The Abdus Salam
International Centre for Theoretical Physics

United Nations
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International Atomic Energy Agency

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Workshop on Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter

24 - 29 July 2011

Anomalous Spin Excitations in La2CuO4 and La2-xSrxCuO4

S. Hayden
University of Bristol
Bristol, U.K.

Strada Costiera 11, 34151 Trieste, Italy - Tel.+39 040 2240 111; Fax +39 040 224 163 - sci_info@ictp.it

Anomalous Spin Excitations in La_2CuO_4 and $La_{2-x}Sr_xCuO_4$

Stephen Hayden
University of Bristol

Collaborators

Baptiste Vignolle (Bristol)
Oliver Lipscombe (Bristol)
Neil Headings (Bristol)

Radu Coldea (Bristol/Oxford)

Toby Perring (ISIS)
Chris Frost (ISIS)

Lipscombe, Vignolle, Perring, Frost, Hayden Phys. Rev. Lett. **102**, 167002 (2009)
Headings, Hayden, Coldea, Perring, Phys. Rev. Lett. **105**, 247001 (2010)

Anomalous Spin Excitations in La_2CuO_4 and $La_{2-x}Sr_xCuO_4$

1) La_2CuO_4

- Introduction and motivation
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Mechanism of high temperature superconductivity

1) The 'holy' trinity: a 1950's paradigm

- Local Density Approximation (LDA – DFT) band structure
- Random Phase Approximation (RPA) spin fluctuation superglue
- Eliasberg equations for the superconductivity

Structured excitations e.g. B. Vignolle, Nat. Phys. (2007); S. M. Hayden, et al., Nature (2004) , C. Stock, et al., PRB (2005); V. Hinkov et al., Nat. Phys. (2007)

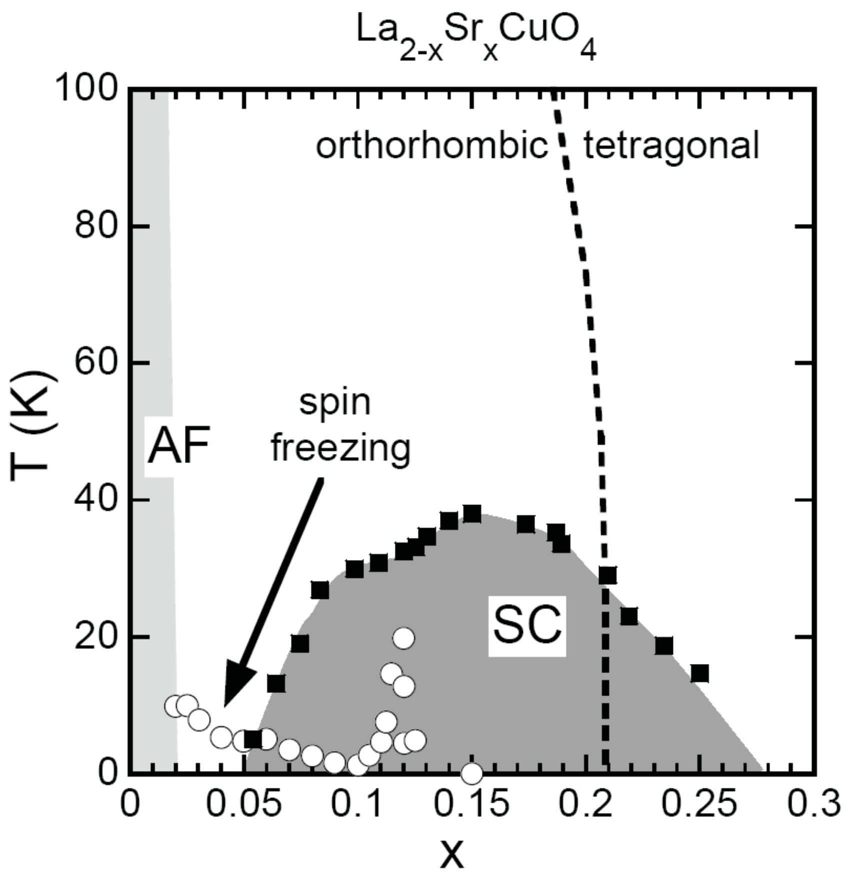
2) The RVB picture: doped Mott insulator

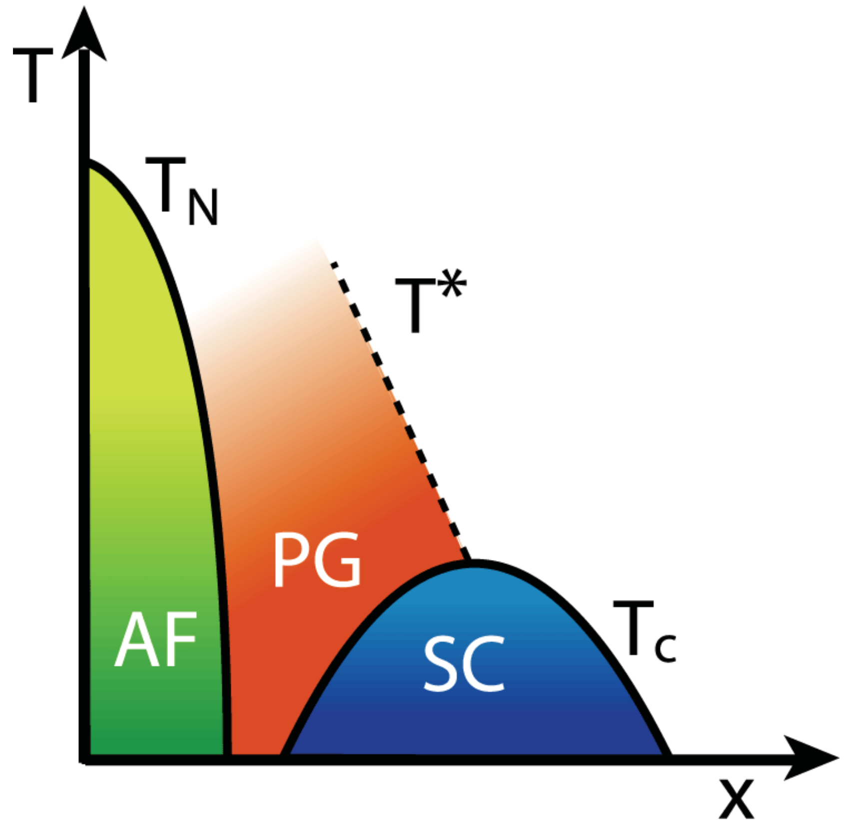
3) Quantum criticality

Competing phase e.g B. Fauque et al., PRL 96, 197001 (2006)

'A modern, but way too short history of the theory of superconductivity at high temperature' (Jan Zaanen 2010)

Generic phase diagram of cuprates





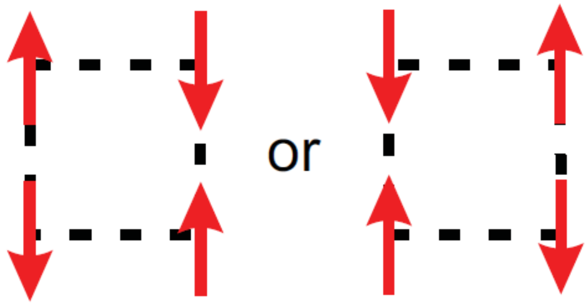
Resonating Valence Bond State in La_2CuO_4

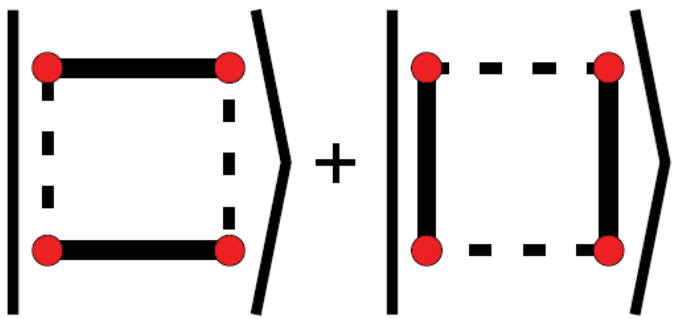
The Resonating Valence Bond State in La_2CuO_4 and Superconductivity

P. W. ANDERSON

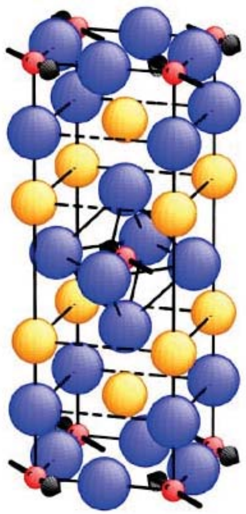
The oxide superconductors, particularly those recently discovered that are based on La_2CuO_4, have a set of peculiarities that suggest a common, unique mechanism: they tend in every case to occur near a metal-insulator transition into an odd-electron insulator with peculiar magnetic properties. This insulating phase is proposed to be the long-sought "resonating-valence-bond" state or "quantum spin liquid" hypothesized in 1973. This insulating magnetic phase is favored by low spin, low dimensionality, and magnetic frustration. The preexisting magnetic singlet pairs of the insulating state become charged superconducting pairs when the insulator is doped sufficiently strongly. The mechanism for superconductivity is hence predominantly electronic and magnetic, although weak phonon interactions may favor the state. Many unusual properties are predicted, especially of the insulating state.

P. W. Anderson,
Science **235**, 1196 (1987)



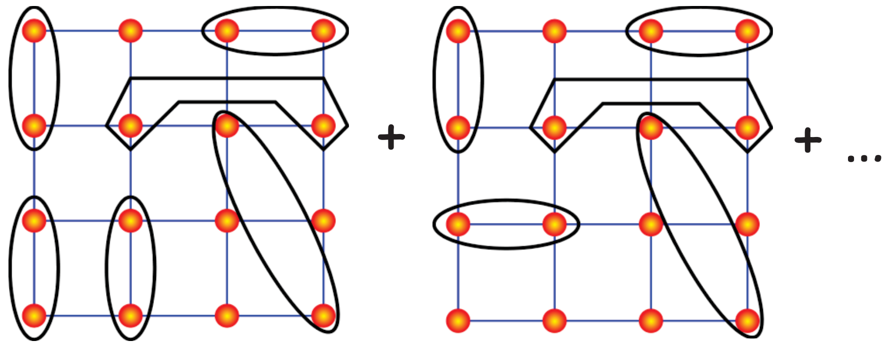


Resonating valence bond theory in 2D



- Spin "liquid" of singlets $\frac{1}{\sqrt{2}}\left\{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right\}$

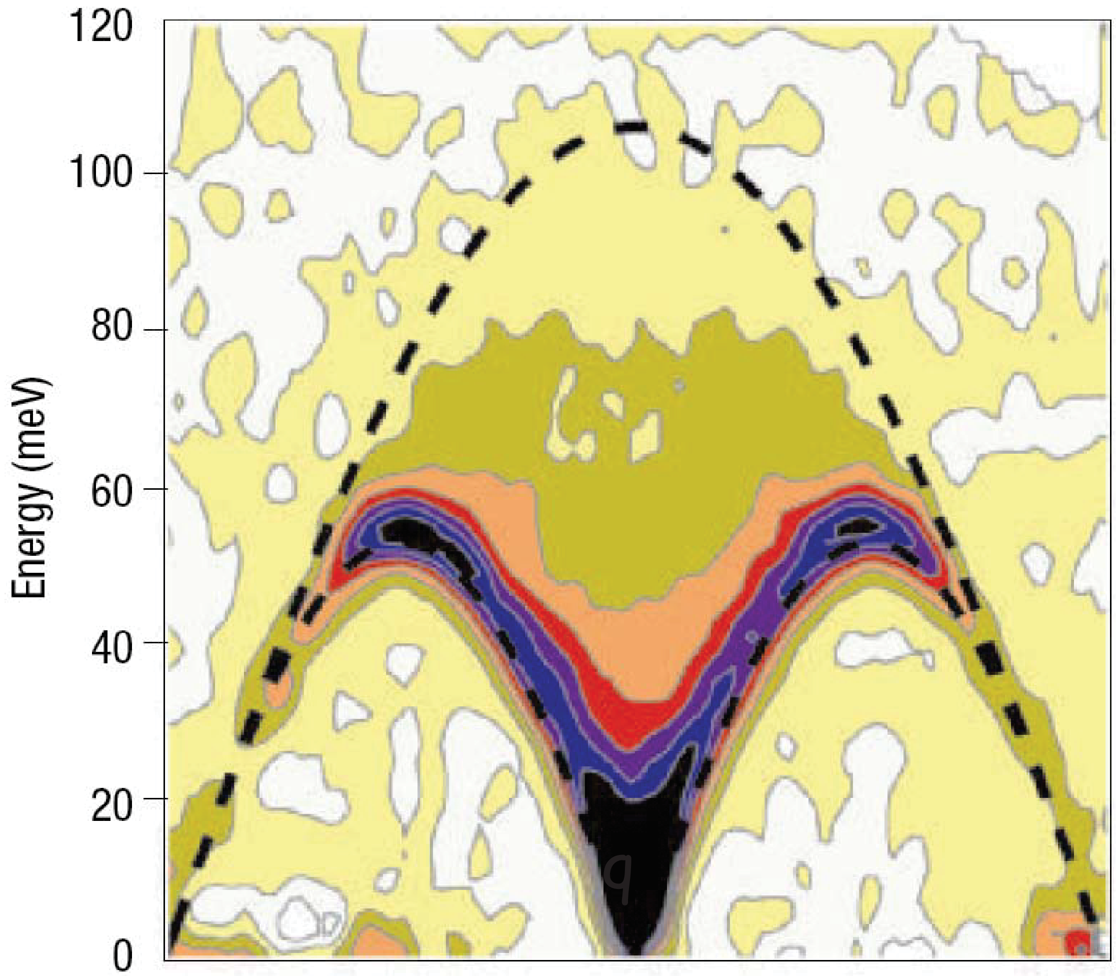
$$|\Psi\rangle =$$



- Broken singlet "releases" 2 spinons

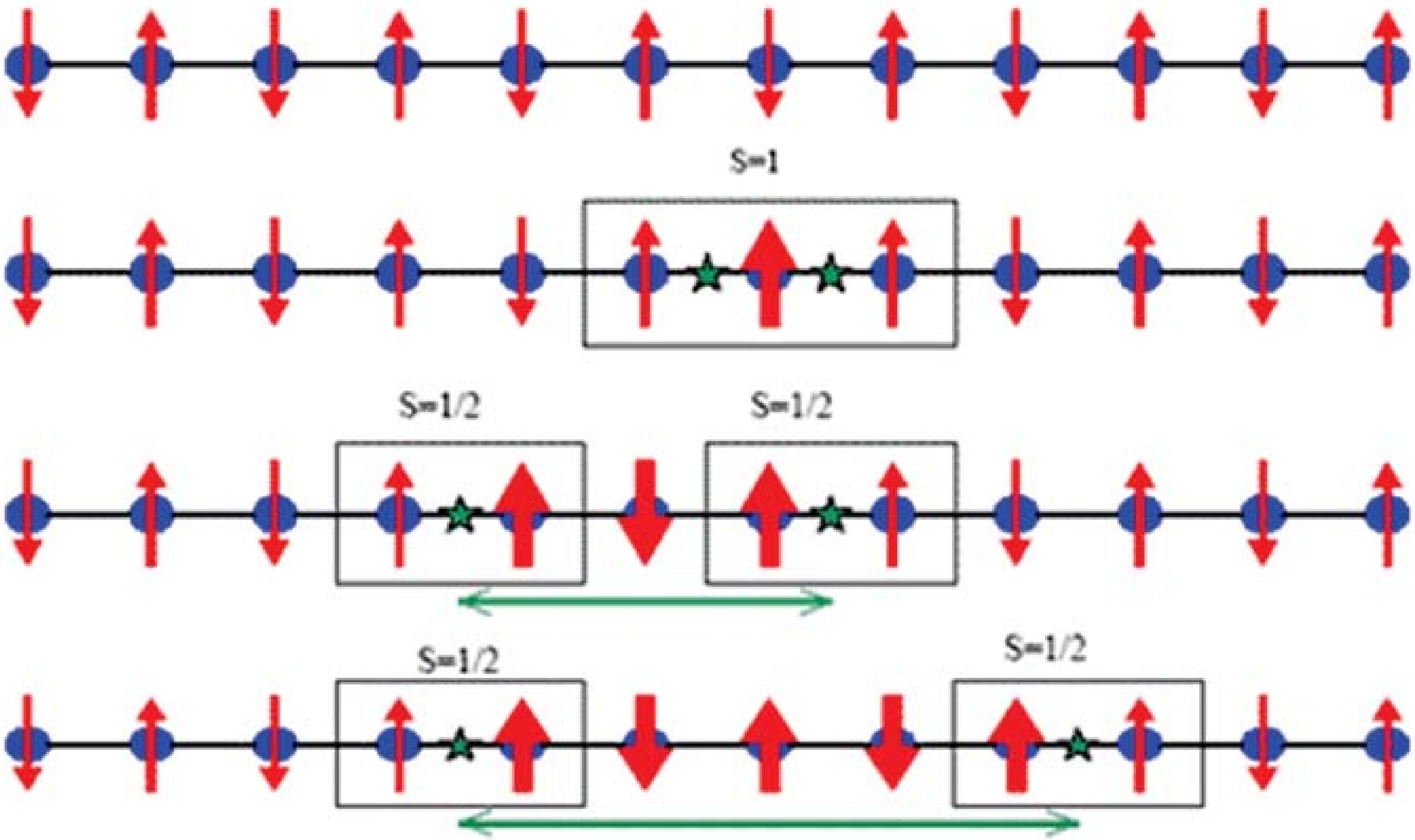
Spinons in 1D antiferromagnets

$KCuF_3$ S=1/2 1D antiferromagnetic chain



Lake et al., Nature Materials 4, 329 (2005)

Spinons in 1D Heisenberg chain



Anomalous Spin Excitations in La_2CuO_4 and $La_{2-x}Sr_xCuO_4$

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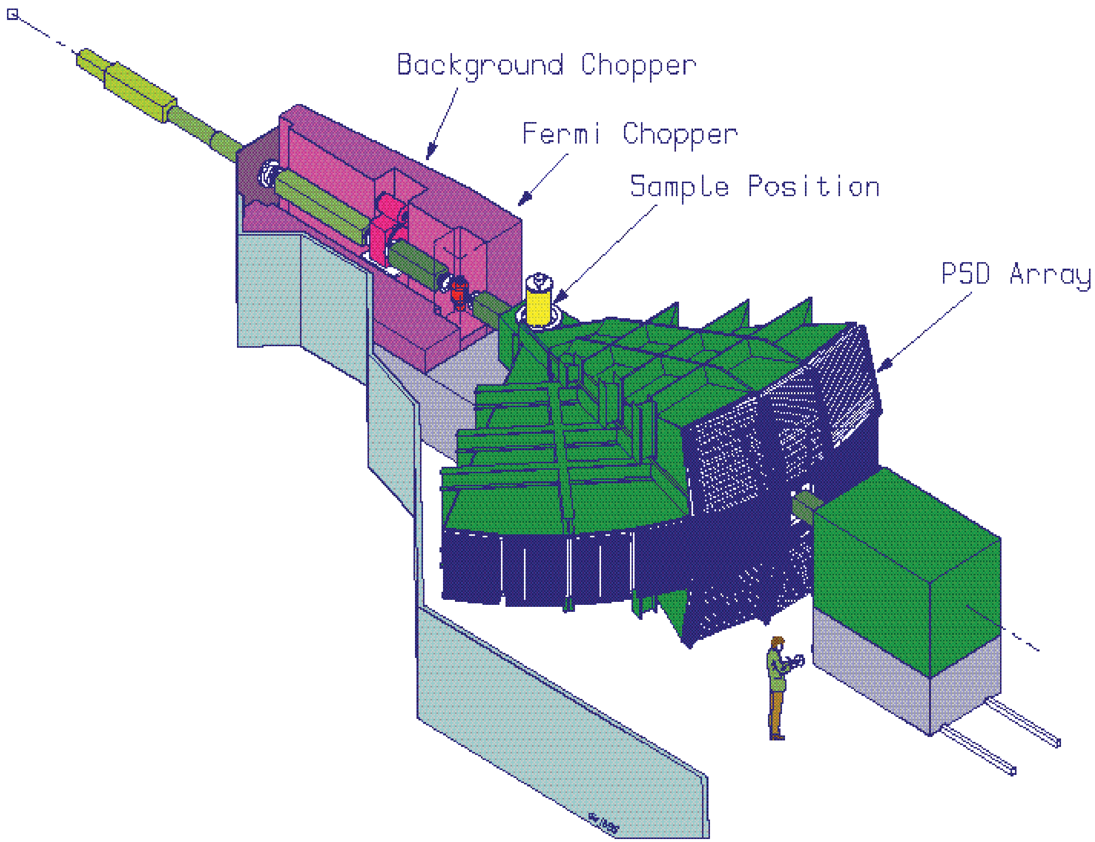
ISIS Spallation Source

Inelastic neutron scattering (INS)

$$\frac{d^2\sigma}{d\Omega\, dE} = (\gamma r_e)^2 \frac{k_f}{k_i} |F(\mathbf{Q})|^2 \left(\frac{2/\pi g^2 \mu_B^2}{1 - \exp(-\hbar\omega/kT)} \right) \chi''(\mathbf{Q},\omega)$$

47.8g La_2CuO_4



MAPS spectrometer

Neutron cross section

$$\sigma_{xx}^{\uparrow\downarrow} = \left(\frac{d^2\sigma}{d\Omega dE}\right)_{\mathbf{H}\|x}^{\uparrow\rightarrow\downarrow} = \frac{k_f}{k_i}\frac{(\gamma r_e)^2}{g^2\mu_B^2}\frac{1}{\pi}F^2(\mathbf{Q})$$

$$\times\ \frac{\chi''_{yy}(\mathbf{q},\hbar\omega) + \chi''_{zz}(\mathbf{q},\hbar\omega)}{1-\exp(-\hbar\omega/kT)}$$

x // **Q**

Neutron cross-section well known

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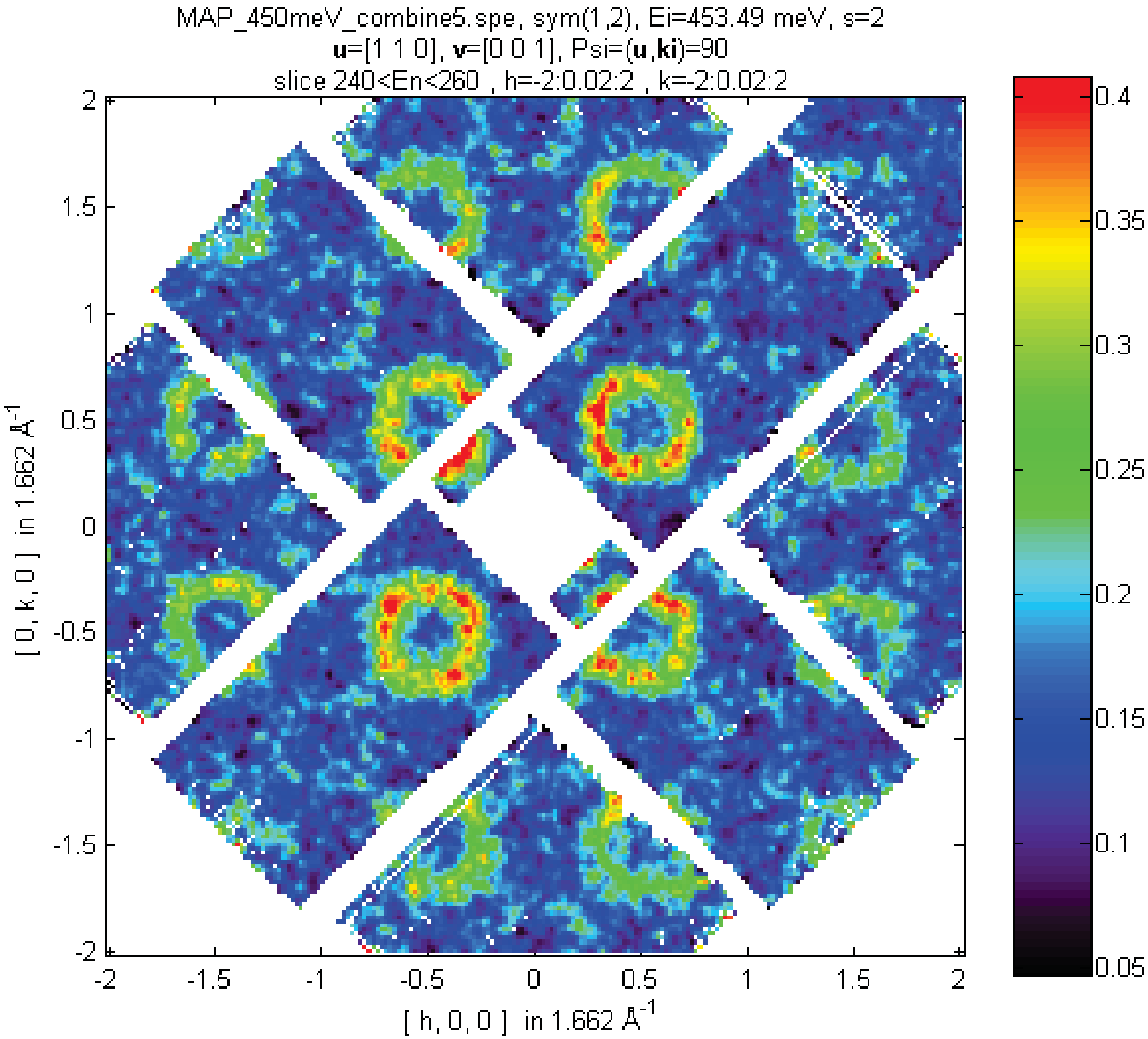
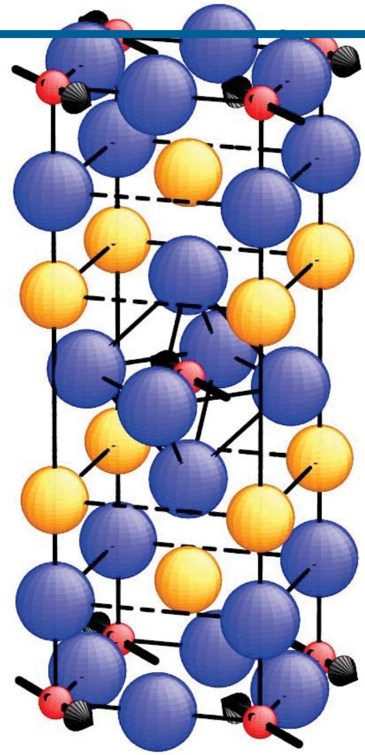
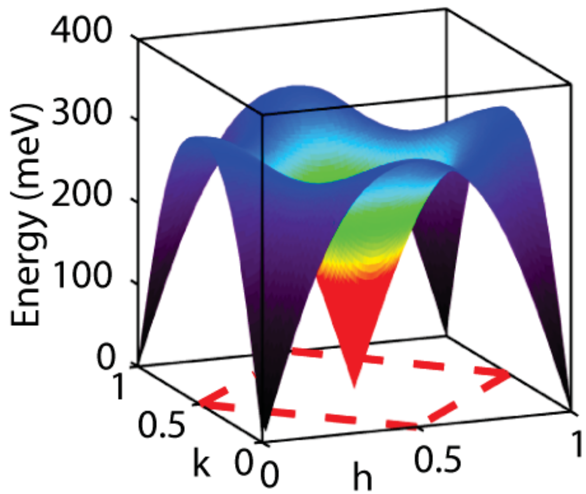
Spin waves in La_2CuO_4 :Example MAPS data

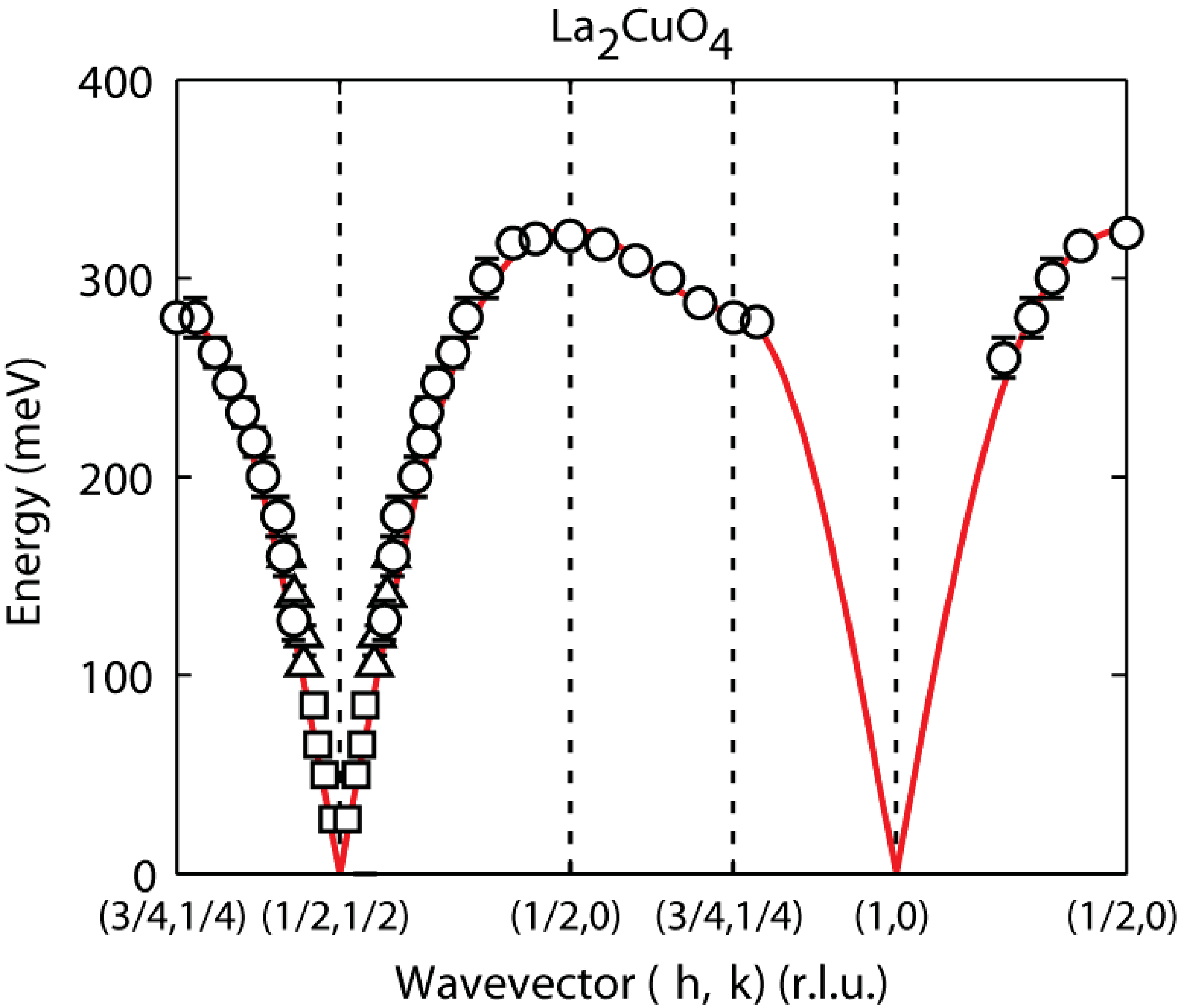
E=250 meV

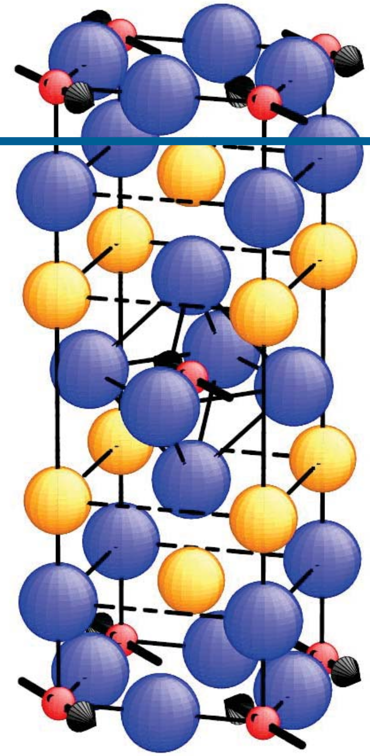


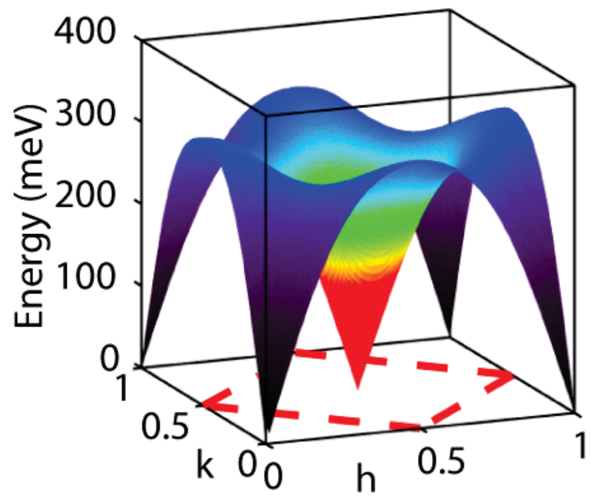




Spin waves in La_2CuO_4





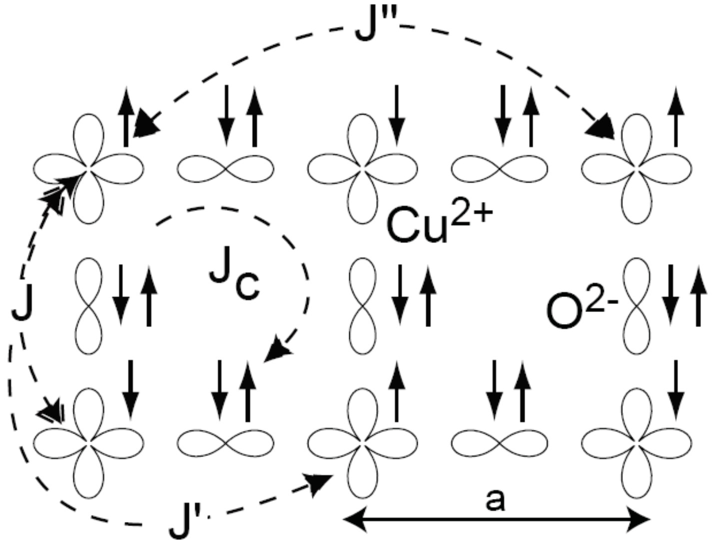


Coldea, Hayden, Aeppli, Perring, Frost, Mason, Cheong, Fisk,PRL **86** 5377 (2001).
Headings, Hayden, Coldea, Perring, Phys. Rev. Lett. **105**, 247001 (2010)

Spin wave dispersion

SW dispersion along BZ (3/4,1/4) to (1/2,0) subject to two competing effects):

1) Quantum fluctuations (beyond SWT) raise (3/4,1/4) wrt (1/2,0)
2) for large *t/U* the opposite happens due to higher order exchange terms.



$$J = 4t^2/U - 24t^4/U^3$$

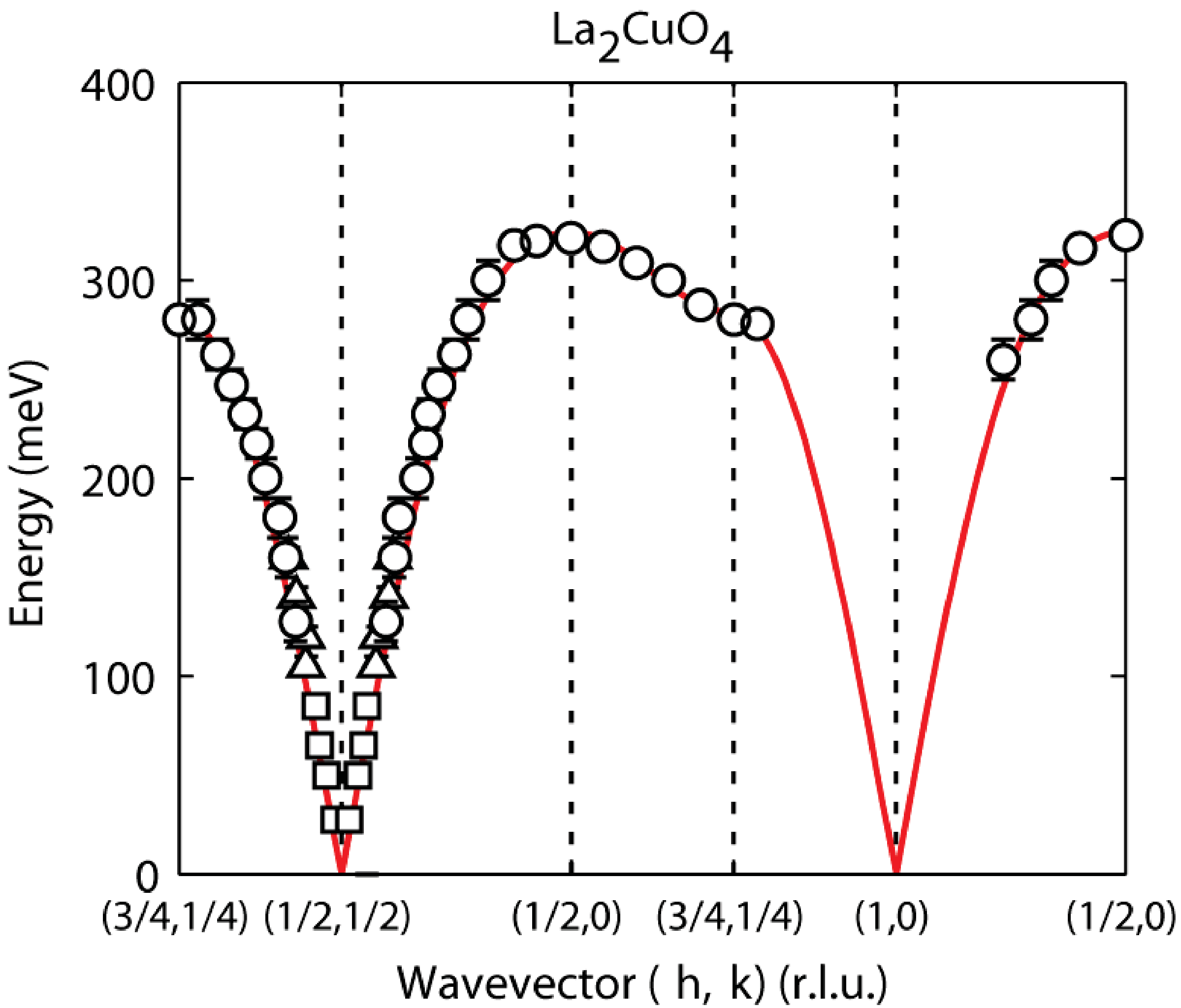
$$J_c = 80\ t^4/U^3$$

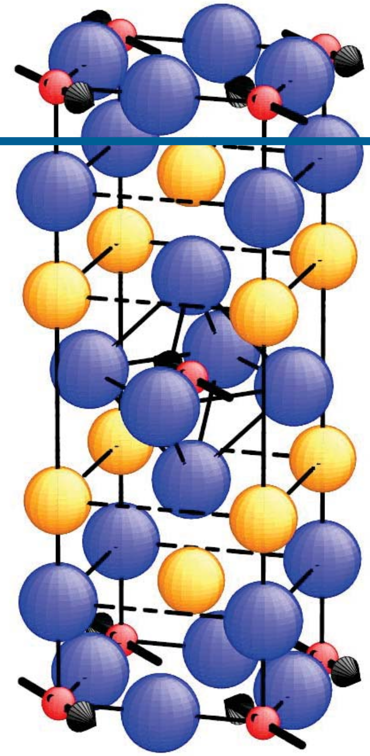
$$J' = J'' = 4t^4/U^3$$

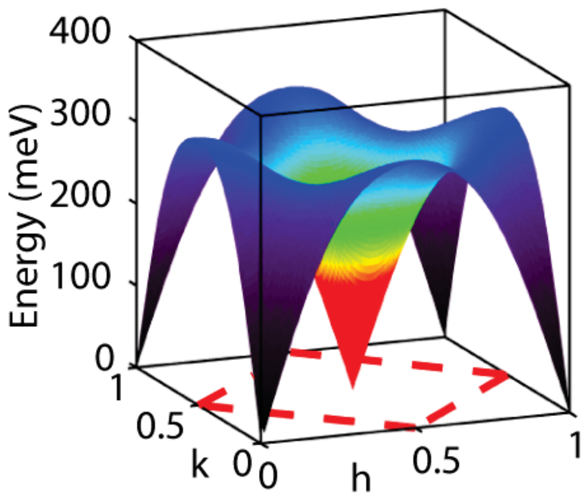
A. H. MacDonald PRB (1990)

t = 0.30 ± 0.02 eV, *U* =2.2 ± 0.4 eV,
J =146 ± 4 meV, and *Jc* = 61 ± 8 meV).

Spin waves in La_2CuO_4



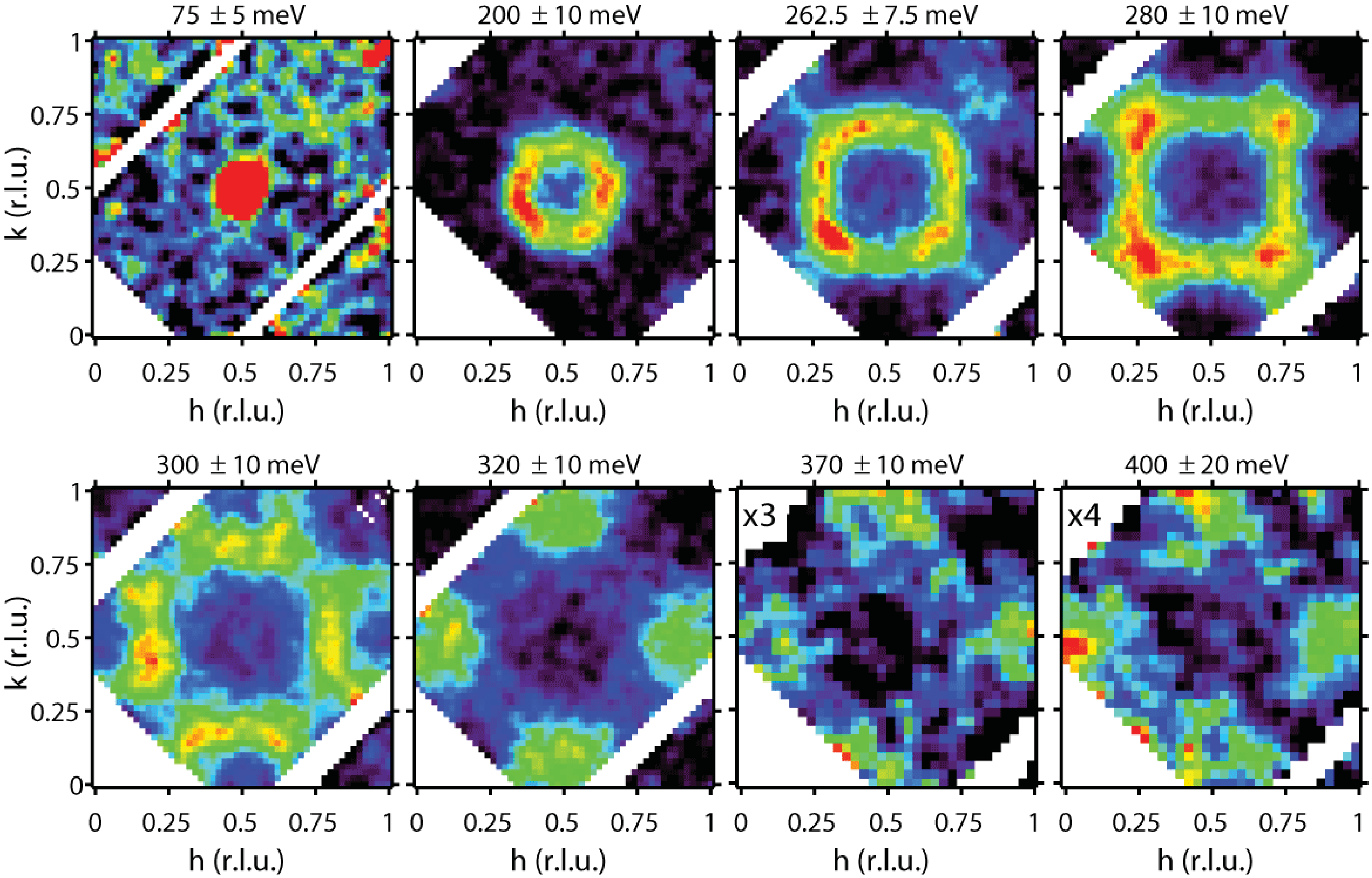




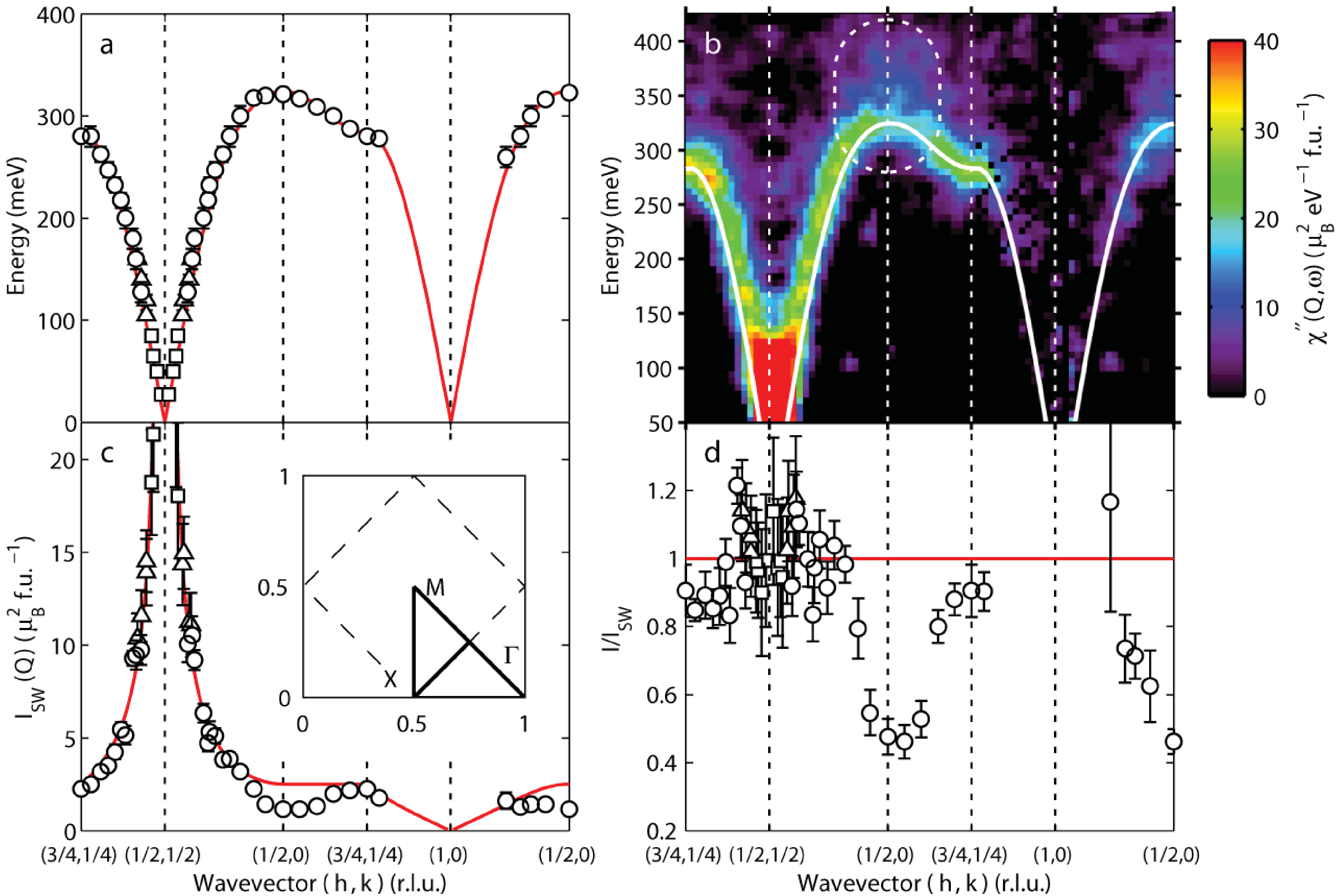
Coldea, Hayden, Aeppli, Perring, Frost, Mason, Cheong, Fisk,PRL **86** 5377 (2001).

Headings, Hayden, Coldea, Perring, Phys. Rev. Lett. **105**, 247001 (2010)

La_2CuO_4 : **q**-dependent slices



Magnetic Excitations in La_2CuO_4



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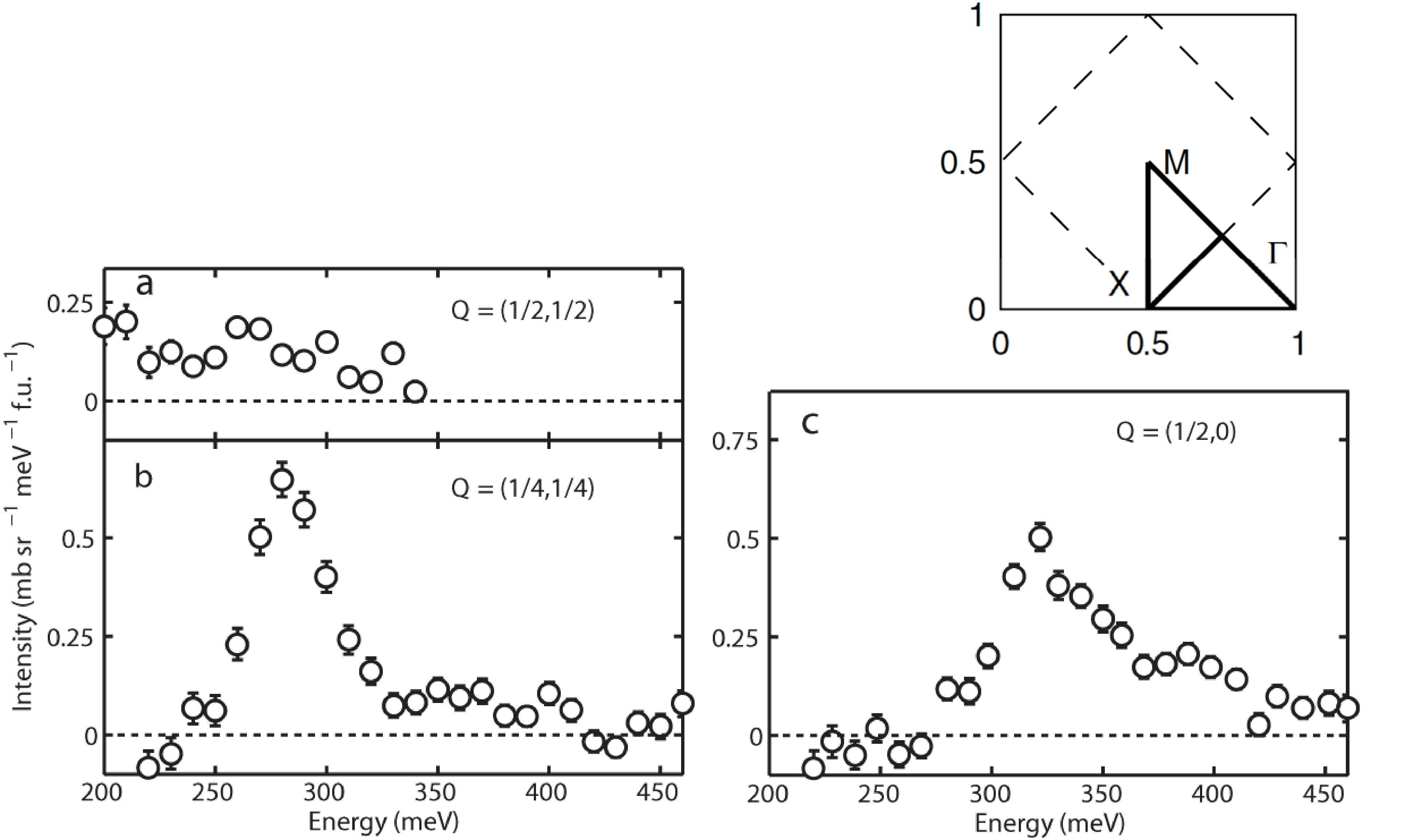
La_2CuO_4: High Energy Excitations



Spin-wave Theory (SWT 1+2 Mag)

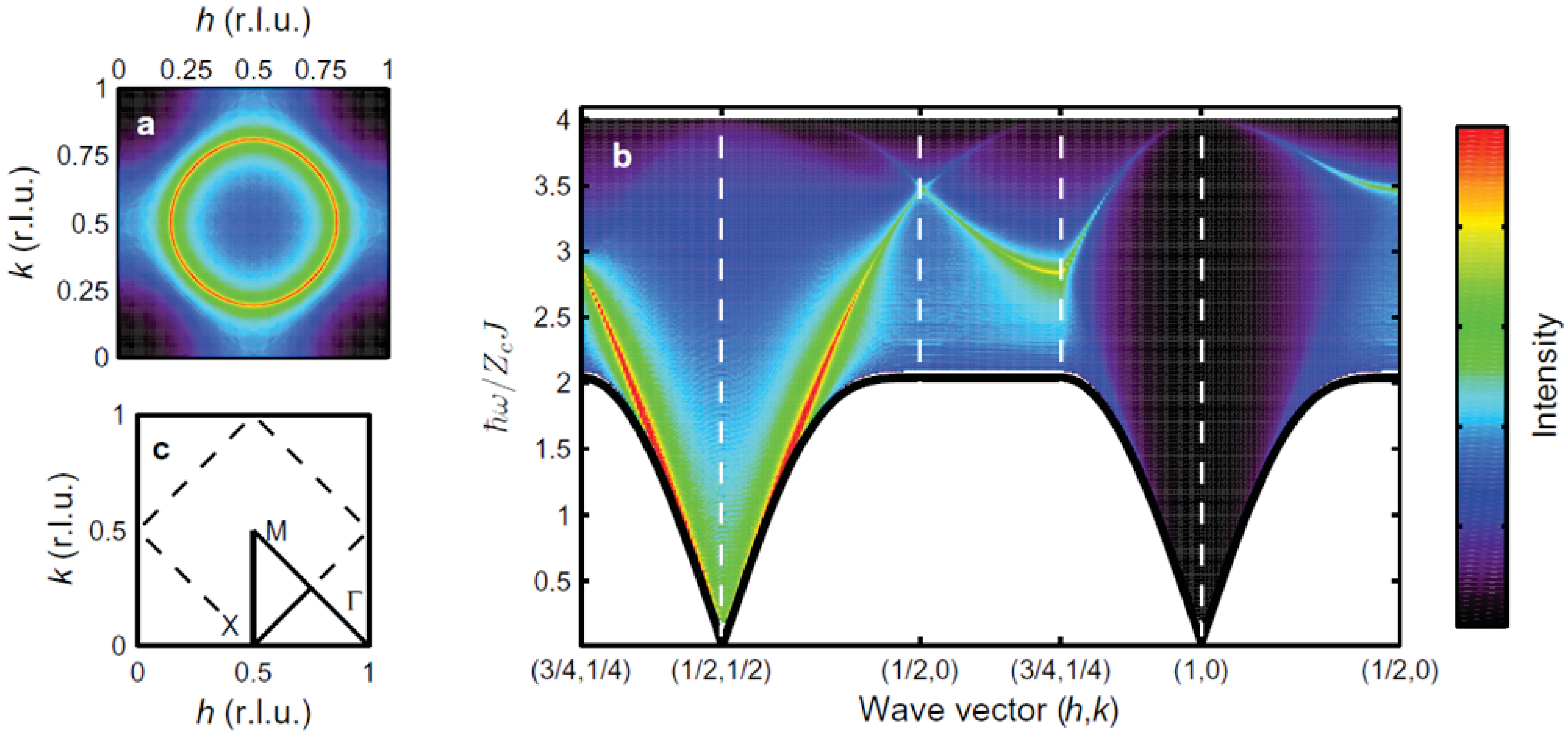
$$\chi''_{\perp}(\mathbf{Q},\hbar\omega) = Z_d(\mathbf{Q})\frac{\pi}{2}g^2\mu_B^2 S\left(u_{\mathbf{Q}} - v_{\mathbf{Q}}\right)^2 \times \delta(\hbar\omega - \hbar\omega_{\mathbf{Q}})$$

1-mag

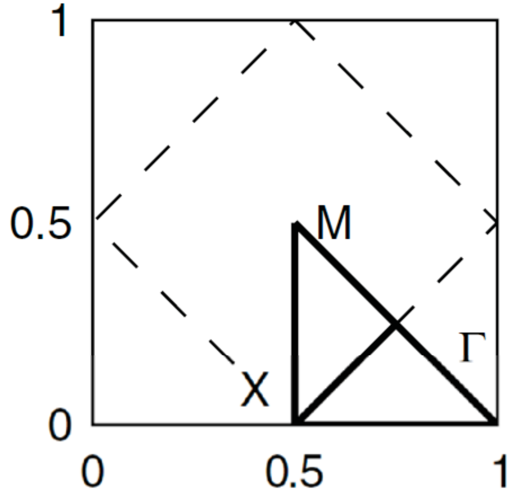
$$\chi''_{\parallel}(\mathbf{Q},\hbar\omega) = Z_{2M}\frac{\pi g^2\mu_B^2}{2N}\sum_{\mathbf{Q}_1,\mathbf{Q}_2} f(\mathbf{Q}_1,\mathbf{Q}_1)$$

$$\times\, \delta(\hbar\omega - \hbar\omega_{\mathbf{Q}_1} - \hbar\omega_{\mathbf{Q}_2})\,\delta(\mathbf{Q} + \mathbf{Q}_1 - \mathbf{Q}_2)$$

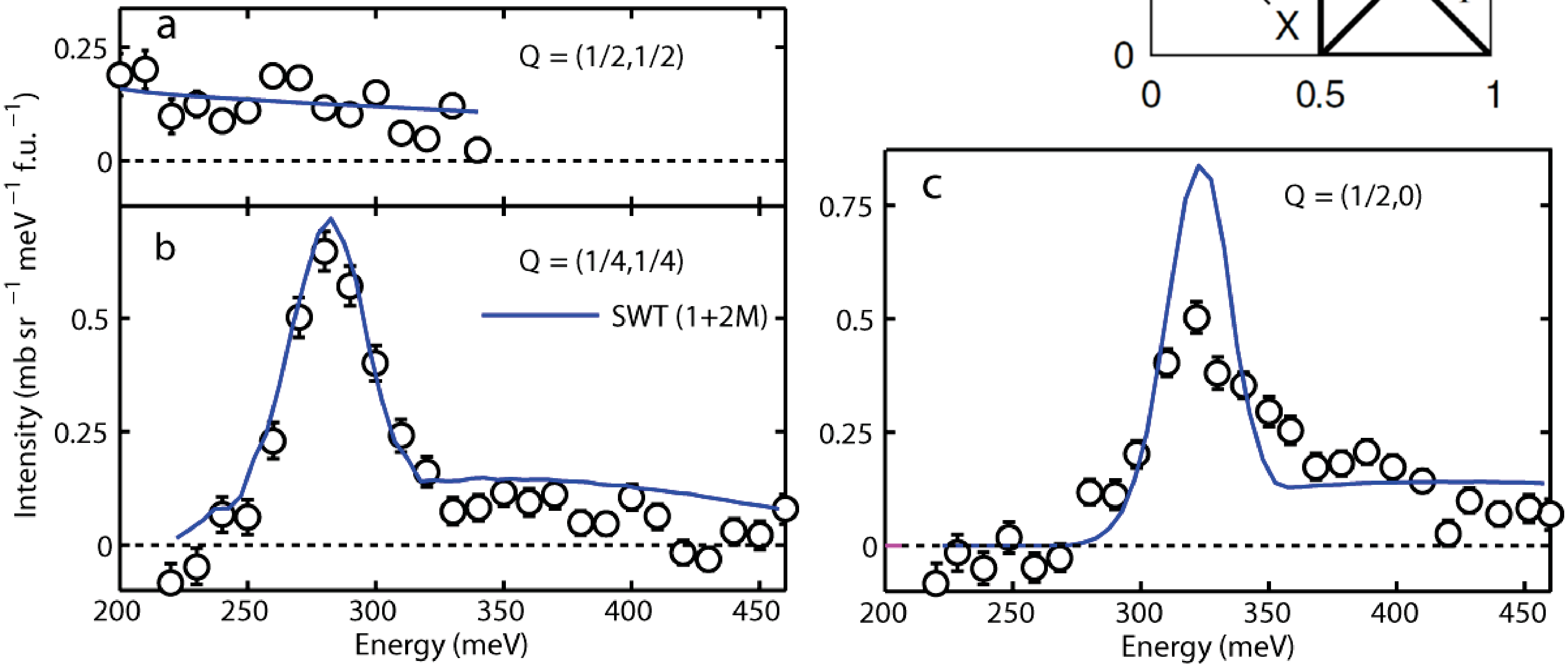
2-mag



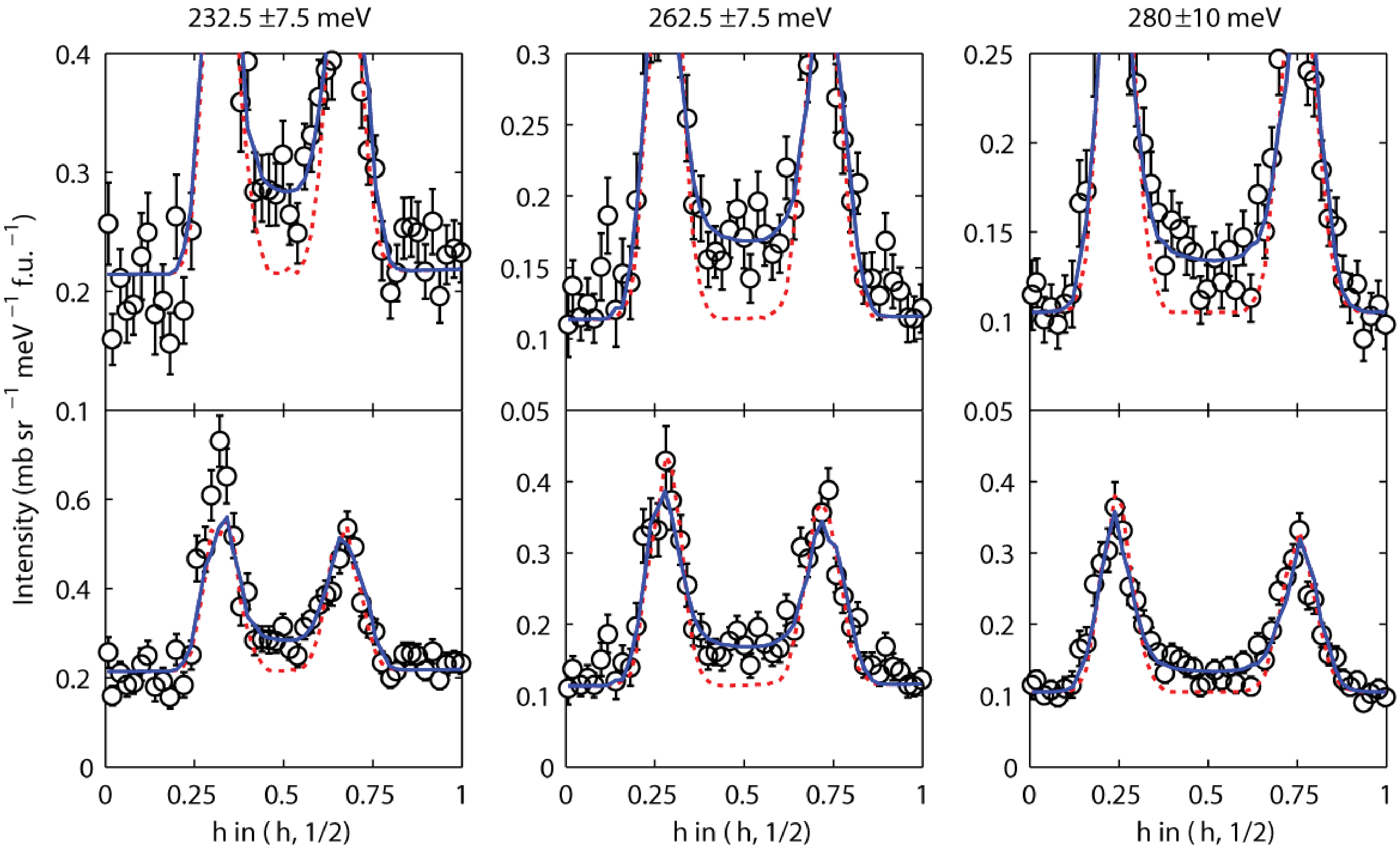
Spin-wave Theory (SWT 1+2 Mag)



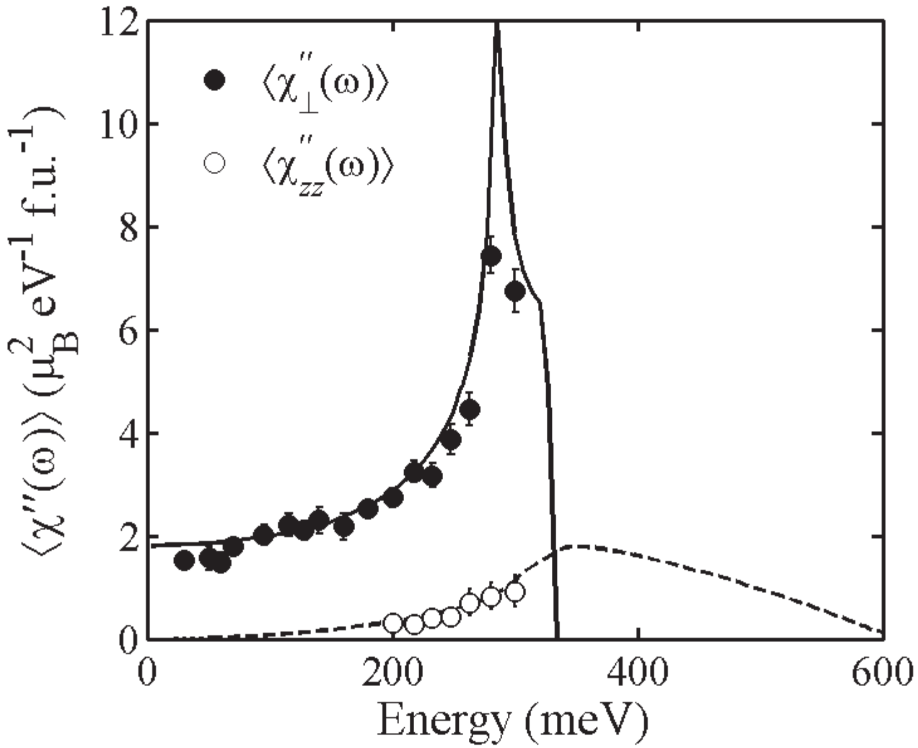
$Z_d = 0.4 \pm 0.04$
$Z_{2M} = 0.47 \pm 0.1$



Continuum (2-magnon) scattering at lower energies

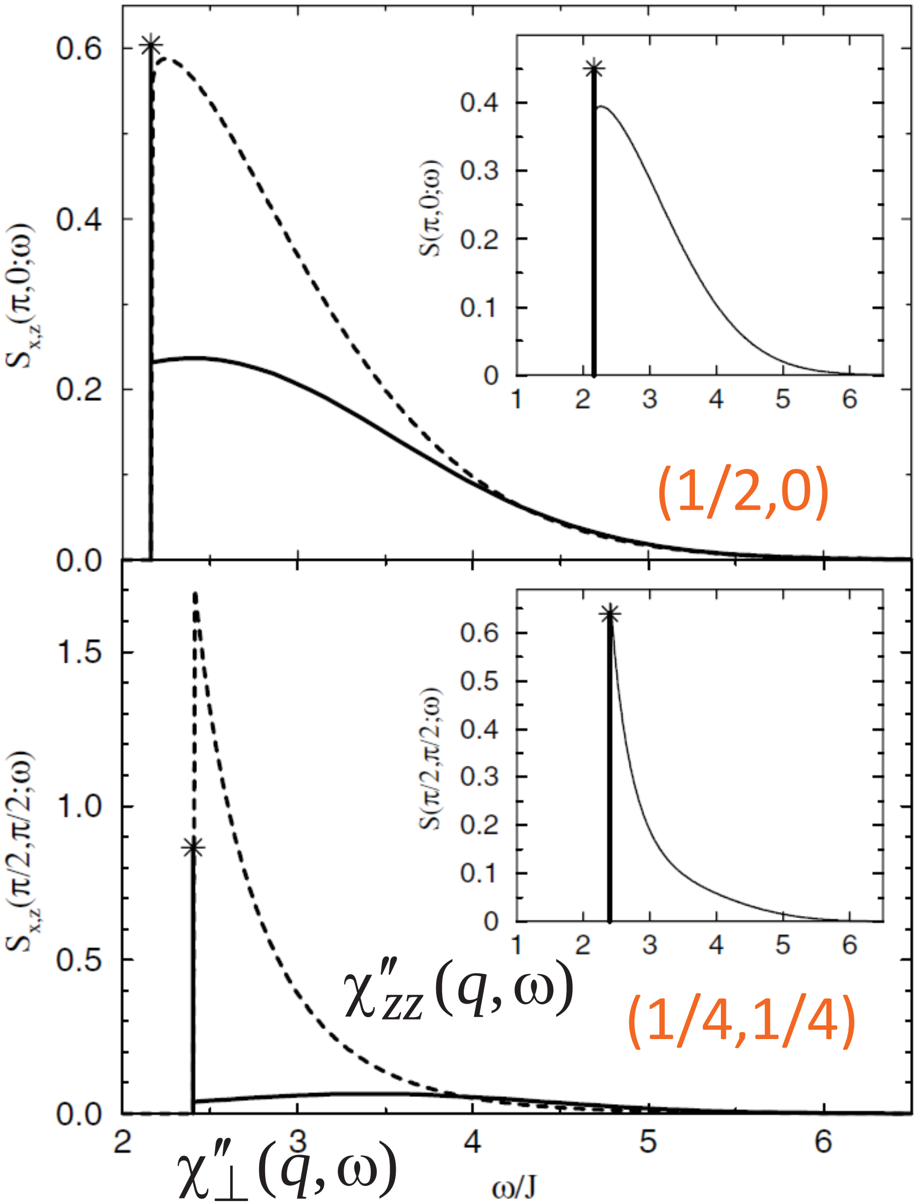


Local susceptibility based on SWT (1+2M)



$$\chi''_{\rm local}(\omega) = \frac{\int_{BZ} \chi''(\mathbf{Q},\omega)\, d\mathbf{Q}}{\int_{BZ} d\mathbf{Q}}$$

Quantum Monte Carlo Simulations



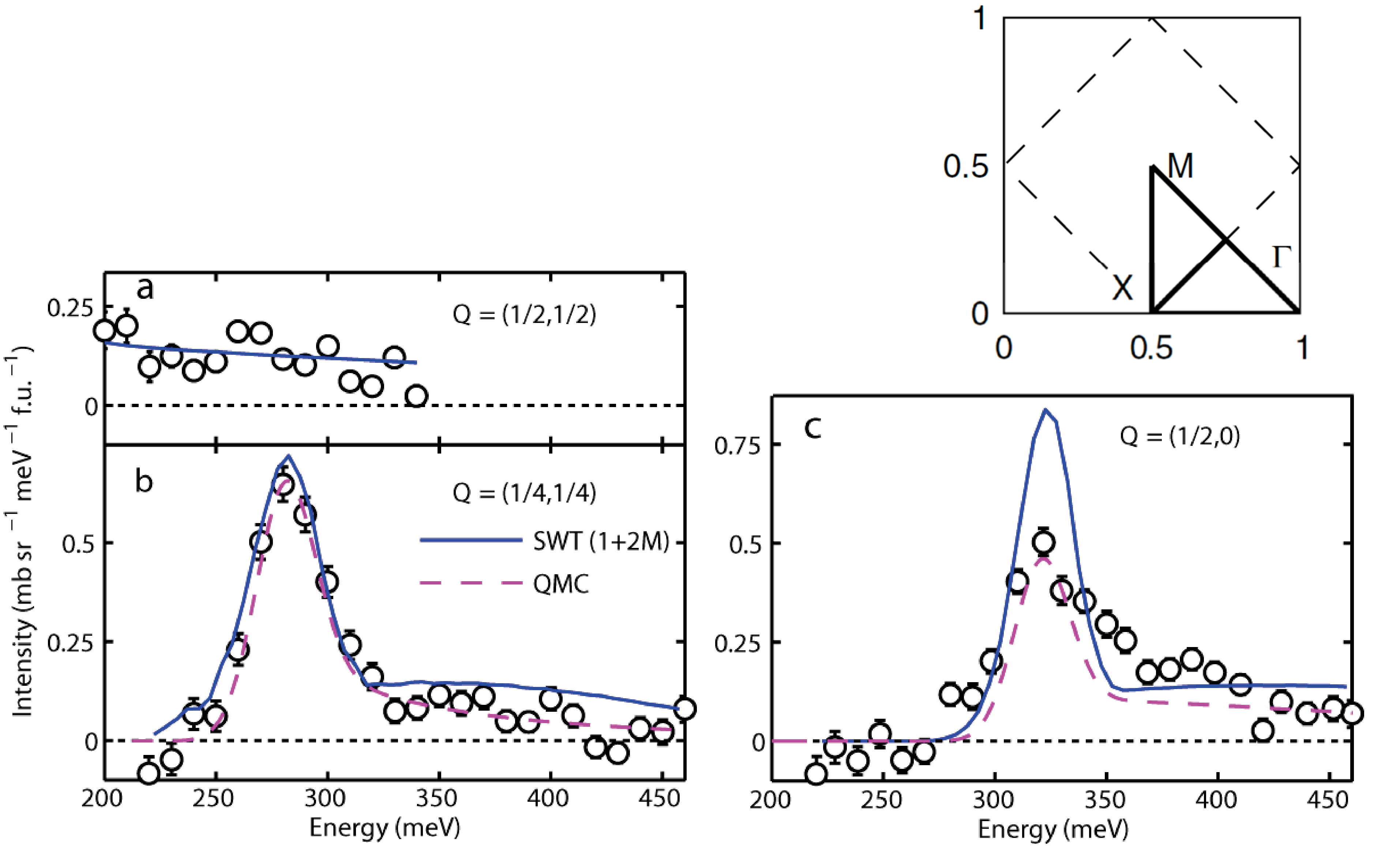
A. W. Sandvik and R. R. P. Singh, PRL 86, 528 (2001)

Points to note:

- QMC includes only J and assumes lineshapes for continuum responses
- profiles shifted to match the measured SW pole positions
- Experiment measures

$$\chi''_{\perp}(q,\omega)+\chi''_{zz}(q,\omega)$$

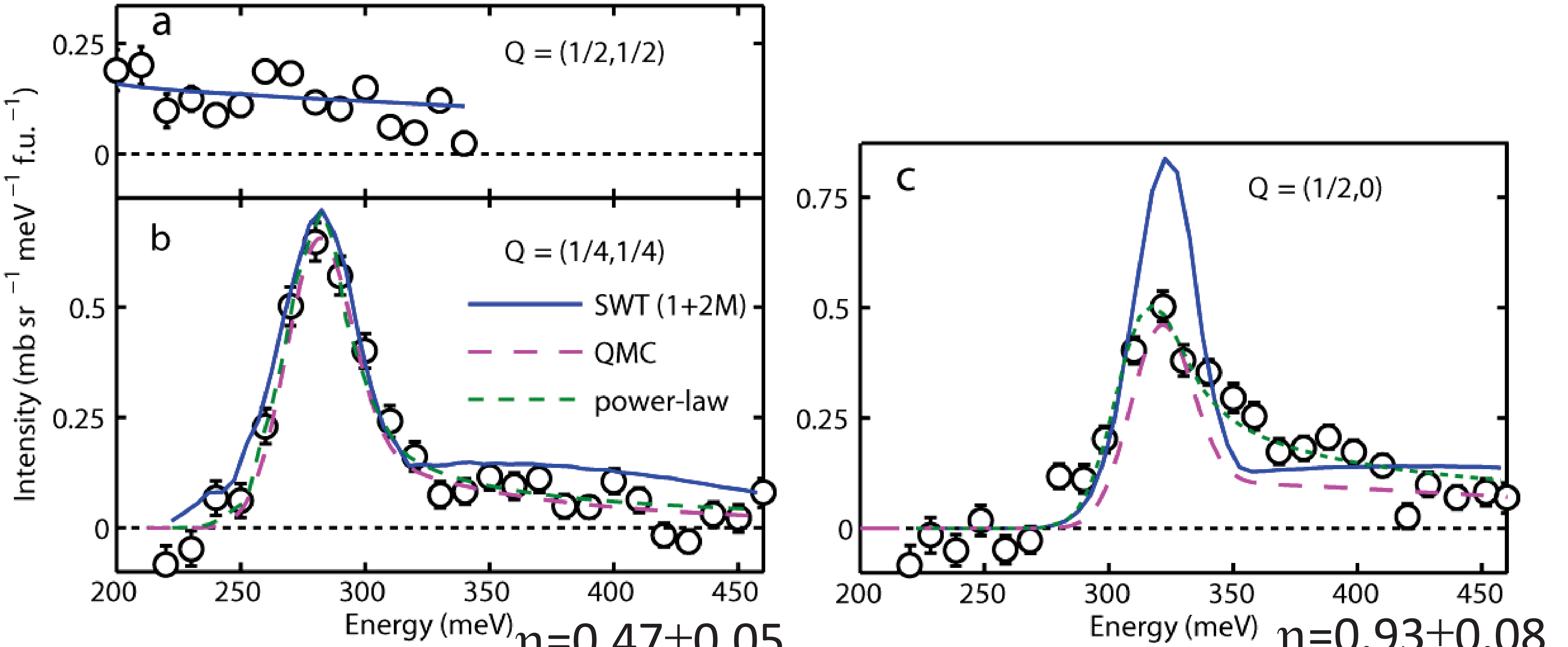
Quantum Monte Carlo Simulations



"Spinon" power law

Generalization of continuum scattering lineshape of the 1D Heisenberg AF chain (η=1)

$$\chi''(\mathbf{q},\omega) = A_{\mathbf{q}} \frac{\theta(\omega-\omega_{\mathbf{q}})}{\left(\omega^2-\omega_{\mathbf{q}}^2\right)^{1-\eta/2}}$$



η=0.47±0.05

η=0.93±0.08

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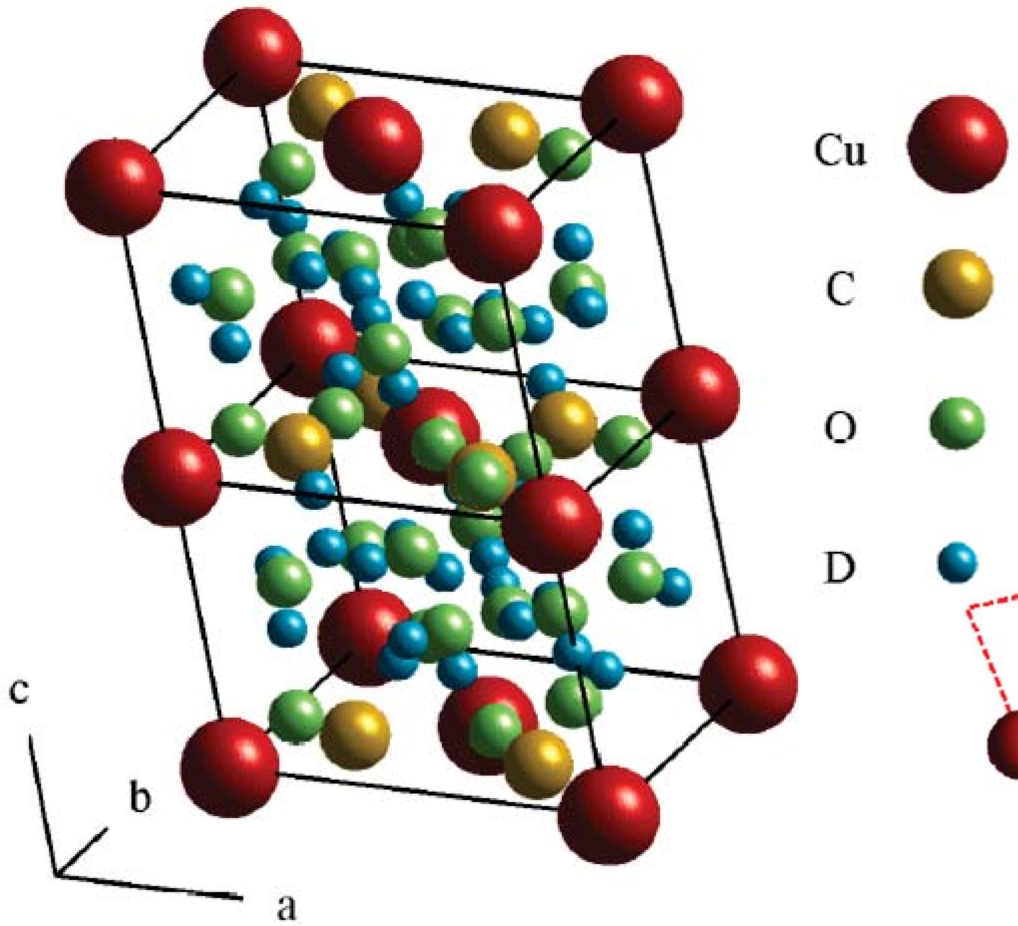
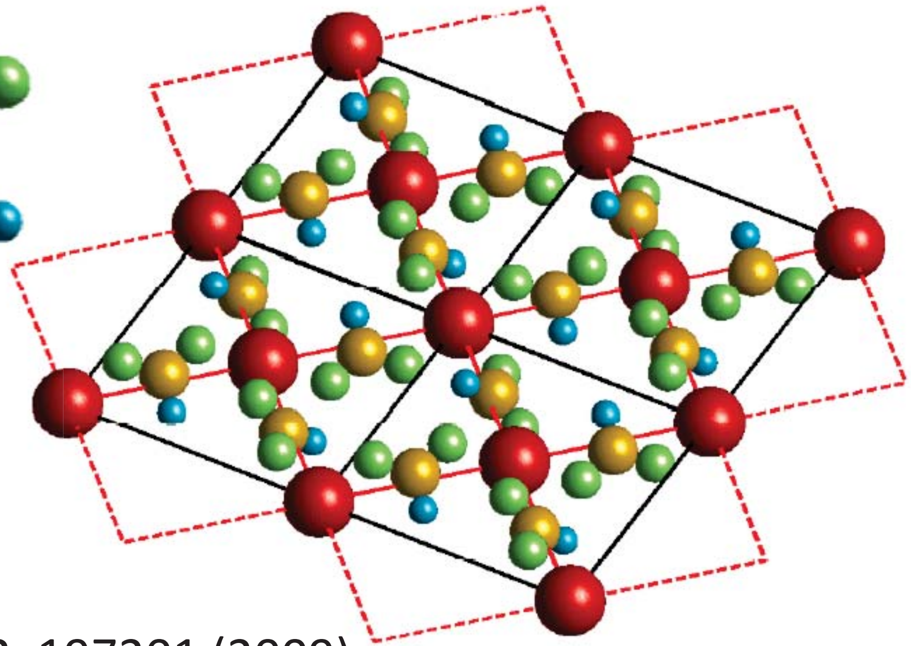
Other S=1/2 Square lattice antiferromagnets

•Reduced (1/2,0) SW intensity and high-energy tail also seen small t/U weak exchange AFs



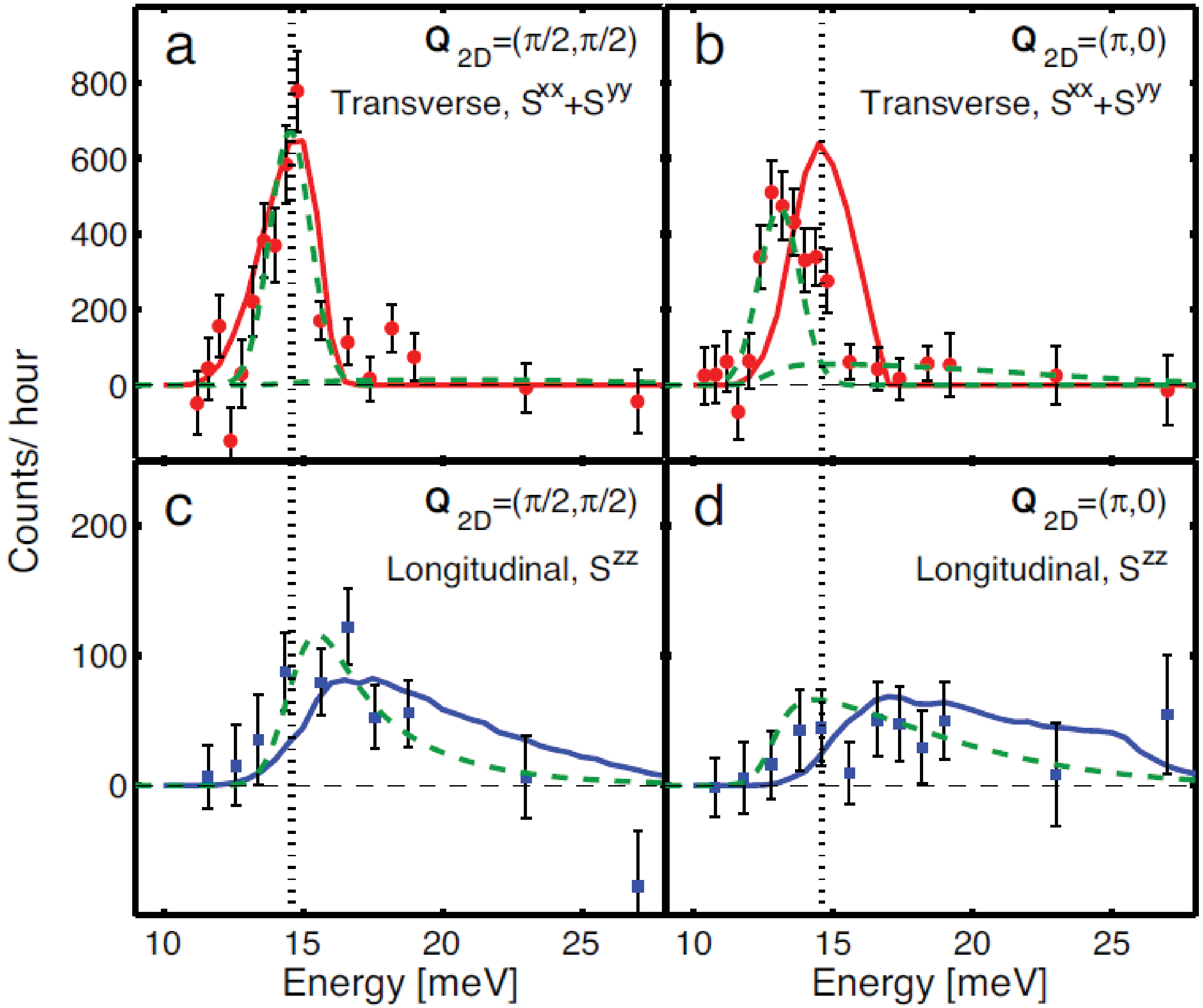
$Cu(DCOO)_2 \cdot 4D_2O$ (CFTD)

N. B. Christensen et al., PNAS 104, 15264 (2007)



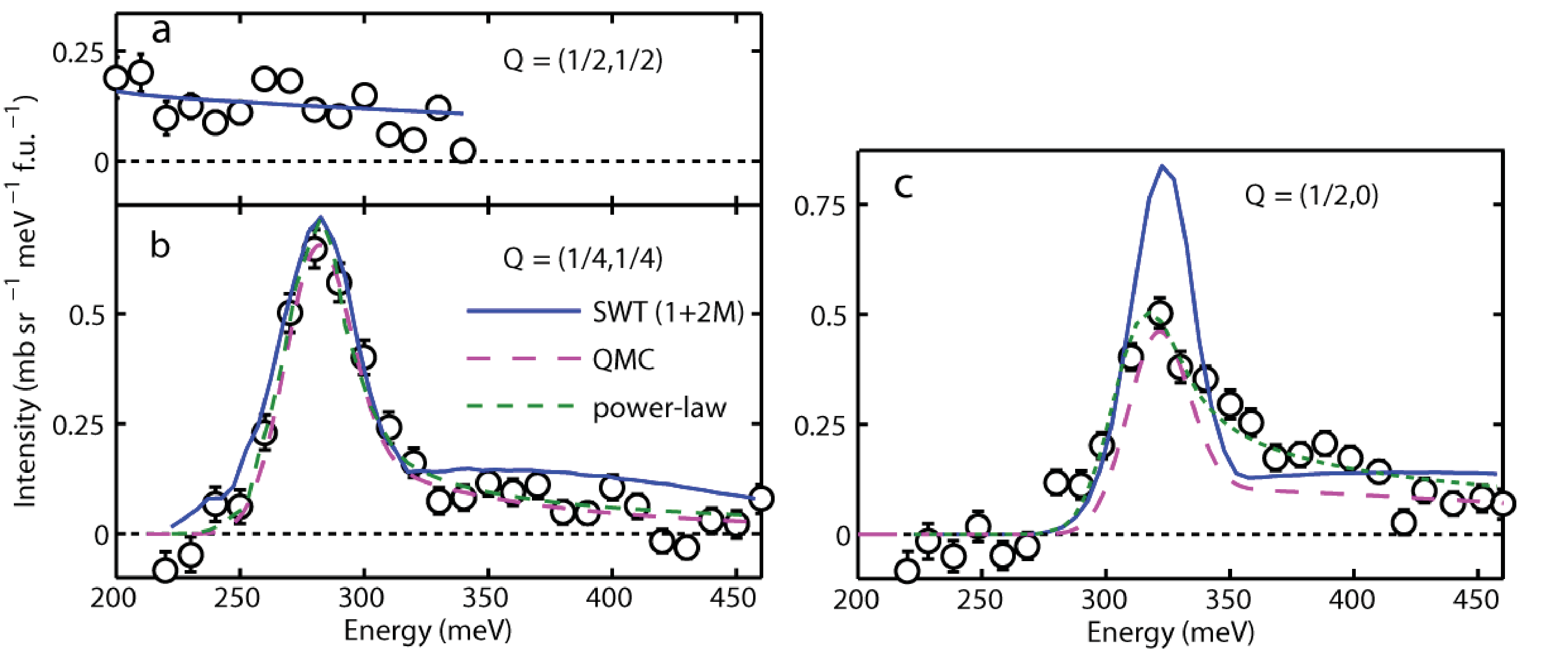
Also Cu(pz)2(ClO4)2 N. Tsyrulin et al, PRL 102, 197201 (2009)

Cu(DCOO)$_2$·4D$_2$O (CFTD)



N. B. Christensen et al., PNAS 104, 15264 (2007)

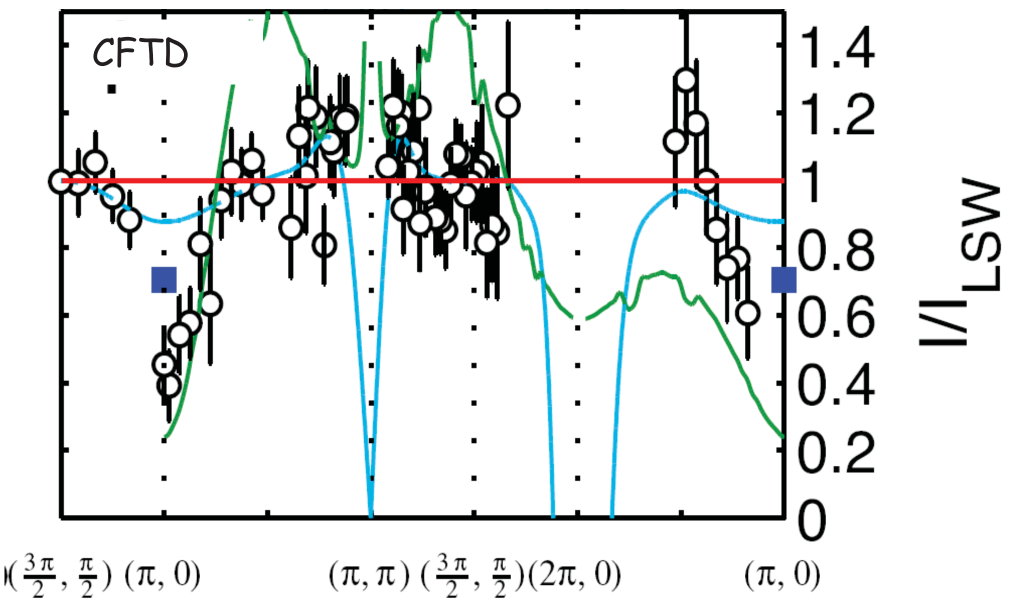
La_2CuO_4



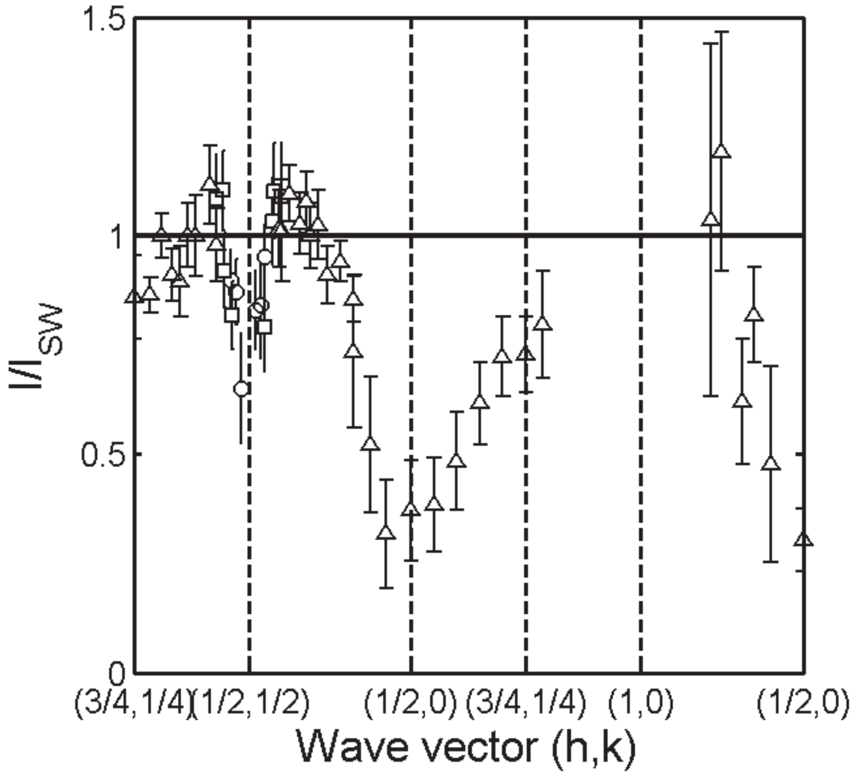
a
Q = (1/2,1/2)
b
Q = (1/4,1/4)
SWT (1+2M)
QMC
power-law
c
Q = (1/2,0)
Intensity (mb sr $^{-1}$ meV $^{-1}$ f.u. $^{-1}$)
Energy (meV)
Energy (meV)

$Cu(DCOO)_2 \cdot 4D_2O$ (CFTD)

SW amplitude dependence



$Cu(DCOO)_2 \cdot 4D_2O$



La_2CuO_4

Christensen et al. PNAS **104** 15264 (2007)

Resonant inelastic x-ray scattering (RIXS)

RIXS at the copper L_3 edge, Cu 2p → 3d

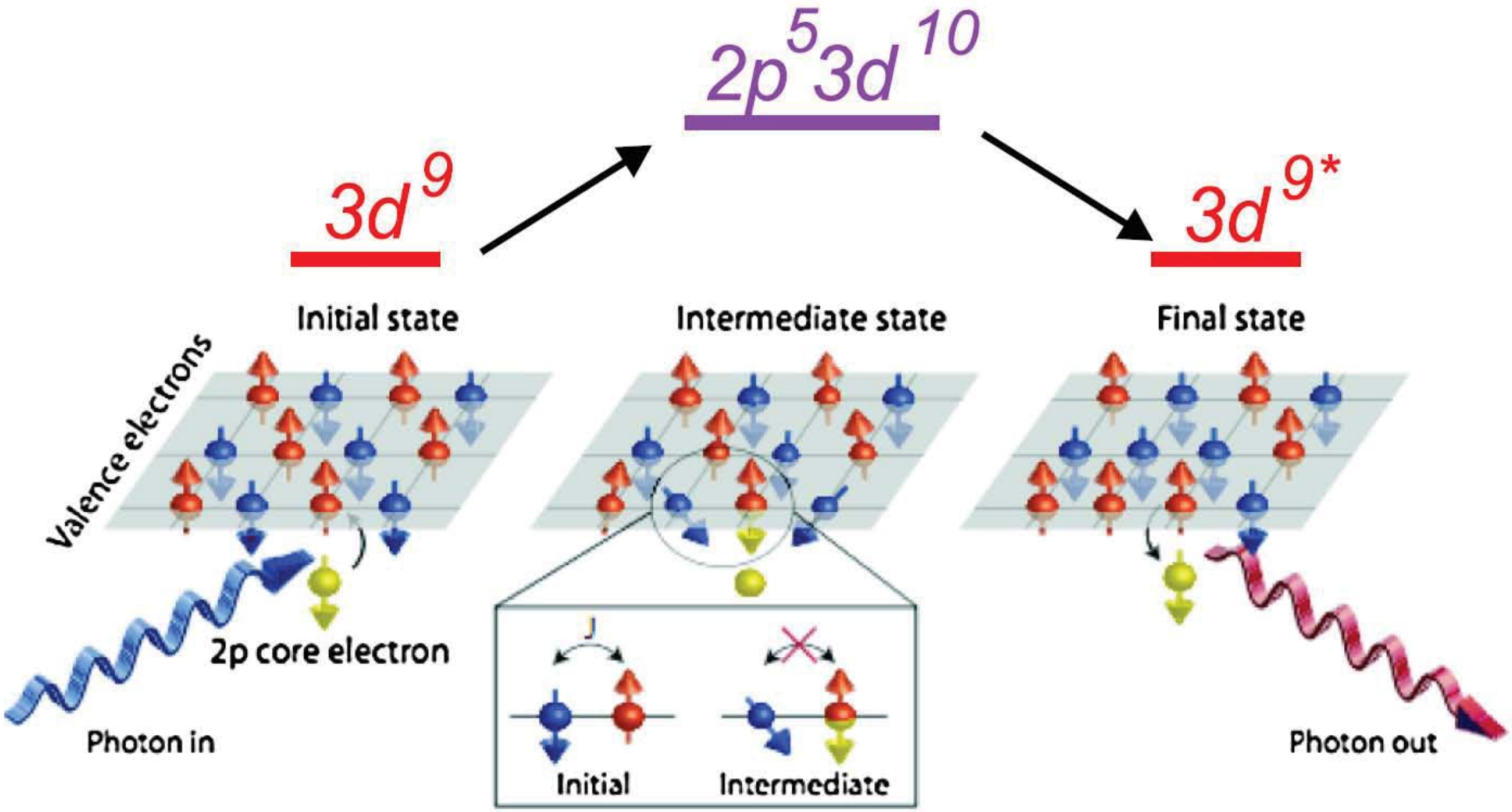
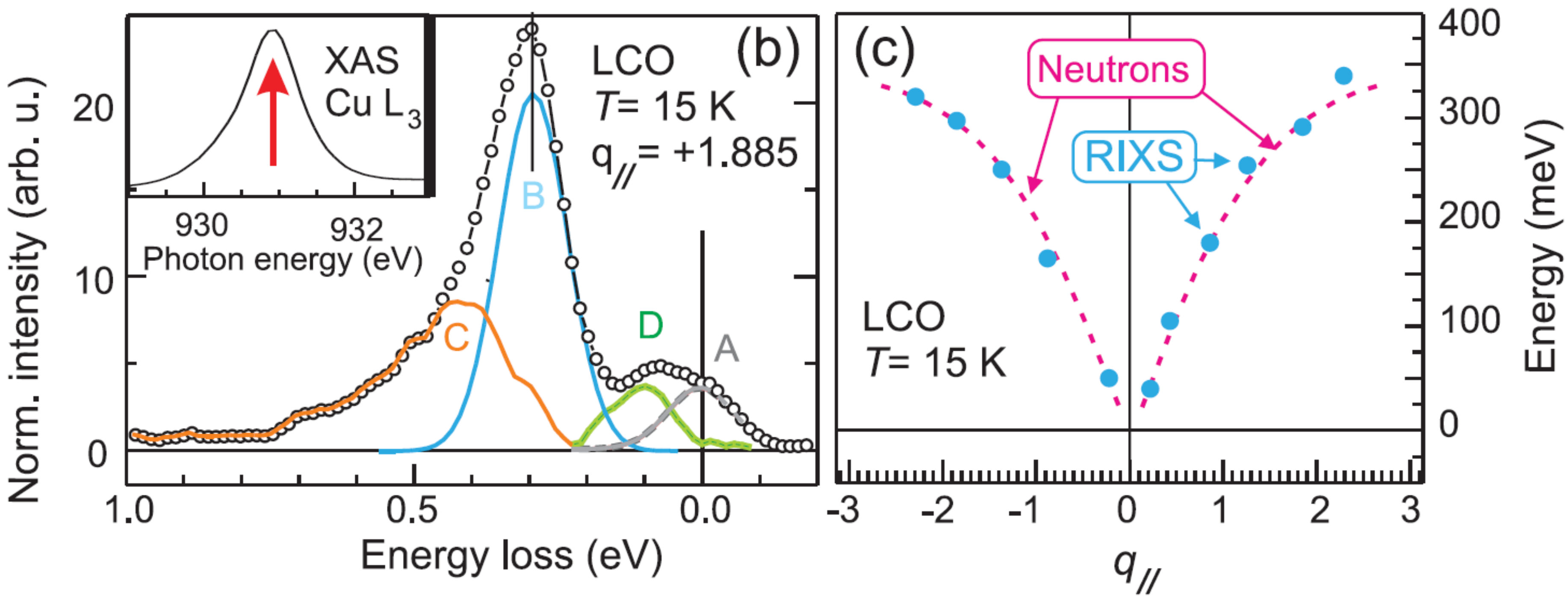
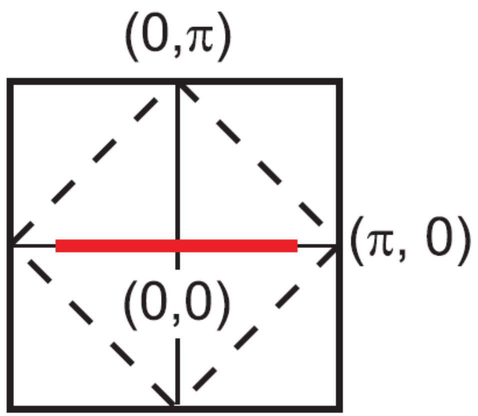


Figure: L. Braicovich et al., PRL 102, 167401 (2009)

RIXS in La_2CuO_4



RIXS at the copper L_3 edge, Cu 2p → 3d



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

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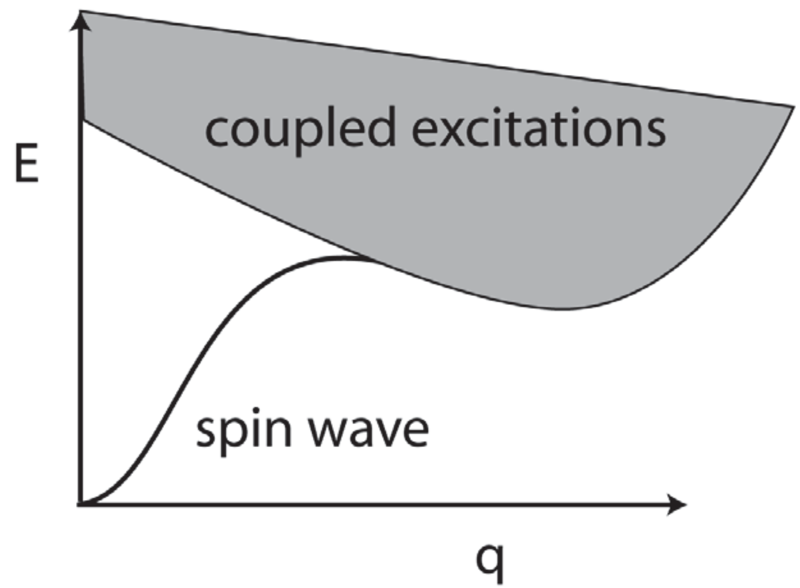
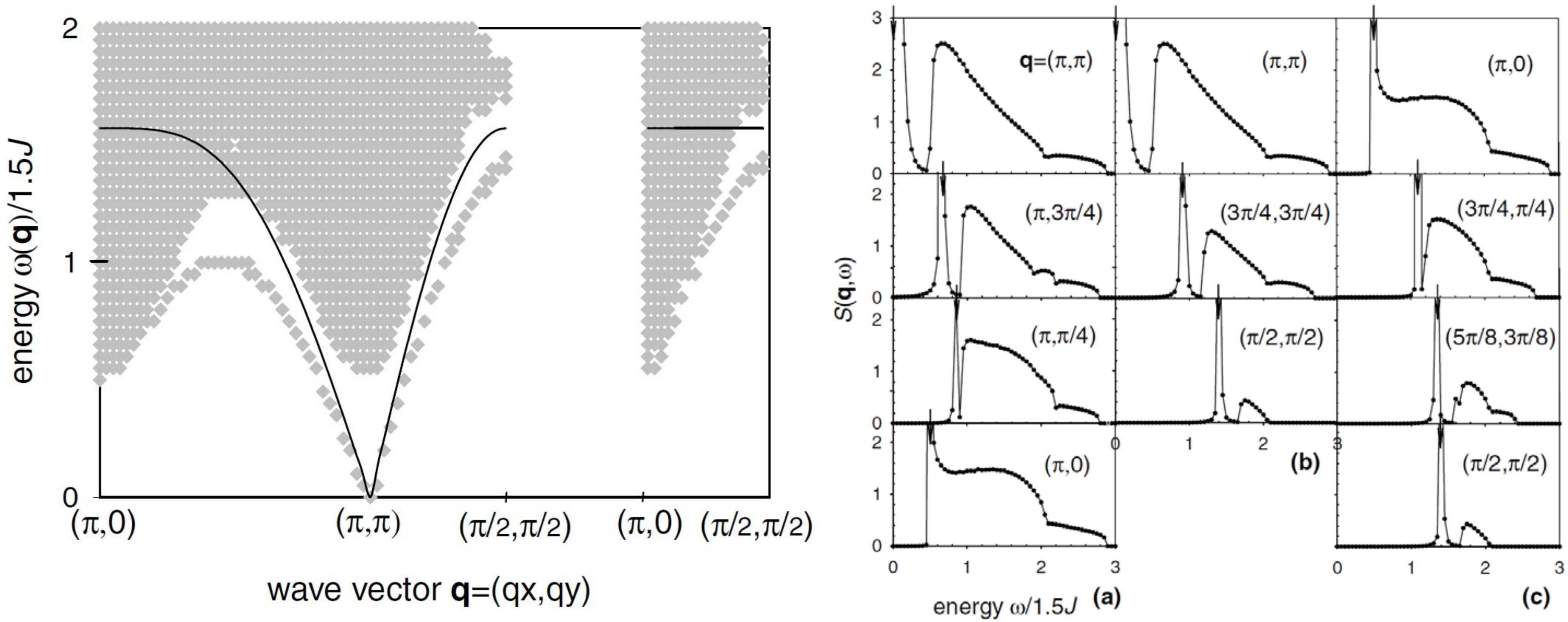
Interpretation

- Low energies: bound spinons ➔ spin waves
- High energies: Evidence for fractionalization. Spin waves unbind into spinons.



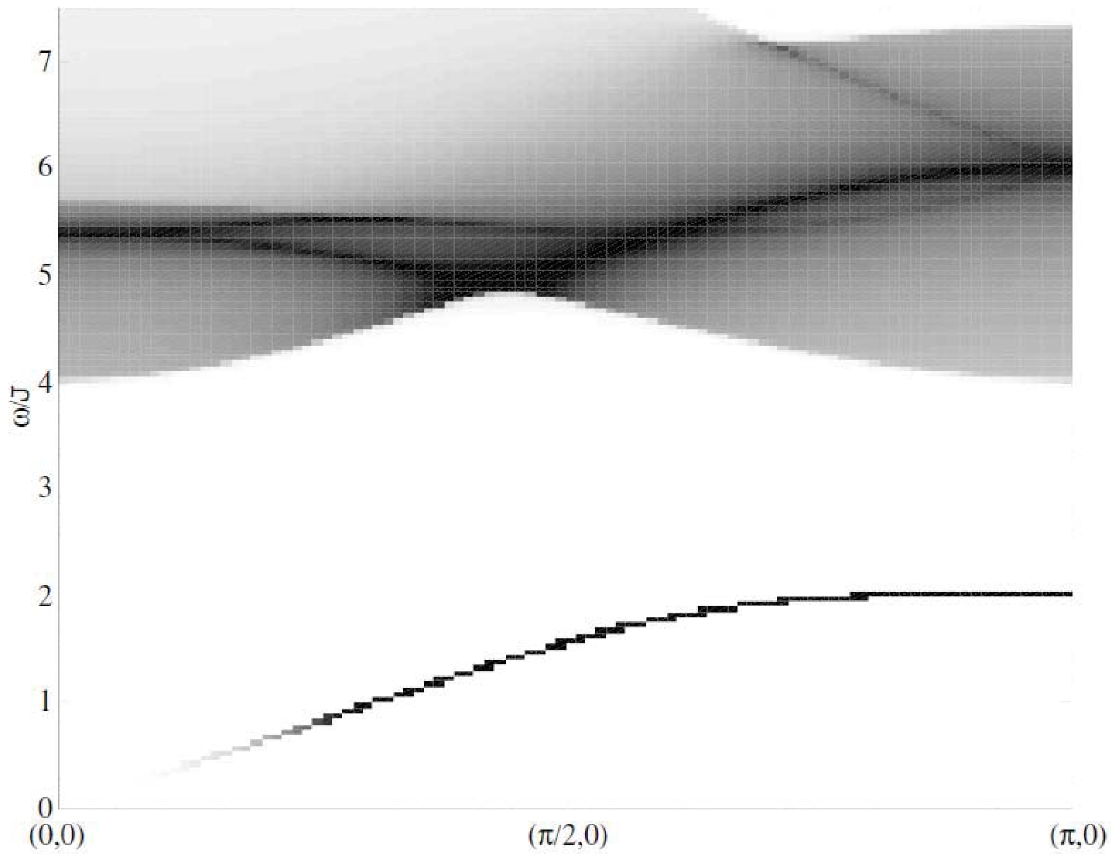
- May also be other explanations (cf reduction of multiband Hubbard model to Heisenberg model only works at low energies.)

Excitations of RVB state: π-flux phase



C.-M. Ho, V. N. Muthukumar, M. Ogata, and P. W. Anderson, Phys. Rev. Lett. **86**, 1626 (2001).

Fractionalized Antiferromagnet (AF*)

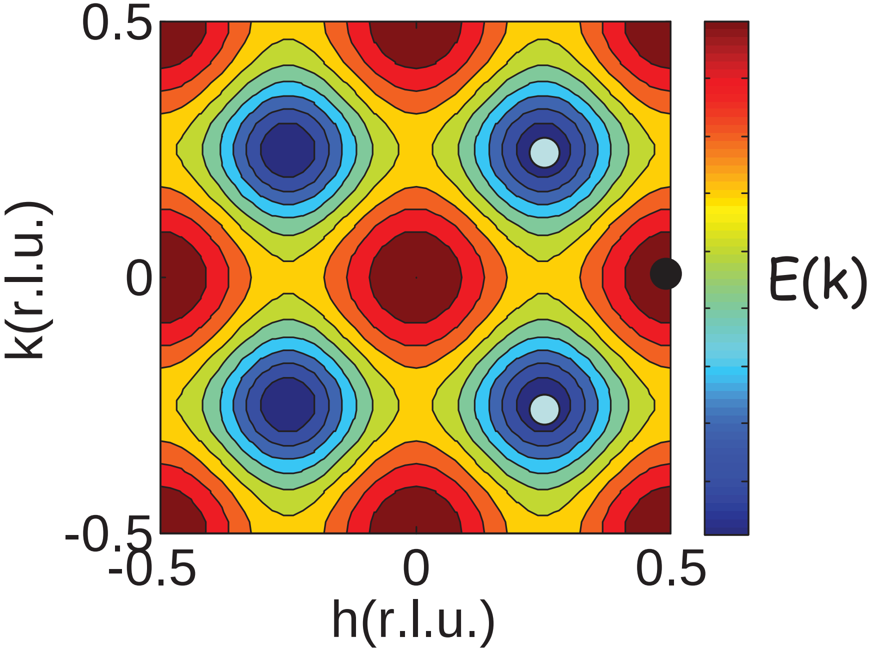


C. Lannert and M. P. A. Fisher, Int. J. Mod. Phys. B 17, 2821 (2003)

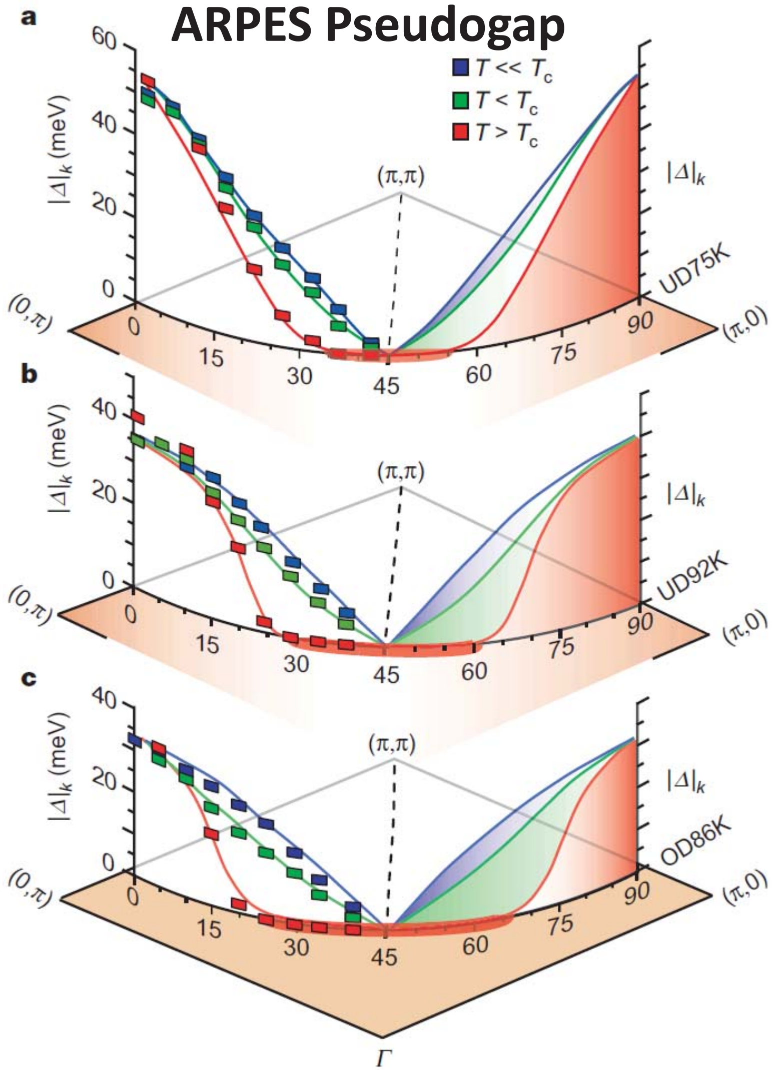
Fermionic Excitations in Cuprates

Spinon Picture

- Spinons are S=1/2 quasiparticles
- (1/2,0) =>two spinons (1/4, ±1/4)
- spinons model would need a d-wave dispersion with minima at (±1/4,1/4) and (1/4, ±1/4)



C-M. Ho et al PRL 2001 π-flux phase



Underdoped $Bi_2Sr_2CaCu_2O_8$

Lee et al., Nature 450, 81 (2007)

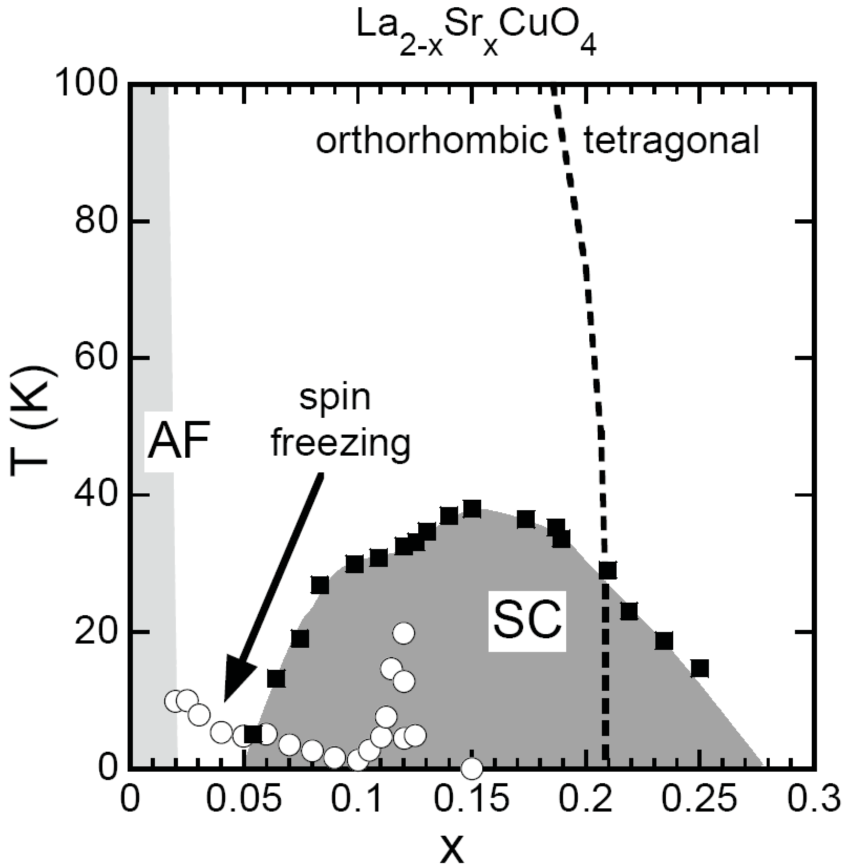
Anomalous Spin Excitations in La_2CuO_4 and $La_{2-x}Sr_xCuO_4$

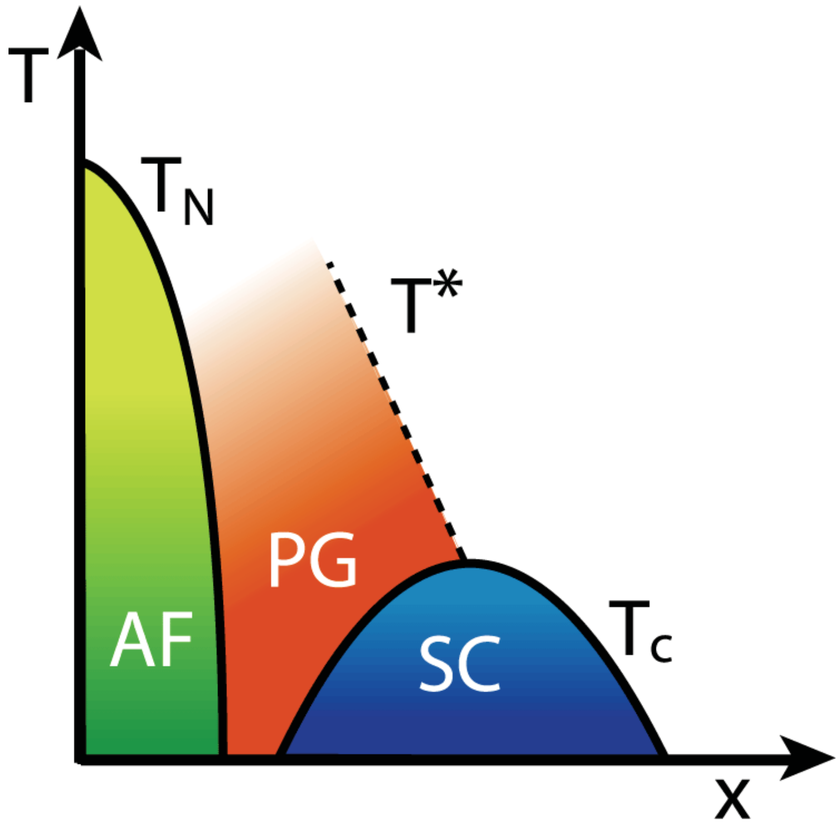
1) La_2CuO_4

- Introduction and motivation
- Experimental
- Spin Excitations in La_2CuO_4
- Comparison with theory
- Other Experiments
- Discussion

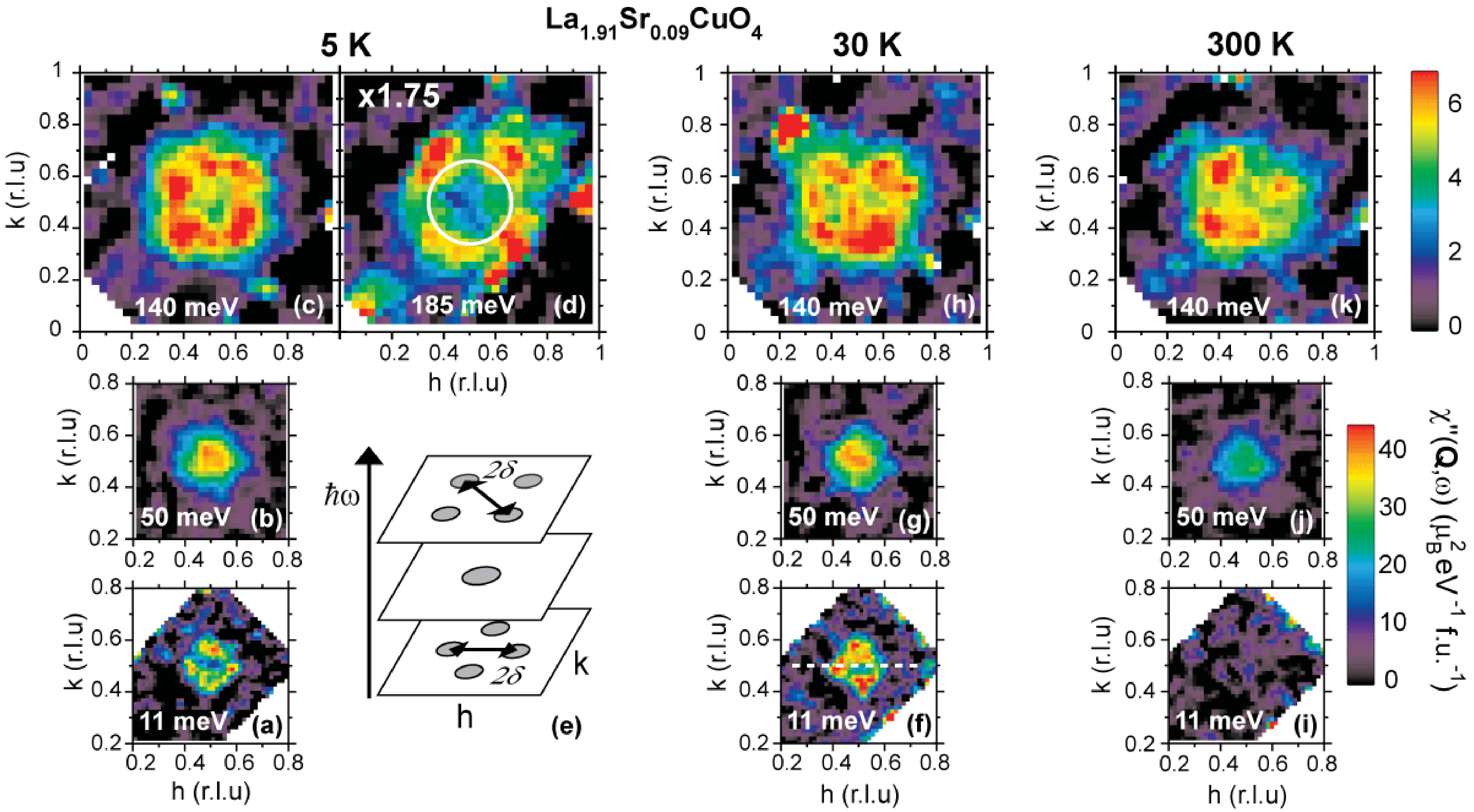
2) The pseudogap and $La_{1.91}Sr_{0.09}CuO_4$ (UD22)

Magnetic excitations in underdoped cuprates

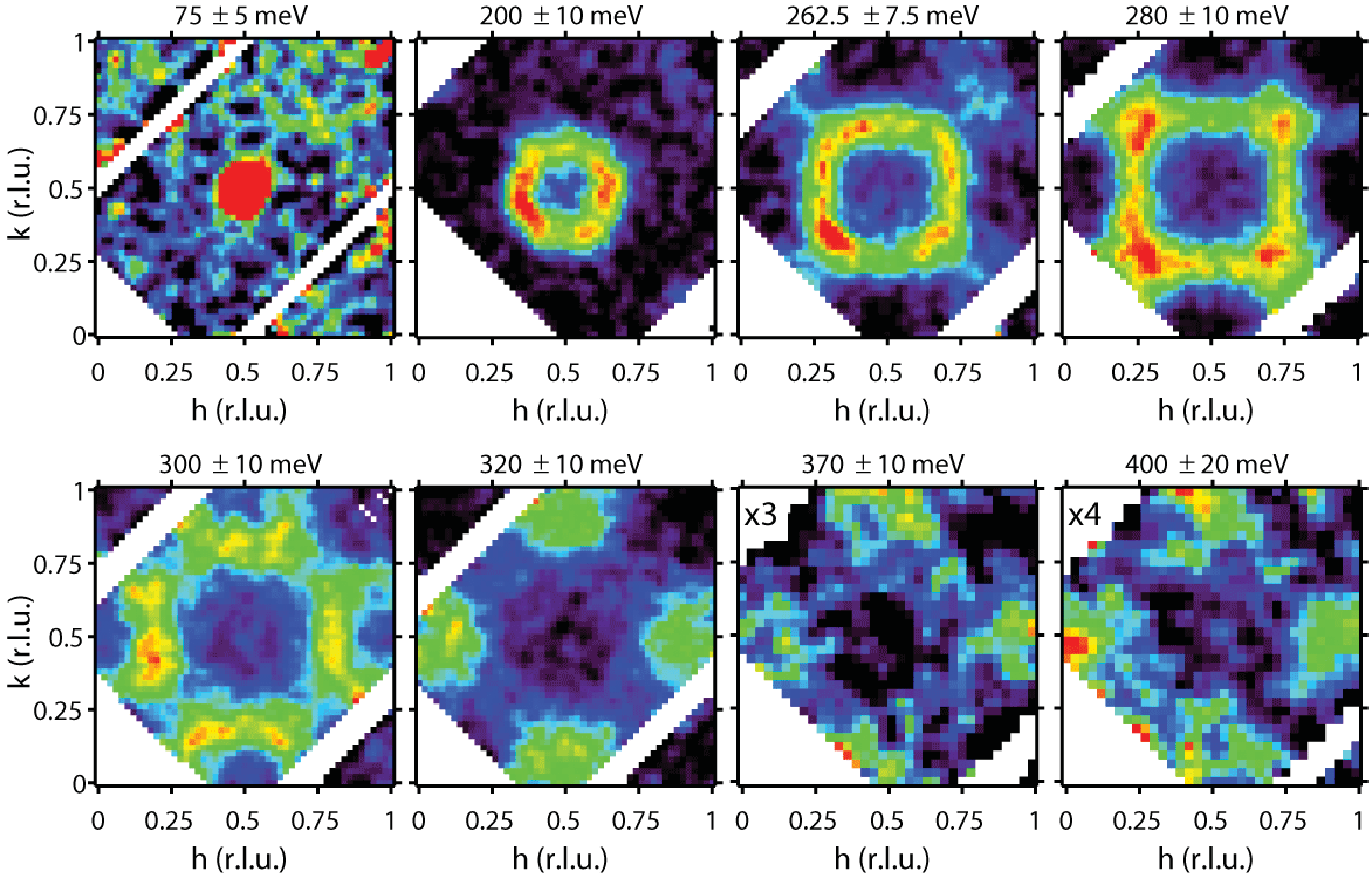




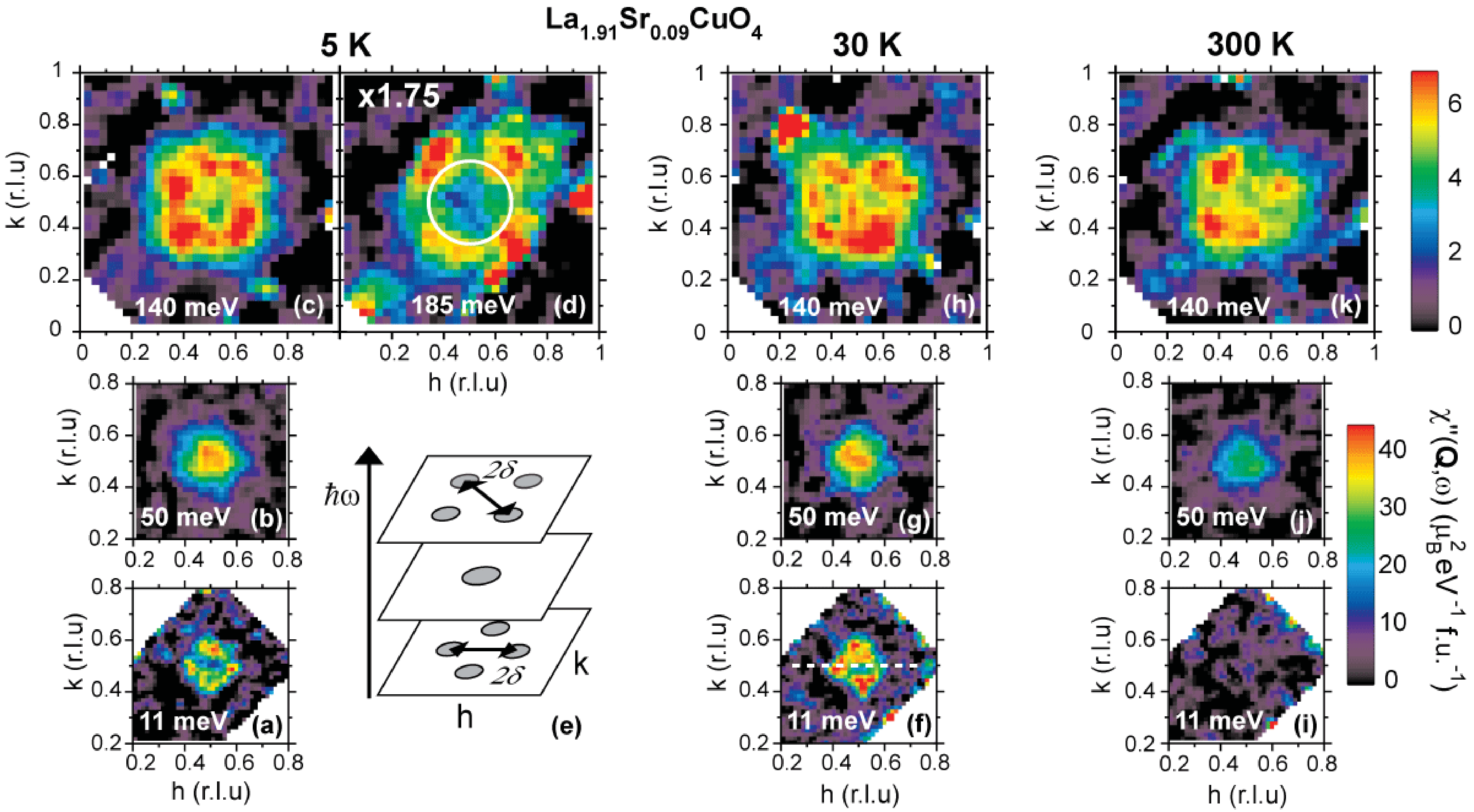
$La_{1.91}Sr_{0.09}CuO_4$ (T_c=22 K): **q**-dependent slices



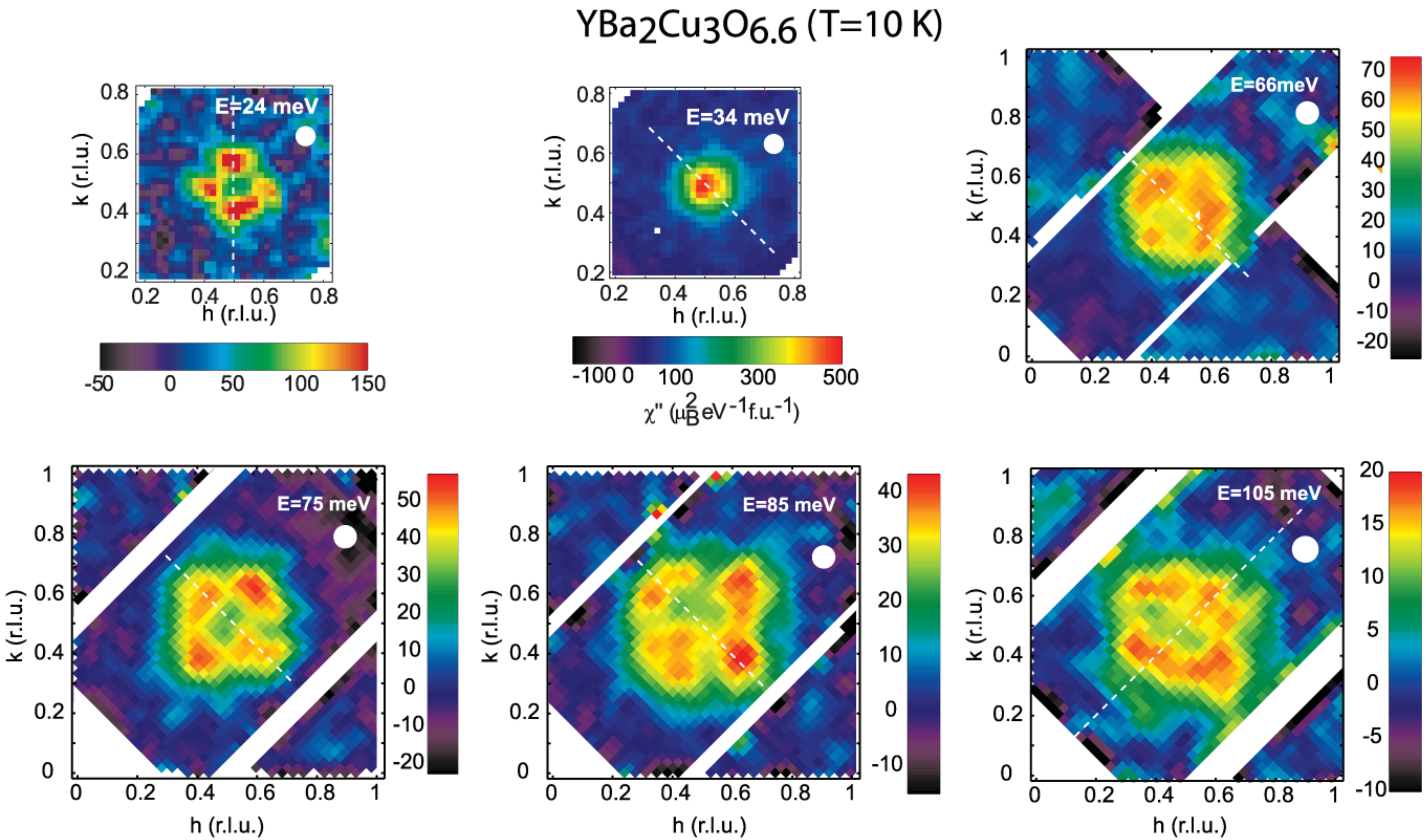
La_2CuO_4 : **q**-dependent slices



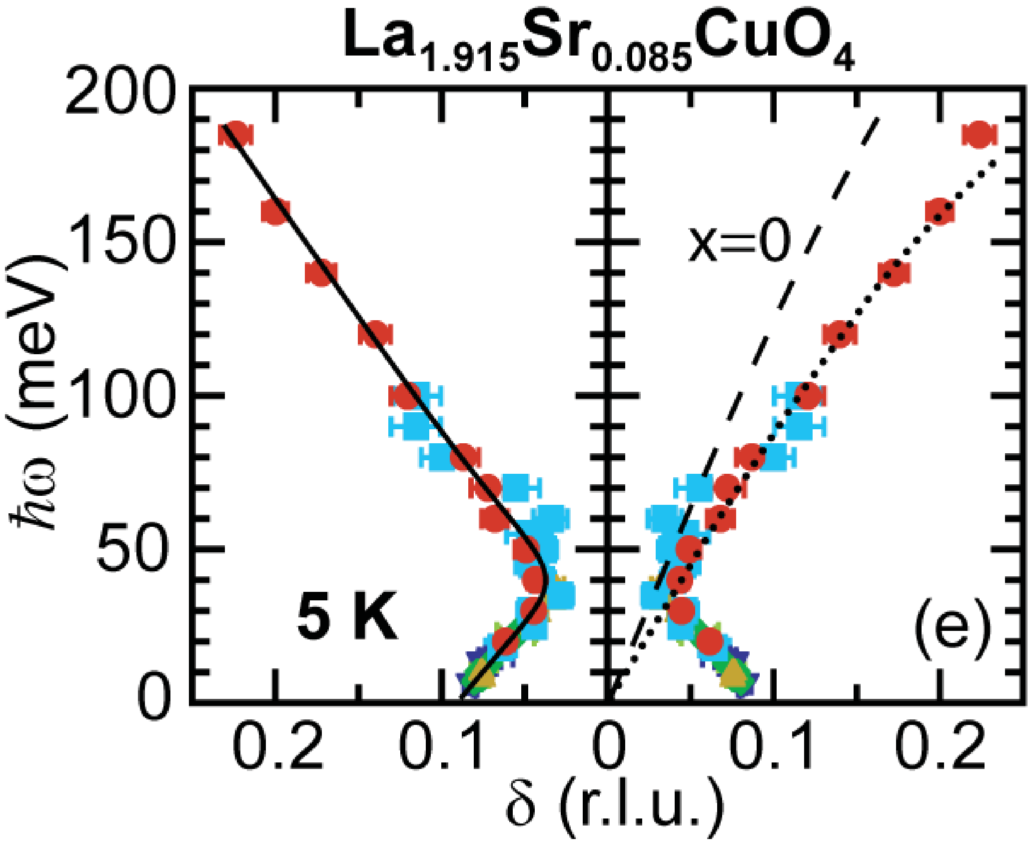
$La_{1.91}Sr_{0.09}CuO_4$ (T_c=22 K): **q**-dependent slices



High-energy magnetic excitations in $YBa_2Cu_3O_{6.6}$

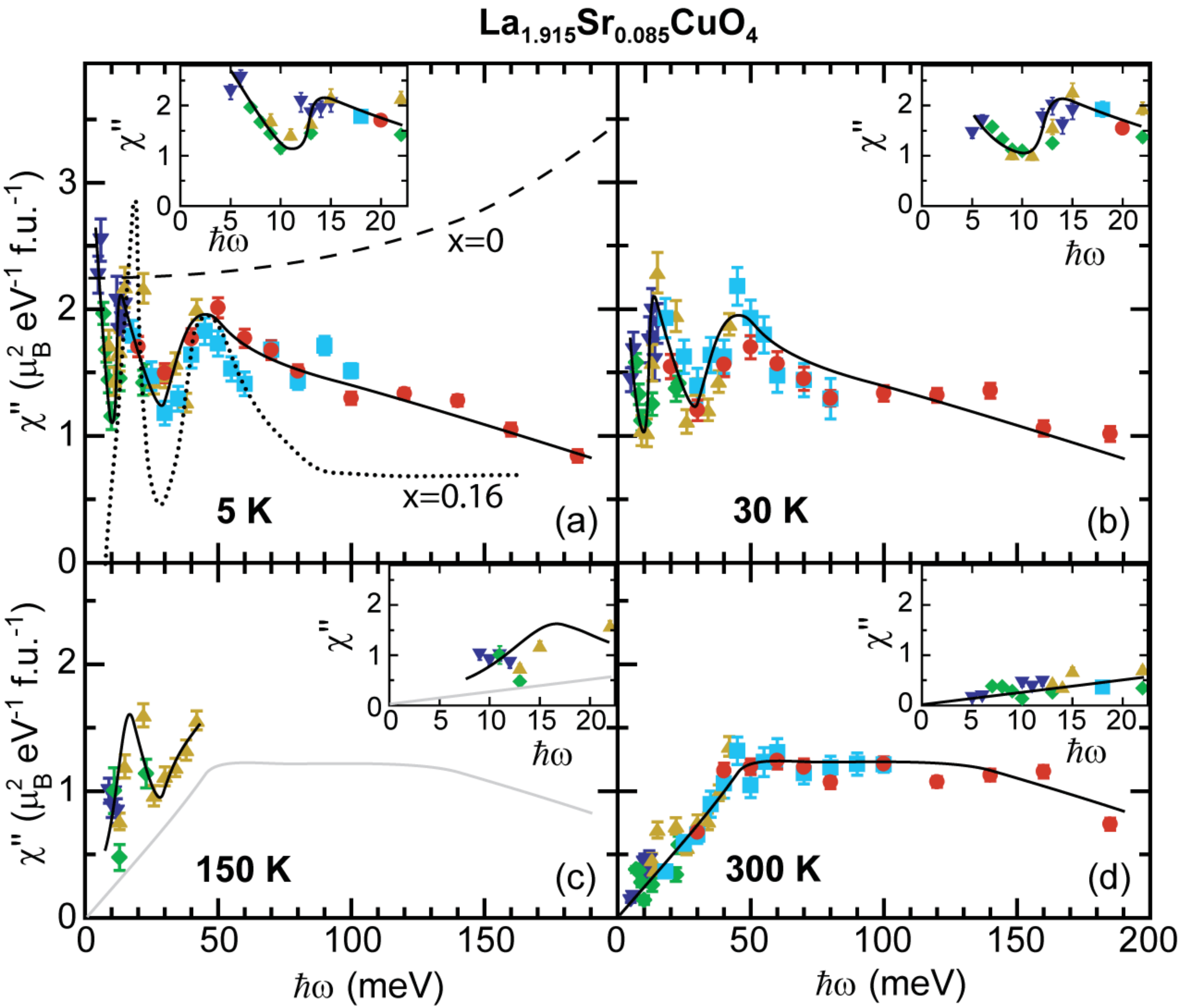


Incommensurability parameter

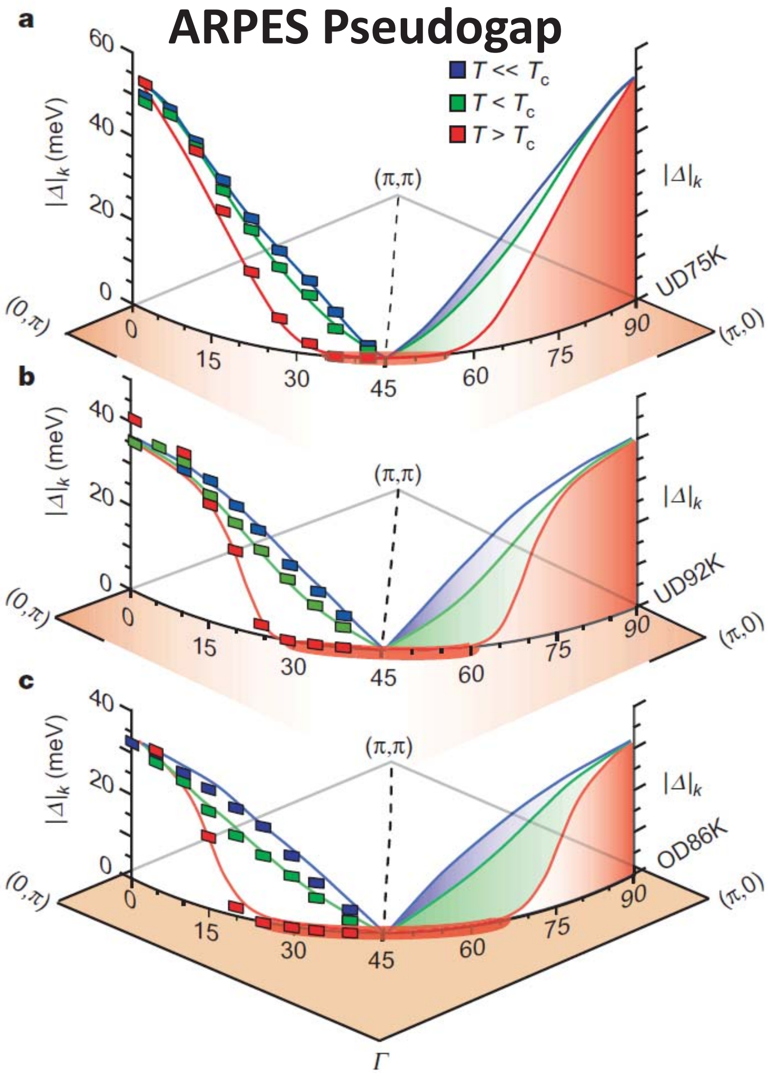


J=87(4) meV [cf J=146 meV in La2CuO4]

Local Susceptibility



Fermionic Excitations in Cuprates



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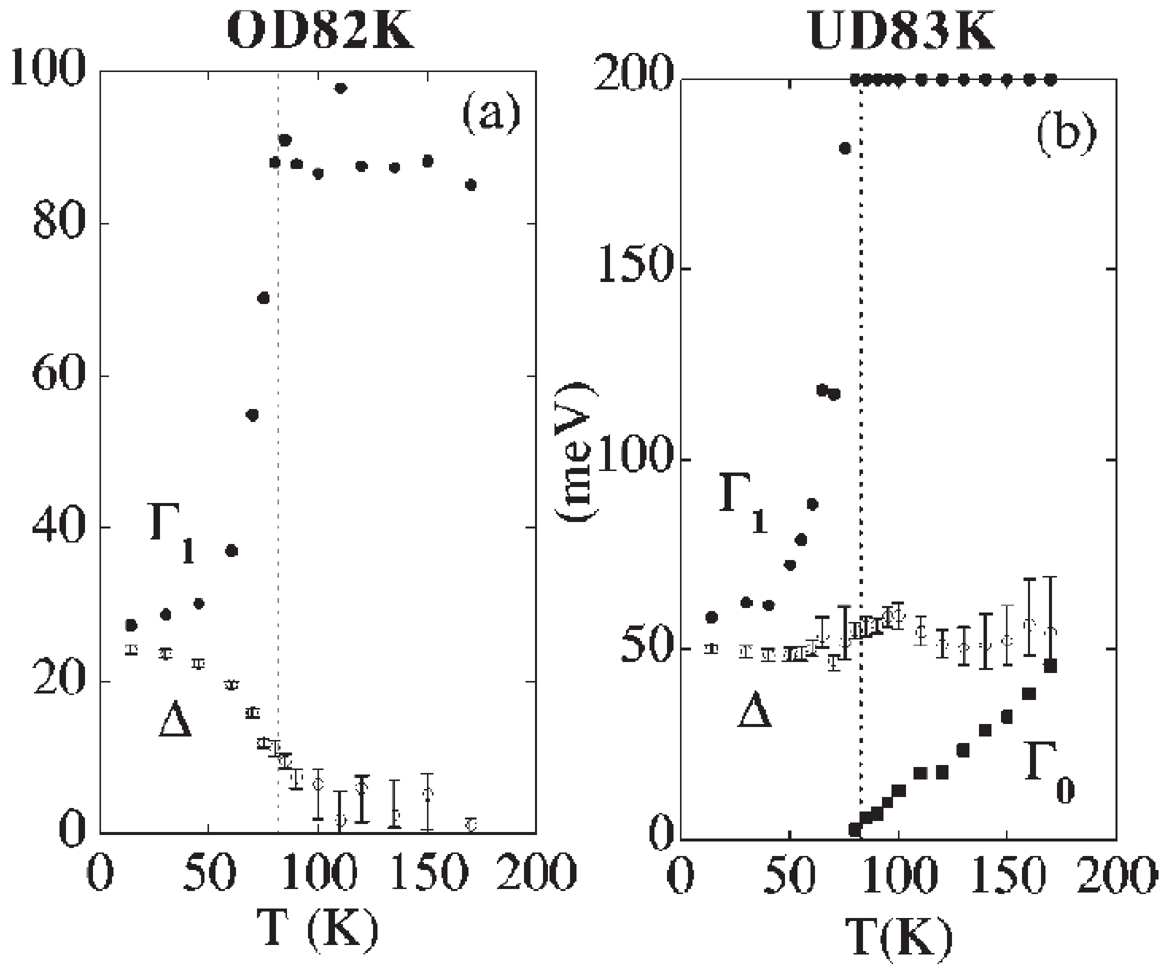
ARPES pseudogap



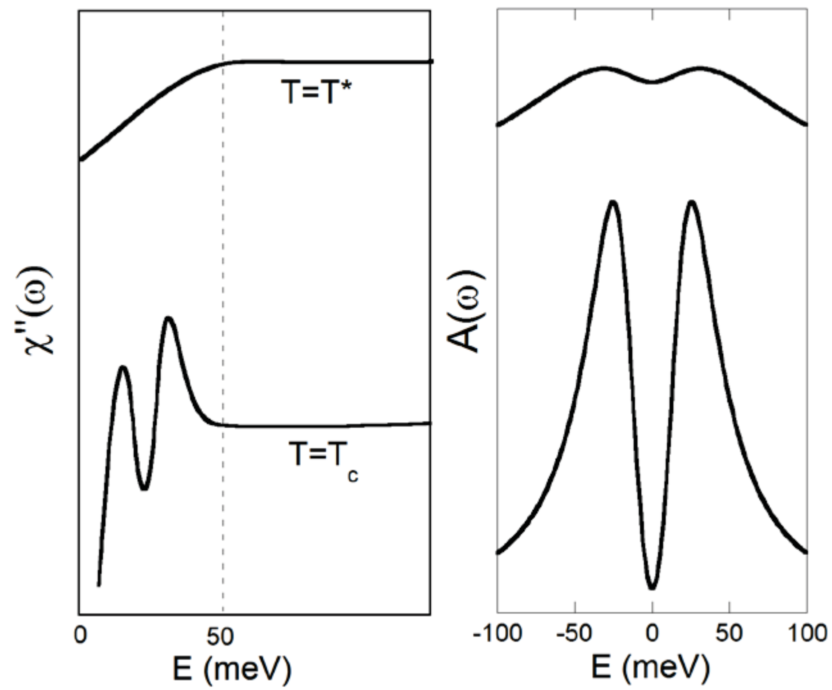
$Bi_2Sr_2CaCu_2O_{8+\delta}$

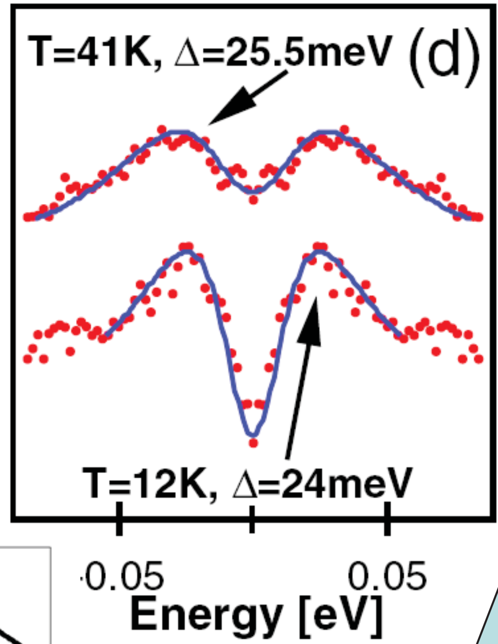
M. R. Norman *et al. PRB* **57**, R11093 (1998).

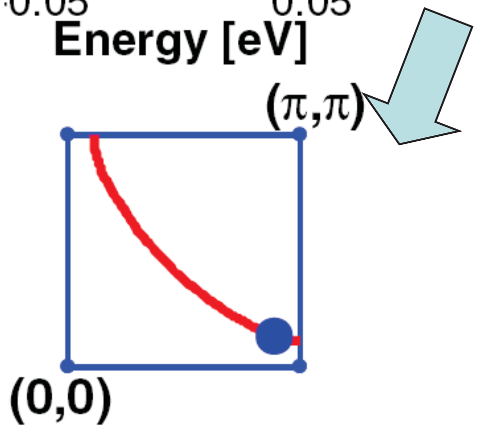
Phenomenological self energy

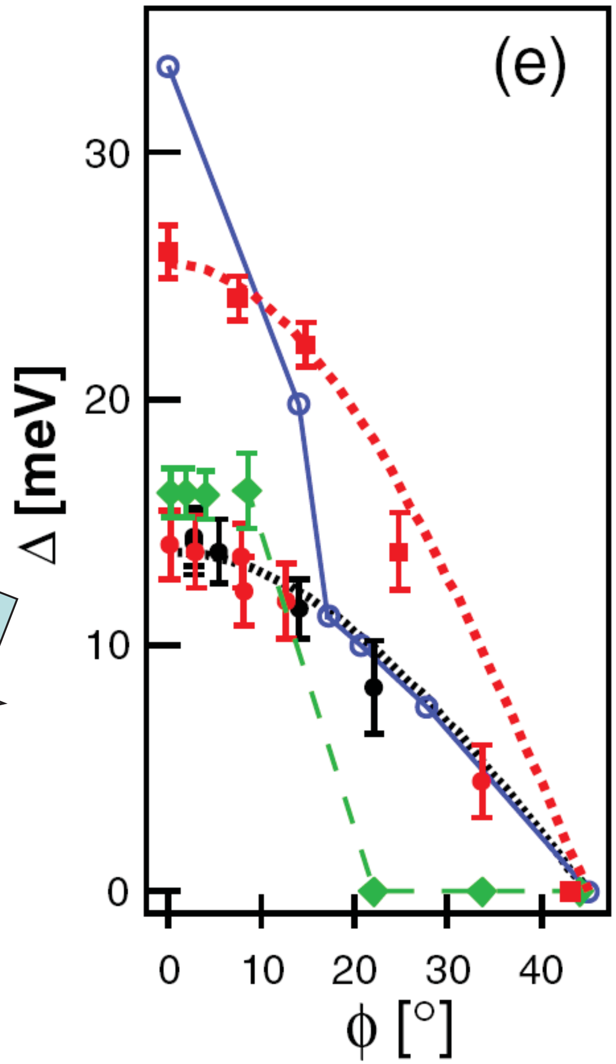
$$\Sigma(\mathbf{k},\omega) = -i\Gamma_1 + \Delta^2/(\omega + i\Gamma_0)$$

Pseudogap and ARPES in $La_{1.895}Sr_{0.105}CuO_4$



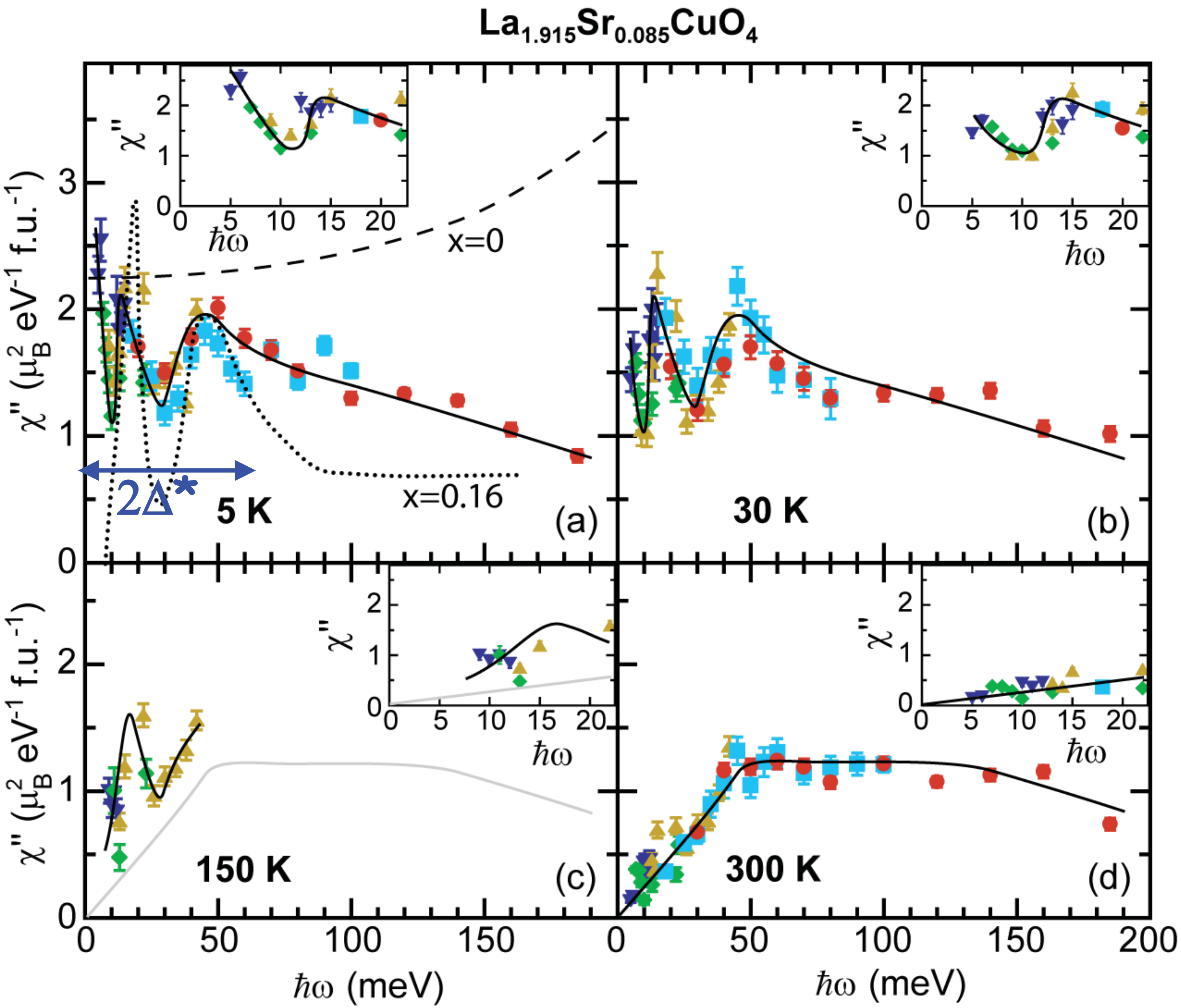






Shi et al. PRL 101, 047002 (2008)

Local Susceptibility



Summary

1) La_2CuO_4

• Néel state may be a "starting point" for ground state, but other wavefunctions must be added

•The deviations from the Néel state are strongest at (1/2,0)

• **Opportunity for comparison of experiment and numerical techniques**

• Open issues: cyclic exchange, difference between systems, relevance to HTC

2) $La_{1.91}Sr_{0.09}CuO_4$ UD22

• Pseudogap manifests itself in the magnetic response as a reduction of damping over wide energy scale.