” at high energies,
softening at low energies !



MAPS

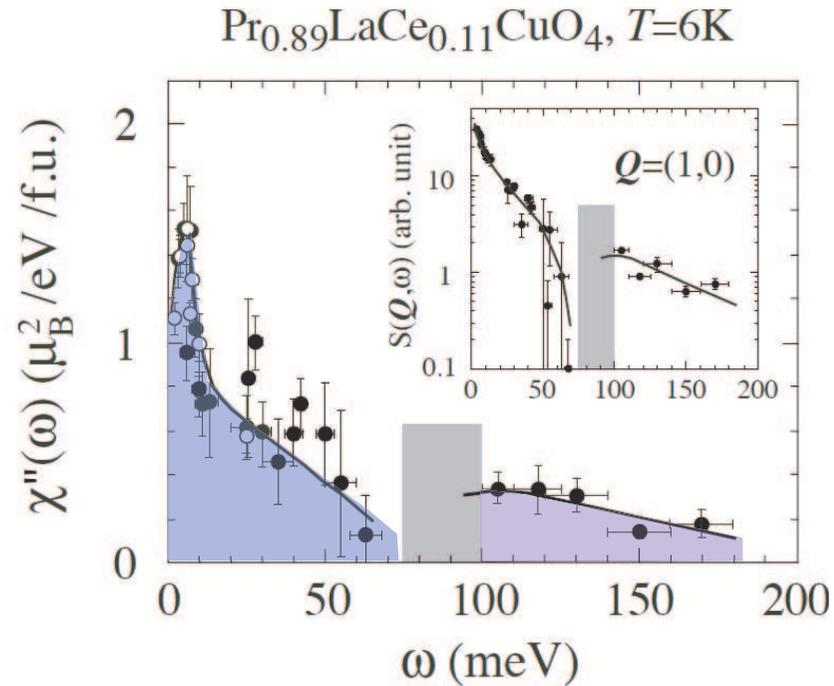


Fujita et al., JPSJ(2006)

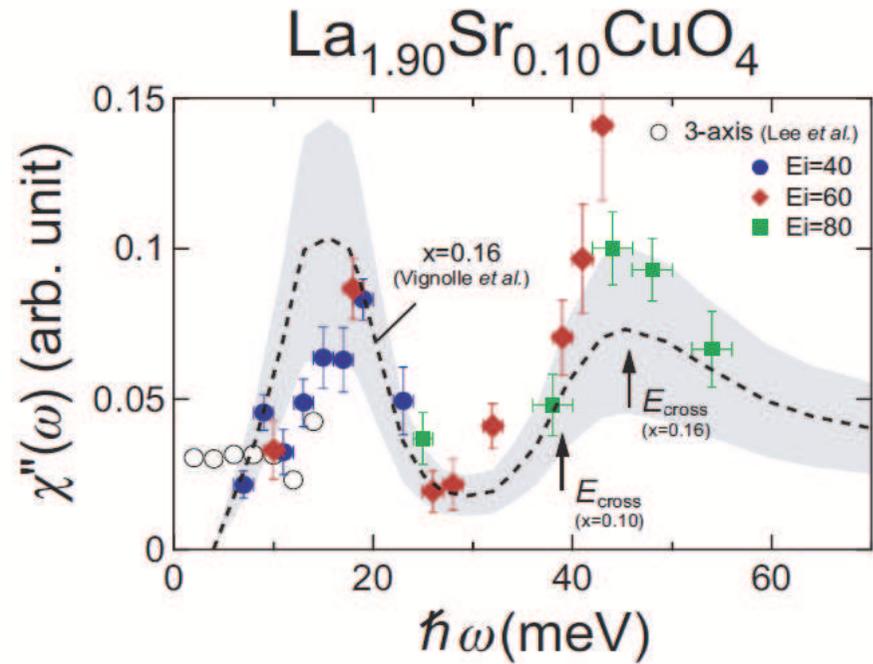
Different from spin-wave-type excitation
in SC phase ?

Pencil shape excitation?

Dual nature in magnetic excitations in n-type?



Fujita et al. JPSJ, 75 ('06)



Future experiment including polarization analysis will clarify this issue

Contents

- 1) Magnetic fluctuation of p-type cuprates (10min.)
- 2) Magnetic fluctuation of n-type cuprates (15min.)
- 3) "Magnetic" impurity-effect in p-type cuprates (15min.)

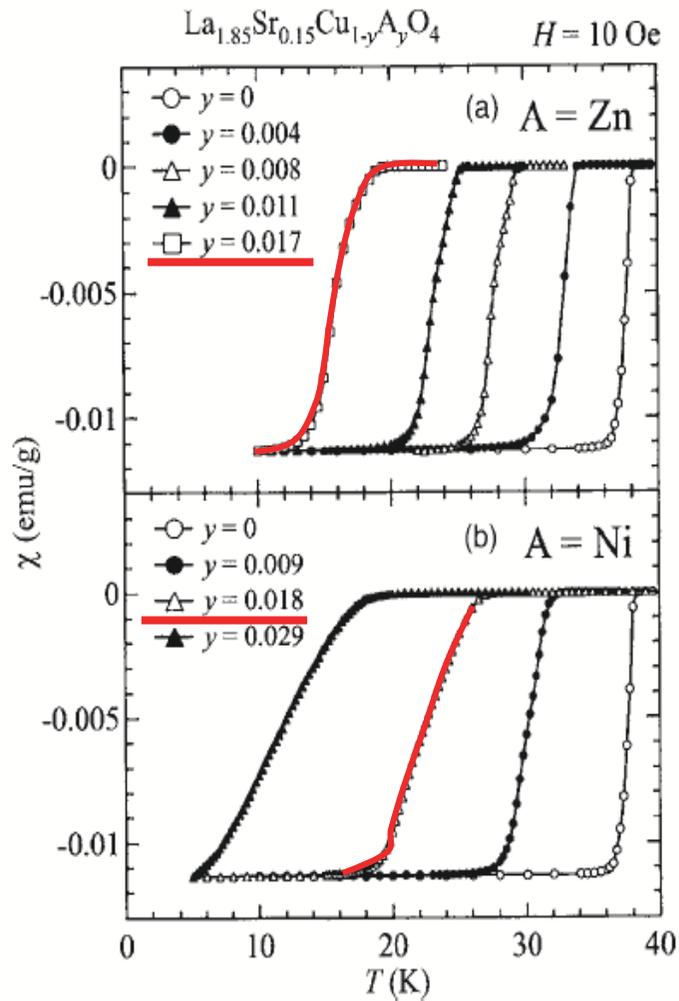
Ni-impurity is not magnetic impurity but charge one

- 4) New pulsed neutron facility in J-PARC (5min.)

Advertisement

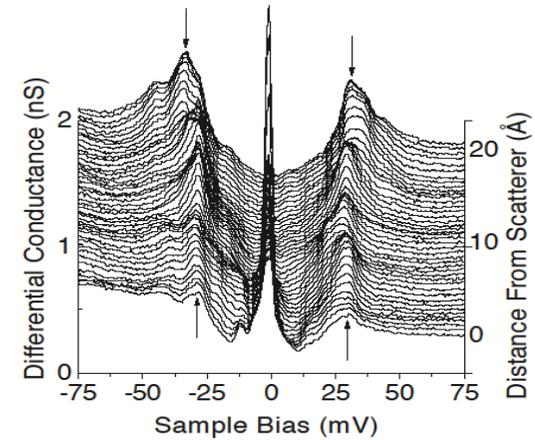
Uniqueness of Ni-impurity in doped cuprates

Robust superconductivity around Ni

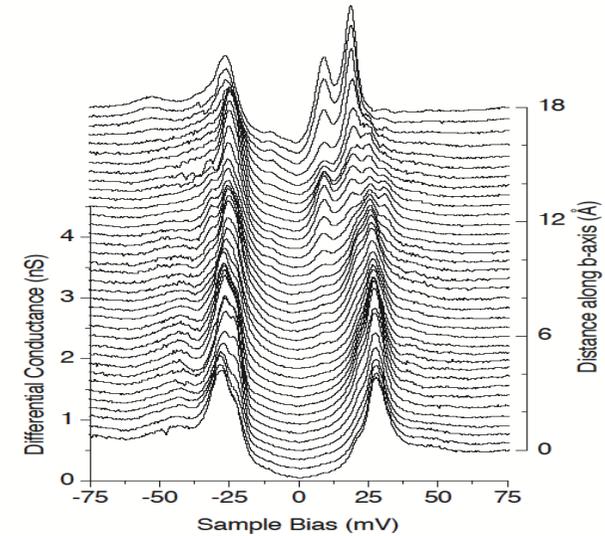


Kofu et al., PRB (2006)

Zn in Bi2212



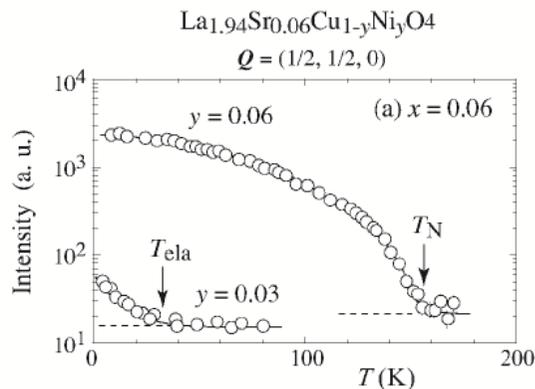
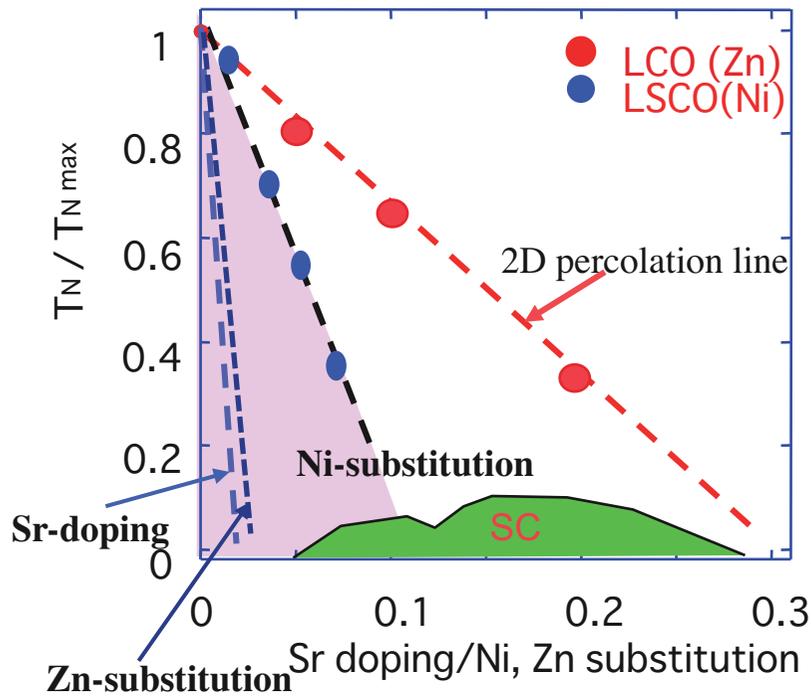
Ni in Bi2212



J.C. Davis's group

Effect of Ni-impurity on spin correlation

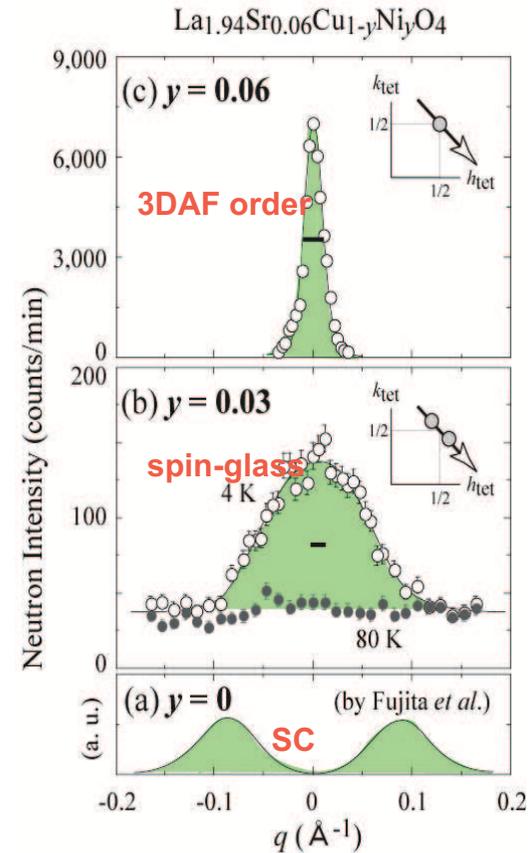
Ni-induced AF order in $\text{La}_{2-x}\text{Sr}_x\text{Cu}_{1-y}\text{Ni}_y\text{O}_4$



Ni-impurity recovers 3DAF order

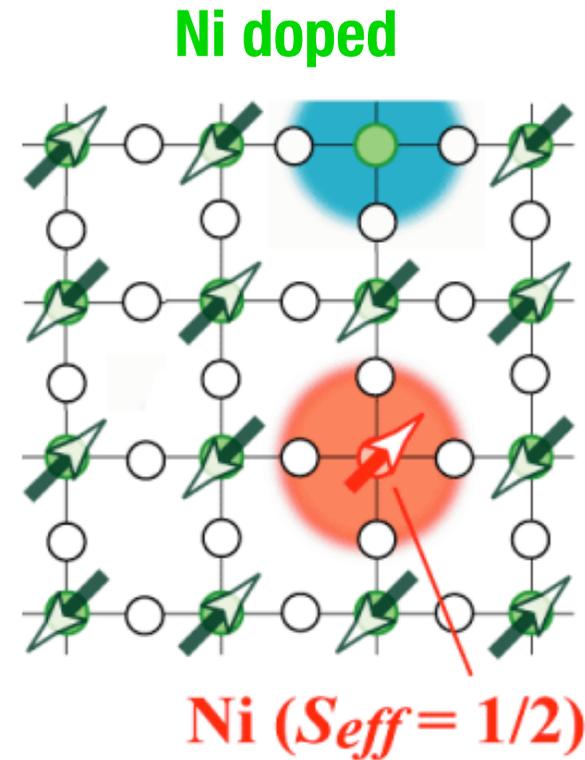
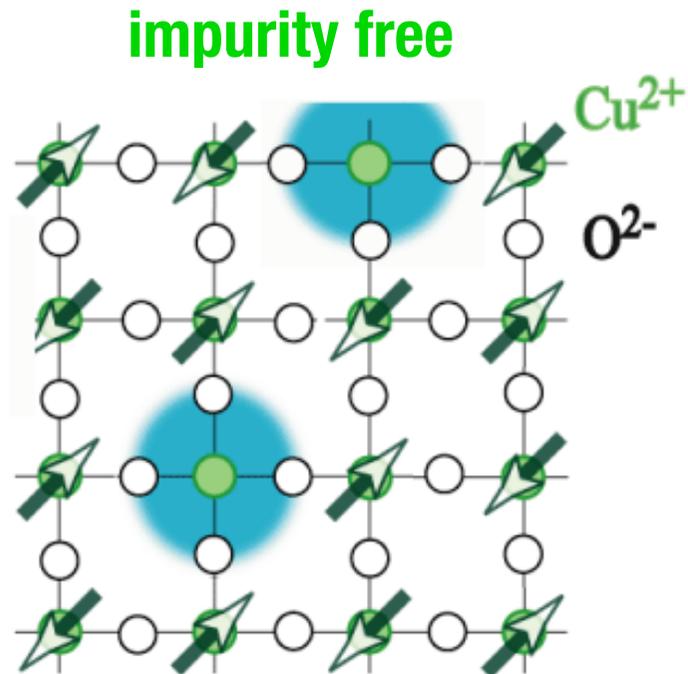
hole-doping 3DAF order \Rightarrow spin-glass \Rightarrow SC

Ni-doping 3DAF order \Leftarrow spin-glass \Leftarrow SC



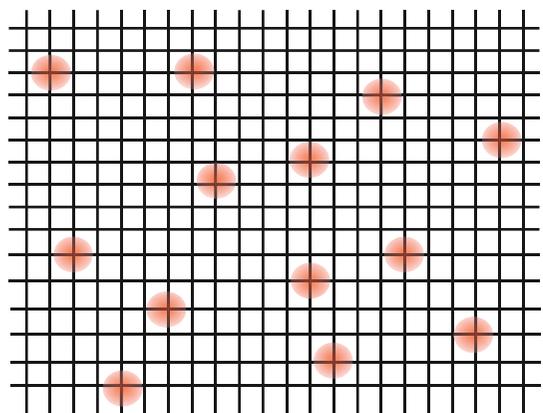
Ni-impurity reduces effective (mobile) hole concentration (Blotter effect)

There must be two types of holes by Ni-doping

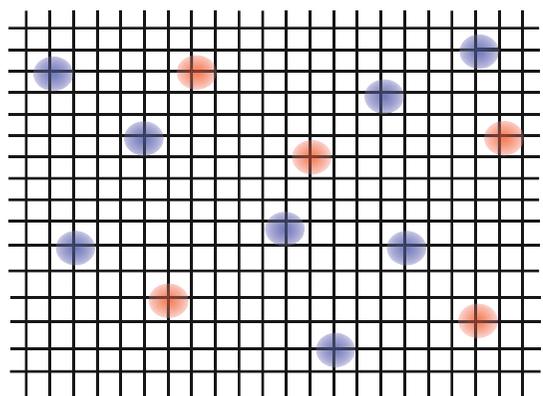


Itinerant Zhang-Rice singlet

Itinerant holes
+ Localized holes

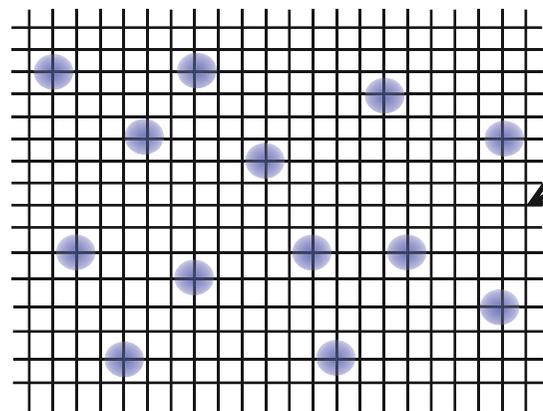


Ni-impurity is not a magnetic impurity but a nearly pure charge impurity in doped cuprates

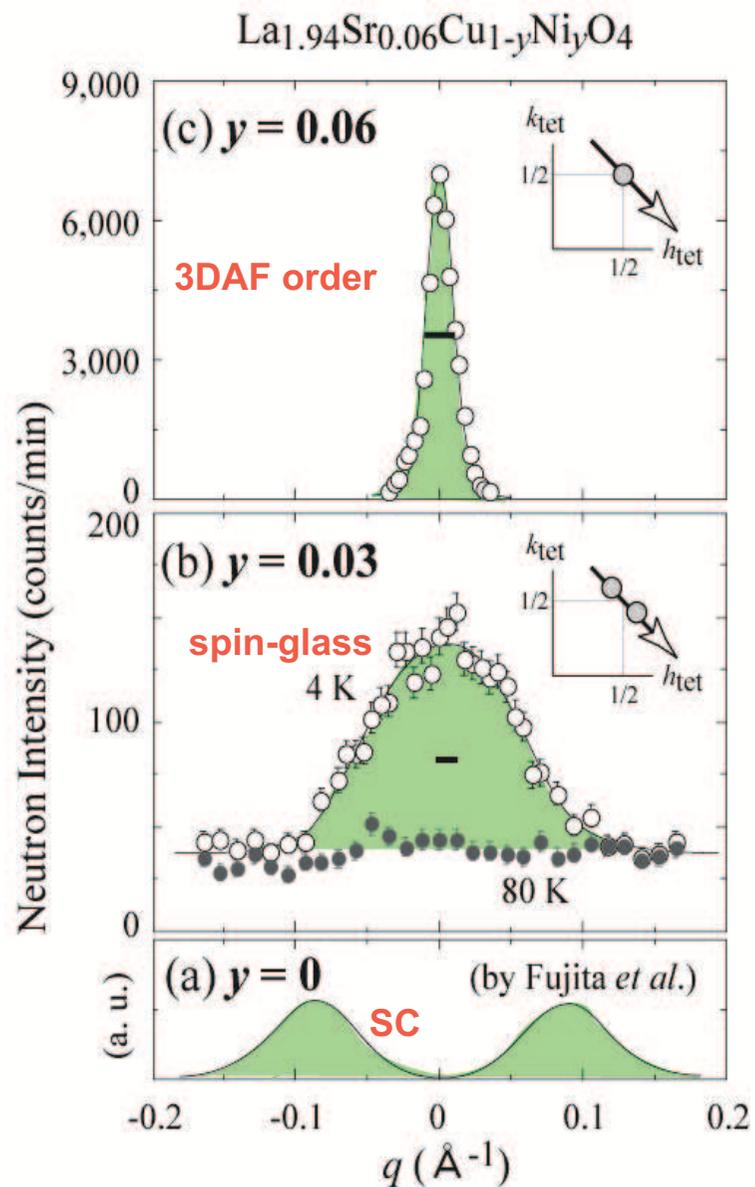


● Localized (Charge 3+) (Spin 1/2)

● Mobile (Singlet)

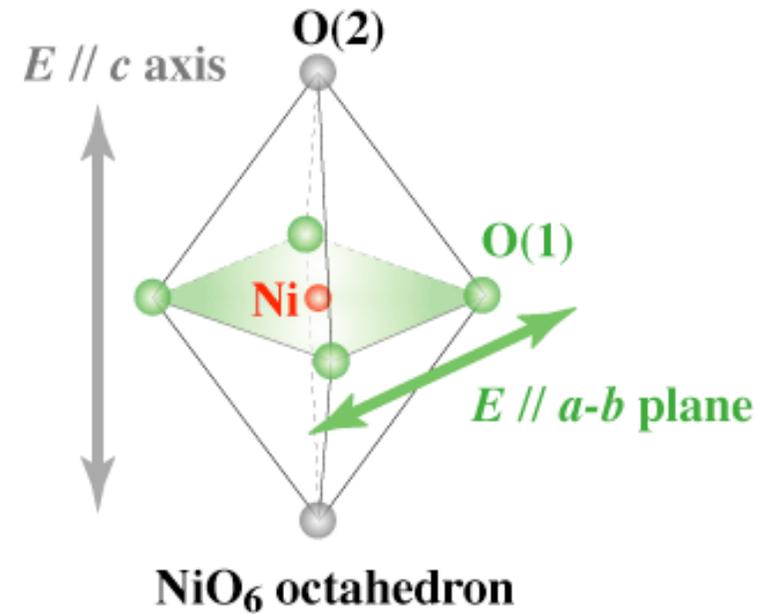
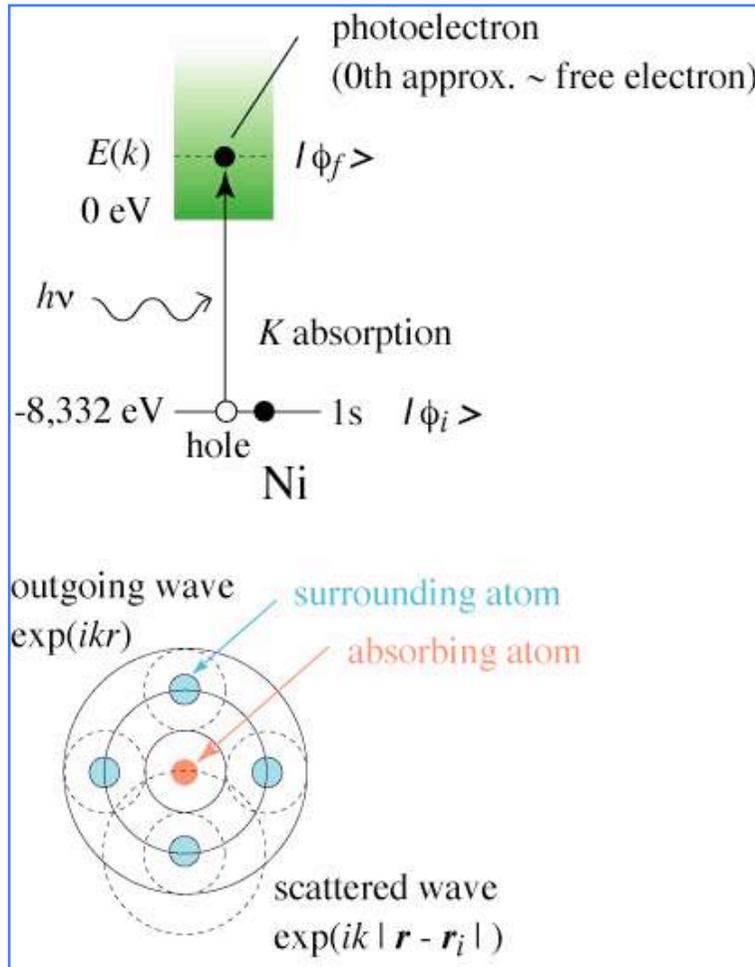


← Cu²⁺(Charge 2+) (Spin 1/2)



XAFS experiment (SPring-8, linearly polarized, Ni K-edge, T=300 K)

Site-selective measurement (local structure around ~1% Ni impurity)



EXAFS raw data

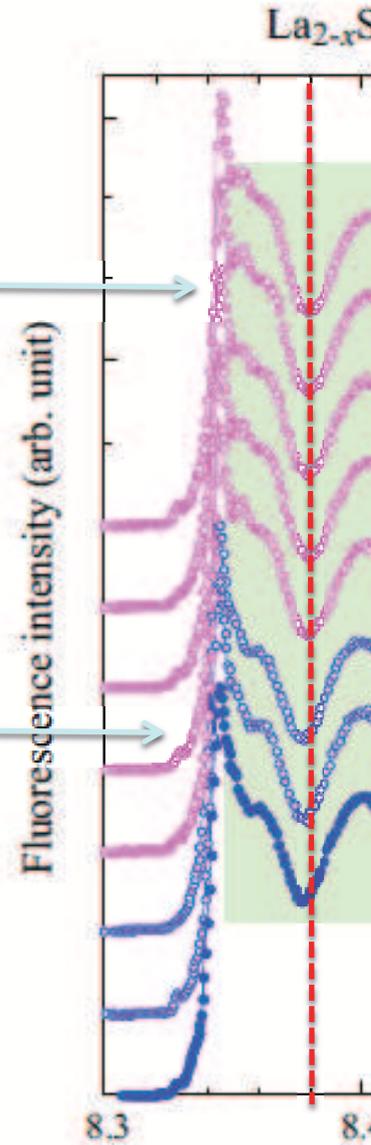
Two groups of single crystal

Hole rich group
(All Ni trap hole)

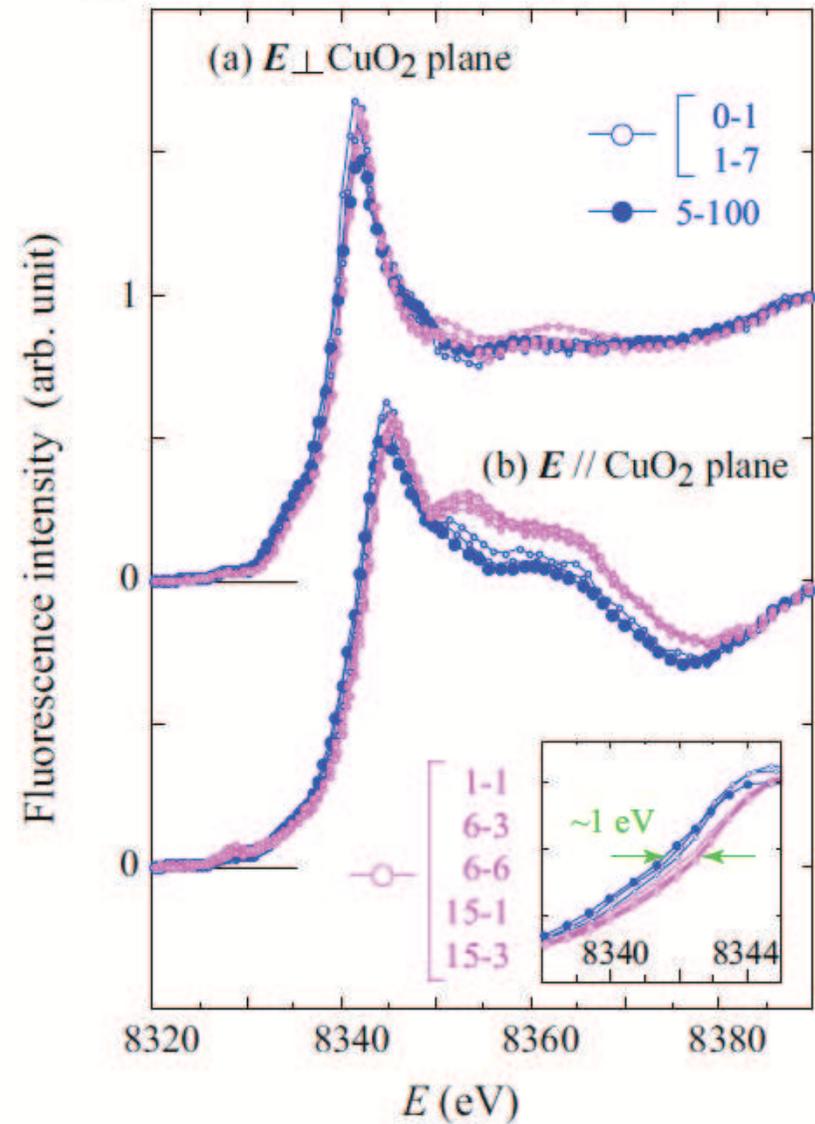
“ 1-1 ” Sr1% & Ni1%

Ni rich group
(Most of Ni does not trap hole)

“ 0-1 ” Sr0% & Ni1%

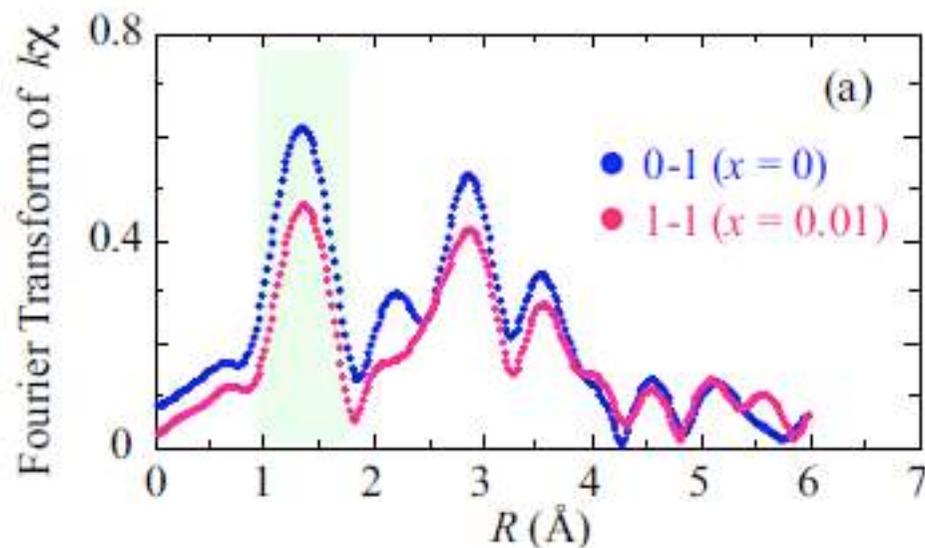


$\text{La}_{2-x}\text{Sr}_x\text{Cu}_{1-y}\text{Ni}_y\text{O}_4$, Ni K -edge, $T = 290$ K



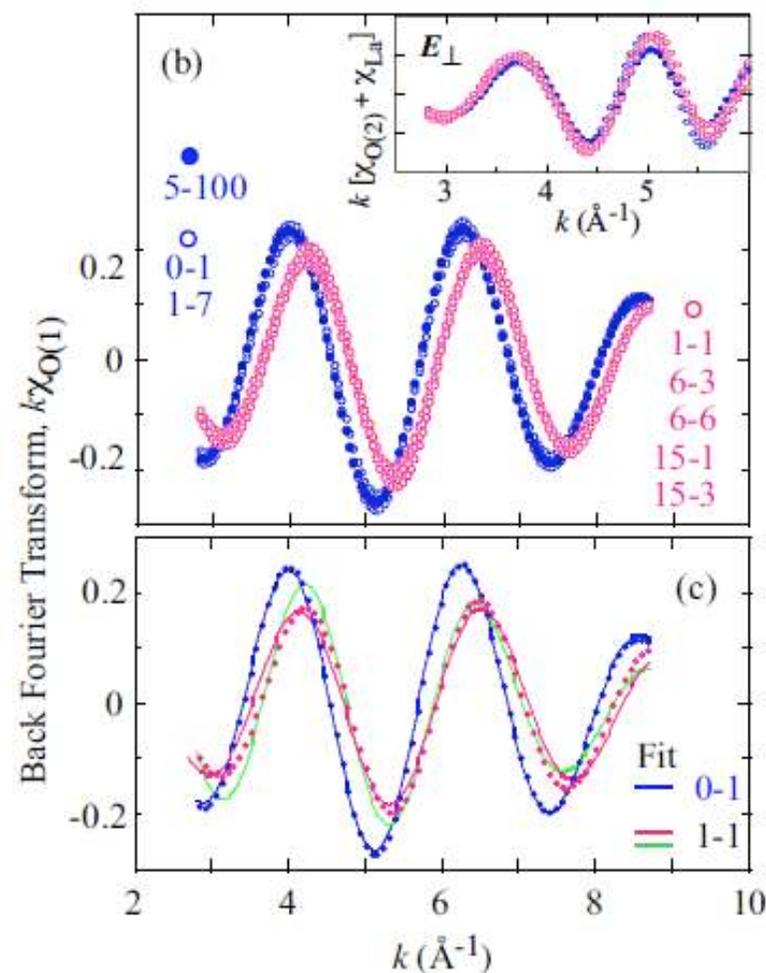
EXAFS analyses

$\text{La}_{2-x}\text{Sr}_x\text{Cu}_{0.99}\text{Ni}_{0.01}\text{O}_4$, $T = 290$ K, Ni K -edge, E_{\parallel}



$$\chi(k) = \sum_{i \text{ shell}} \chi_i(k), \quad (1)$$

$$\chi_i(k) = C_i F_i(k) \exp(-2\sigma_i^2 k^2) \frac{\sin(2kR_i + \Phi_i(k))}{kR_i^2} \quad (2)$$



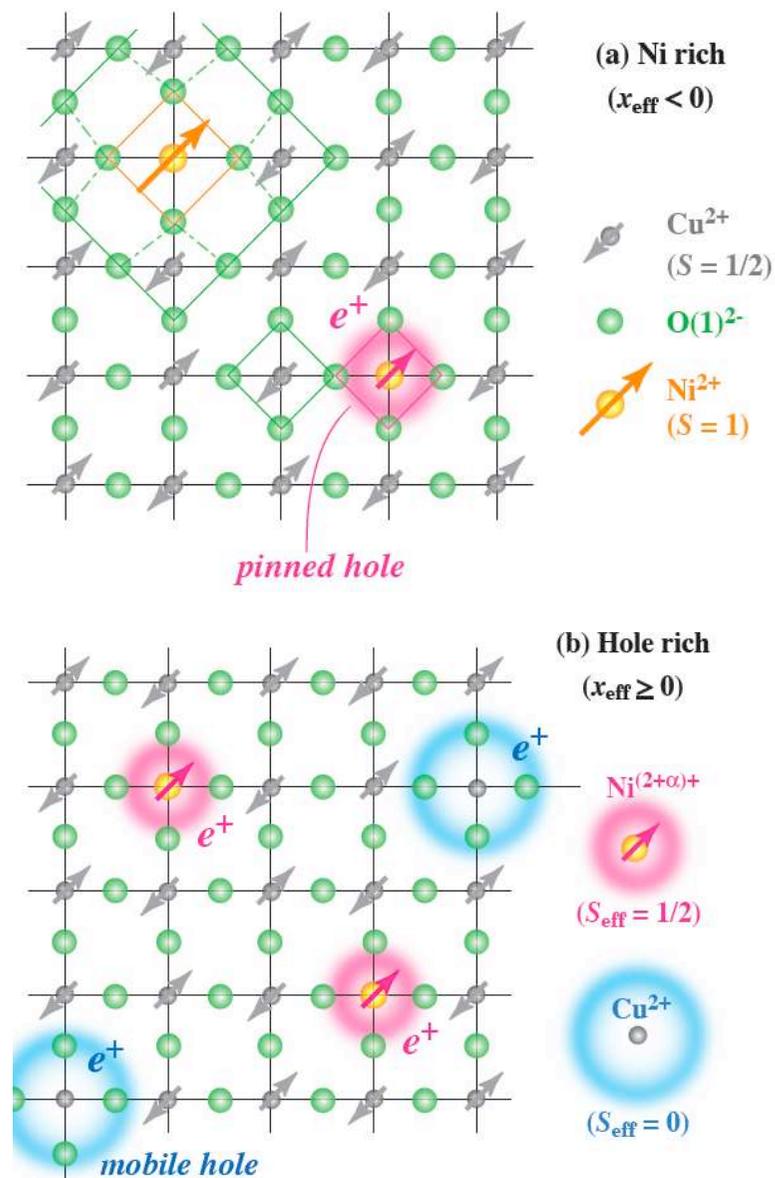
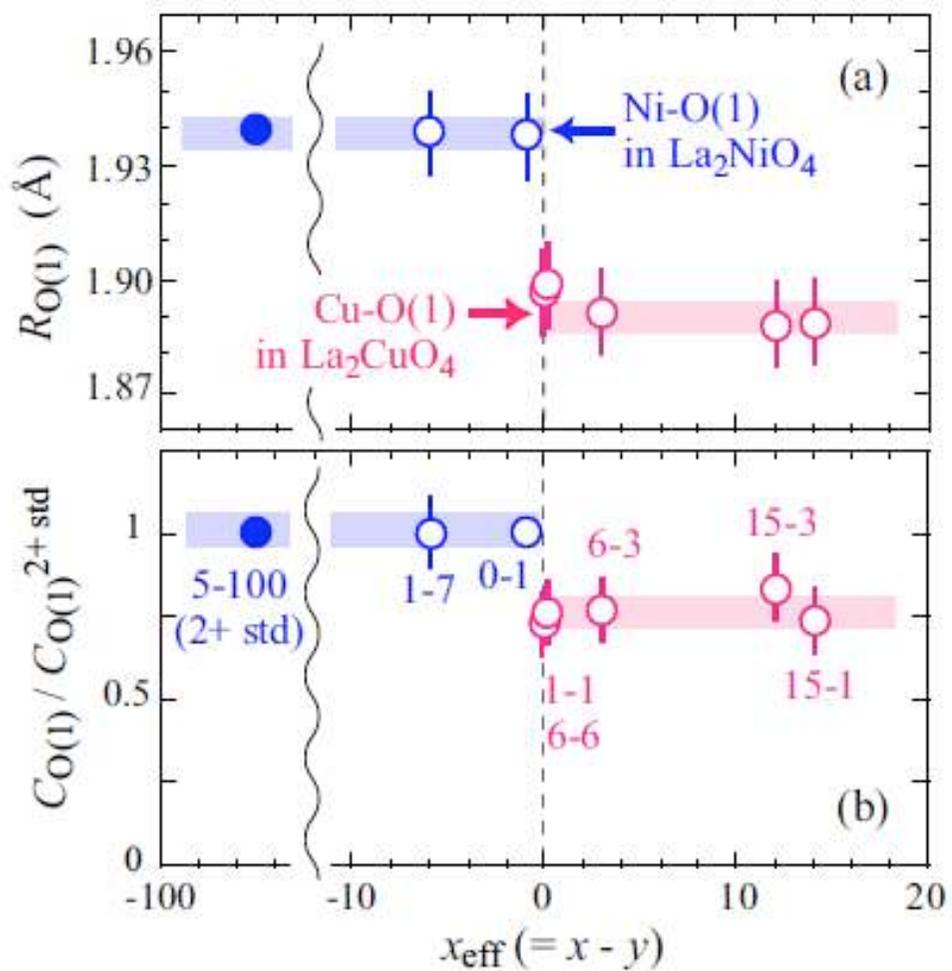
2 types of local in-plane structure around Ni impurity

----→ **two types of Ni states** Ni^{2+} and $\text{Ni}^{(2+\alpha)+}$

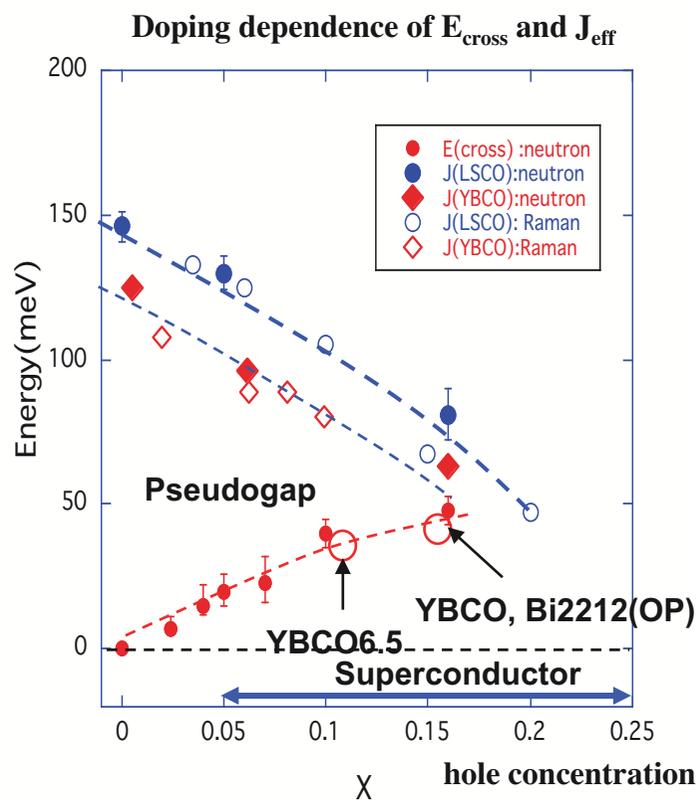
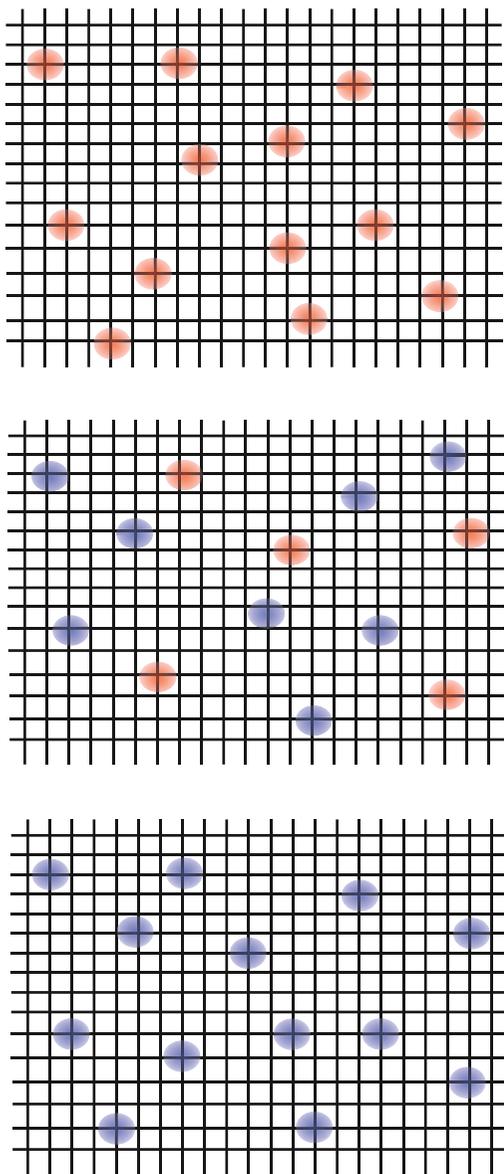
EXAFS results

hole-trapped state of $\text{Ni}=3d^7$ or $3d^8\text{L}$
 $\rightarrow S = 1/2$ with similar local structure around Cu

Ni-O(1) parameter



Ni-substitution effect on magnetic excitation

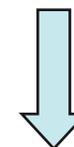


Increase of J_{eff}

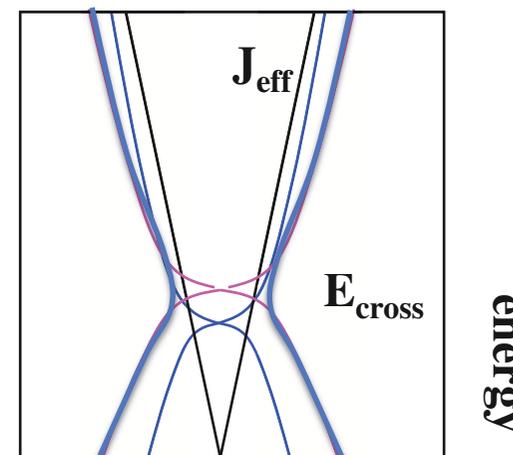


?

reduction of effective hole concentration

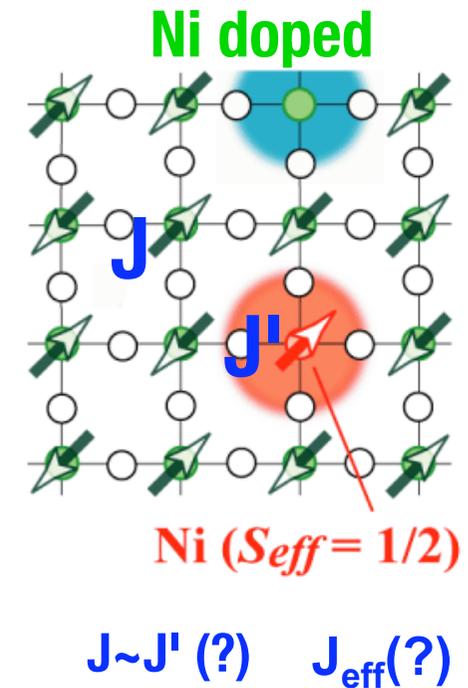
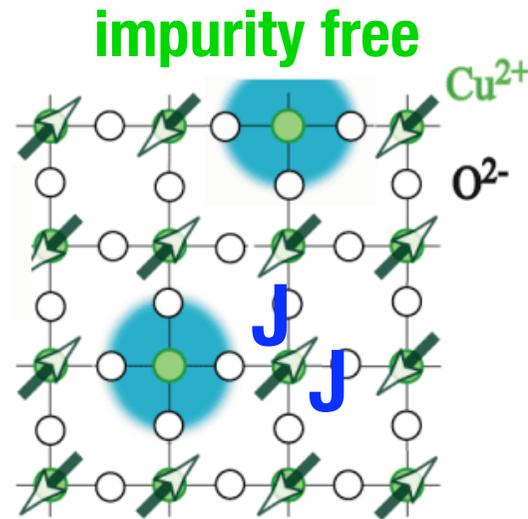
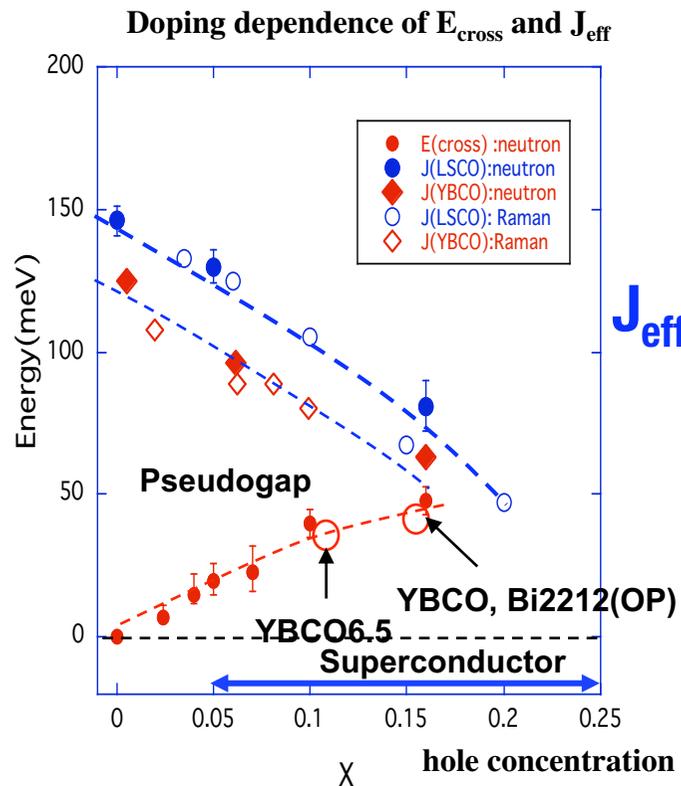


reduction of E_{cross} ?



Unique feature of Ni-impurity including the robust SC against Ni can be qualitatively explained by the blotter effect of Ni-impurity in the doped cuprates

In order to sustain high-Tc SC, 2D antiferromagnetic framework with $s=1/2$ is necessary



Thank you for attention

