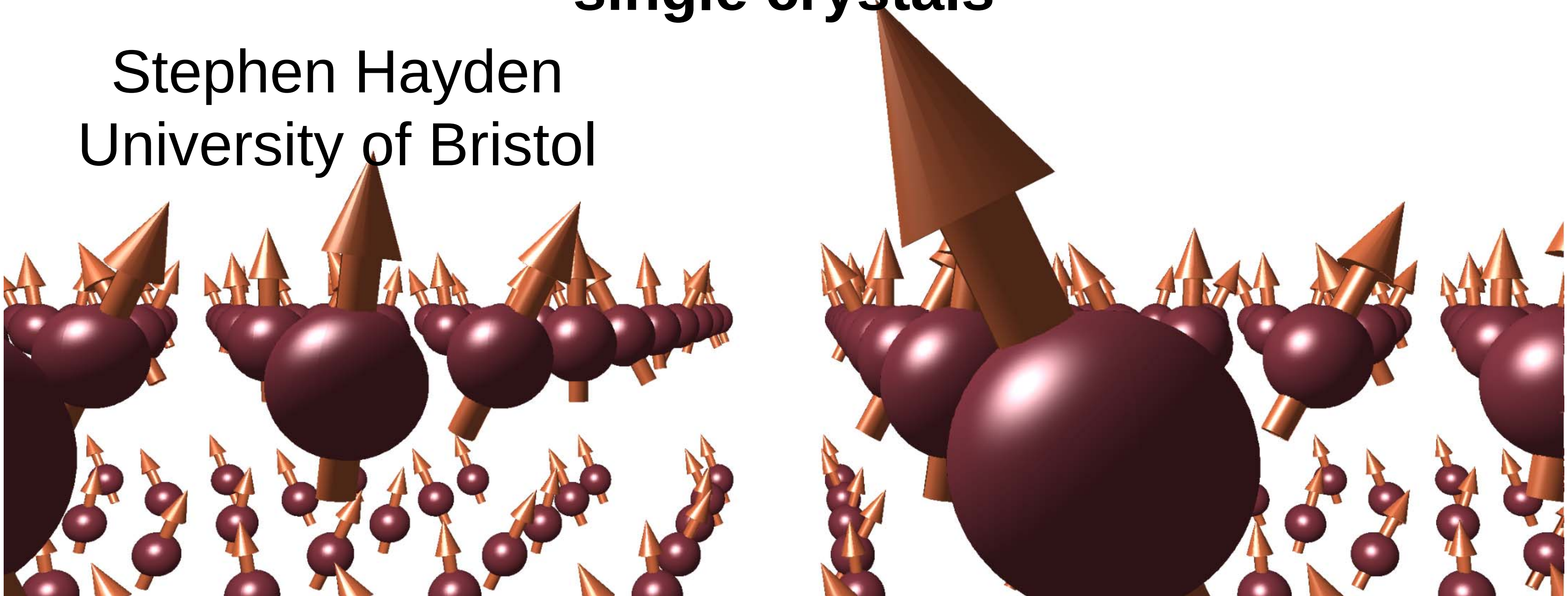
University of BRISTOL

Neutron spectroscopy of collective excitations in single crystals

Stephen Hayden
University of Bristol



Summer school on condensed matter research, Zuoz, August 2015.

Talk plan

I. Thinking about resolution (Three axis)
II. Direct geometry time-of-time Spectroscopy
III. Magnetic excitations in cuprates
IV. Magnetic excitations in $Sr_3Ru_2O_7$

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IV. Magnetic excitations in $Sr_3Ru_2O_7$

The story so far......

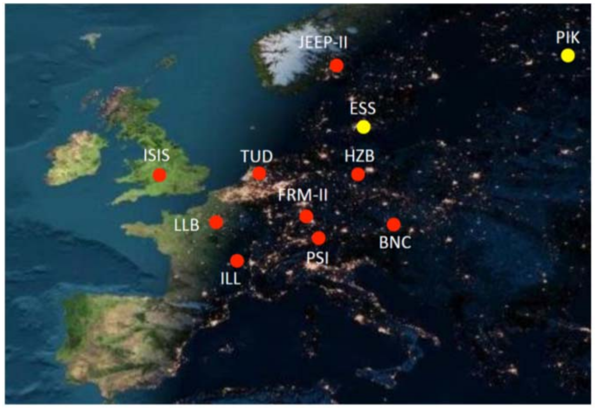
Summerschool on Condensed Matter Research, Zuoz, 15. August 2015 – 21. August 2015
Spectroscopy with Neutrons, Muons and Photons

	Sunday 16 Aug 2015	Monday 17 Aug 2015	Tuesday 18 Aug 2015	Wednesday 19 Aug 2015	Thursday 20 Aug 2015	Friday 21 Aug 2015
09:00 – 10:15	Neutron and Muon Sources - (HIPA, target E, SINQ and ESS) Mike Seidel	Introduction to MuSr practical - scientific problem to be analysed Rustem Khasanov	Using X-rays – general introduction and science examples Phil Willmott	Excursion	Practicals (in parallel) 1) Multiplet analysis (F. de Groot) 2) EXAFS analysis (C. Borca)	Neutron spectroscopy of collective excitations in single crystals Stephen Hayden
10:15 – 10:45	COFFEE	COFFEE	COFFEE		COFFEE	COFFEE
10:45 – 12:00	MuSr - techniques and instrumentation Hubertus Luetkens	Introduction to Neutron practical - scientific problem to be analysed Sandor Toth	Generating X-rays – the machines Riccardo Bartolini		Practicals (in parallel) 1) Multiplet analysis (F. de Groot) 2) EXAFS analysis (C. Borca)	New Developments (neutron optics mm) Peter Böni
12:15 – 15:30	Lunch and Free Afternoon	Lunch and Free Afternoon	Lunch and Free Afternoon		Lunch and Free Afternoon	Closing remarks Lunch Departure
15.30 – 16.00	COFFEE	COFFEE	COFFEE	COFFEE	COFFEE	
16:00 – 17:15	Neutrons – techniques and instrumentation Ken Anderson	Practicals (in parallel) 1) Muon Analysis (Z. Guguchia, P. Biswas) 2) Spin wave analysis (C. Rüegg, S. Toth)	Using X-rays – Instrumentation for spectroscopy Jan Dreiser	Introduction to Exafs practical – scientific problem to be analysed Camelia Borca	New developments photons: High brightness sources Christoph Quitmann	
17:15 – 17:30	SHORT BREAK	SHORT BREAK	SHORT BREAK	SHORT BREAK	SHORT BREAK	
17:30 – 18:15	CAMEA Henrik Rønnow	Practicals (in parallel) 1) Muon Analysis (Z. Guguchia, P. Biswas) 2) Spin wave analysis (C. Rüegg, S. Toth)	XFEL – techniques and instrumentation (time-resolved spectroscopy) Chris Milne	Introduction to Multiplet practical – scientific problem to be analysed Frank de Groot	Complementary methods, Optical spectroscopy Leonardo Degiorgi	
18.:15 – 18.45	Short poster presentation		Short poster presentation			
19:00 – 20:00	DINNER	DINNER	DINNER	DINNER	Apéro	
20:00 – 21:00	FREE EVENING	Supercomputing Thomas Schulthess	POSTER SESSION	Monitoring landcover / landuse with satellites and airborne systems Charlotte Steinmeier	BANQUET	

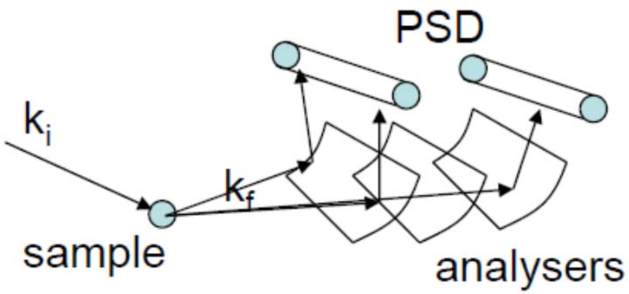
The story so far......

16:00 – 17:15	Neutrons – techniques and instrumentation **Ken Anderson**
17:15 – 17:30	SHORT BREAK
17:30 – 18:15	CAMEA **Henrik Rønnow**

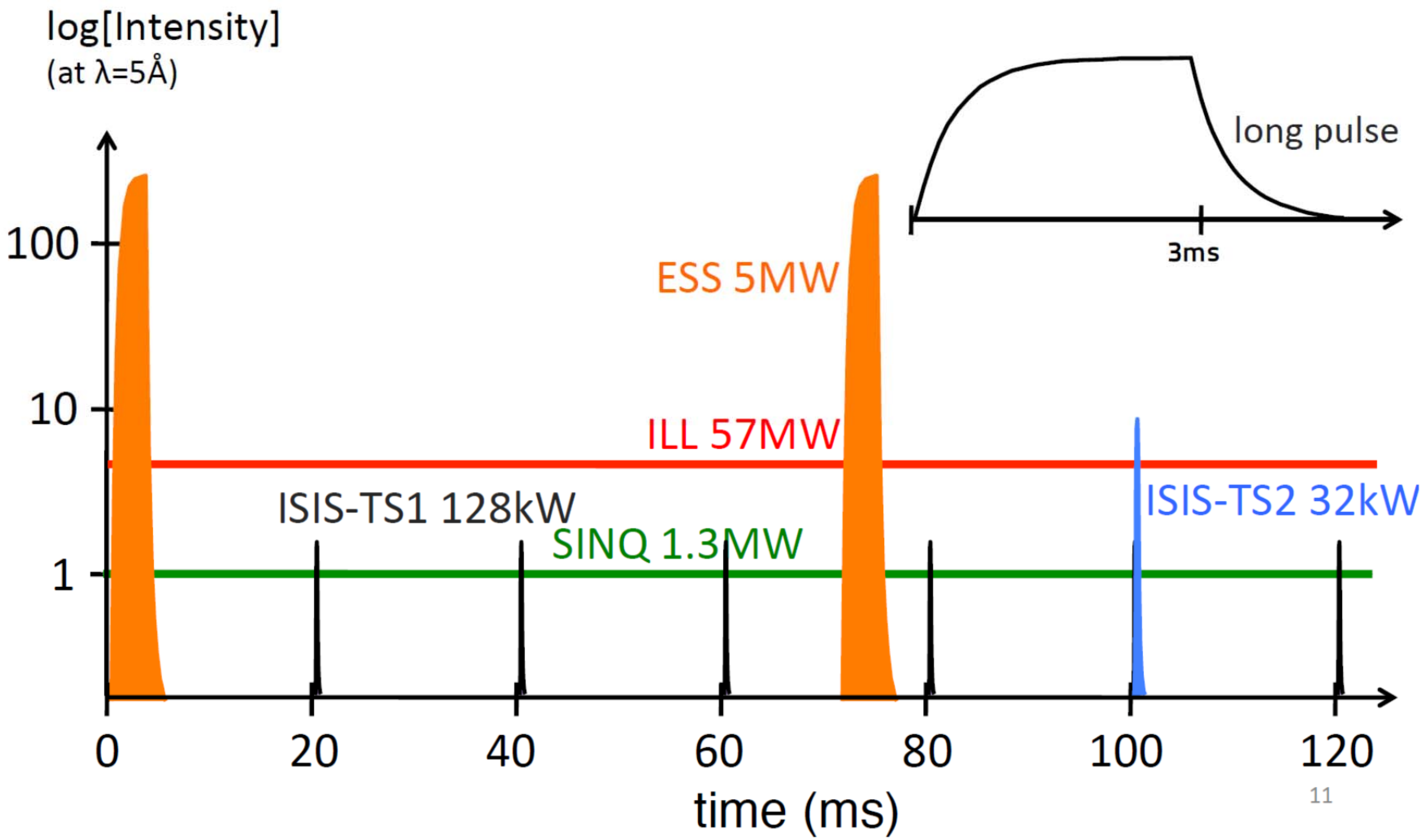
Neutron
Techniques and Instrumentation



CAMEA



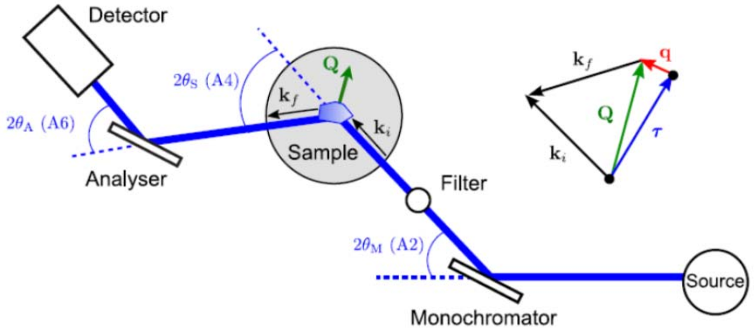
Time structure of neutron sources



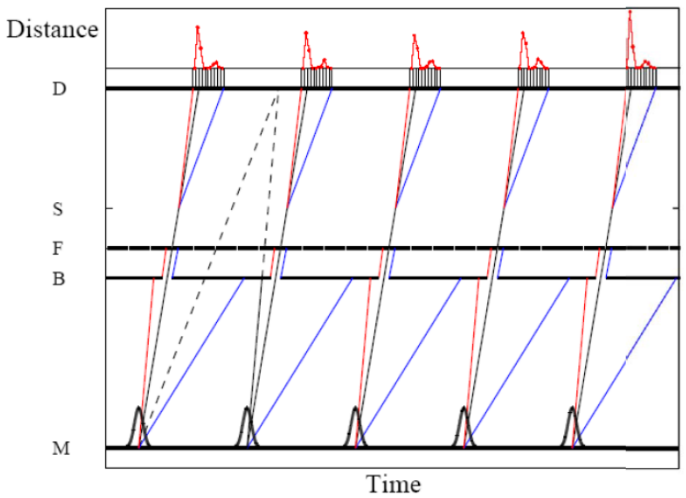
from K Anderson

TAS and ToF

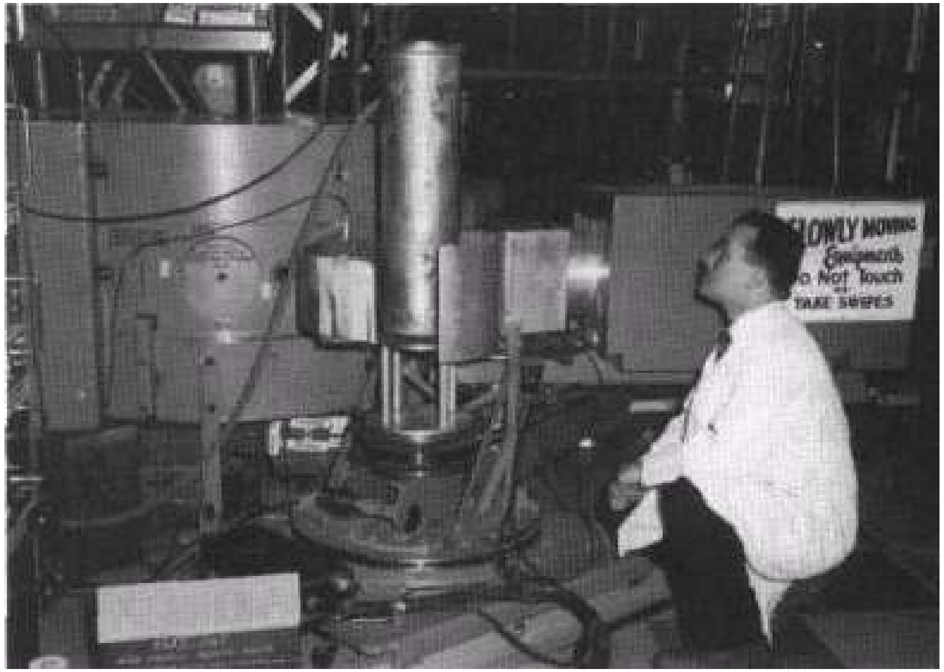
Triple axis spectrometer



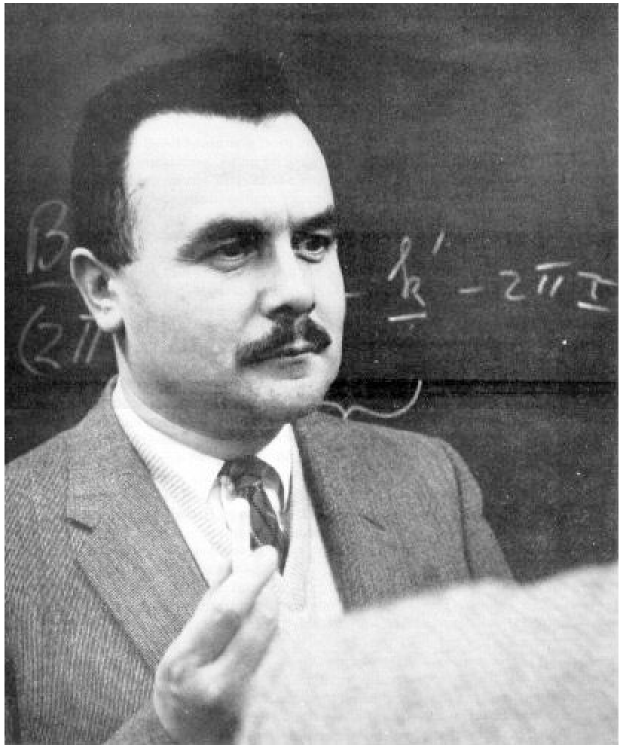
Time of flight spectrometer



Triple Axis Spectrometer

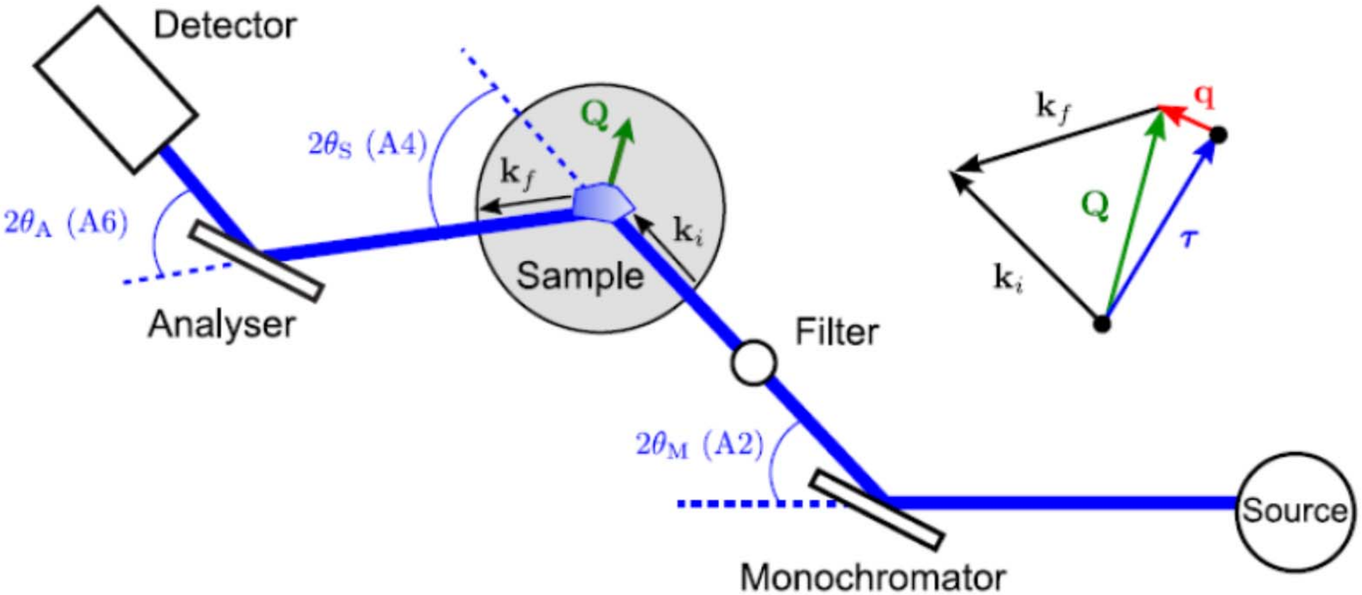


Triple-axis spectrometer installed at NRU in Chalk River, 1958



Bert Brockhouse (1918 –2003), Noble prize, 1994

Triple Axis Spectrometer



$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$$

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

$(\mathbf{Q}, \omega)$ refer to the *excitation*.

Typical cross sections

Phonons vs. magnetic excitations

Phonons

$$\left(\frac{\partial^2\sigma}{\partial\Omega\partial E'}\right)_{phonon} \propto \frac{\sigma_{coh}}{4\pi}\frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}\frac{1}{2M}\exp(-2W)x$$

$$\sum_s\sum_\tau \frac{(\vec{Q}\cdot\vec{e}_s)^2}{\omega_s}\left[(n(\omega_s)+1)\delta(\omega-\omega_s)\delta(\vec{Q}-\vec{q}-\vec{\tau})+n(\omega_s)\delta(\omega+\omega_s)\delta(\vec{Q}+\vec{q}-\vec{\tau})\right]$$

Increases with **Q**

Increases with T

$$\left(\frac{\partial^2\sigma}{\partial\Omega\partial E'}\right)_{mag} \propto \frac{k_f}{k_i}\left\{\frac{1}{2}gF(\vec{Q})\right\}^2\sum_{\alpha\beta}\left(\delta_{\alpha\beta}-\hat{Q}_\alpha\hat{Q}_\beta\right)\sum_{ll'}\exp\left(i\vec{Q}\cdot(\vec{l}-\vec{l}')\right)\int\left\langle S_0^\alpha(0)S_l^\beta(t)\right\rangle\exp(-i\omega t)dt$$

Decreases with **Q**

Bose statistics for simple ordered systems (FM, AFM, etc.).
Spreads in **Q** and ħω at high T
Limited by sum-rules

+ Neutron polarisation analysis

from H Ronnow

Scattering Law

We can write the neutron scattering cross section using the general form:

$$\frac{d^2\sigma}{d\Omega\, dE_f} = \frac{k_f}{k_i} S(\mathbf{q}, \hbar\omega)$$

or

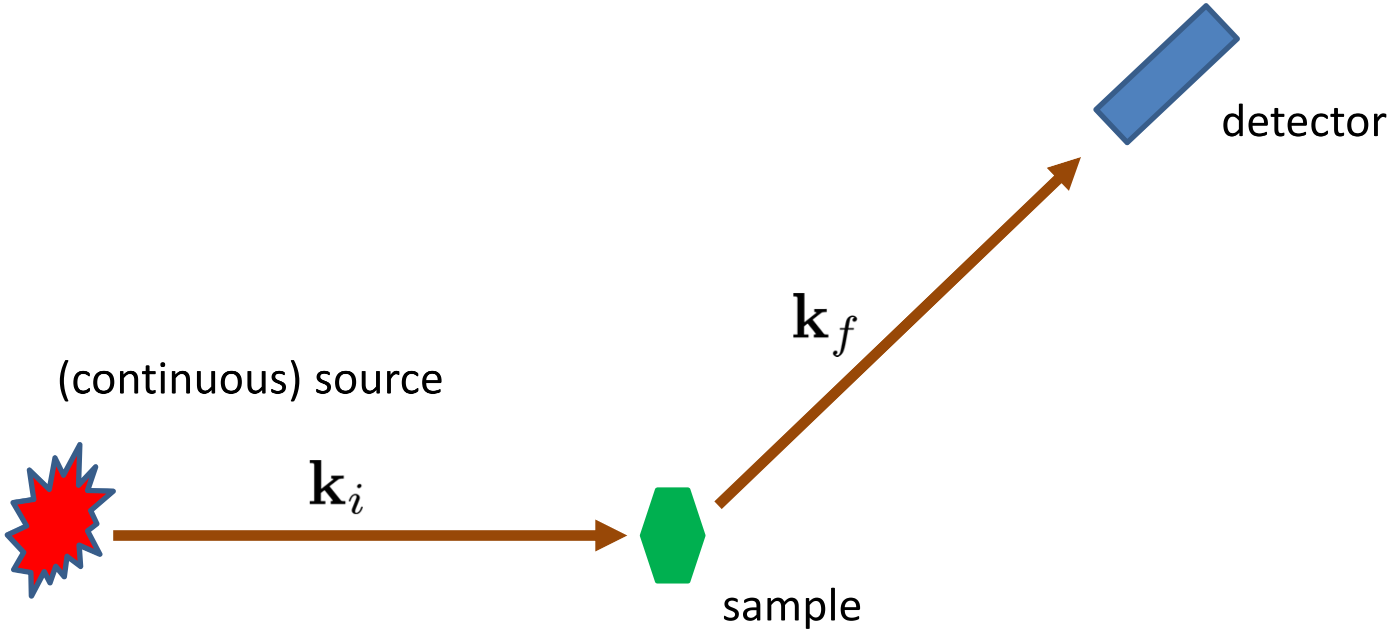
$$\frac{k_i}{k_f} \frac{d^2\sigma}{d\Omega\, dE_f} = S(\mathbf{q}, \hbar\omega)$$

six coordinates $(\mathbf{k}_i, \mathbf{k}_f)$

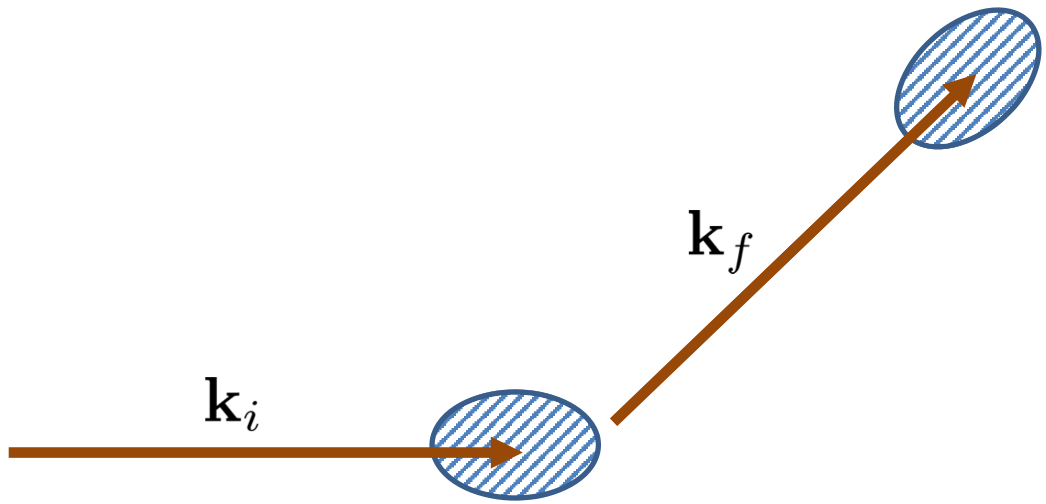
four coordinates $(\mathbf{Q}, \hbar\omega)$

$$\left.\begin{aligned} \mathbf{Q} &= \mathbf{k}_i - \mathbf{k}_f \\ \hbar\omega &= E_i - E_f \end{aligned}\right\}$$ Transform with Jacobian

Schematic of inelastic scattering experiment



Resolutions and Phase Space



Definitions

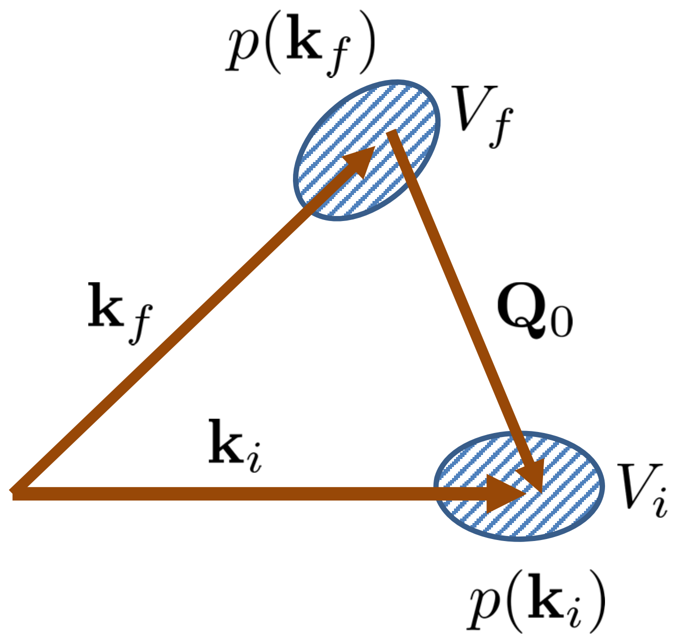
$$d\Omega_f = \frac{dk_{f,x}\, dk_{f,y}}{k_f^2}; \quad dE_f = \frac{\hbar^2 k_f}{m} dk_{f,z}$$

- $p(\mathbf{k}_i)$ is the probability that a neutron leaves the source and hits the sample with wavevector $\mathbf{k}_i$
- $p(\mathbf{k}_f)$ is the probability that a neutron with wavevector $\mathbf{k}_f$ passes the analyer system an is detected.
- $S(\mathbf{Q}, \omega)$ is proportional to the probablity that a neutron is scattered from $\mathbf{k}_i$ to $\mathbf{k}_f$

Resolutions and Phase Space

$$\begin{aligned} I &\propto S(\mathbf{Q},\omega)p_i(\mathbf{k}_i)p_f(\mathbf{k}_f)\, dk_{ix}\, dk_{iy}\, dk_{iz}\, dk_{fx}\, dk_{fy}\, dk_{fz} \\ &\propto S(\mathbf{Q},\omega)\, p_i(\mathbf{k}_i)\, p_f(\mathbf{k}_f)\, dV_i\, dV_f \end{aligned}$$

small deviations

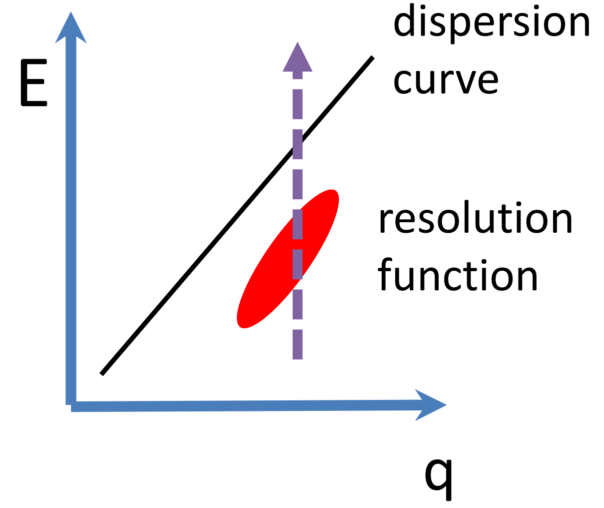


$$I(\mathbf{Q}_0,\omega_0) = A \int S(\mathbf{Q},\omega)\, R(\mathbf{Q}-\mathbf{Q_0},\omega-\omega_0)\, d^3Q\, d\omega$$

See B. Dorner Acta Cryst. A28, 319 (1972).

Qualitative properties of the resolution function

- resolution volumes increase with k_i and k_f. $V_i \propto k_i^3 \cot\theta_M$
- convolution of volumes can lead to focussing
- vertical focussing leads to poor resolution along z.



Programs to calculate resolution function:

RESTRAX	http://neutron.ujf.cas.cz/restrax/
McStas	http://www.mcstas.org/

Key references:

MAIER-LEIBNITZ, H. (1966). Nukleonik, 8, 61.
COOPER, M. J. and NATHANS, R. (1967). Acta Cryst. 23, 357.

Talk plan

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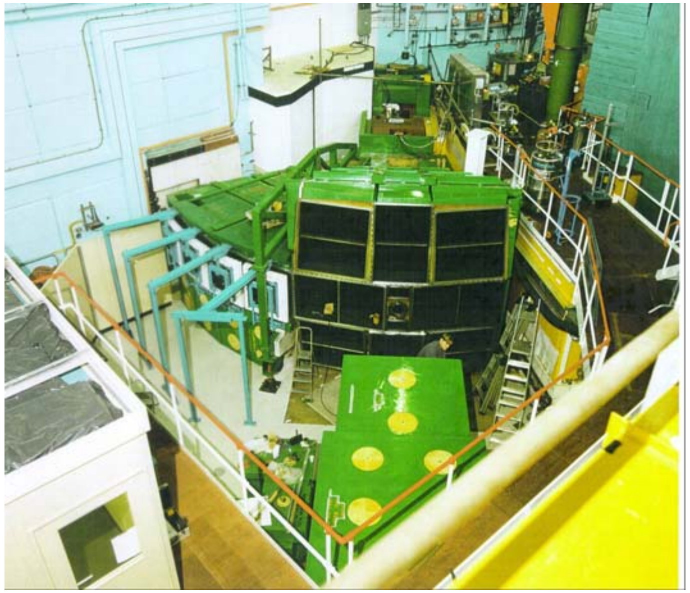
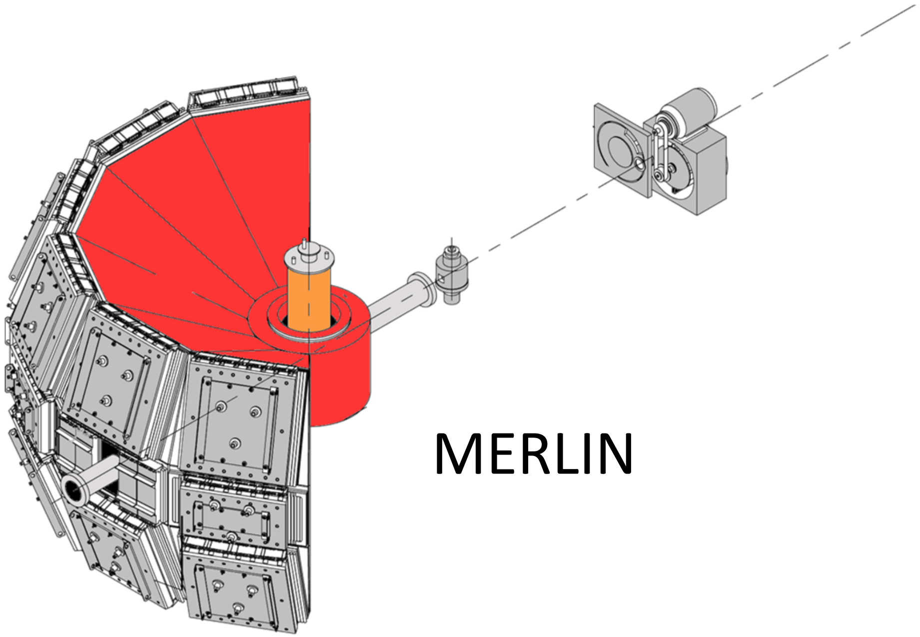
Direct geometry Time-of-time Spectroscopy

Spectrometers at ISIS



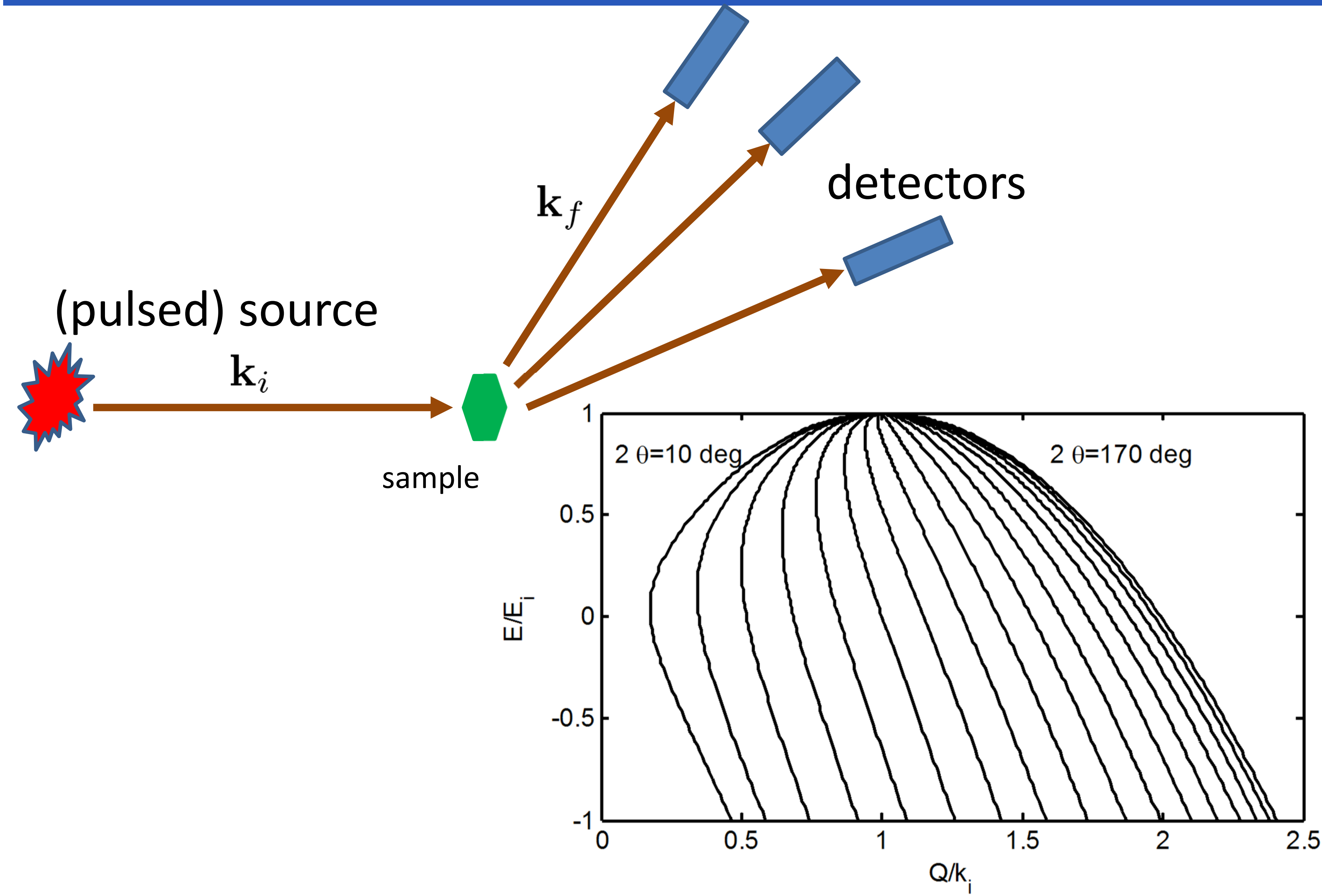
MAPS



MERLIN

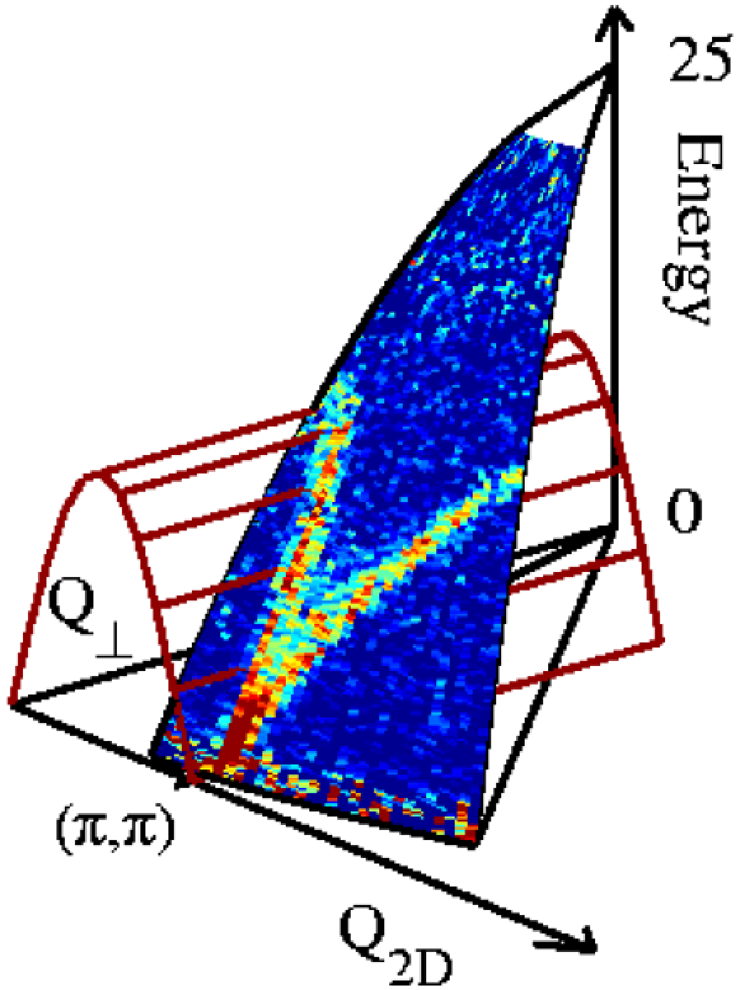
LET

Direct geometry ToF (one detector or a line)



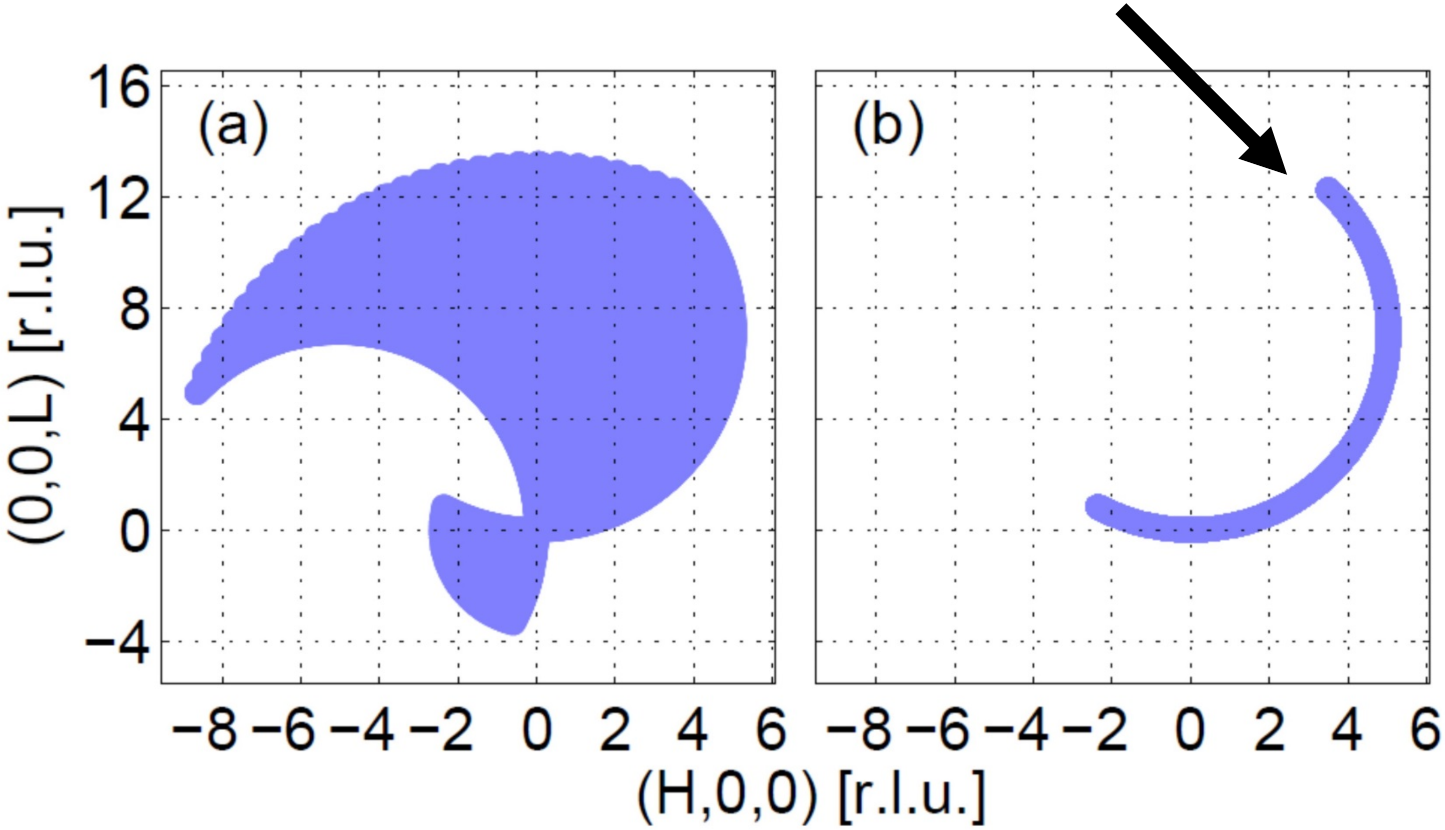
Direct geometry ToF (line of detectors)

and 1D system...



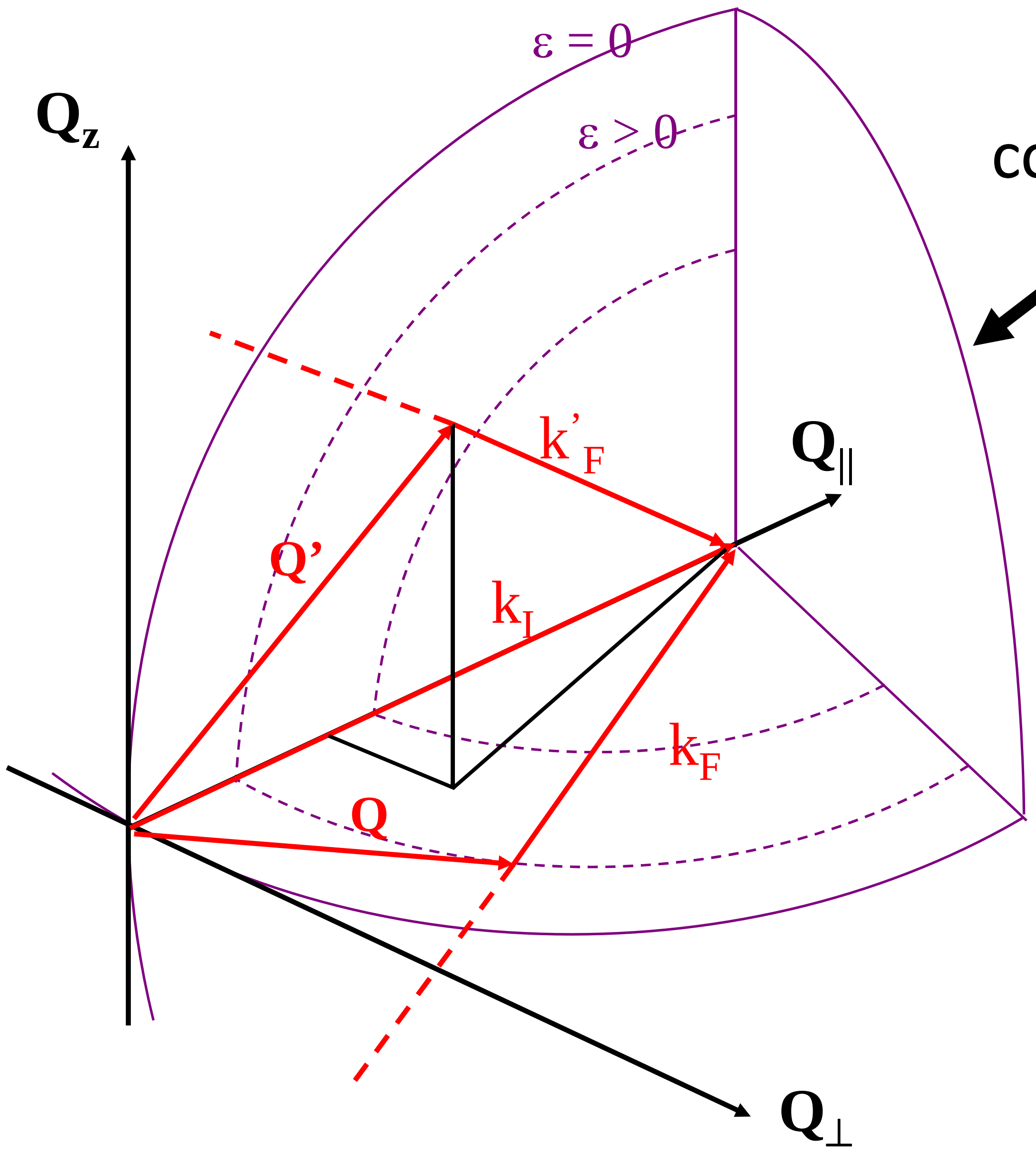
Rotating sample

constant energy transfer



credit: R Ewings

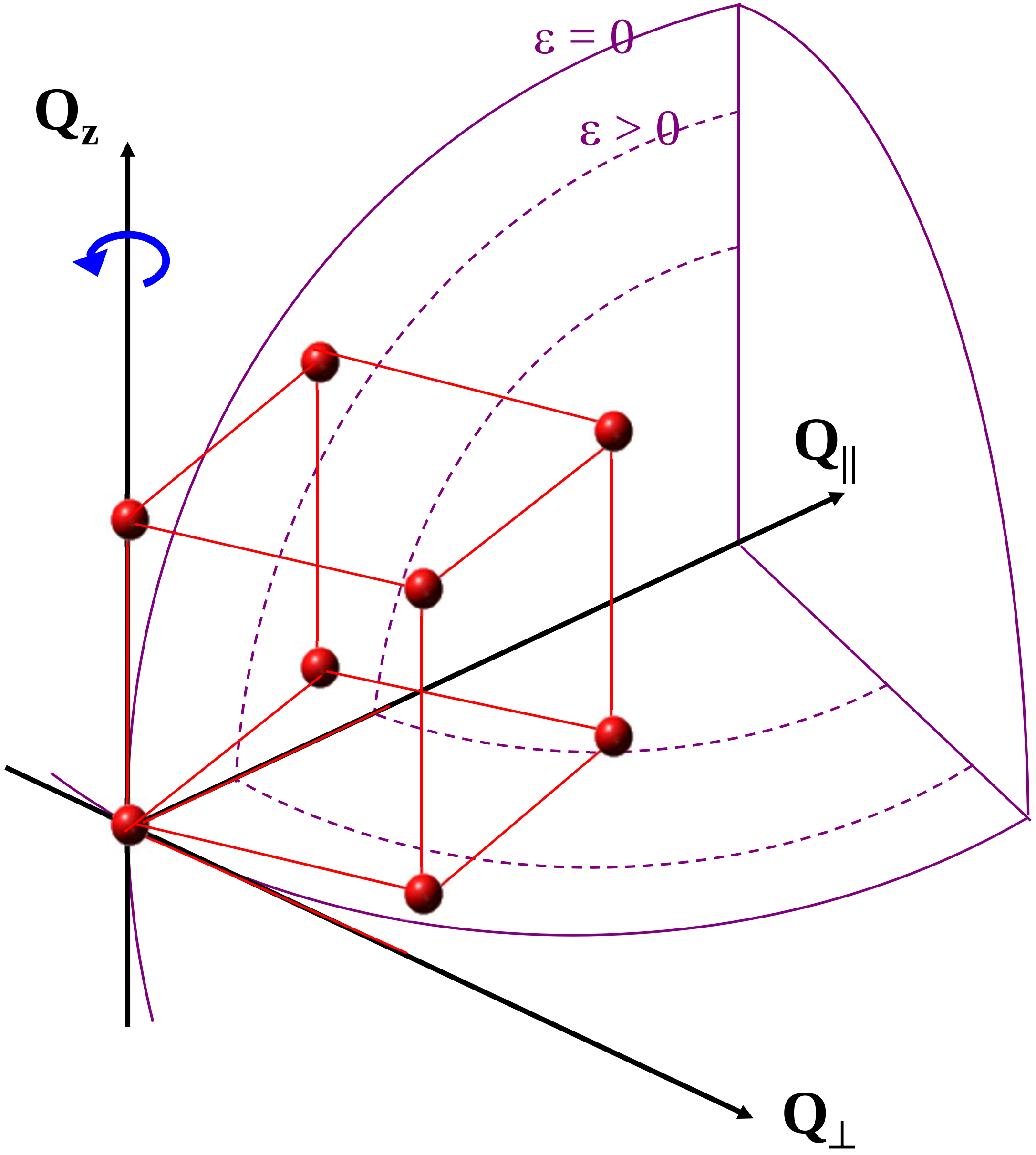
2-D (area) of detectors



constant energy spheres

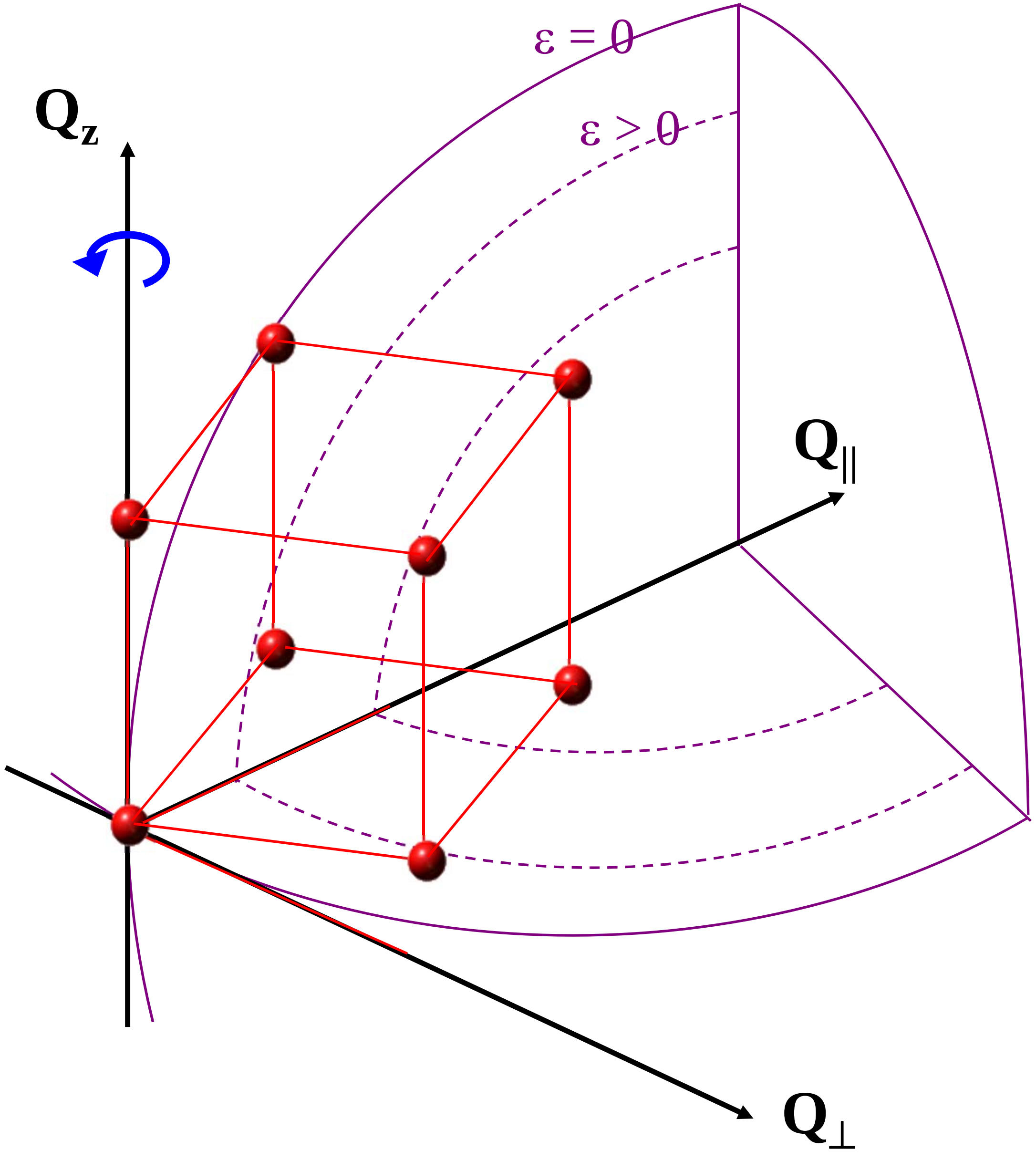
credit: T Perring

2-D (area) of detectors : rotate sample



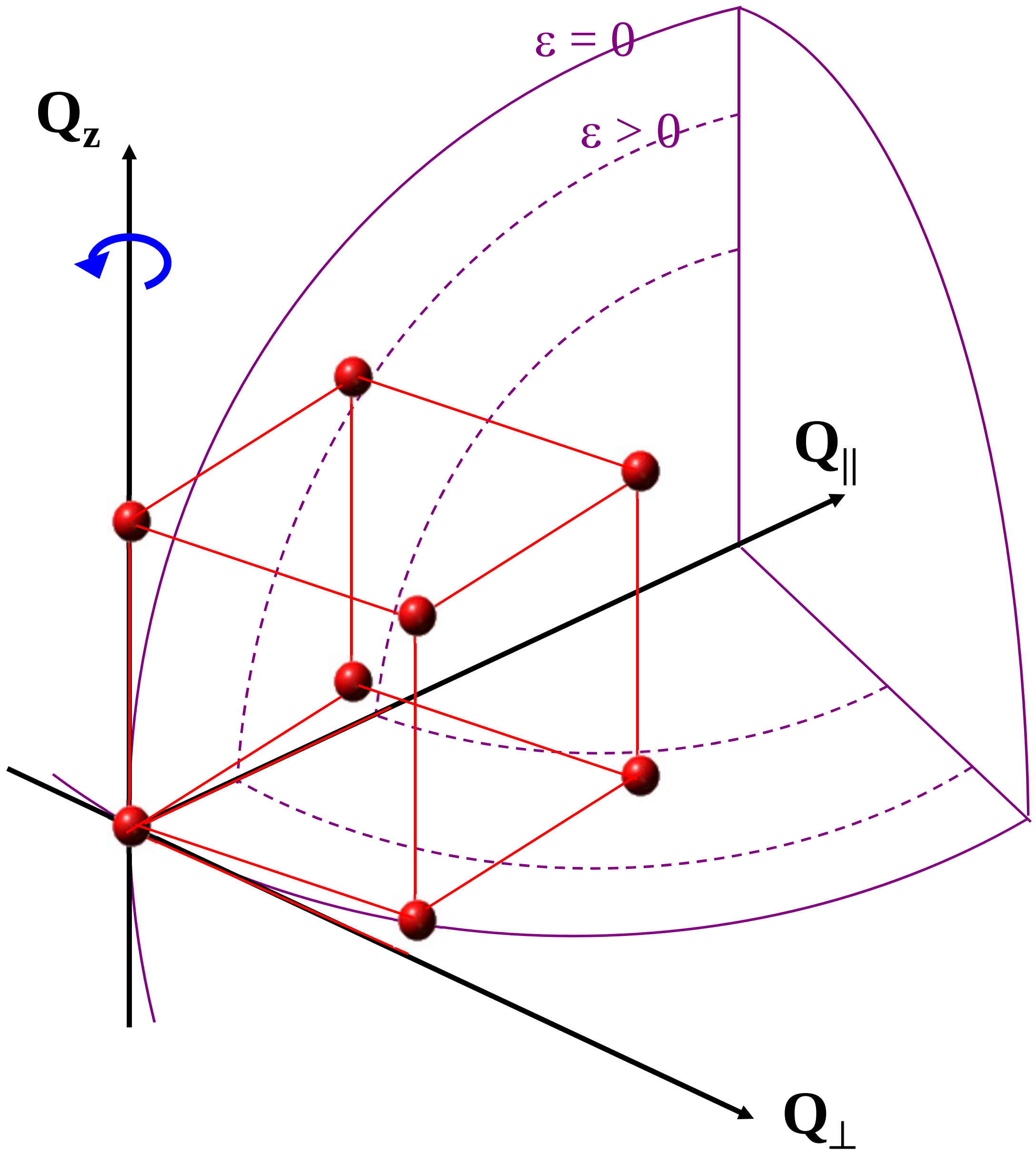
credit: T Perring

2-D (area) of detectors : rotate sample



credit: T Perring

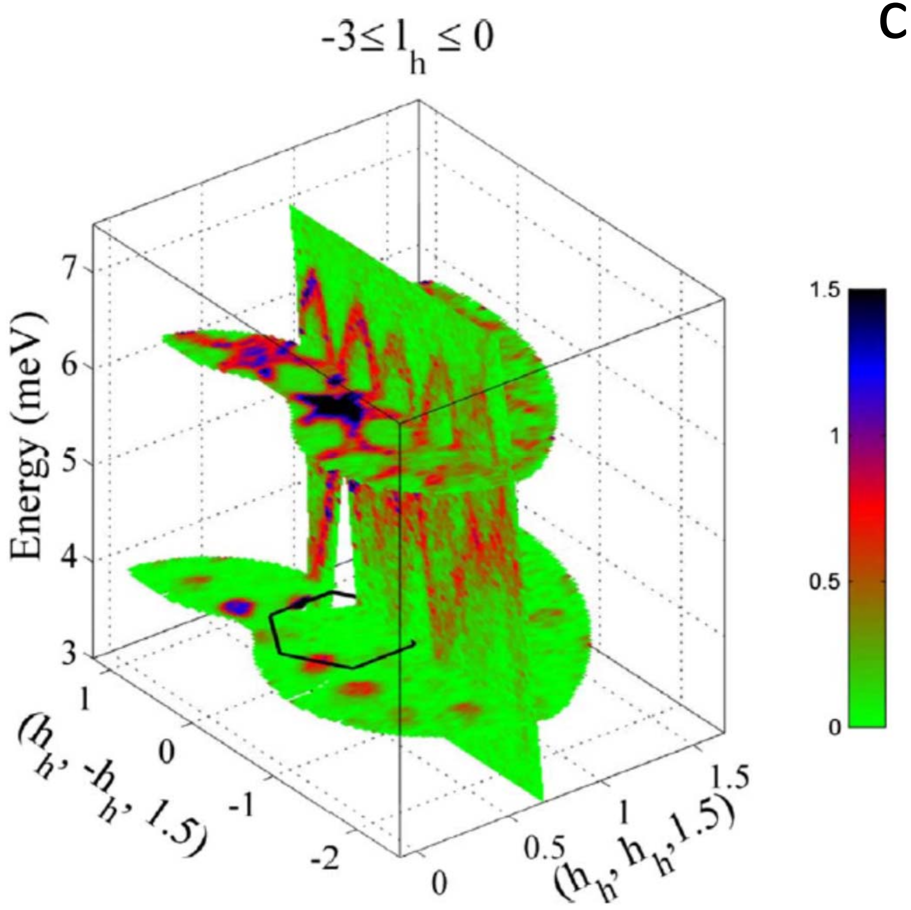
2-D (area) of detectors : rotate sample



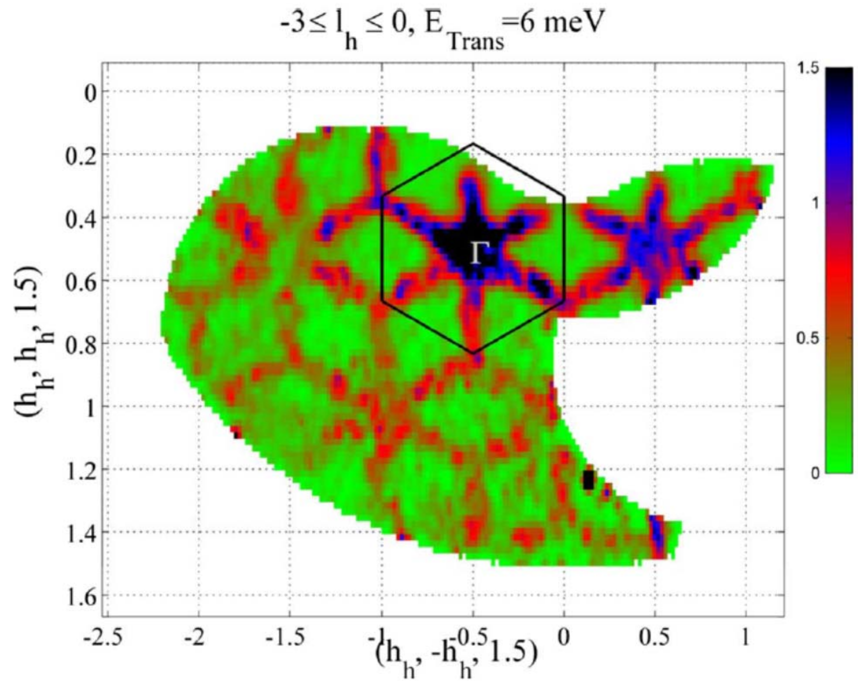
credit: T Perring

Example of 'Horaced' data

Spin dimer antiferromagnet $Sr_3Cr_2O_8$ MERLIN



cut through 4-D space of data



D. L. Quintero-Castro et al., PRB **81**, 014415 (2010)

Talk plan

I. Thinking about resolution (Three axis)
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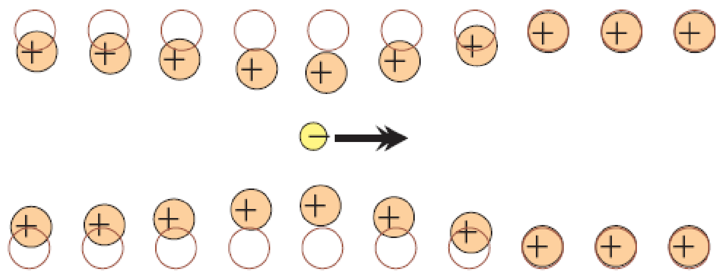
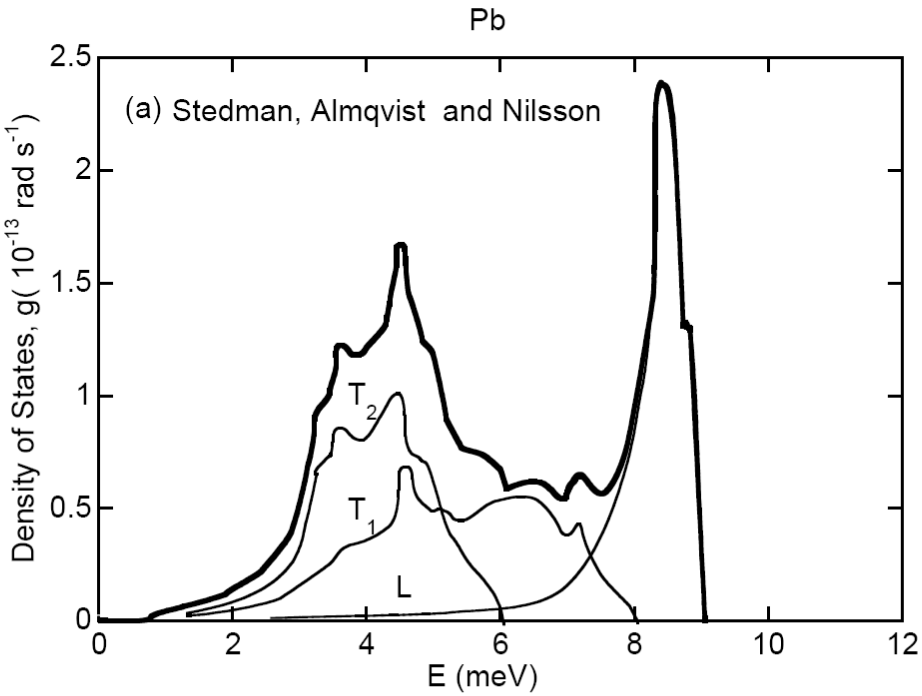
III. Magnetic excitations in cuprates
IV. Magnetic excitations in $Sr_3Ru_2O_7$

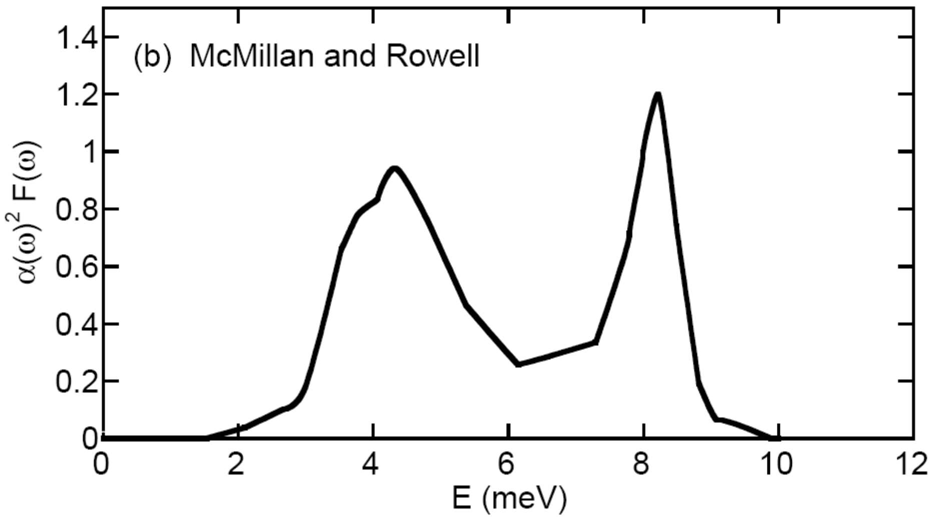
Magnetic excitations in cuprates

I. The pairing glue
II. Neutron scattering in $La_{2-x}Sr_xCuO_4$
III. Parent antiferromagnet
IV. Optimal doping
V. Overdoped
VI. Summary

"Phonon glue" in lead







- phonon DOS, $F(\omega)$

- $\alpha^2(\omega)\,F(\omega)$ from SIS tunnelling

SIS Tunnelling in Conventional Superconductors

Magnetically mediated pairing

$$V_{kk'} = g^2 \chi(q)$$

Pairing Interaction

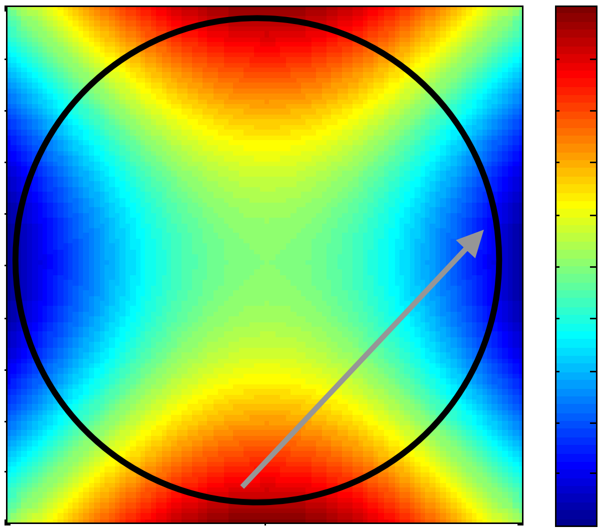
$$\Delta_k = -\sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2\sqrt{\varepsilon_{k'}^2 + \Delta_{k'}^2}}$$

Gap equation

favours states where Δ_k changes sign over Fermi surface

Gap functions

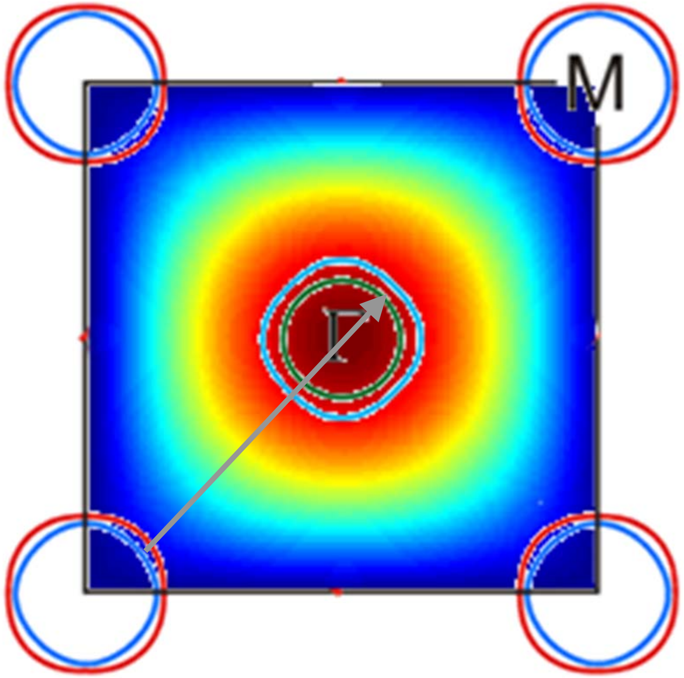
cuprates



$d_{x^2-y^2}$

$$\Delta_k = \Delta_0(\cos k_x - \cos k_y)$$

pnictides



$s_\pm$

$$\Delta_k = \Delta_0 \cos k_x \cos k_y$$

Mazin et al, PRL 08

Magnetic excitations in cuprates

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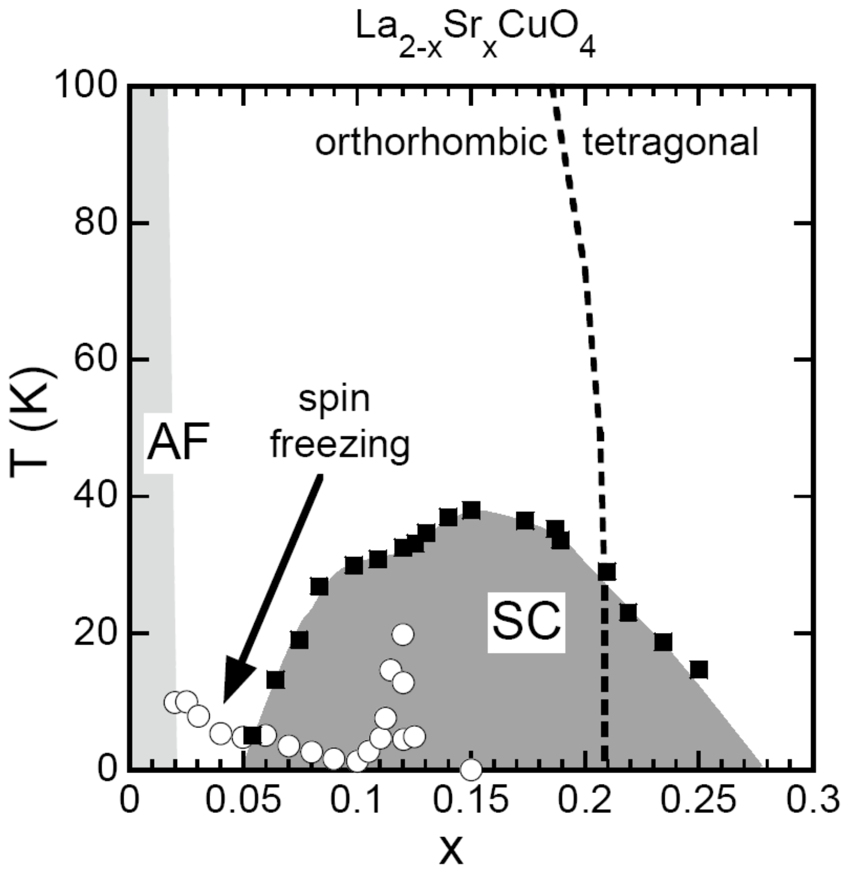
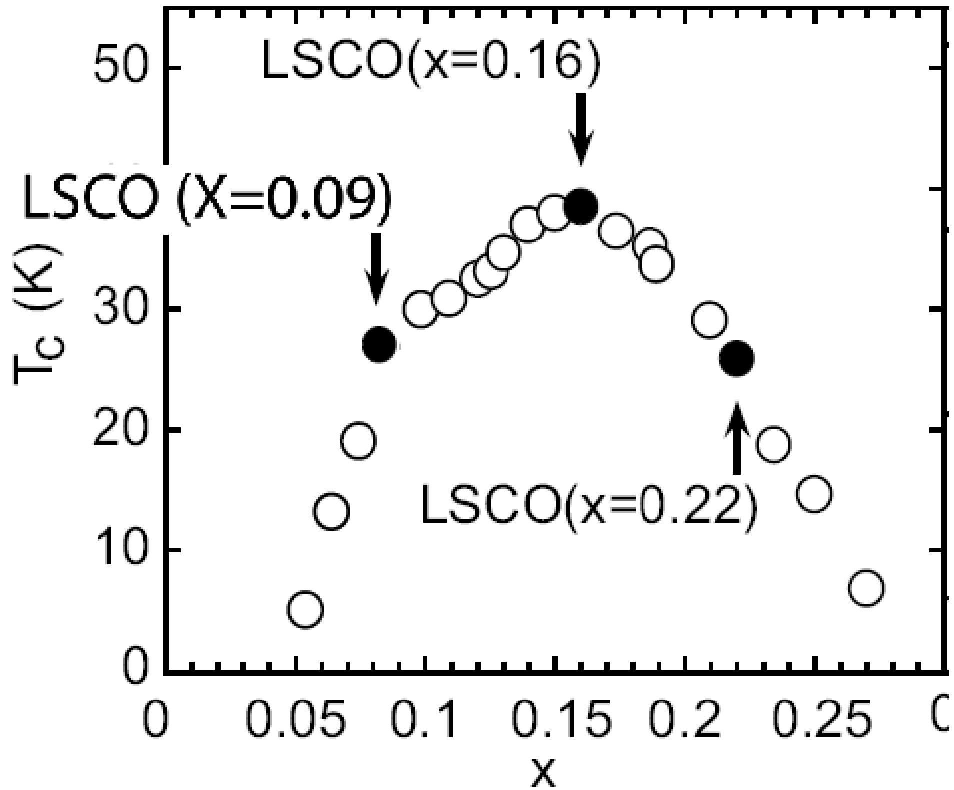
Spin fluctuations in $La_{2-x}Sr_xCuO_4$

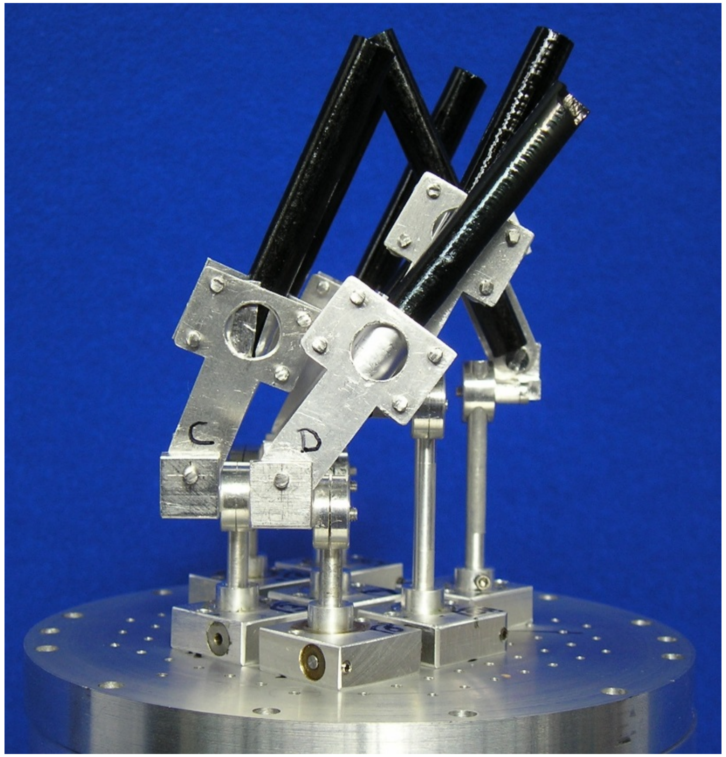


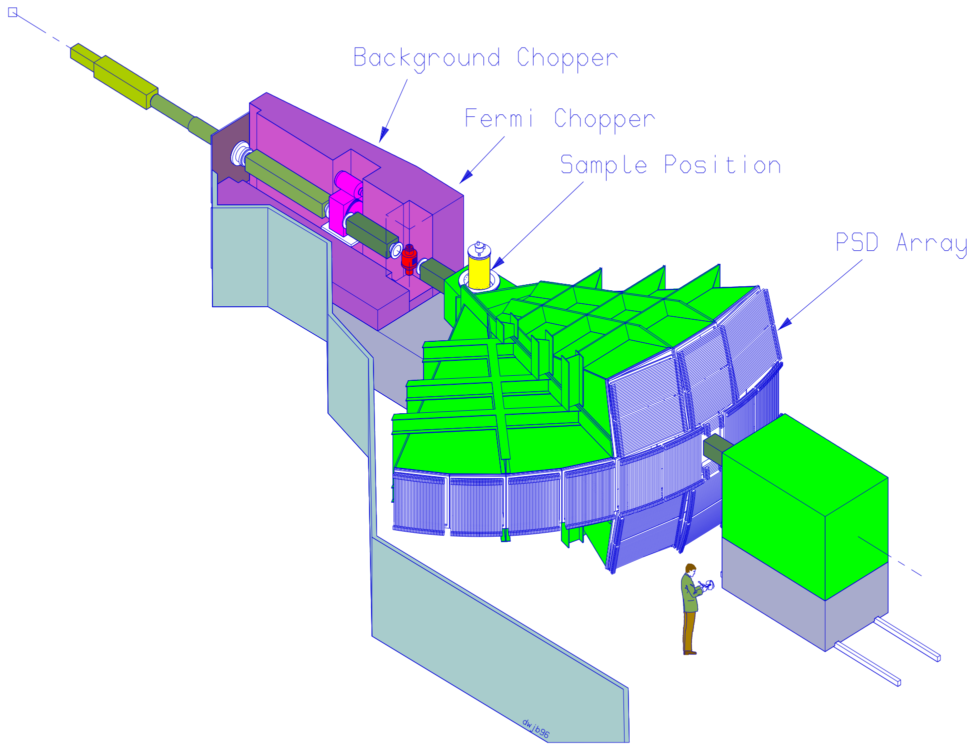


Inelastic neutron scattering

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

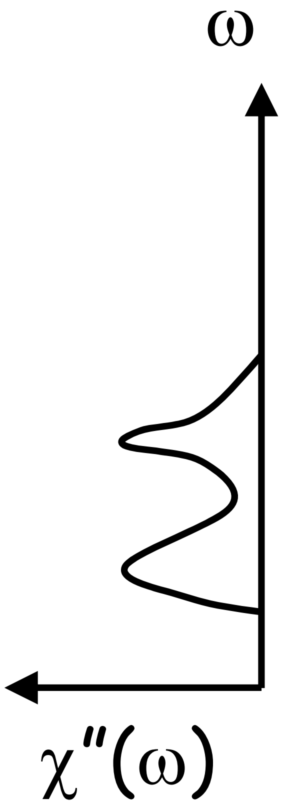
$$\chi''_{\mathrm{local}}(\omega) = \frac{\int_{BZ} \chi''(\mathbf{Q}, \omega)\, d\mathbf{Q}}{\int_{BZ} d\mathbf{Q}}$$

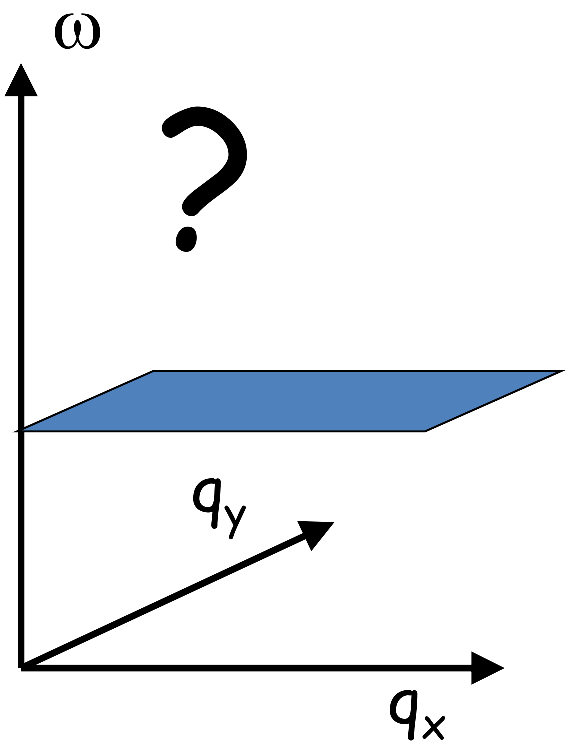


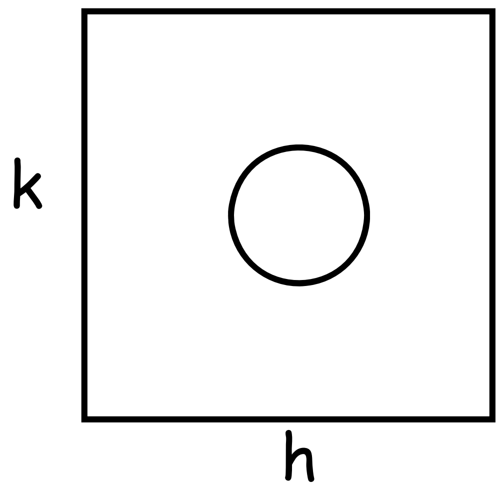


The response function $\chi''(q,\omega)$

things we would like to know ....







Magnetic excitations in cuprates

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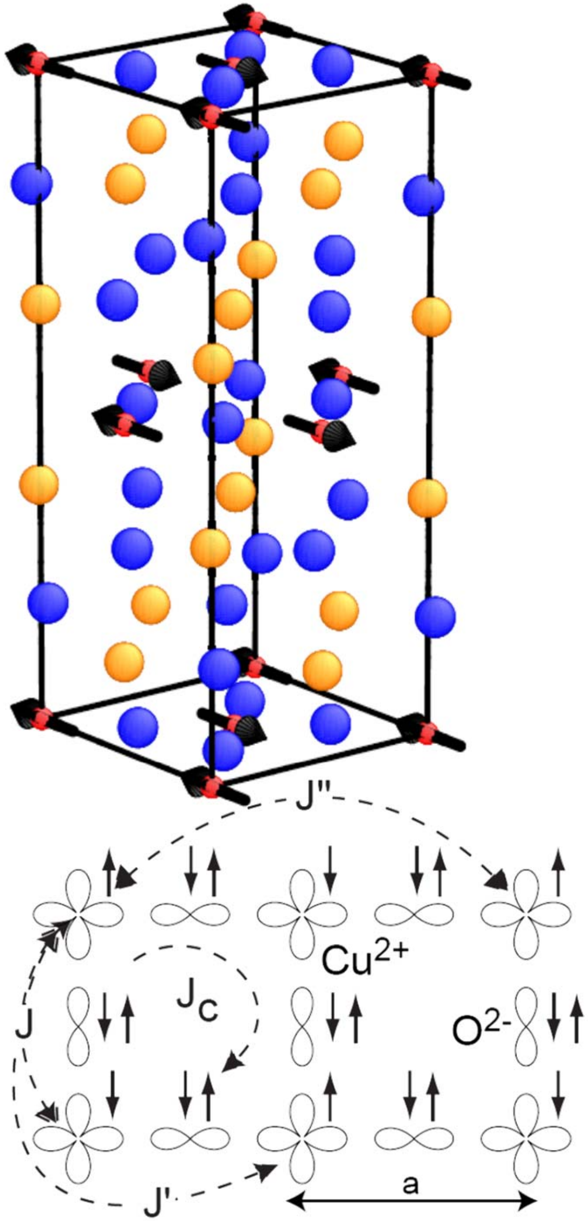
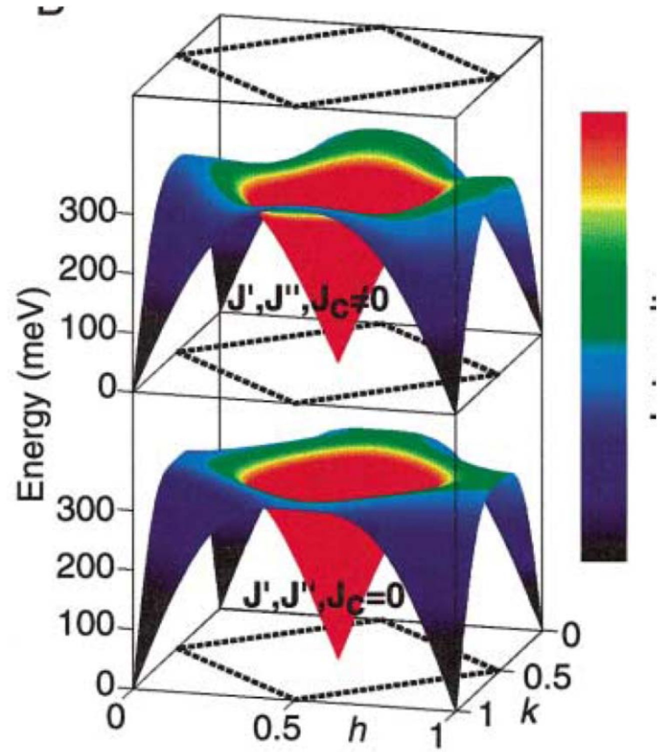
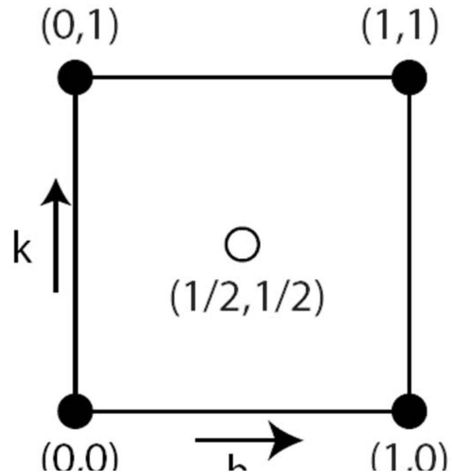
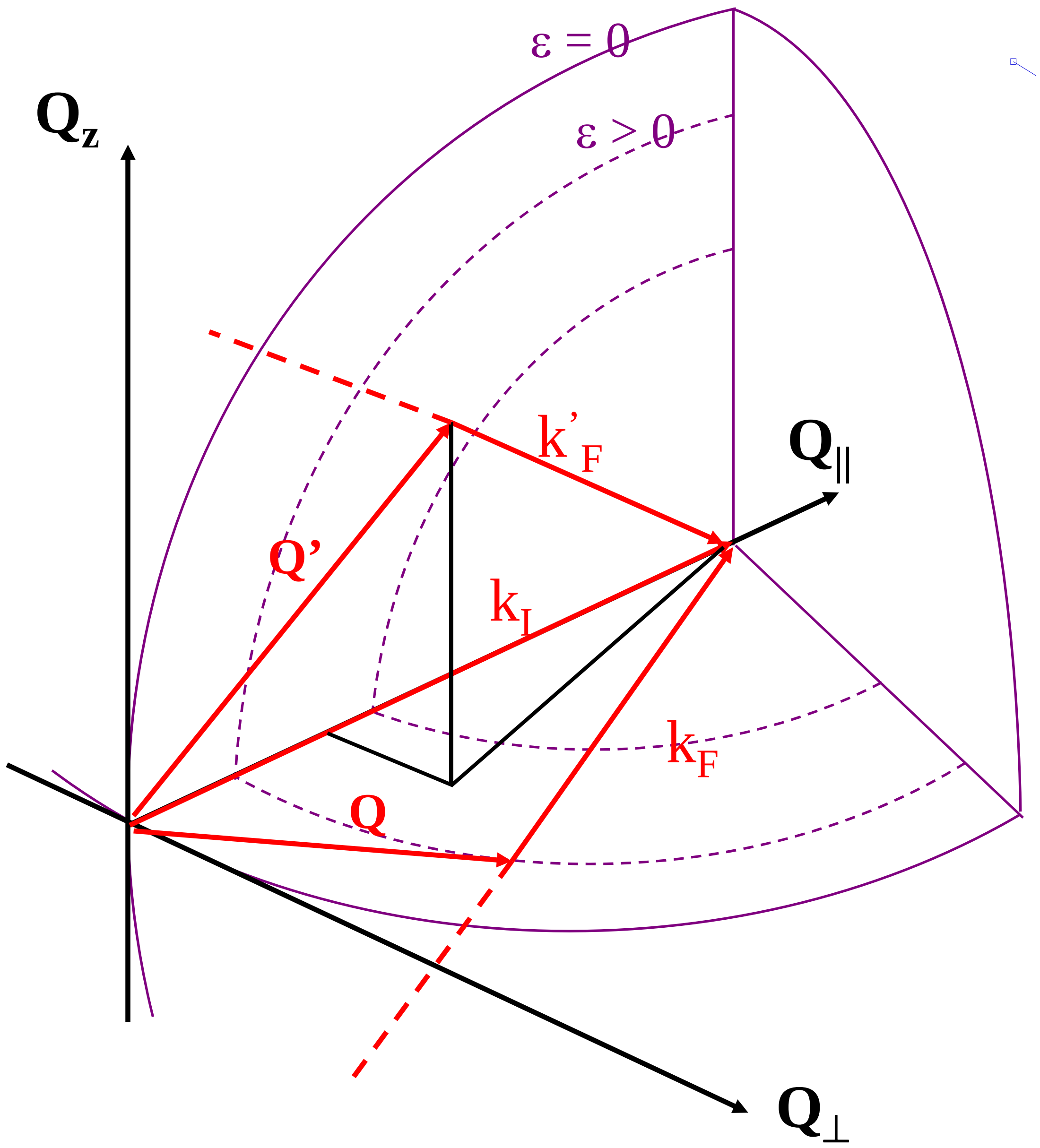
Magnetic Excitations in La_2CuO_4

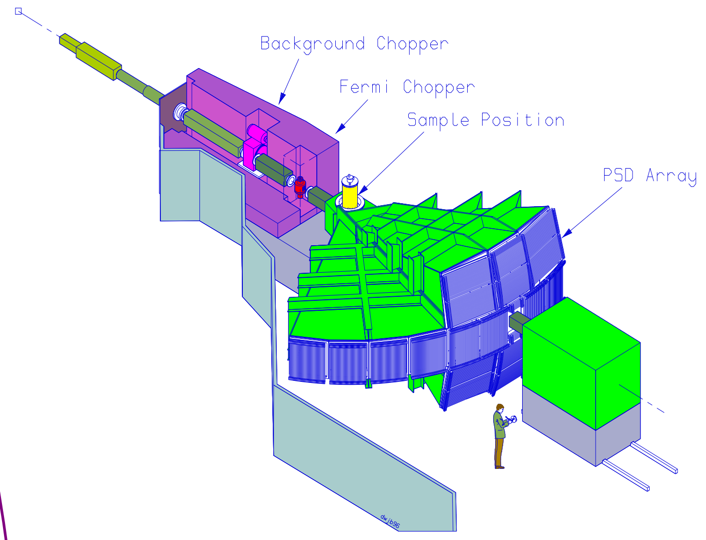






MAPS with 2-D system





credit: T Perring

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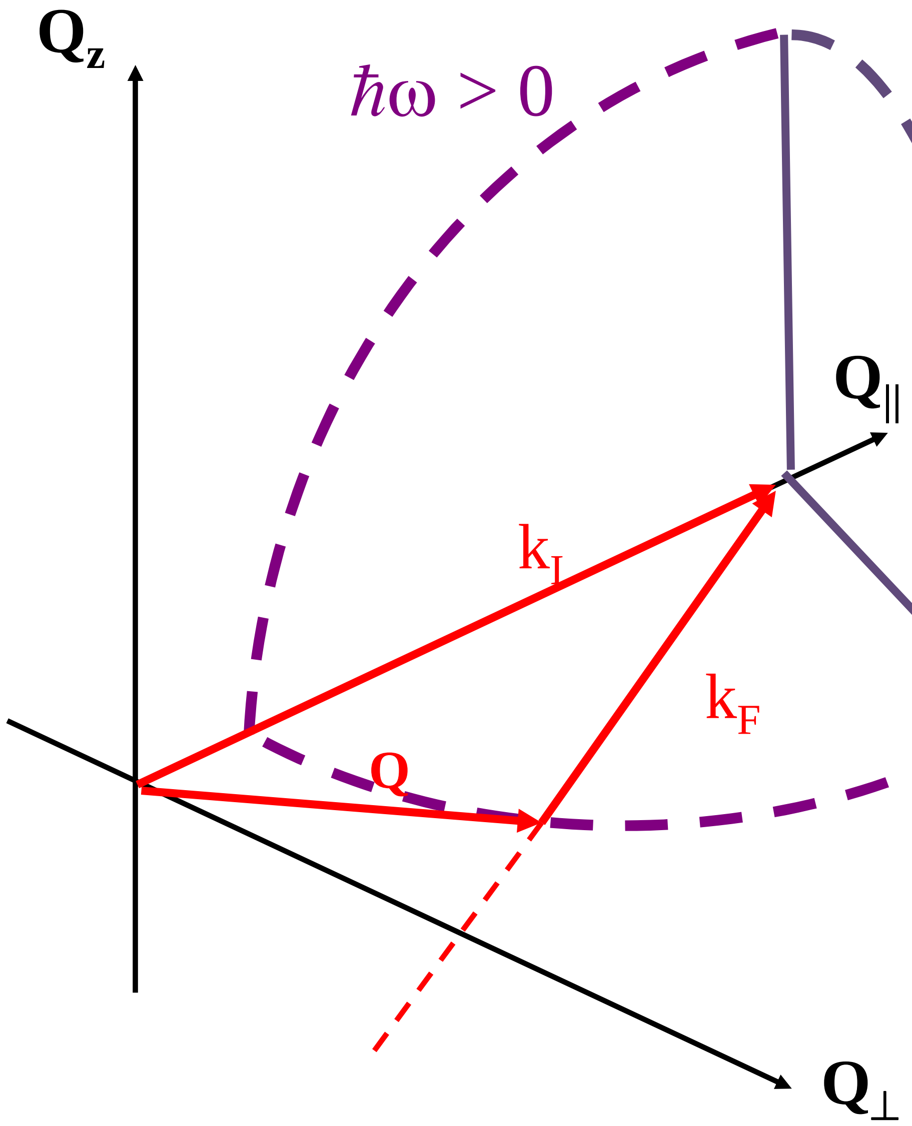
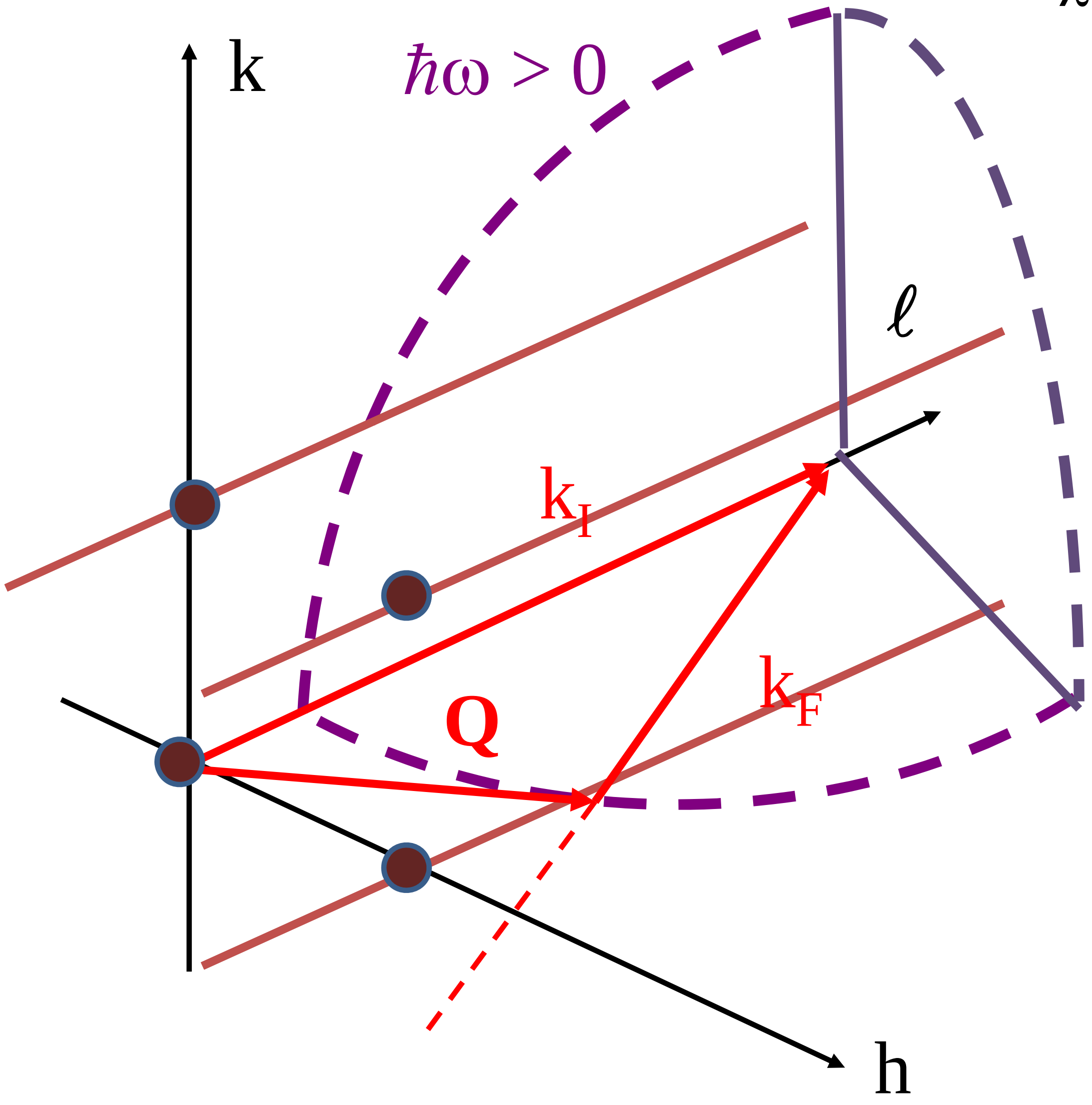


credit: T Perring

MAPS with 2-D system

if $\chi''(\mathbf{q},\omega)$ does not depend on ℓ



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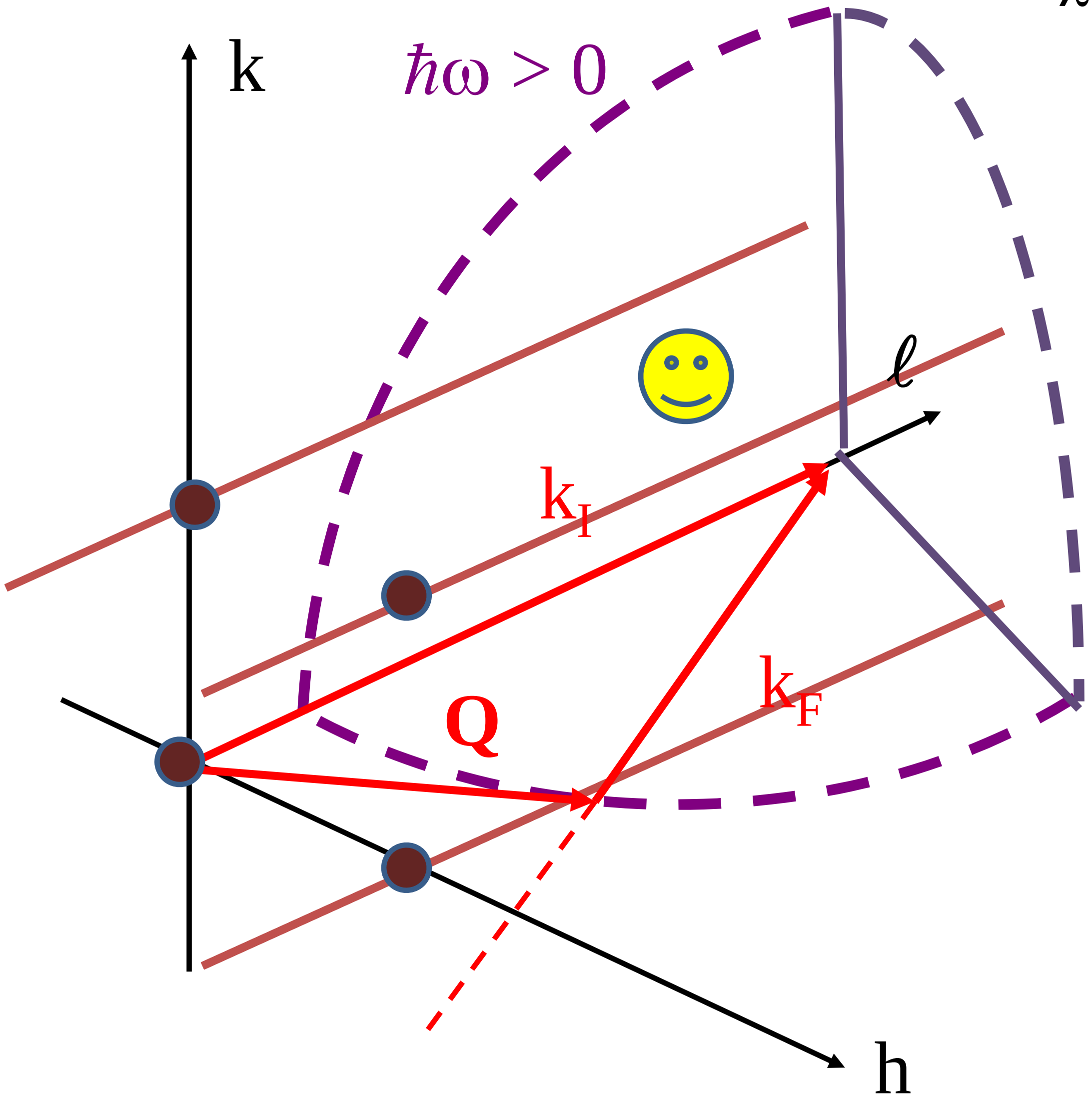

credit: T Perring

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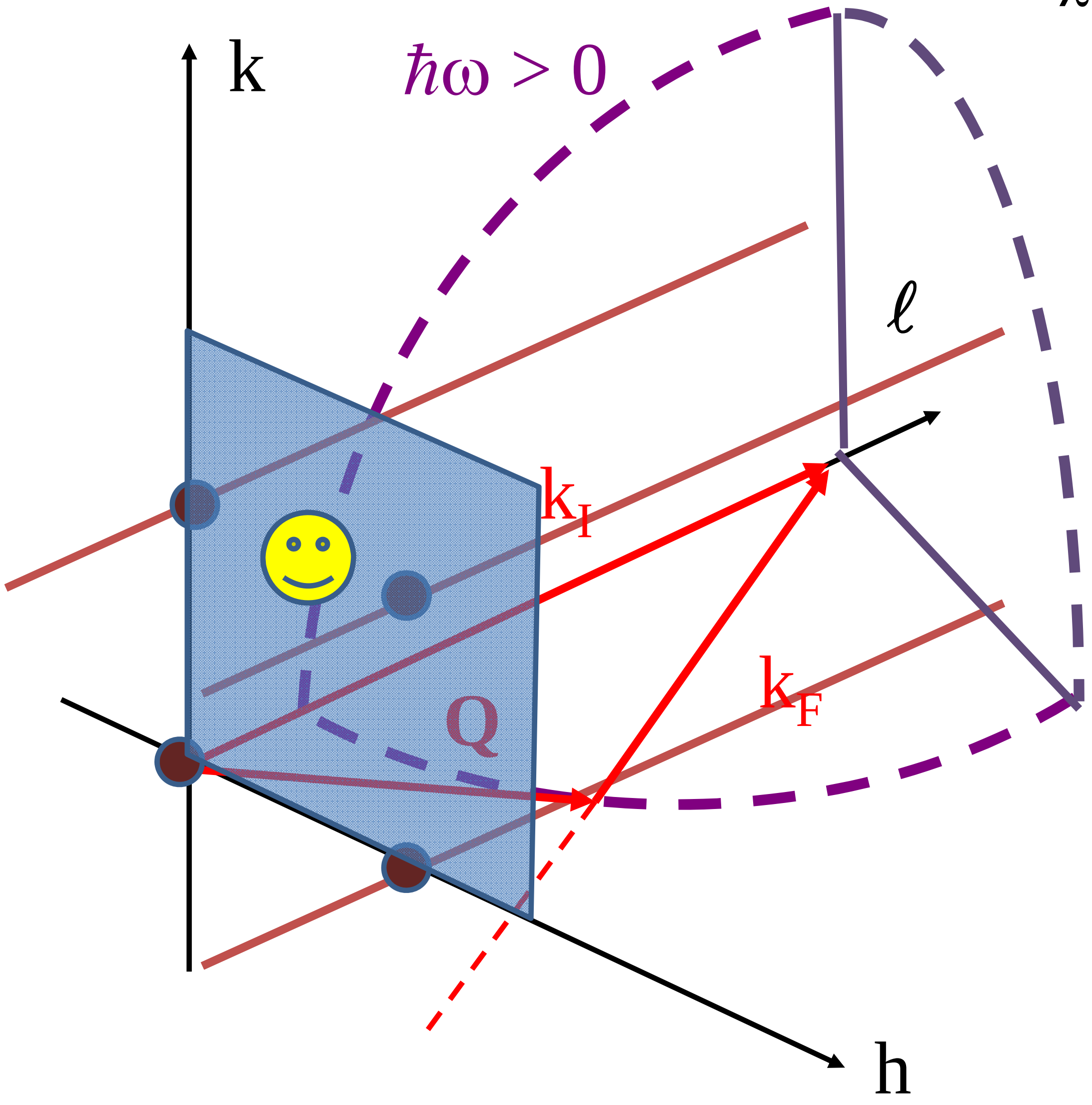
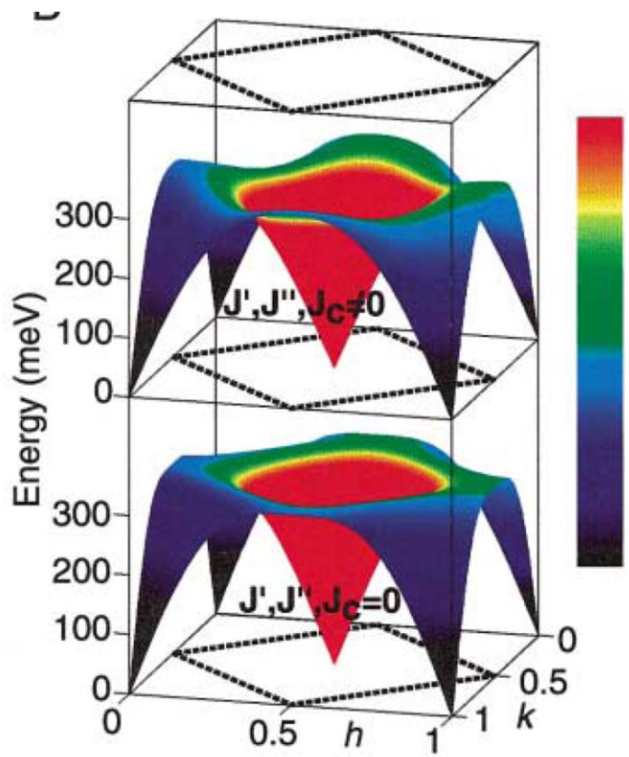
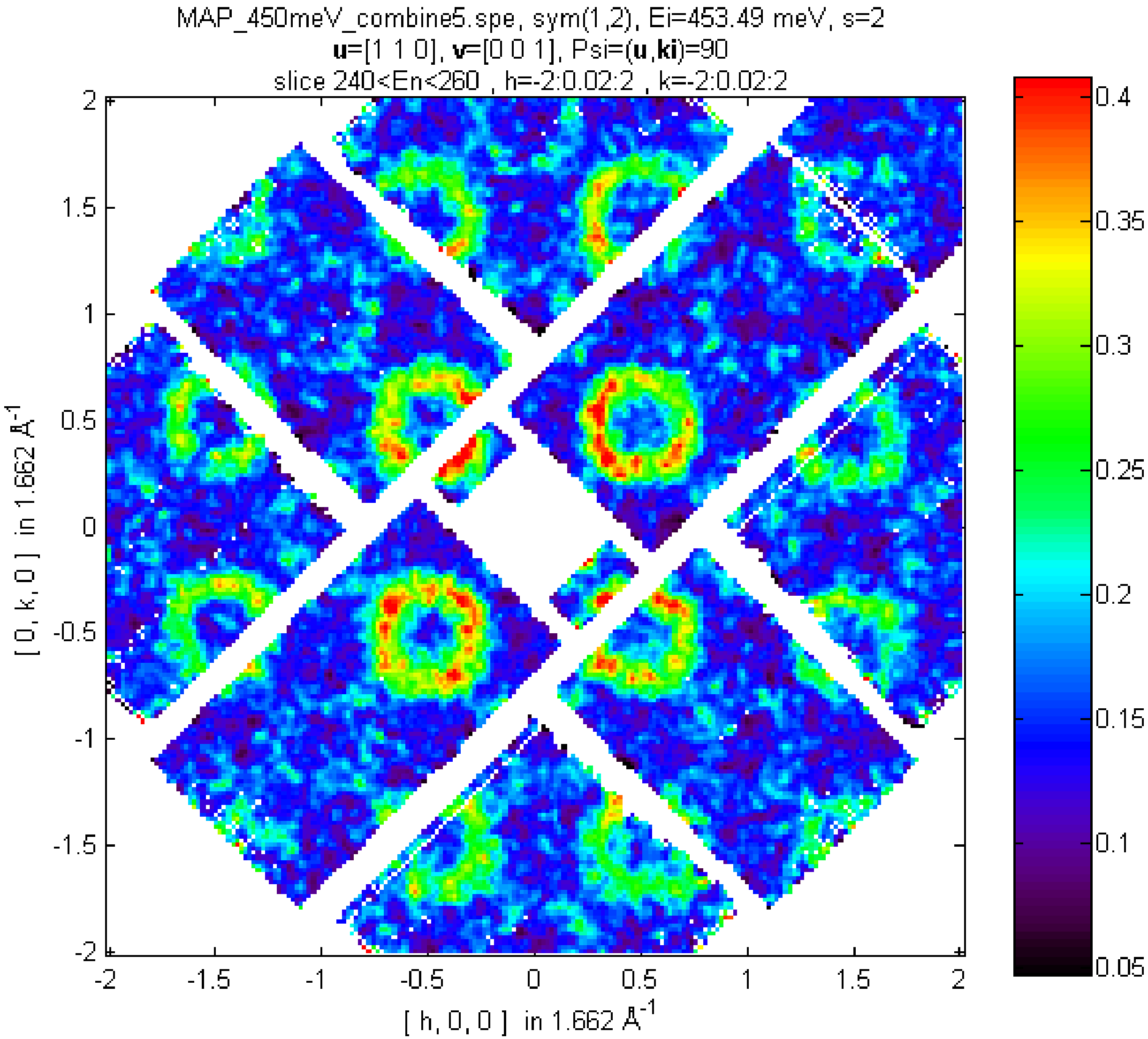
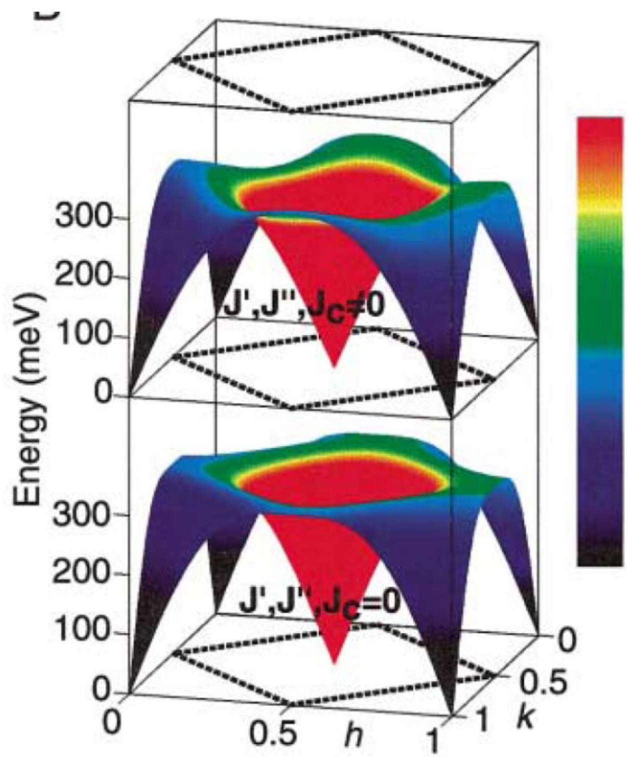




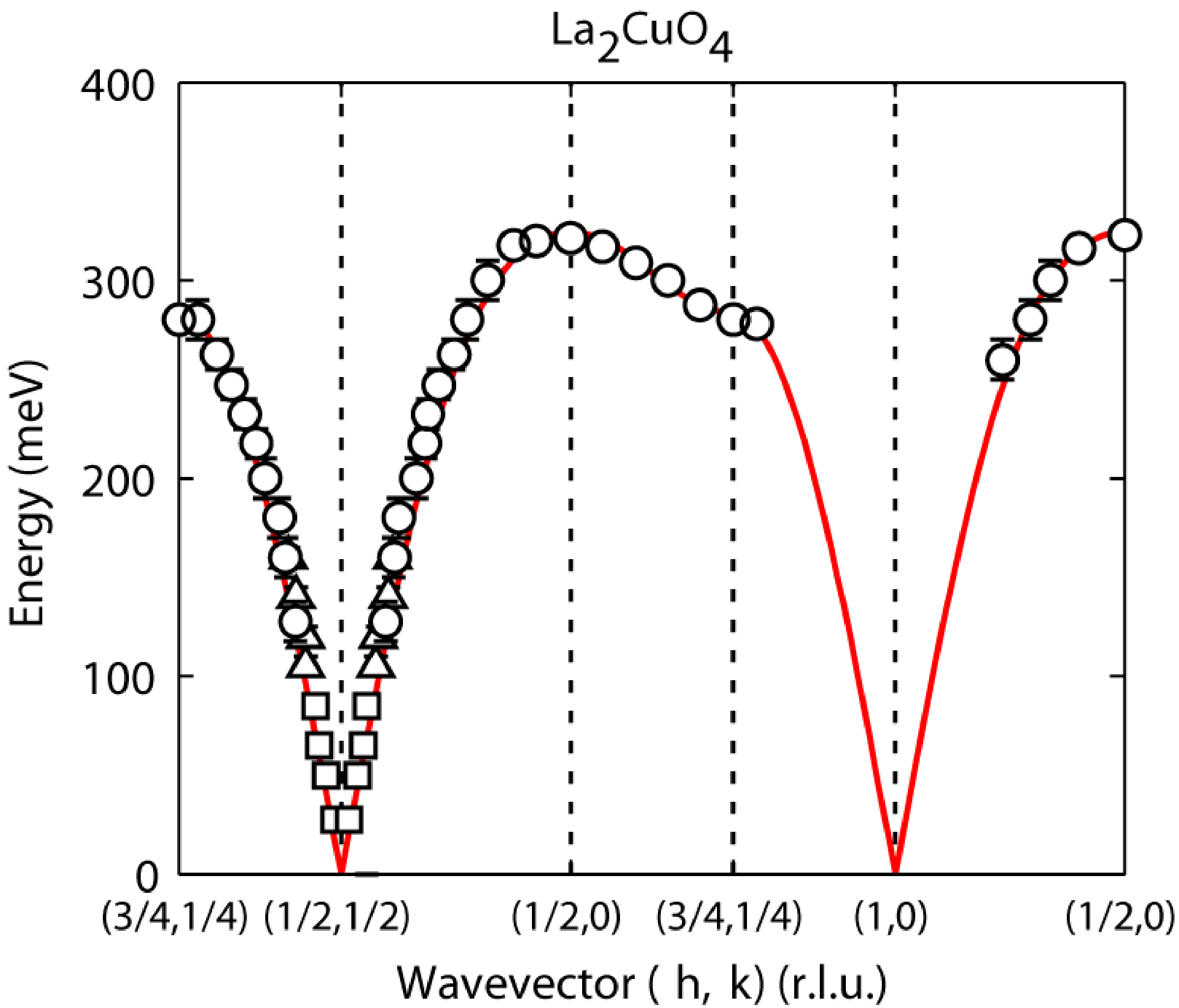
Spin waves in La_2CuO_4 :MAPS

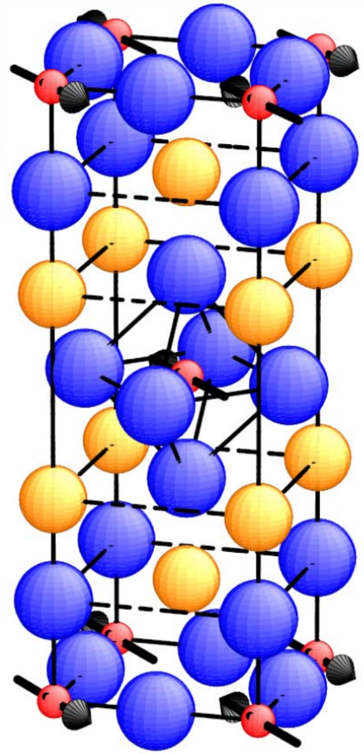


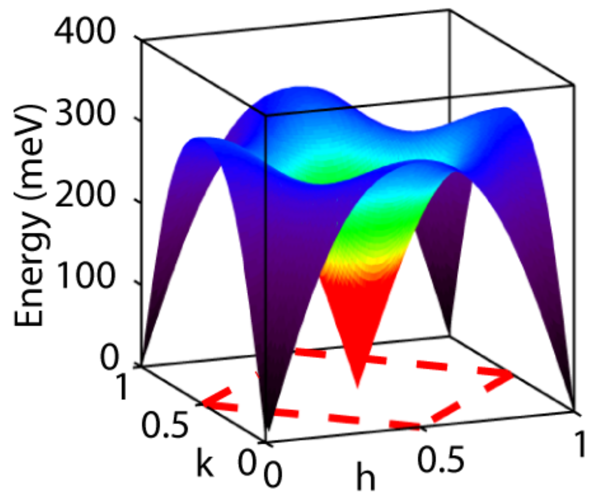
E=250 meV



Spin waves in La_2CuO_4







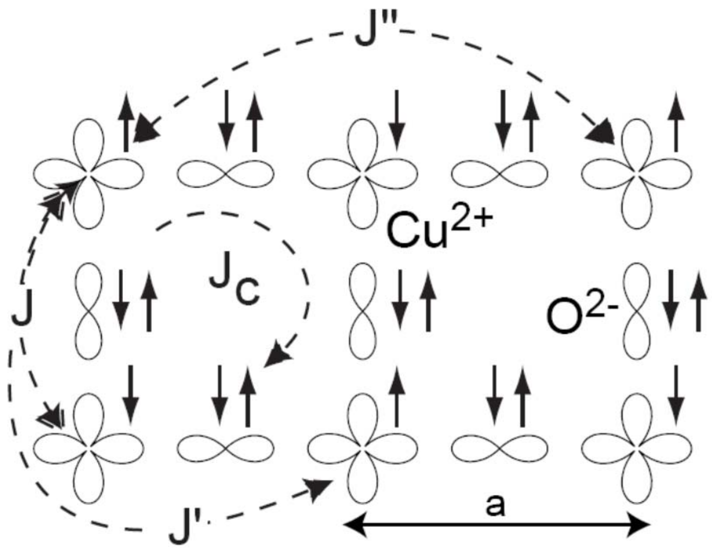
Coldea, Hayden, Aeppli, Perring, Frost, Mason, Cheong, Fisk,PRL **86** 5377 (2001).

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.



A. H. MacDonald PRB (1990)

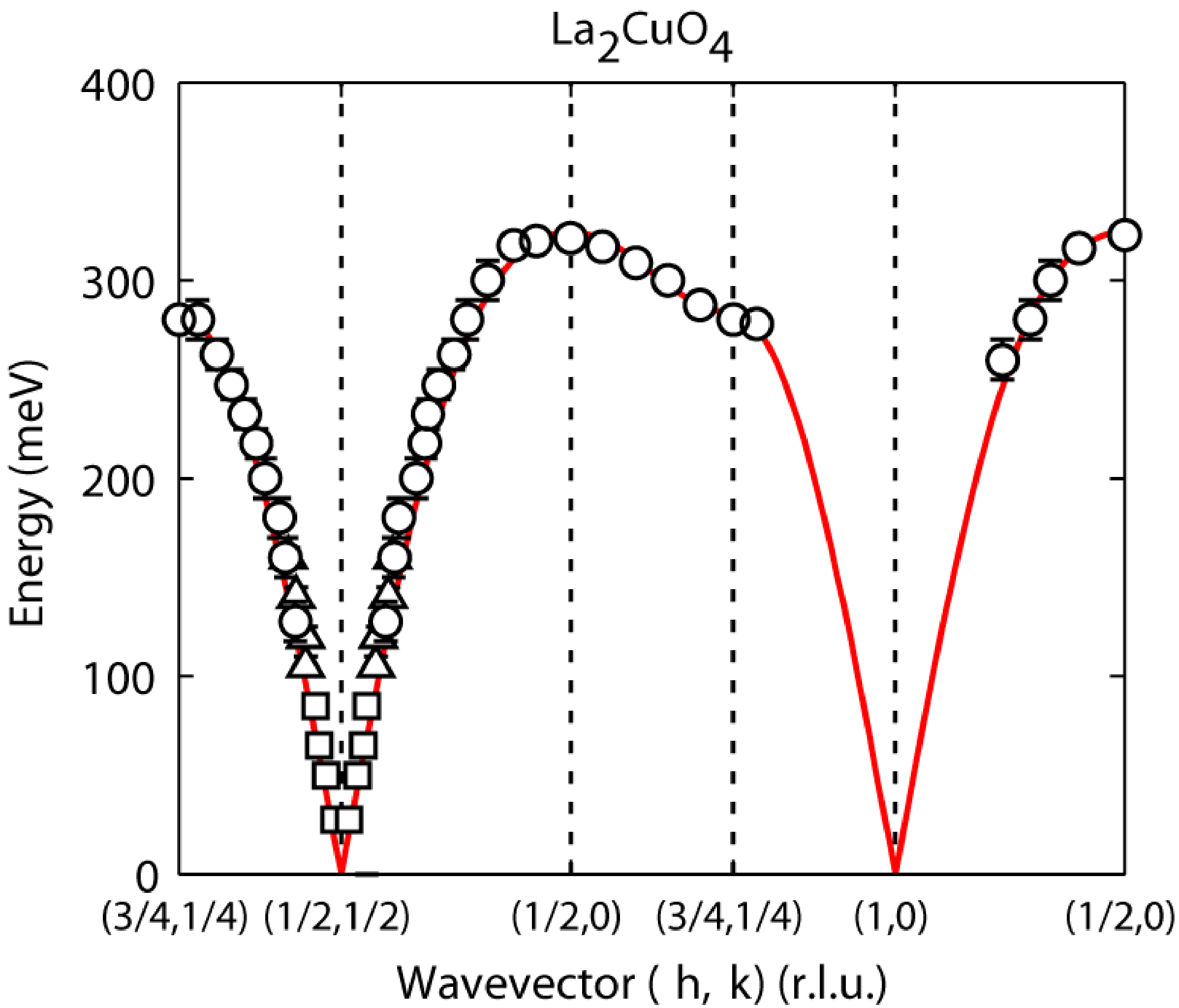
$$J = 4t^2/U - 24t^4/U^3$$

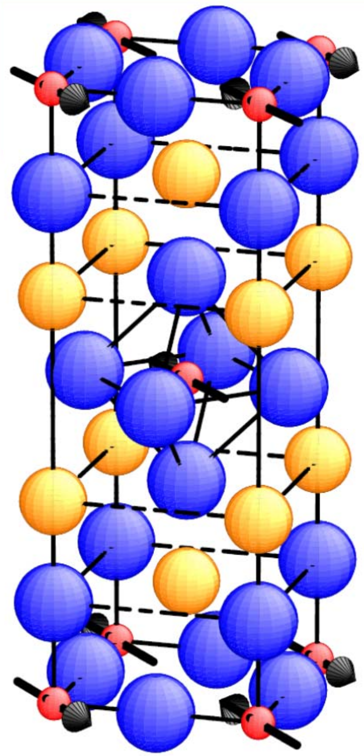
$$J_c = 80\ t^4/U^3$$

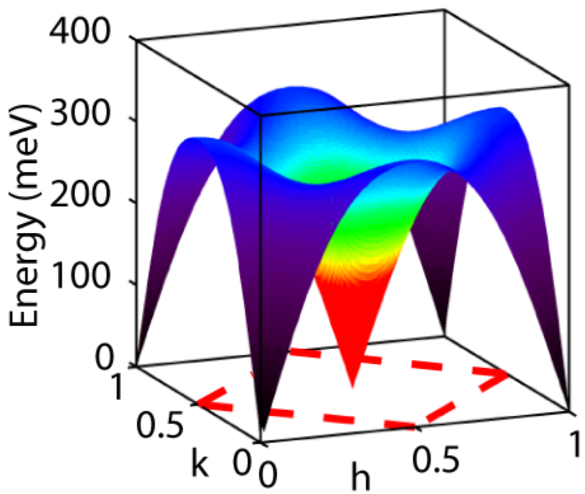
$$J' = J'' = 4t^4/U^3$$

t = 0.30 $\pm$ 0.02 eV, U =2.2 $\pm$ 0.4 eV,
J =146 $\pm$ 4 meV, and J_c = 61 $\pm$ 8 meV).

Spin waves in La_2CuO_4



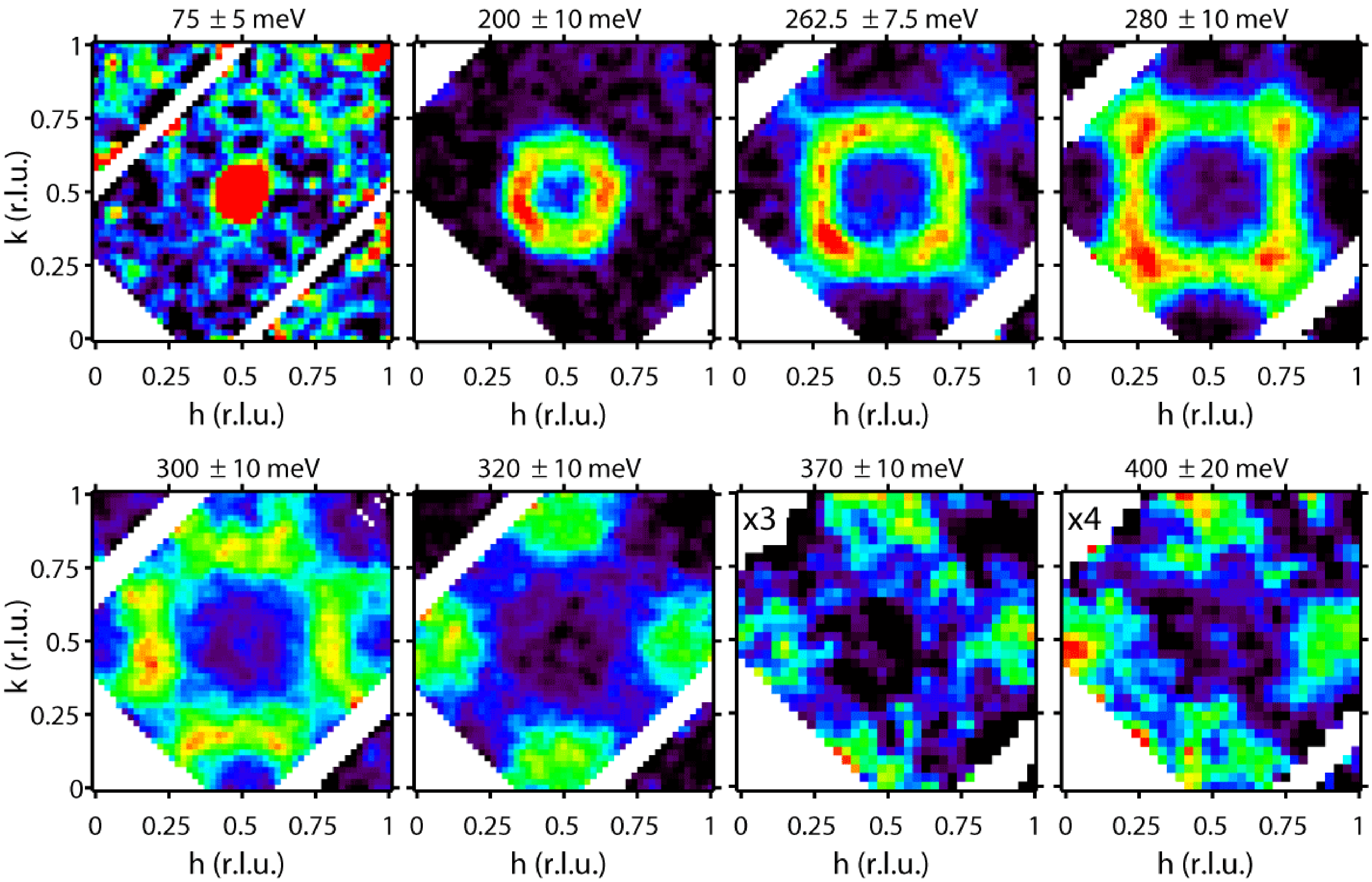




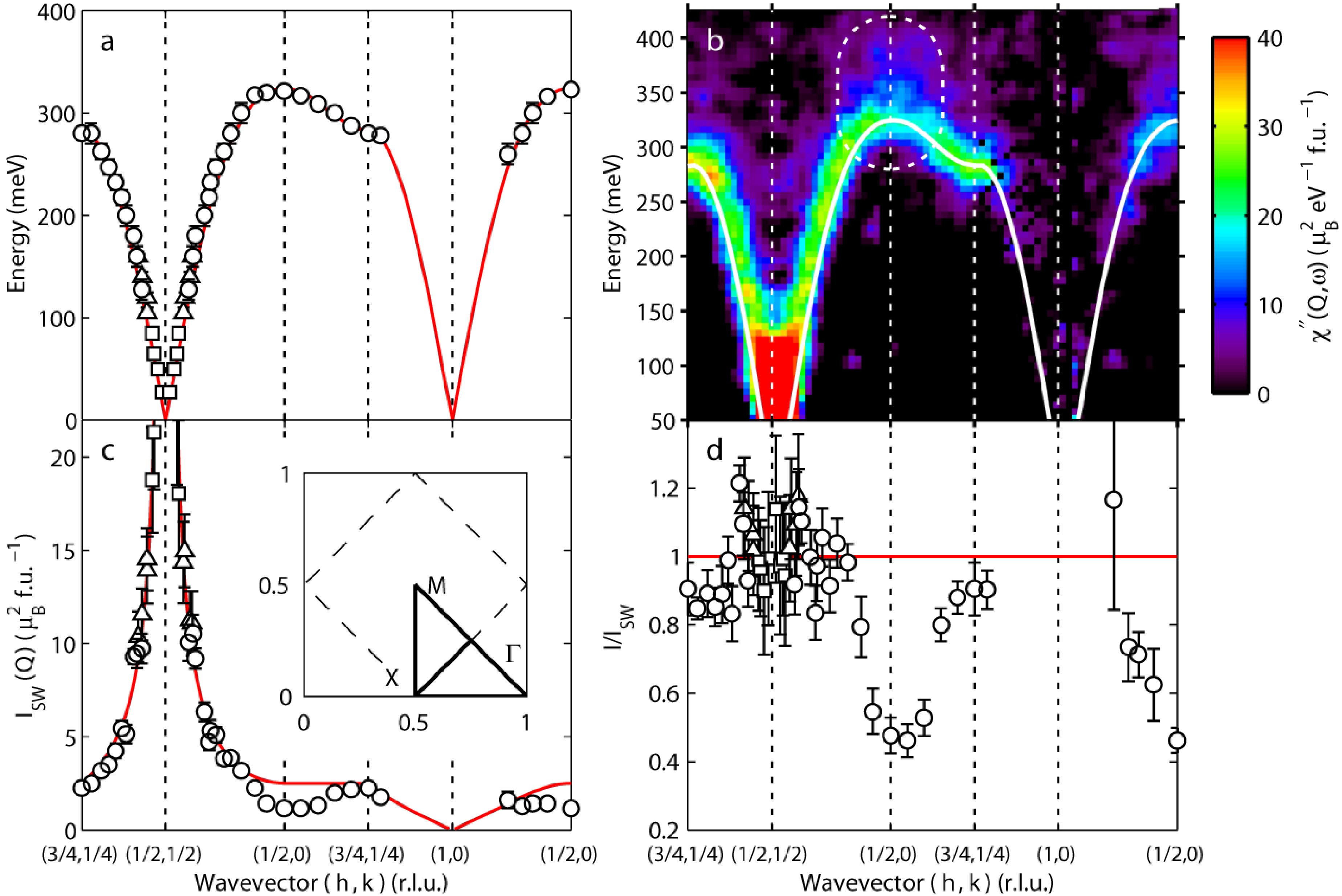
Coldea, Hayden, Aeppli, Perring, Frost, Mason, Cheong, Fisk,PRL **86** 5377 (2001).

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

La_2CuO_4 : **q**-dependent slices



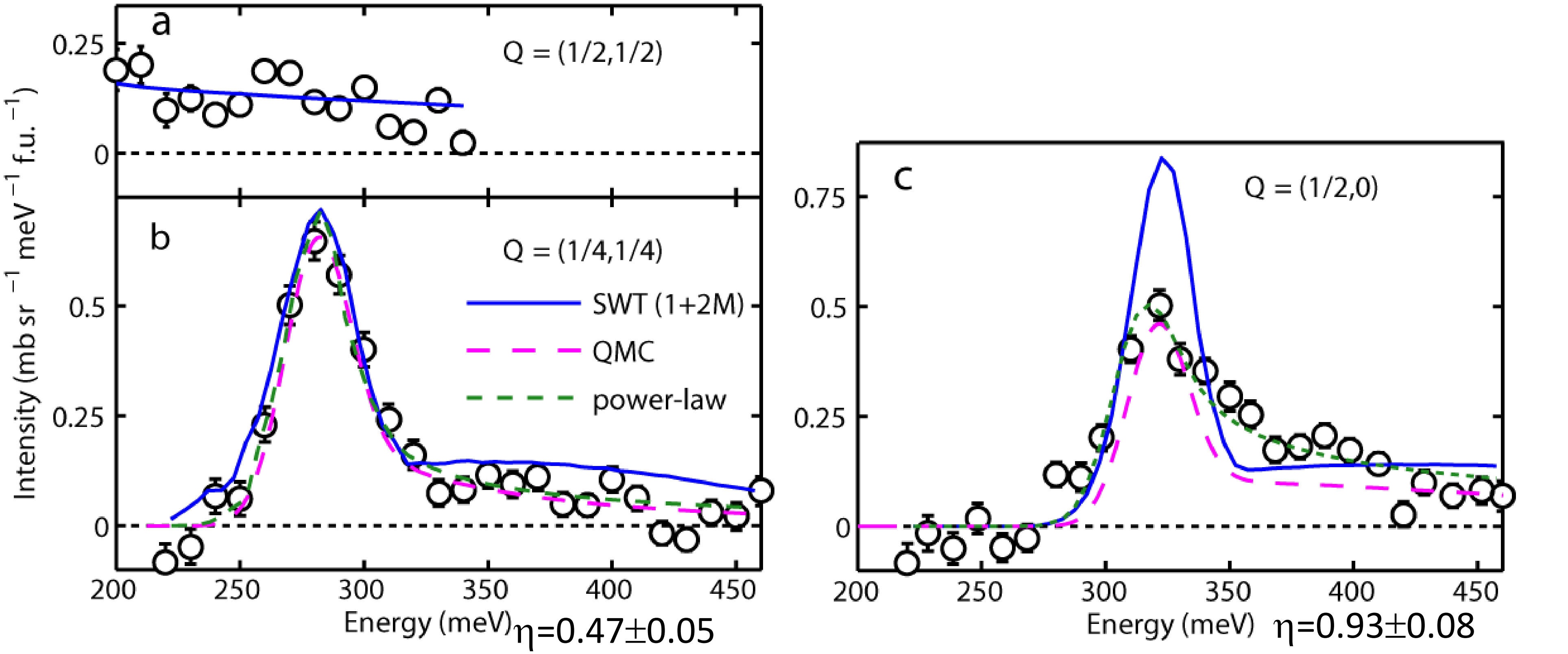
Magnetic Excitations in La_2CuO_4



"Spinon" power law

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

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



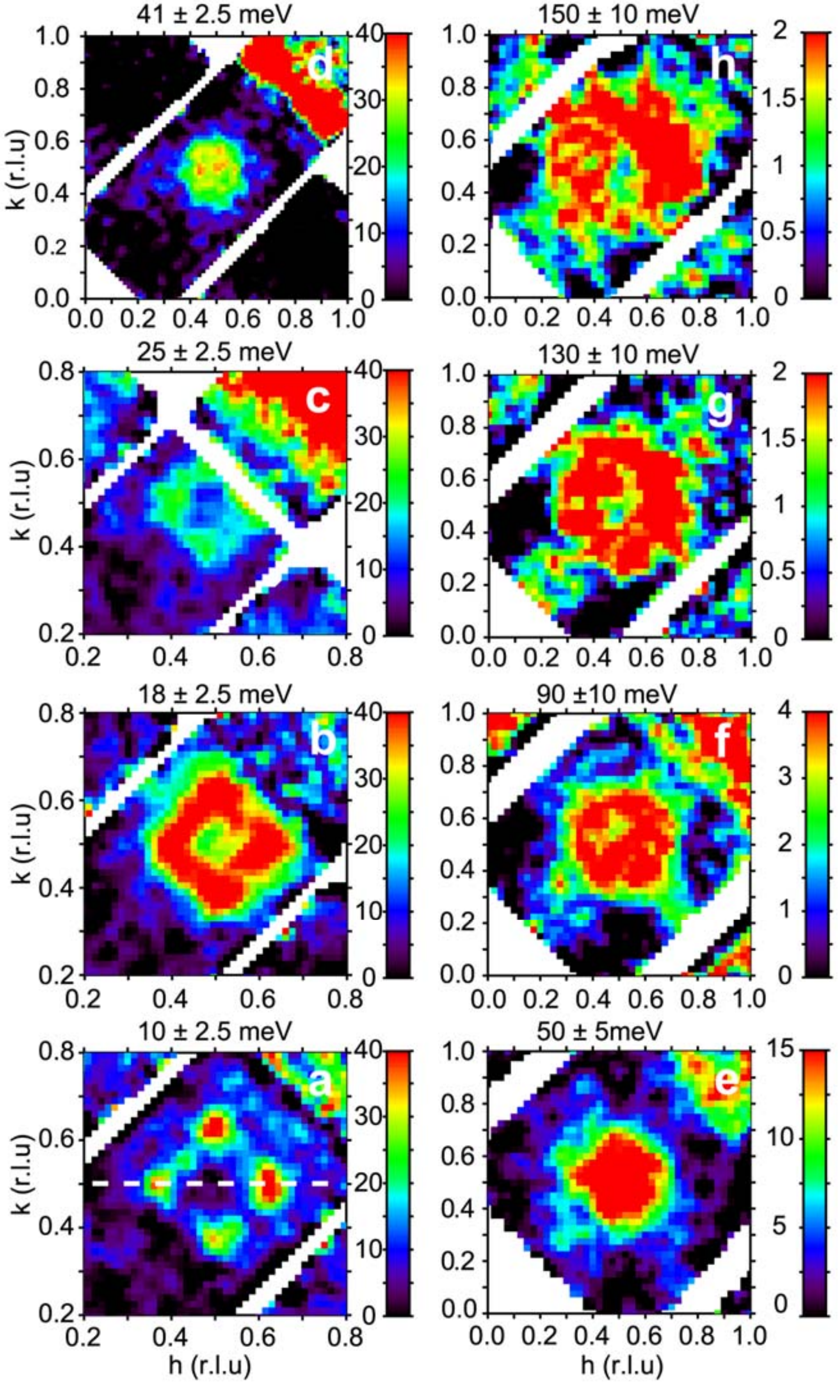
η=0.47±0.05

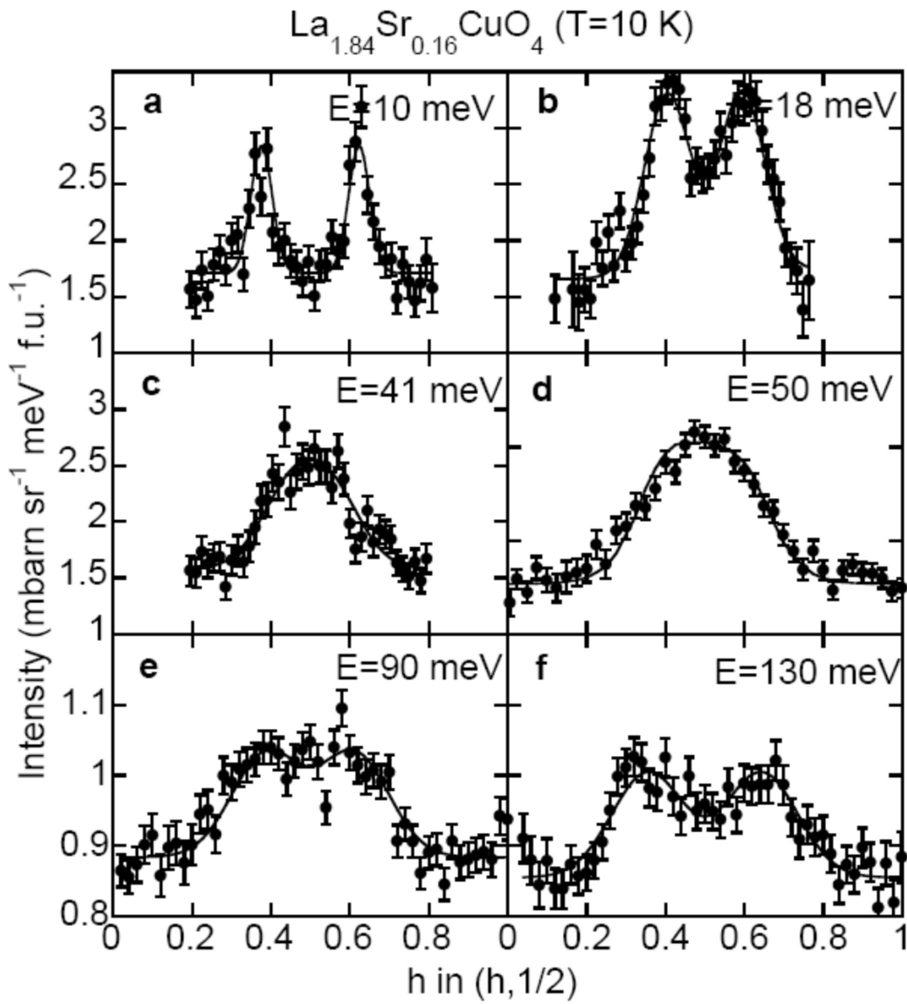
η=0.93±0.08

Magnetic excitations in cuprates

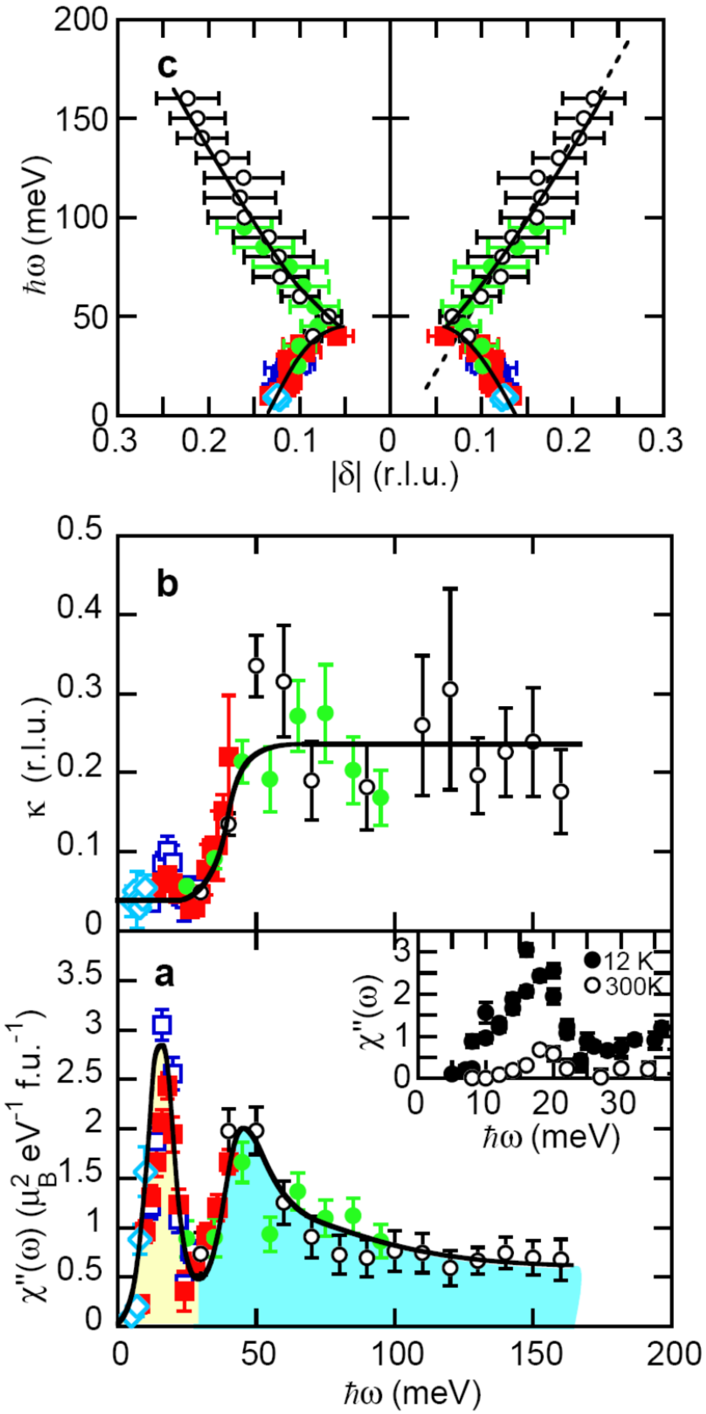
I. The pairing glue
II. Neutron scattering in $La_{2-x}Sr_xCuO_4$
III. Parent antiferromagnet
IV. Optimal doping
V. Overdoped
VI. Summary

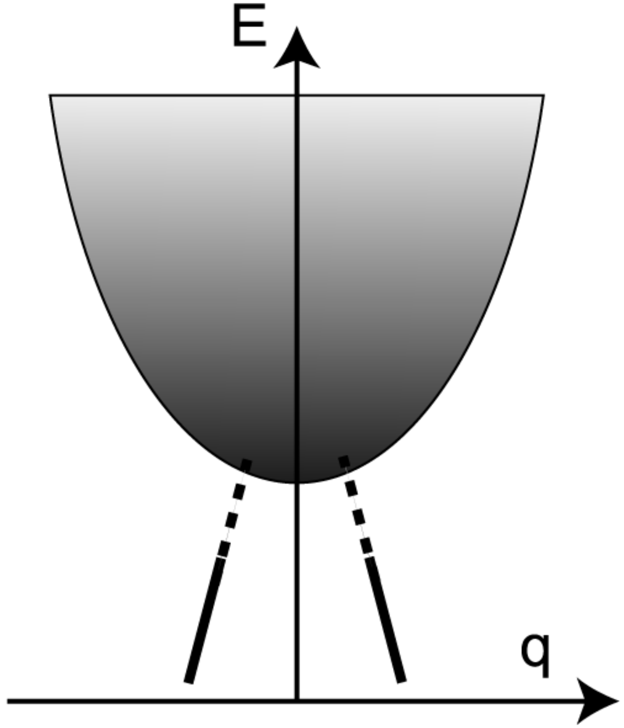
$La_{1.84}Sr_{0.16}CuO_4$ (T_c=38.5 K, MAPS





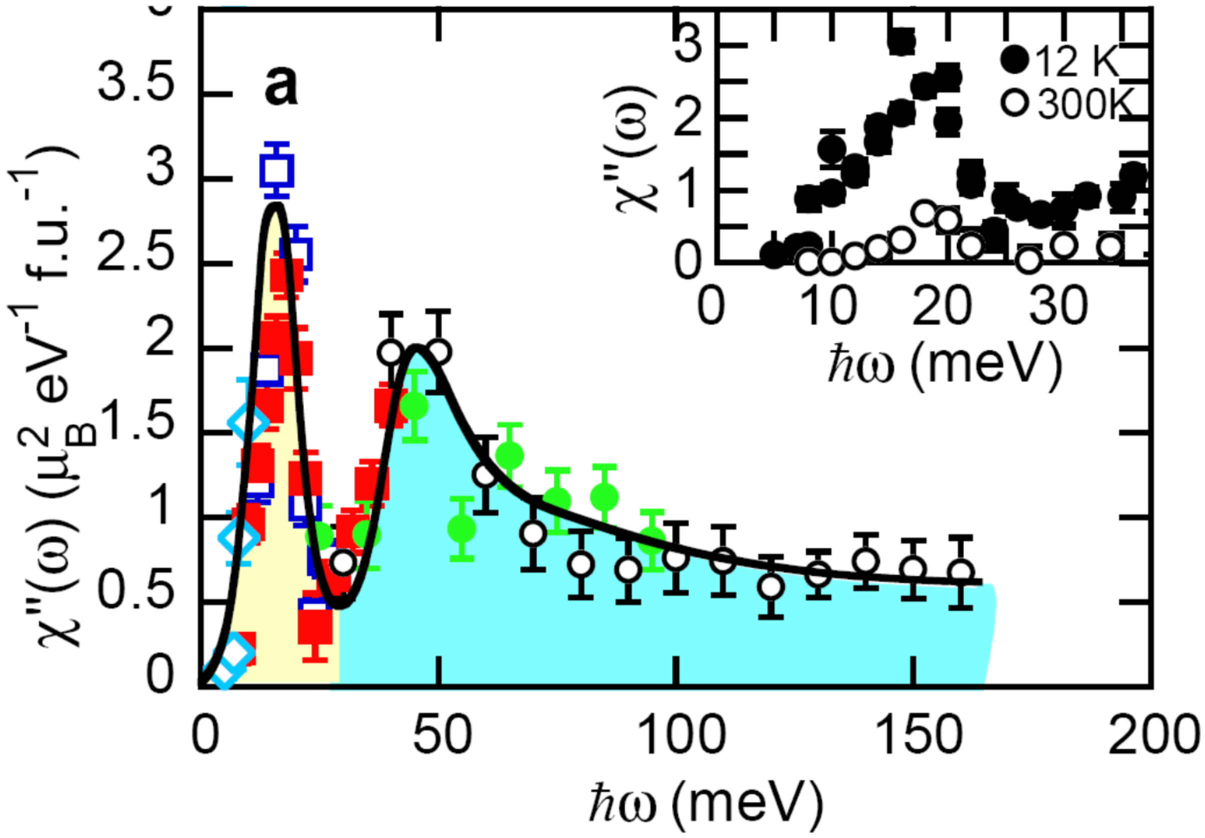
fitted parameters (x=0.16)





$$\chi''(\omega) = \int \chi''(\mathbf{Q},\omega)d^3Q / \int d^3Q$$

$La_{1.84}Sr_{0.16}CuO_4$



key features

- double-peaked structure (two energy scales 18,50 meV)
- rapid broadening of pattern near 40 meV
- possible "rotation of pattern" at high energies

Magnetic excitations in cuprates

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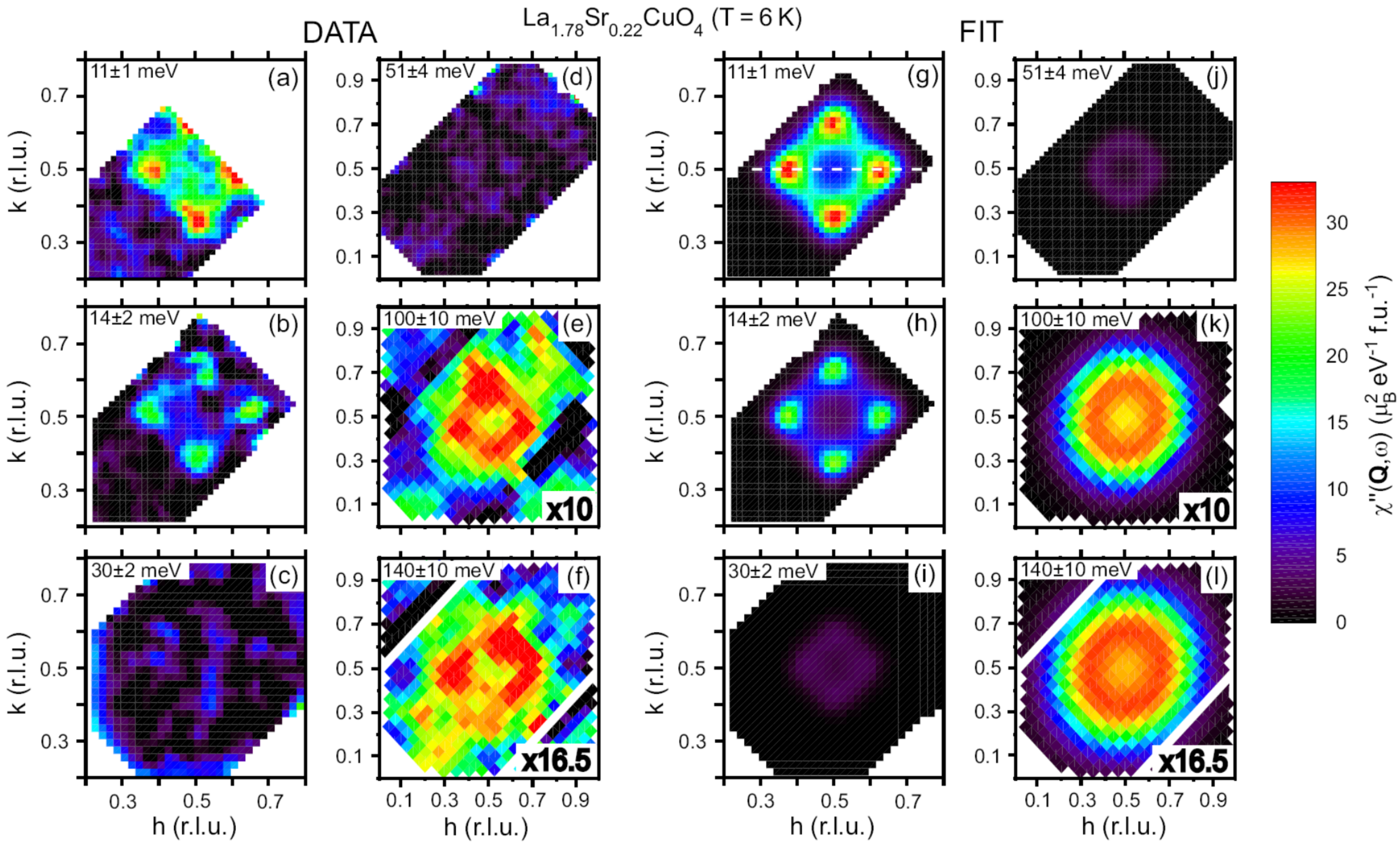
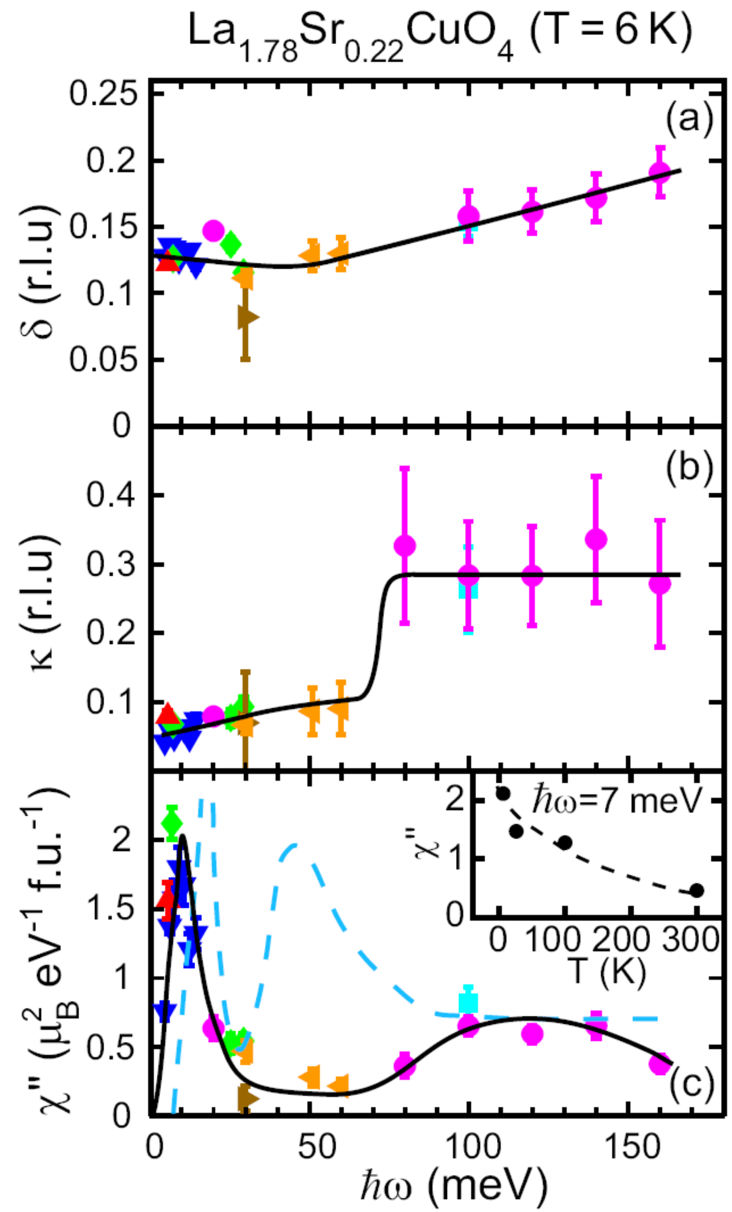
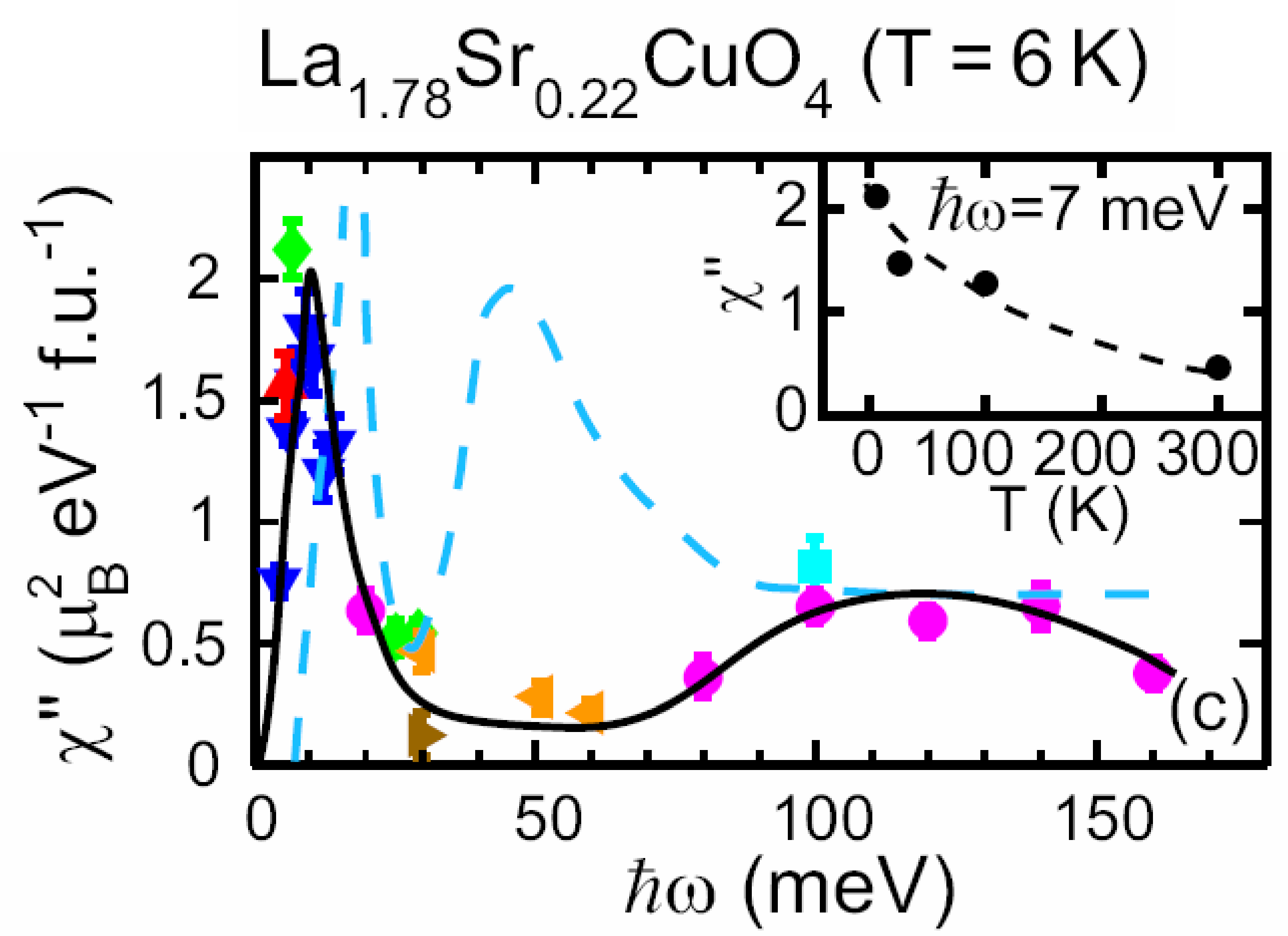
Overdoped Sample $La_{2-x}Sr_xCuO_4$ (x=0.22, T_c=26K)



Overdoped Sample $La_{2-x}Sr_xCuO_4$ (x=0.22, T_c=26K)



Collapse of intermediate frequencies



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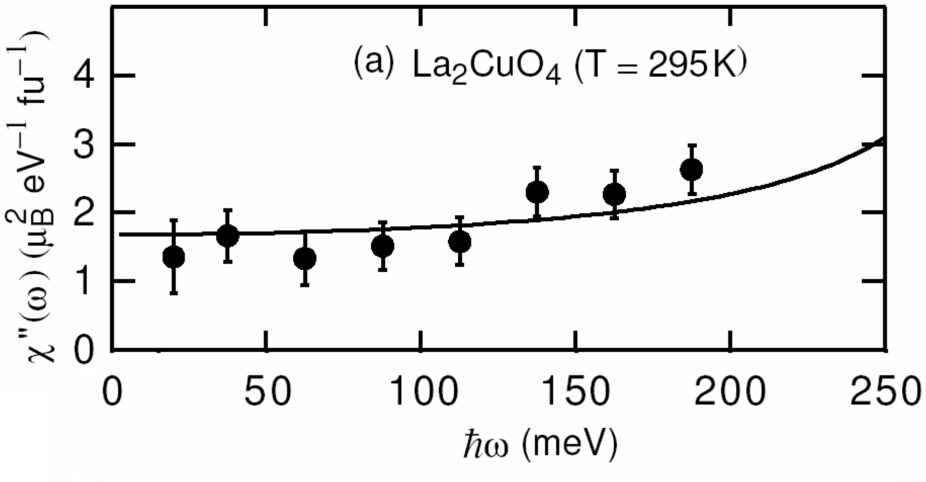
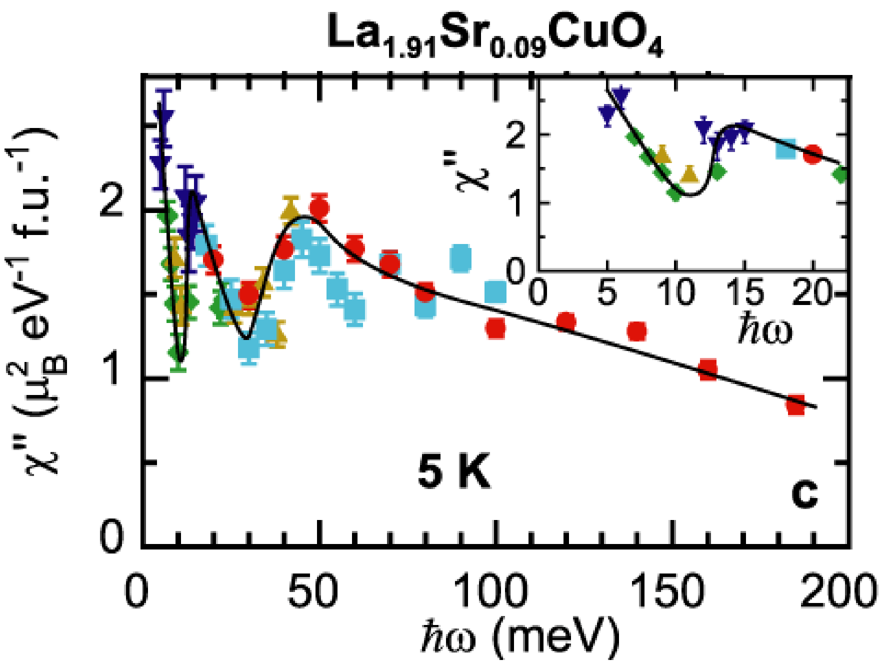
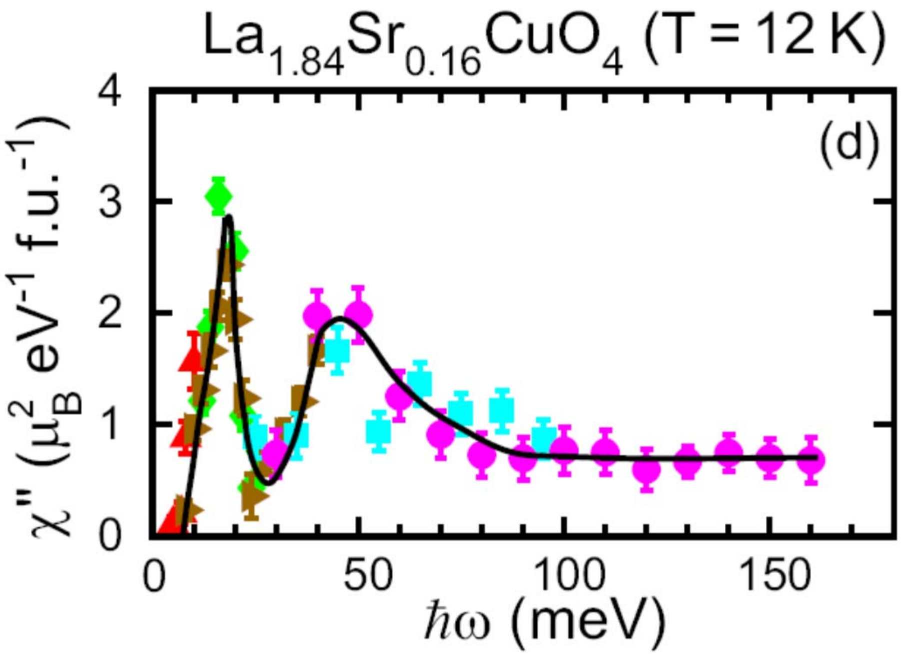
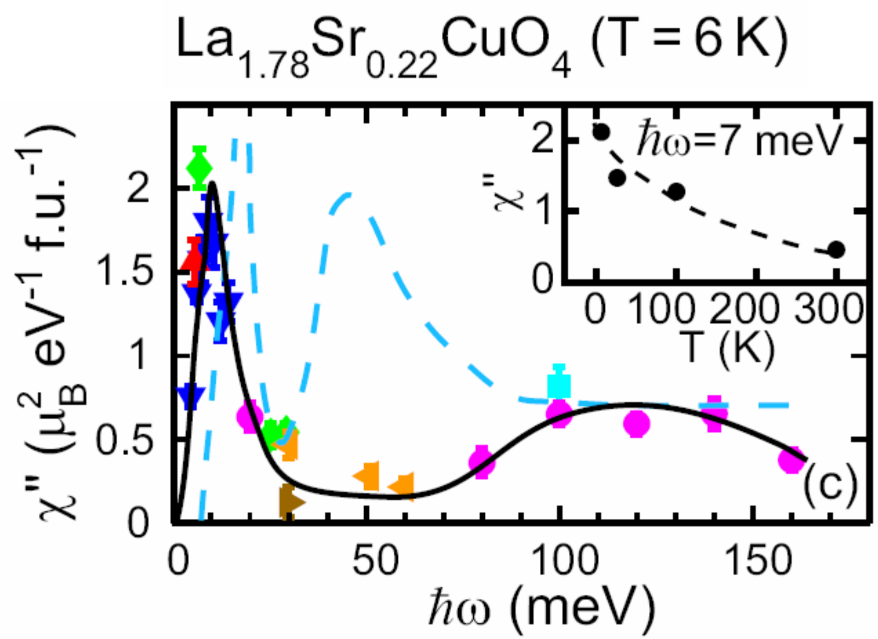
Evolution with doping

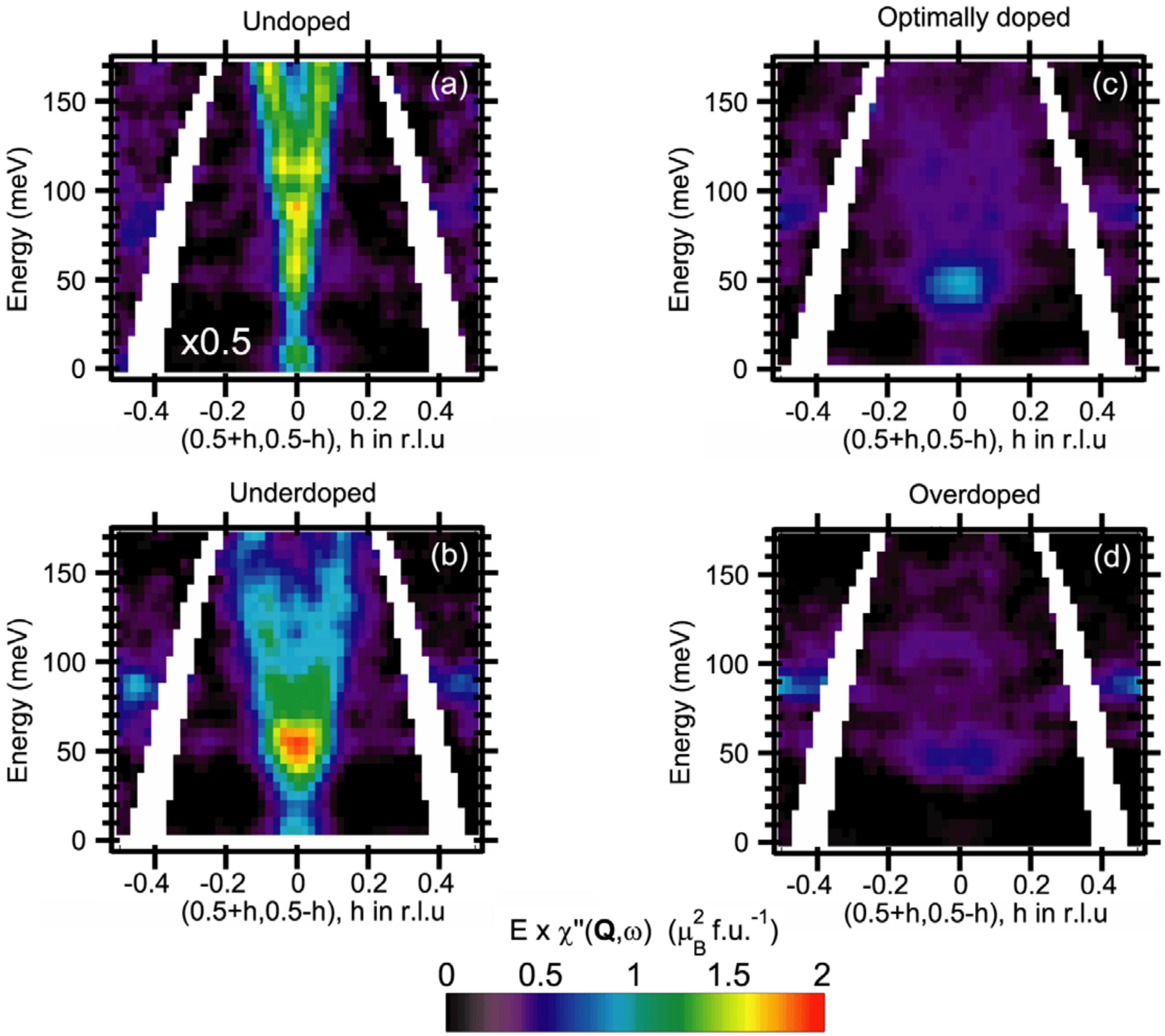




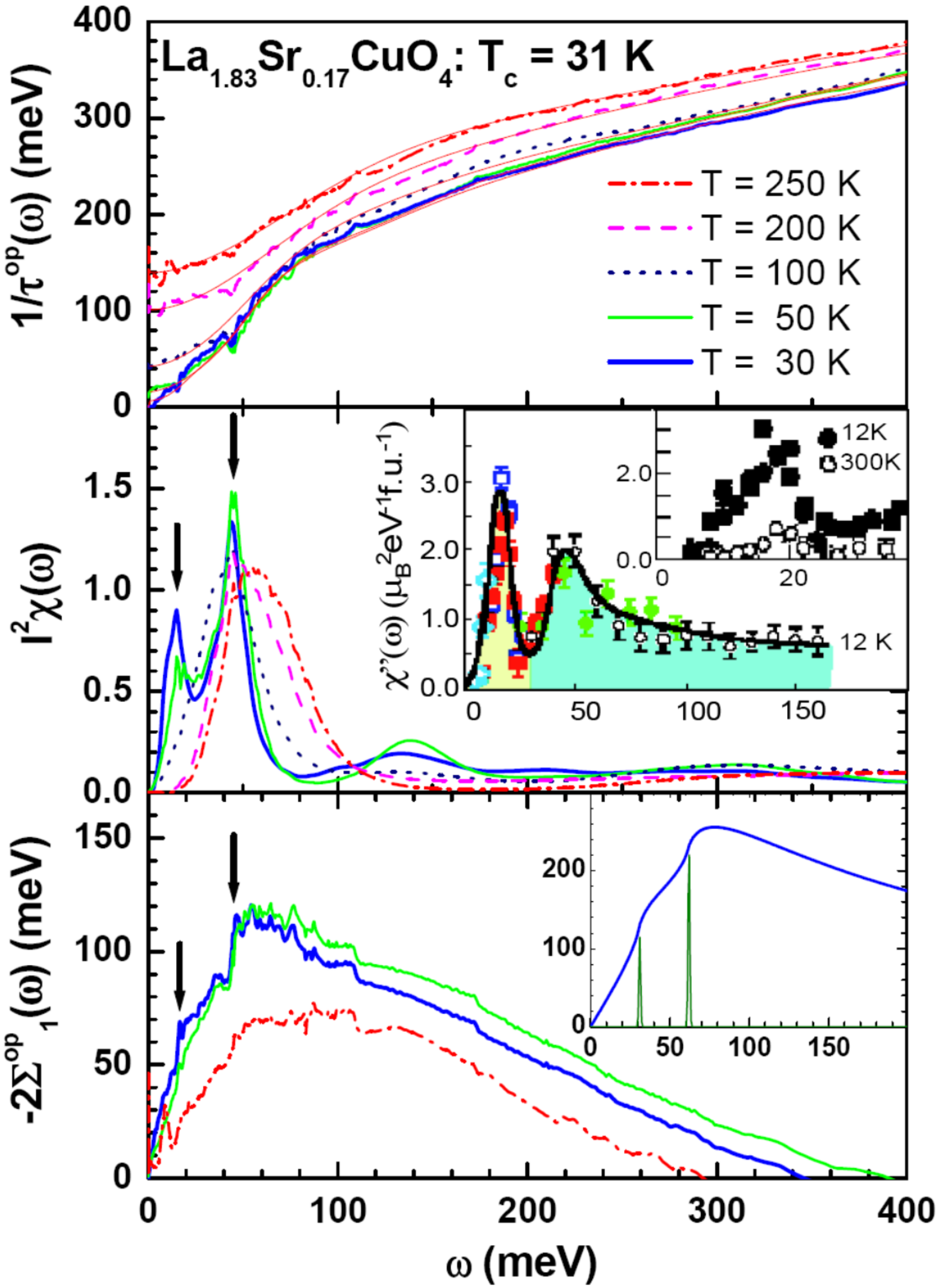




The evolution of $\chi''(q,\omega)$ in $La_{2-x}Sr_xCuO_4$ with doping



Optical Conductivity



J. Hwang et al.,
PRL **100**, 137005 (2008)

$$\sigma(\omega) = i\frac{\omega_p^2}{4\pi}\frac{1}{\omega[1+\lambda^{op}(\omega)]+i/\tau^{op}(\omega)}$$

$$= i\frac{\omega_p^2}{4\pi}\frac{1}{\omega - 2\Sigma^{op}(\omega)}$$

$$\frac{1}{\tau^{op}} \simeq \frac{2\pi}{\omega}\int_0^\infty d\Omega\alpha^2F(\Omega)\int_0^{\omega-\Omega} d\omega'\tilde{N}(\omega')$$

spin fluctuations probably the glue...

fin