

Anisotropic dispersion of the spin excitations in a cuprate superconductor

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Outline

Introduction

- Resonant Inelastic X-ray Scattering (RIXS)
- RIXS on cuprates

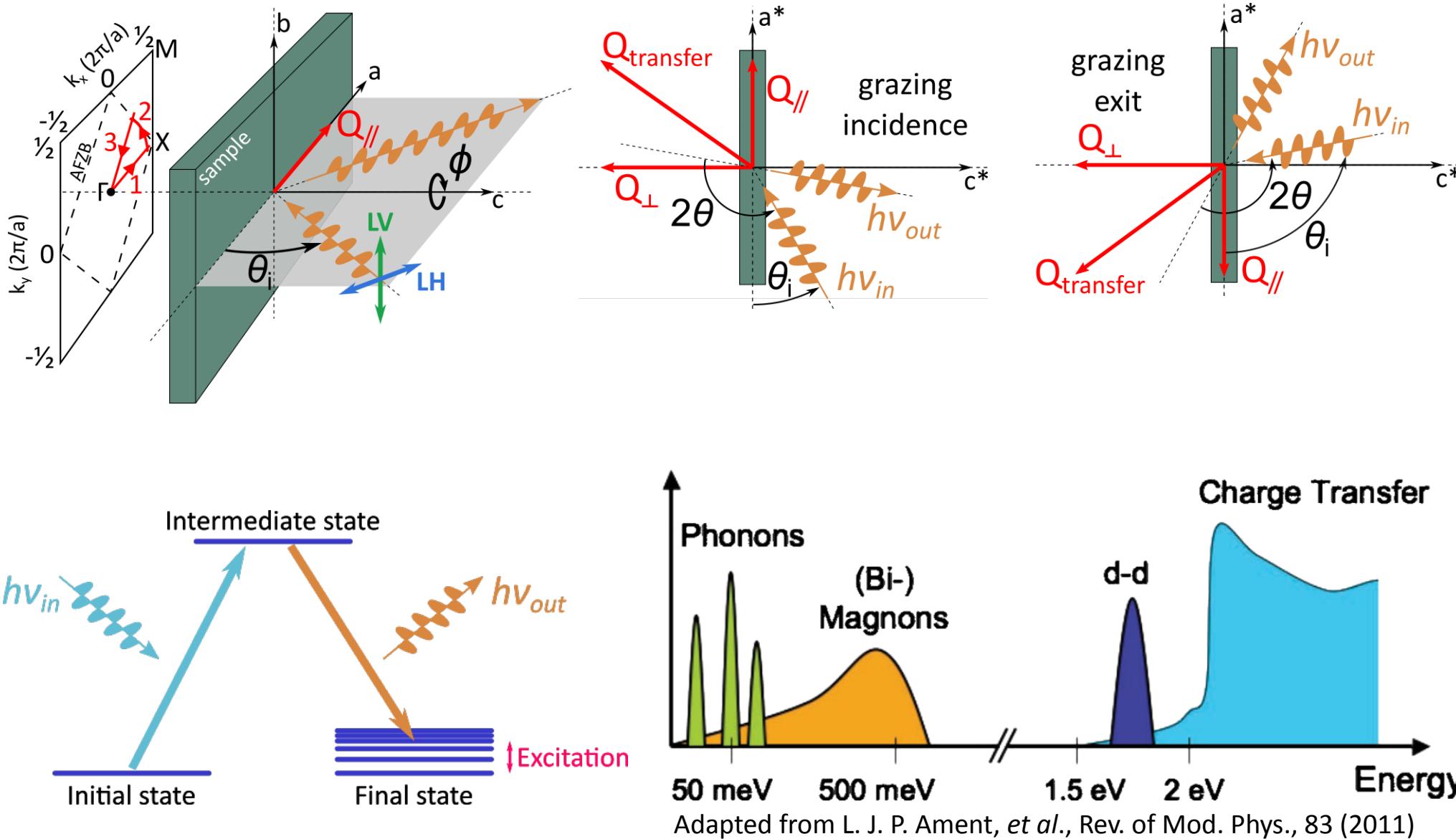
Magnetic excitations on LSCO 12%

- Overview of the data
- Extraction of the magnetic-excitations dispersion
- Hubbard model
- LSCO vs. LCO comparison

Two orbital model & data interpretation

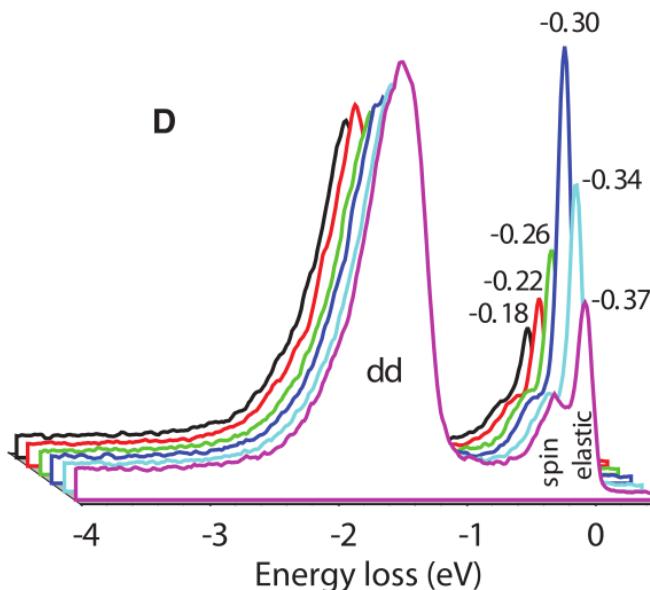
Conclusions

Introduction: RIXS

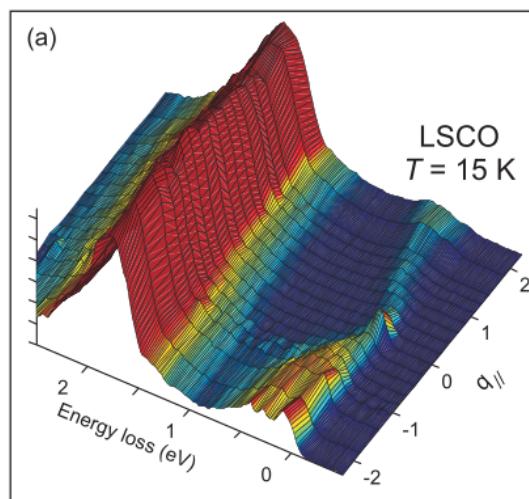


Adapted from L. J. P. Ament, et al., Rev. of Mod. Phys., 83 (2011)

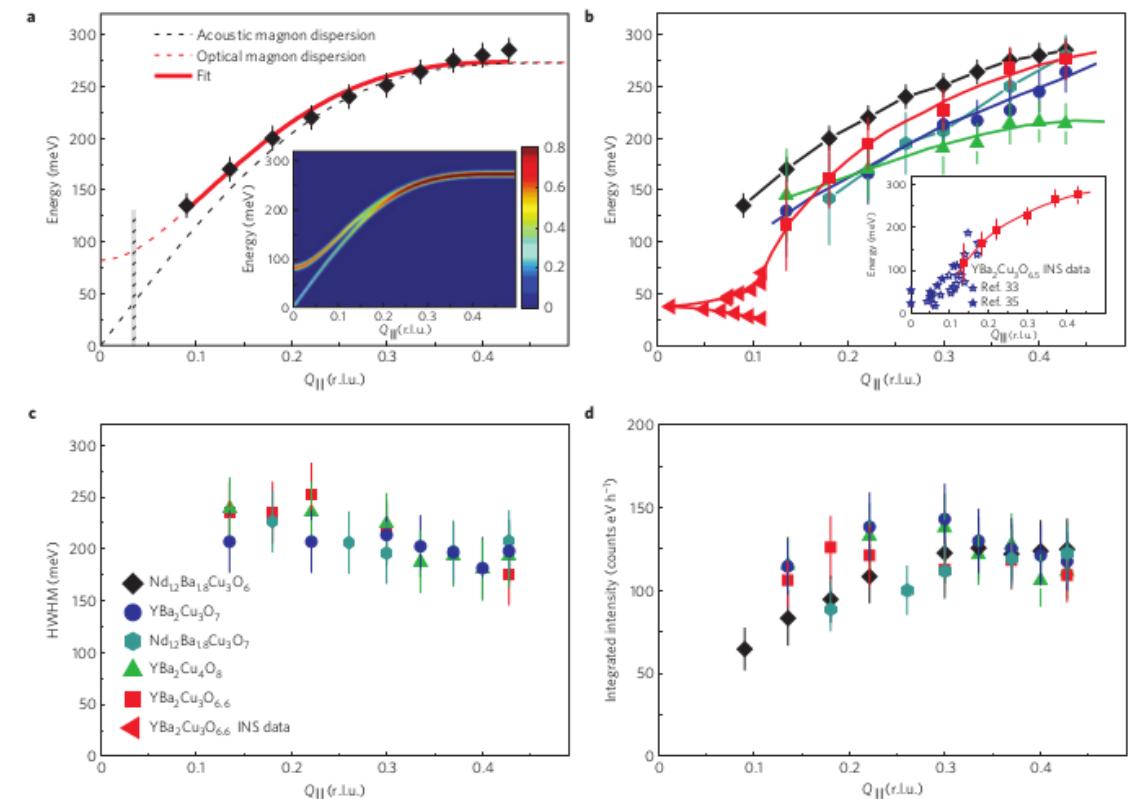
Introduction: RIXS on cuprates



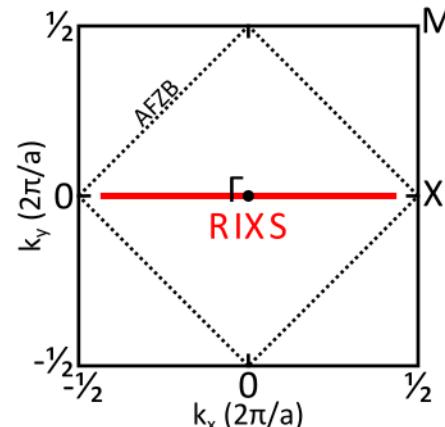
G. Ghiringhelli *et al.*, Science 6096, 821 (2012)



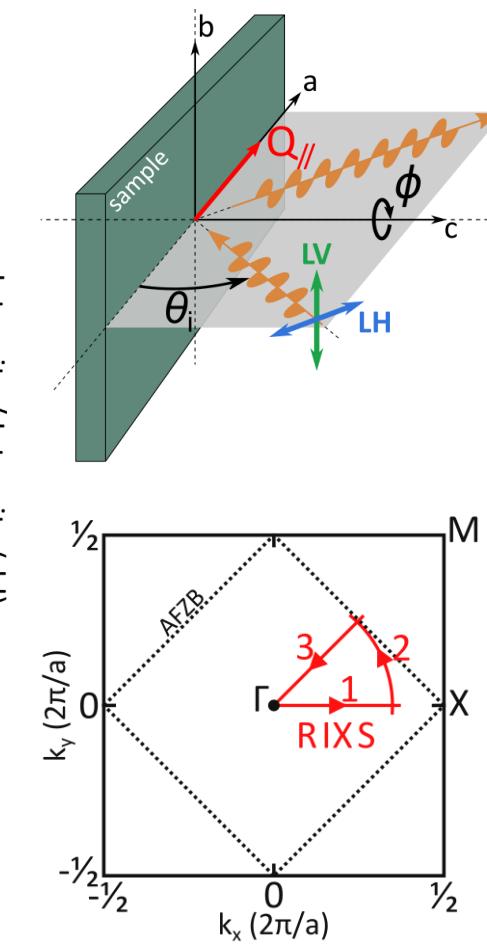
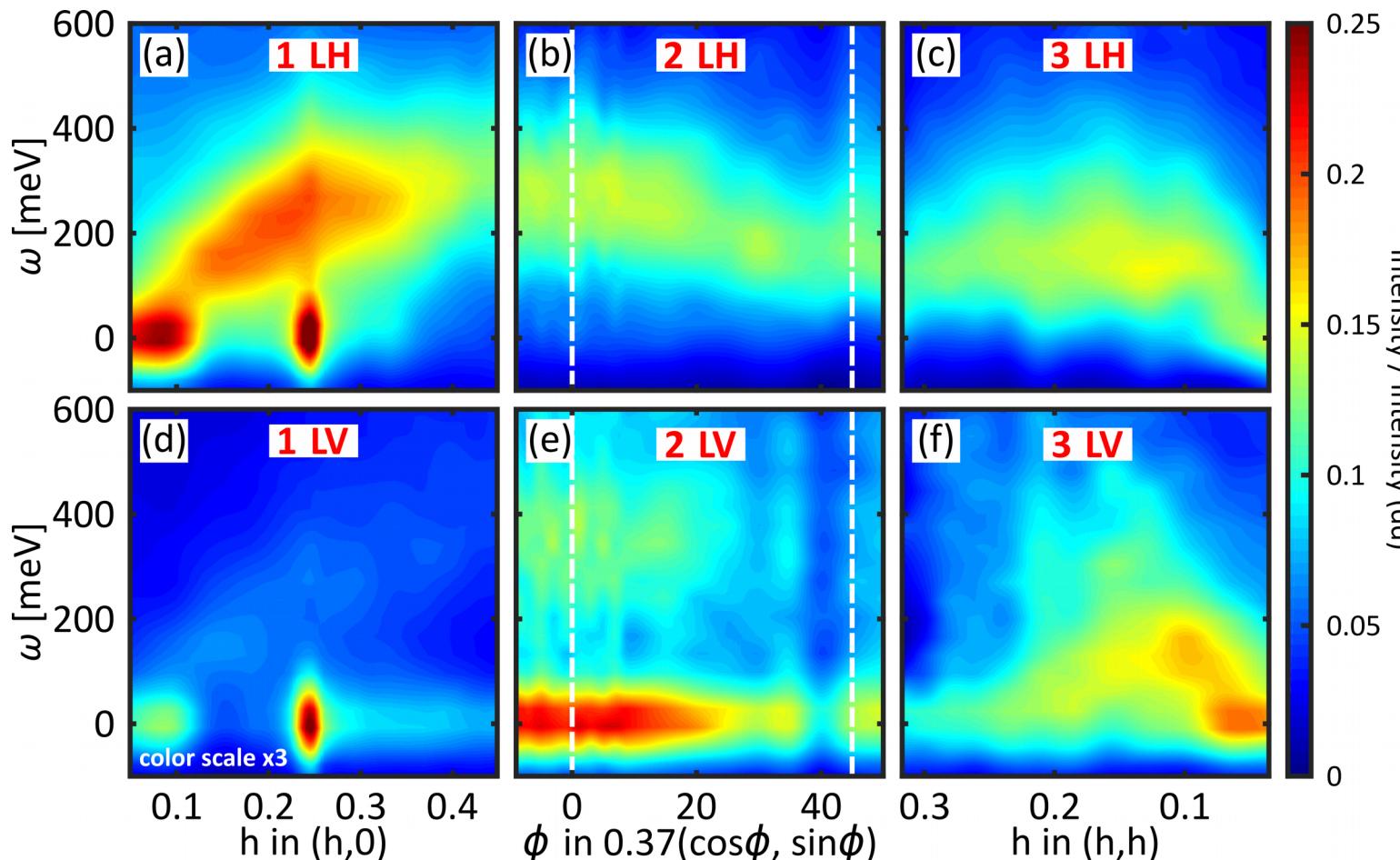
L. Braicovich *et al.*, PRL 104, 077002 (2010)



M. Le Tacon *et al.*, Nature Physics 7, 725–730 (2011)



Magnetic excitations on LSCO 12%: Overview of the data



$$Q_{CDW} = (\pm\delta_1, \delta_2)$$

$$\delta_1 = 0.24(6) \text{ rlu}$$

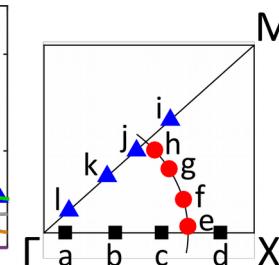
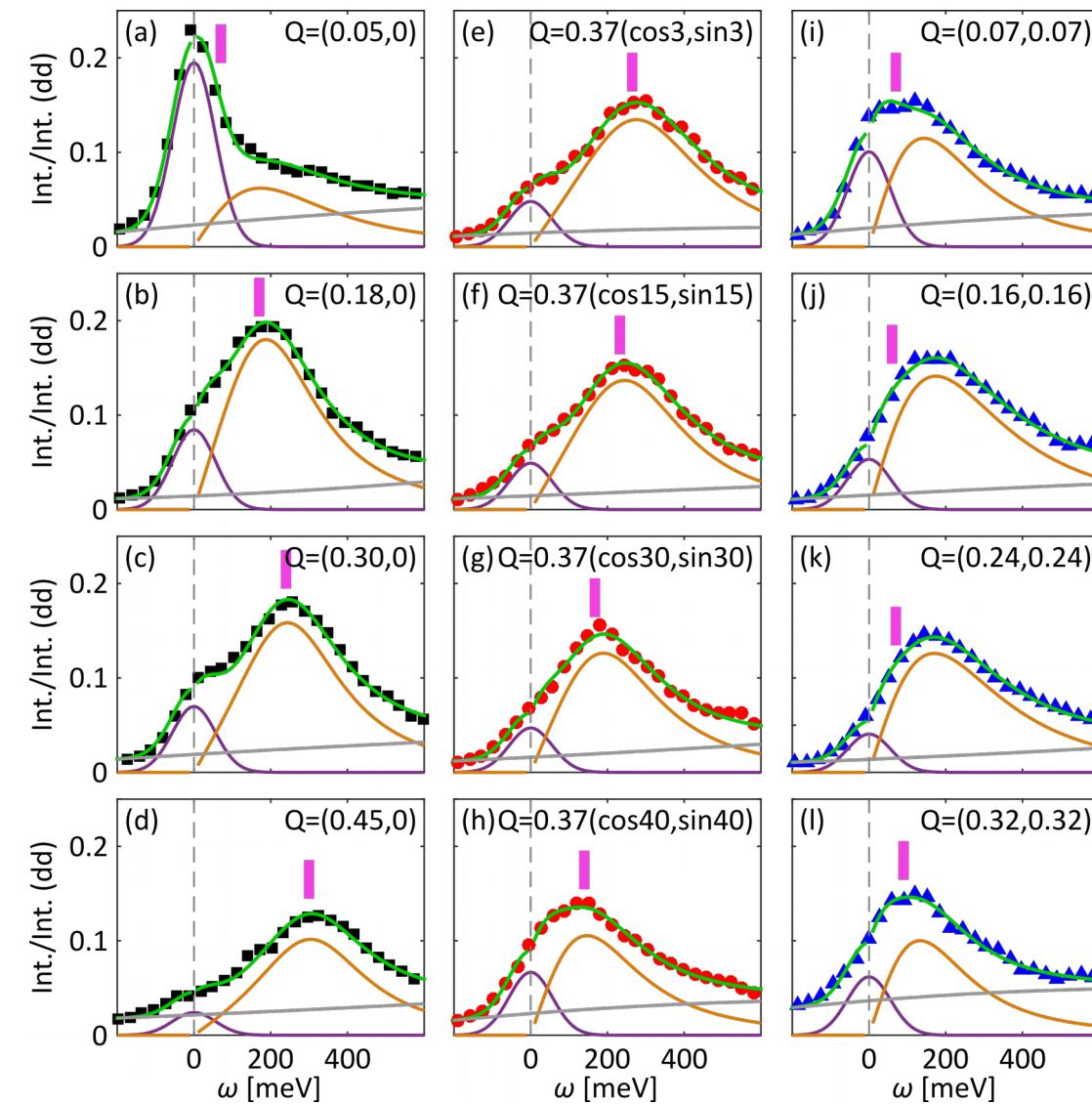
$$\delta_2 \approx 0.01 \text{ rlu}$$

V. Thampy *et al.*, PRB 90, 100510 (2014)
 T. P. Croft *et al.*, PRB 89, 224513 (2014)

Magnetic excitations stronger for LH light
 under grazing exit scattering conditions

M. Le Tacon *et al.*, Nature Physics 7, 725–730 (2011)

Magnetic excitations on LSCO 12%: Paramagnons



Damped harmonic oscillator response function

$$\chi'' = \chi_0 \frac{\gamma \omega}{[\omega^2 - \omega_0^2]^2 + \omega^2 \gamma^2}$$

Damping coefficient

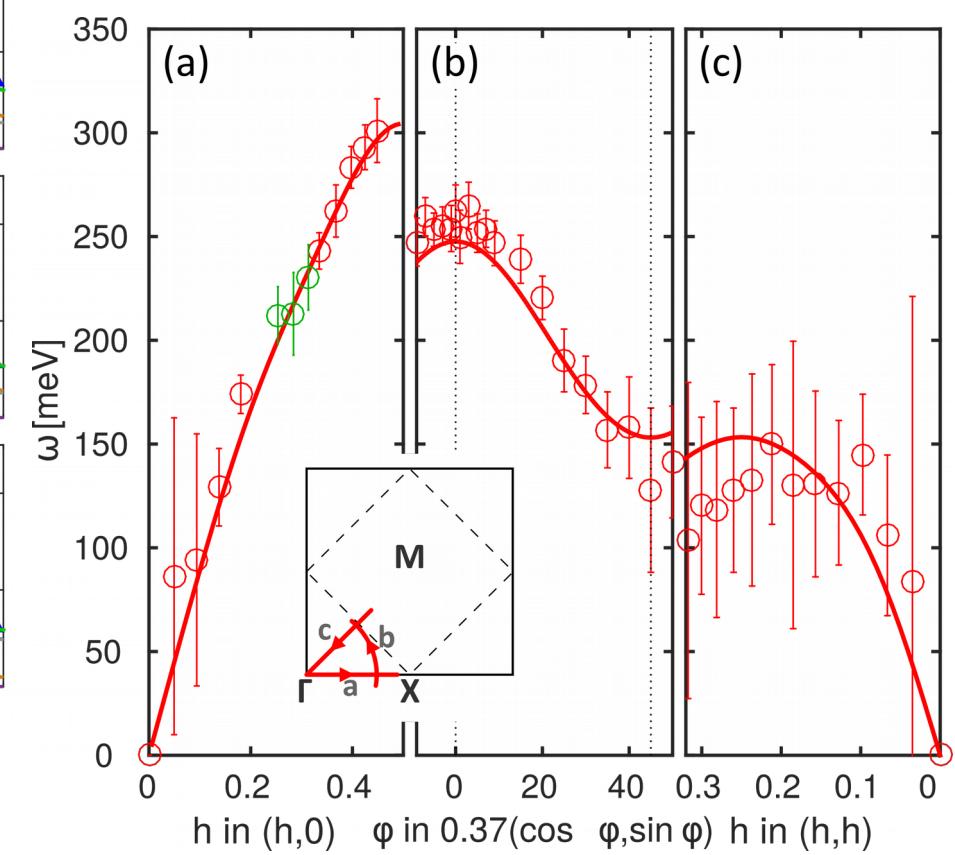
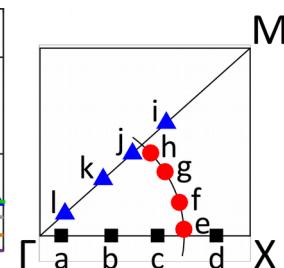
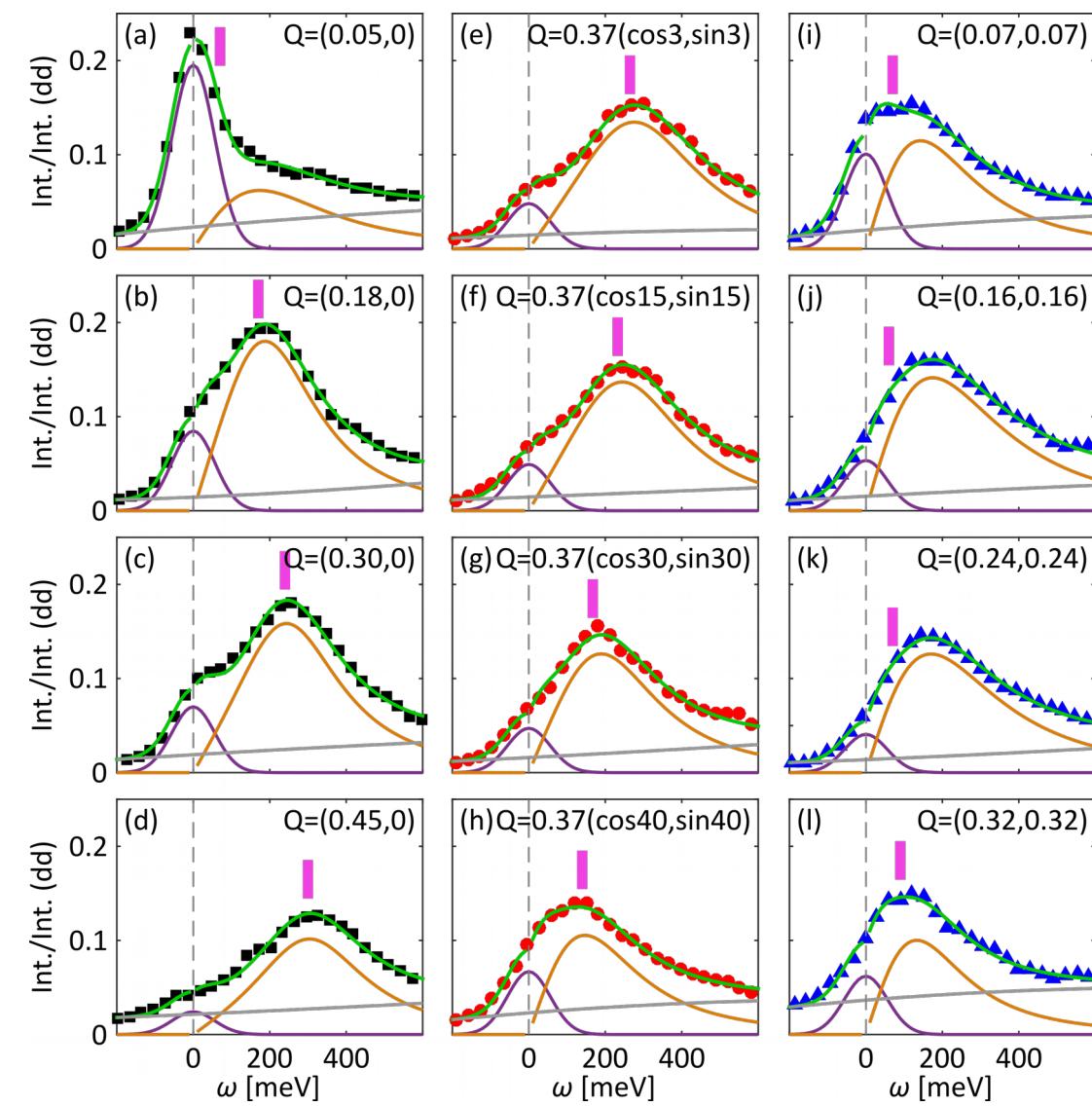
$$(\gamma/2) = \sqrt{\omega_0^2 - \omega_1^2}$$

Dynamical Structure Factor

$$S(Q, \omega) = \frac{1}{1 - \exp(\hbar \omega / k_B T)} * \chi''(Q, \omega)$$

C. Monney, et al., PRB 93, 075103 (2016); J. Lamsal and W. Montfrooij, PRB 93, 214513 (2016)

Magnetic excitations on LSCO 12%: Paramagnons



Magnetic excitations on LSCO 12%: Hubbard model

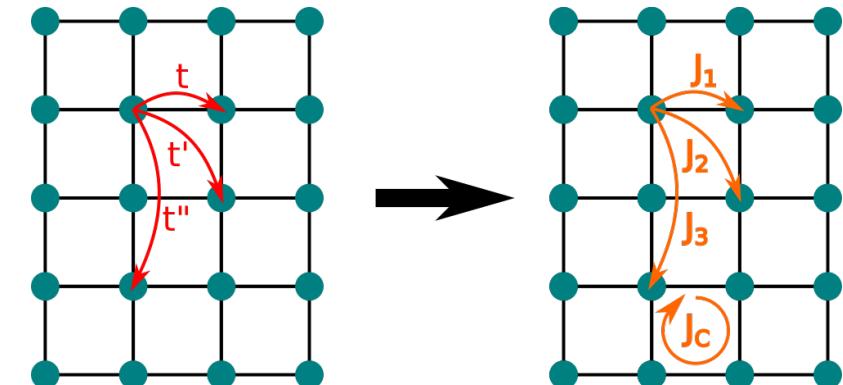
Hamiltonian

$$H_H = -t \sum_{i,j_1;\sigma} c_{i,\sigma}^\dagger c_{j_1,\sigma} - t' \sum_{i,j_2;\sigma} c_{i,\sigma}^\dagger c_{j_2,\sigma} - t'' \sum_{i,j_3;\sigma} c_{i,\sigma}^\dagger c_{j_3,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$



Dispersion relation

$$\omega(\mathbf{q}) = Z \sqrt{A(\mathbf{q})^2 - B(\mathbf{q})^2}, Z = 1.219$$

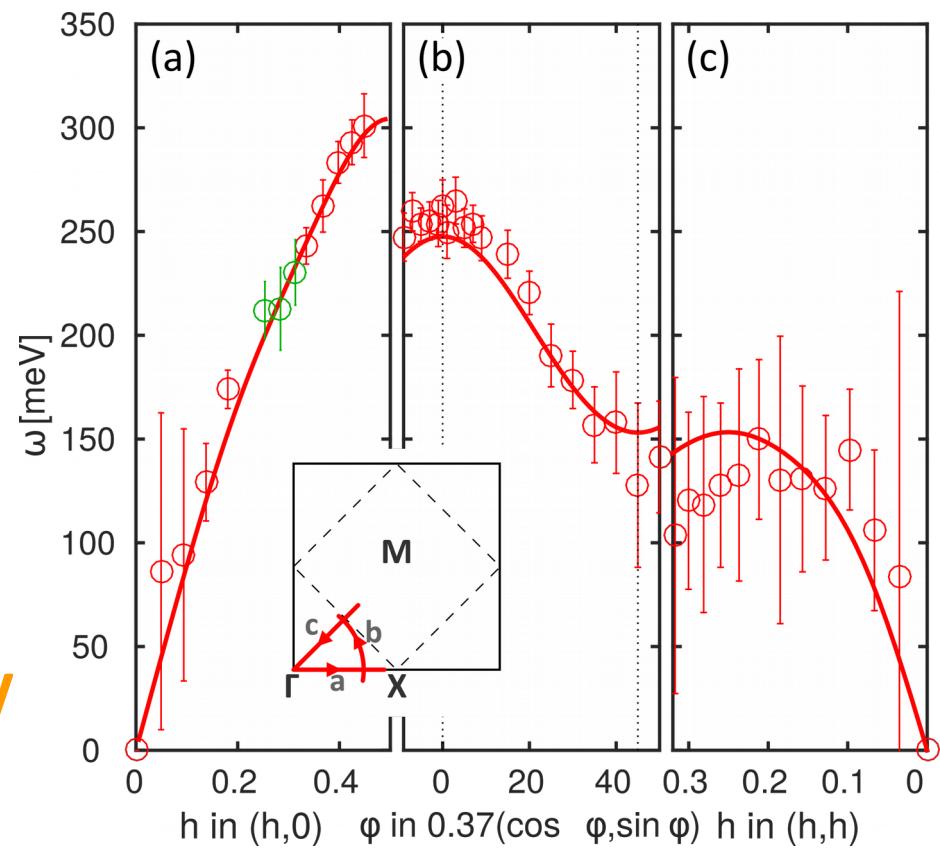


Zone-boundary dispersion

$$E_{ZB} = \omega\left(\frac{1}{2}, 0\right) - \omega\left(\frac{1}{4}, \frac{1}{4}\right)$$

Case (1) $E_{ZB} = 12 Z J_B, \quad J_B = \frac{4t^4}{U^3}$
for $t' = t'' = 0$

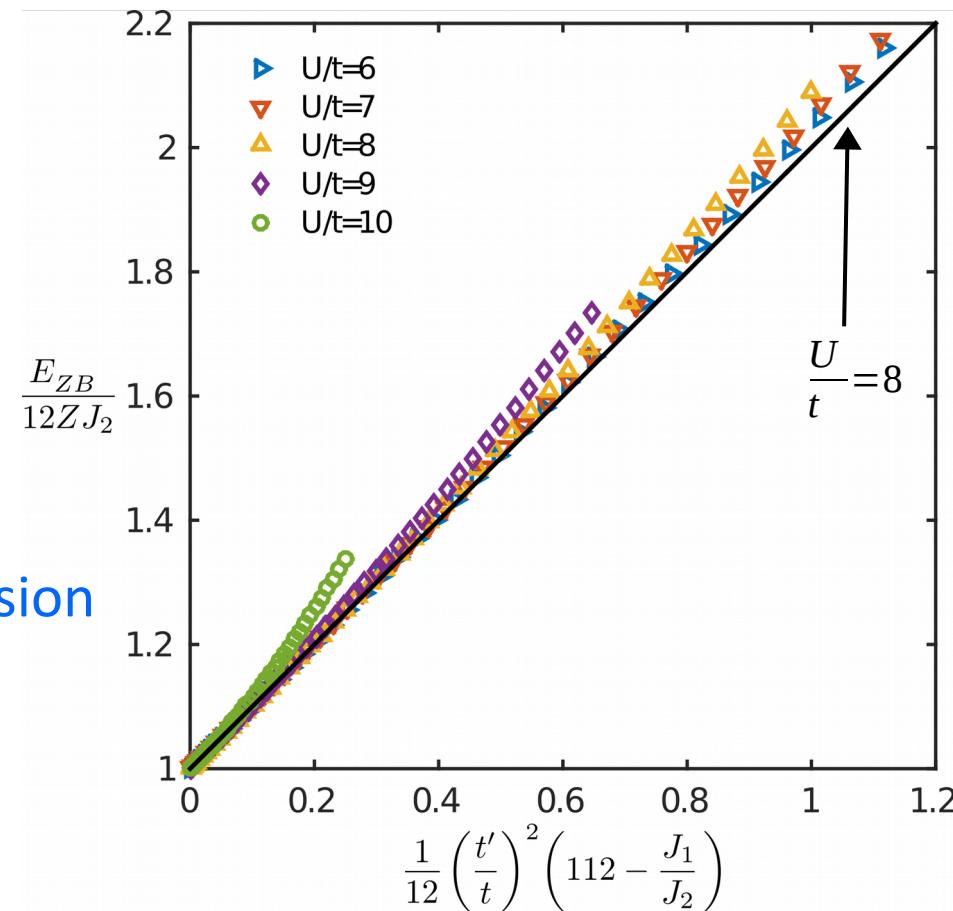
If $t = 430$ meV, $U/t = 8 \rightarrow E_{ZB} \approx 50$ meV



J.-Y. P. Delannoy *et al.*, PRB 79, 235130 (2009); O. Ivashko *et al.*, PRB 95, 214508 (2017)

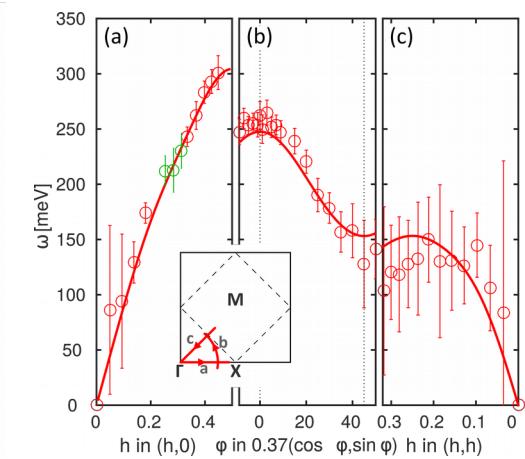
Magnetic excitations on LSCO 12%: Hubbard model

Zone-boundary dispersion
 $E_{ZB} = \omega\left(\frac{1}{2}, 0\right) - \omega\left(\frac{1}{4}, \frac{1}{4}\right)$

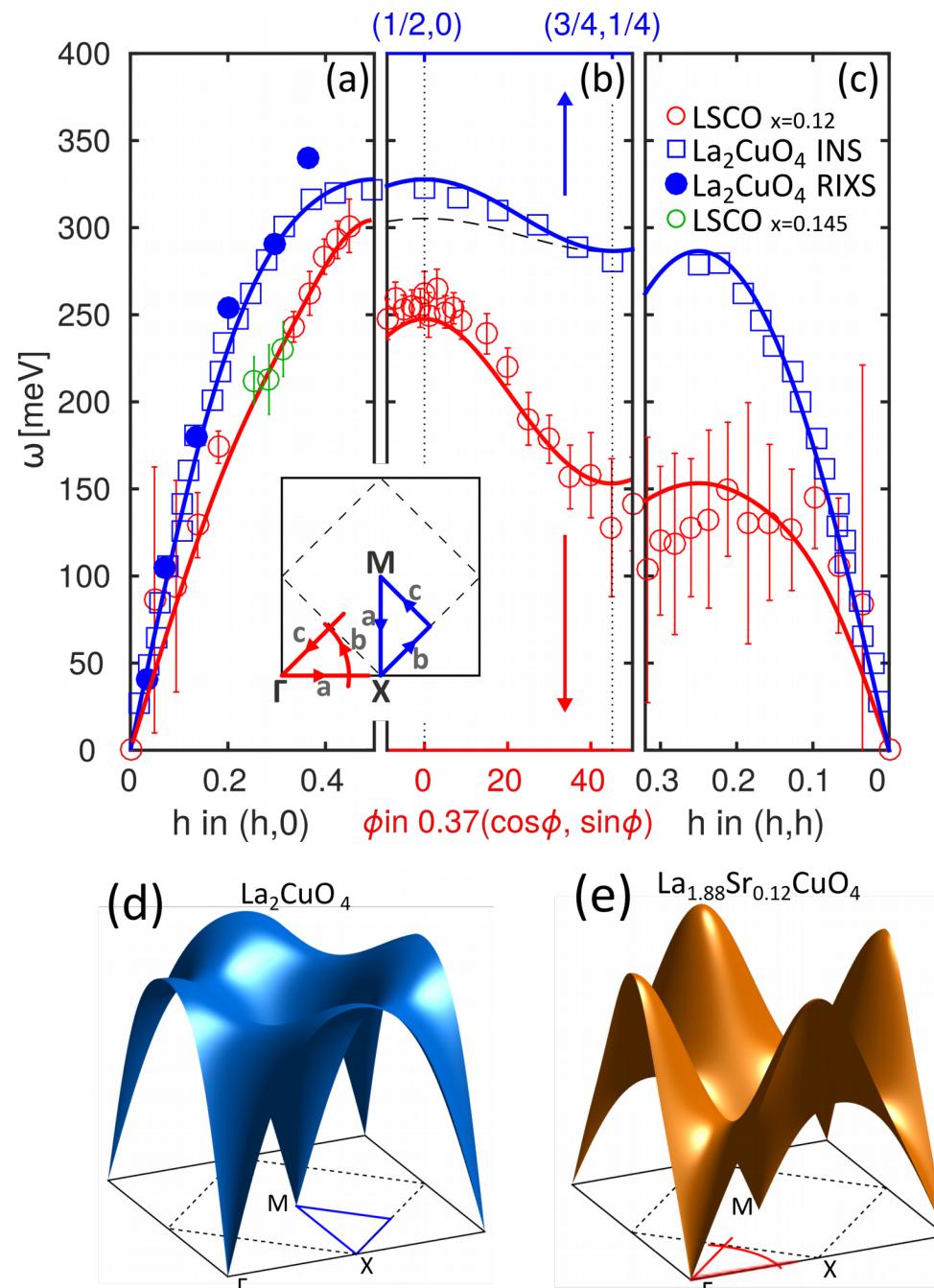


Case (2) $\frac{E_{ZB}}{12ZJ_B} \approx 1 + \frac{1}{12} \left(112 - \frac{J_A}{J_B} \right) \left(\frac{t'}{t} \right)^2, \quad J_A = \frac{4t^2}{U}, \quad J_B = \frac{4t^4}{U^3}$

for $\frac{U}{t} \approx 8, \left| \frac{t'}{t} \right| \leq 0.5, -\frac{t''}{t'} = 0.5$



Magnetic excitations on LSCO 12%: LSCO vs. LCO



ARPES
 $4t = 1720 \text{ meV}$ and $-t'/t = 0.16$ ($-t''/t = 0.5$)
C. G. Fatuzzo *et al.*, PRB 89, 205104 (2014); J. Chang *et al.*, Nat. Comm. 4, 2559 (2013); T. Yoshida *et al.*, PRB 74, 224510 (2006)

\downarrow

$U/t \sim 5$ & $Z \sim 0.7$

$4t = 1720 \text{ meV}$ and $Z = 1.219$ ($-t''/t = 0.5$)

$\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$	U (eV)	U/t	t'/t	t''/t	Z	Ref.
$x = 0$	2.2	7.4	0	0	1.18	1
$x = 0$	3.6	8.3	-0.313	0.167	1.219	2
$x = 0$	3.9	9.1	-0.308	0.154	1.219	3
$x = 0.12$	2.9	6.8	-0.405	0.202	1.219	3

- 1 N. S. Headings *et al.*, PRL 105, 247001 (2010)
R. Coldea *et al.*, PRL 86, 5377 (2001)
2 J.-Y. P. Delannoy *et al.*, PRB 79, 235130 (2009)
3 O. Ivashko *et al.*, PRB 95, 214508 (2017)

Two orbital model & data interpretation

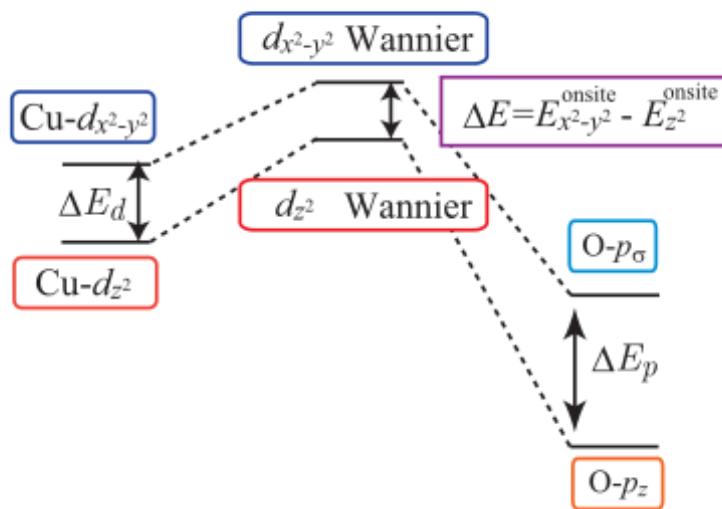
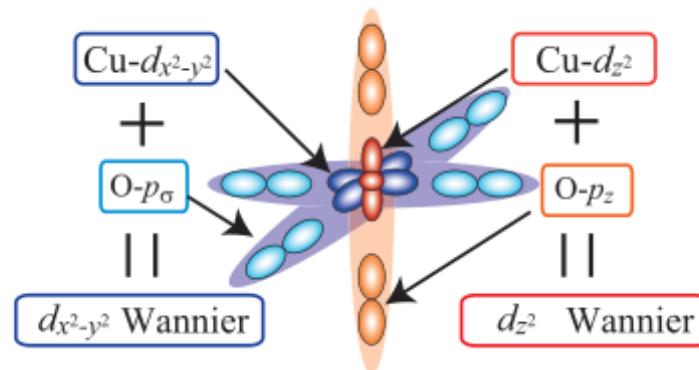
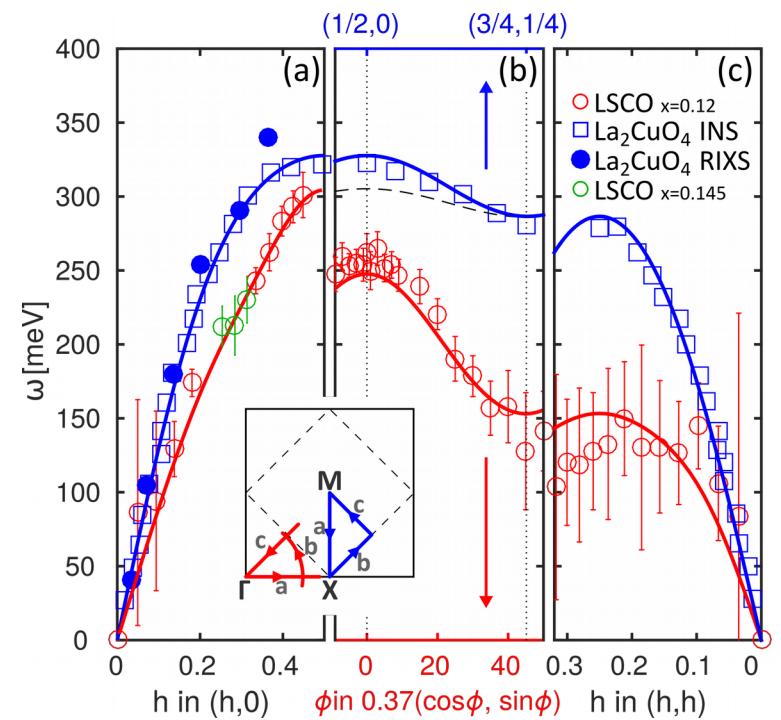
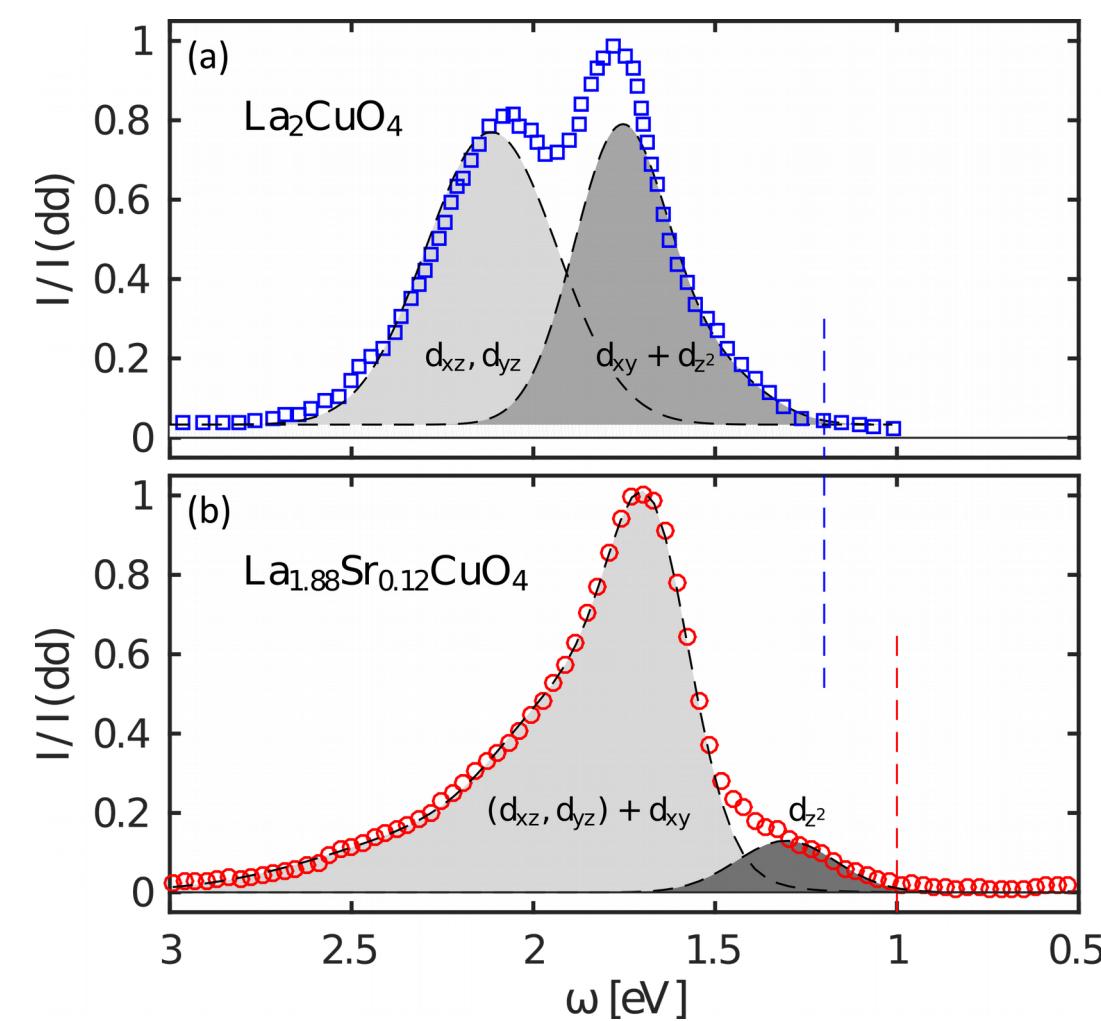


TABLE I. Hopping integrals within the $d_{x^2-y^2}$ orbital for the single- and two-orbital models (upper half), interorbital hopping (middle), and $\Delta E \equiv E_{x^2-y^2} - E_{z^2}$ (bottom).

	One-orbital		Two-orbital	
	La	Hg	La	Hg
$t(d_{x^2-y^2} \rightarrow d_{x^2-y^2})$				
t_1 (eV)	-0.444	-0.453	-0.471	-0.456
t_2 (eV)	0.0284	0.0874	0.0932	0.0993
t_3 (eV)	-0.0357	-0.0825	-0.0734	-0.0897
$(t_2 + t_3)/ t_1 $	0.14	0.37	0.35	0.41
$t(d_{x^2-y^2} \rightarrow d_{z^2})$				
t_1 (eV)			0.178	0.105
t_2 (eV)			Small	Small
t_3 (eV)			0.0258	0.0149
ΔE (eV)			0.91	2.19

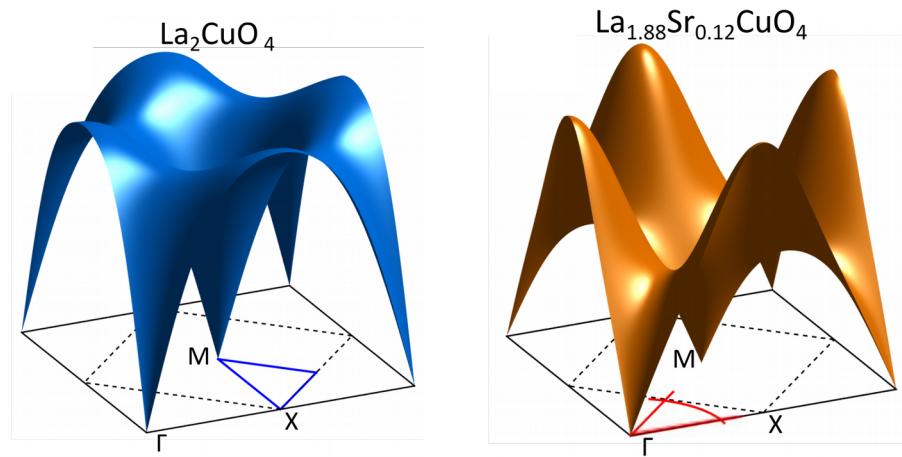
H. Sakakibara *et al.*, PRL 105, 057003 (2010)
H. Sakakibara *et al.*, PRB 85, 064501 (2012)

Two orbital model & data interpretation



$$E_{z^2} \downarrow \Rightarrow |t'|, |t''| \uparrow \Rightarrow E_{ZB} \uparrow$$

Conclusions



- Magnetic excitations in LSCO are strongly anisotropic compared to the ones on LCO
- Hubbard type model reveals a non negligible value of t' (and t'') in contrast with ARPES data
- This discrepancy between RIXS and ARPES data is solved within the frame of two-orbital model
- Cu d_{z^2} orbital reveals to be important for the description of the antiferromagnetic zone-boundary dispersion of the magnetic excitations

O. Ivashko *et al.*, PRB 95, 214508 (2017)