Resonant Inelastic X-ray Scattering on Elementary Excitations

Jeroen van den Brink

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TECHNISCHE UNIVERSITÄT DRESDEN

PSI Summer School
Zugerberg 12.08.2014

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Ament, van Veenendaal, Devereaux, Hill & JvdB
Rev. Mod. Phys. 83, 705 (2011)

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Outline

1. Introducing RIXS

2. Magnetic RIXS on low dimensional magnets

1. Introducing RIXS

Basic Scattering Process

Direct & Indirect RIXS

5 features of RIXS

Elementary Excitations Accessible to RIXS

Progress in past decade

2. Magnetic RIXS on low dimensional magnets

Quasi 2D cuprates

Quasi 1D cuprates

Quasi 2D iron pnictide

Quasi 2D iridate

Doped Cu & Fe systems

Basic Scattering Process

Direct and Indirect RIXS

What is

Resonant

Inelastic

X-ray scattering

RIXS

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X-ray scattering

RIXS

X-ray scattering: photon in→ solid → photon out

inelastic: $\omega_{out} < \omega_{in}$

resonant: tune ω_{in} *to an atomic absorption edge*

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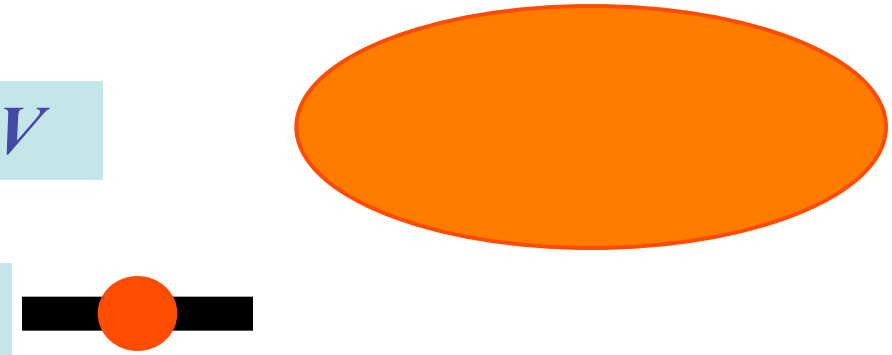
Cu
K-edge

4 p

~9 KeV

1 s



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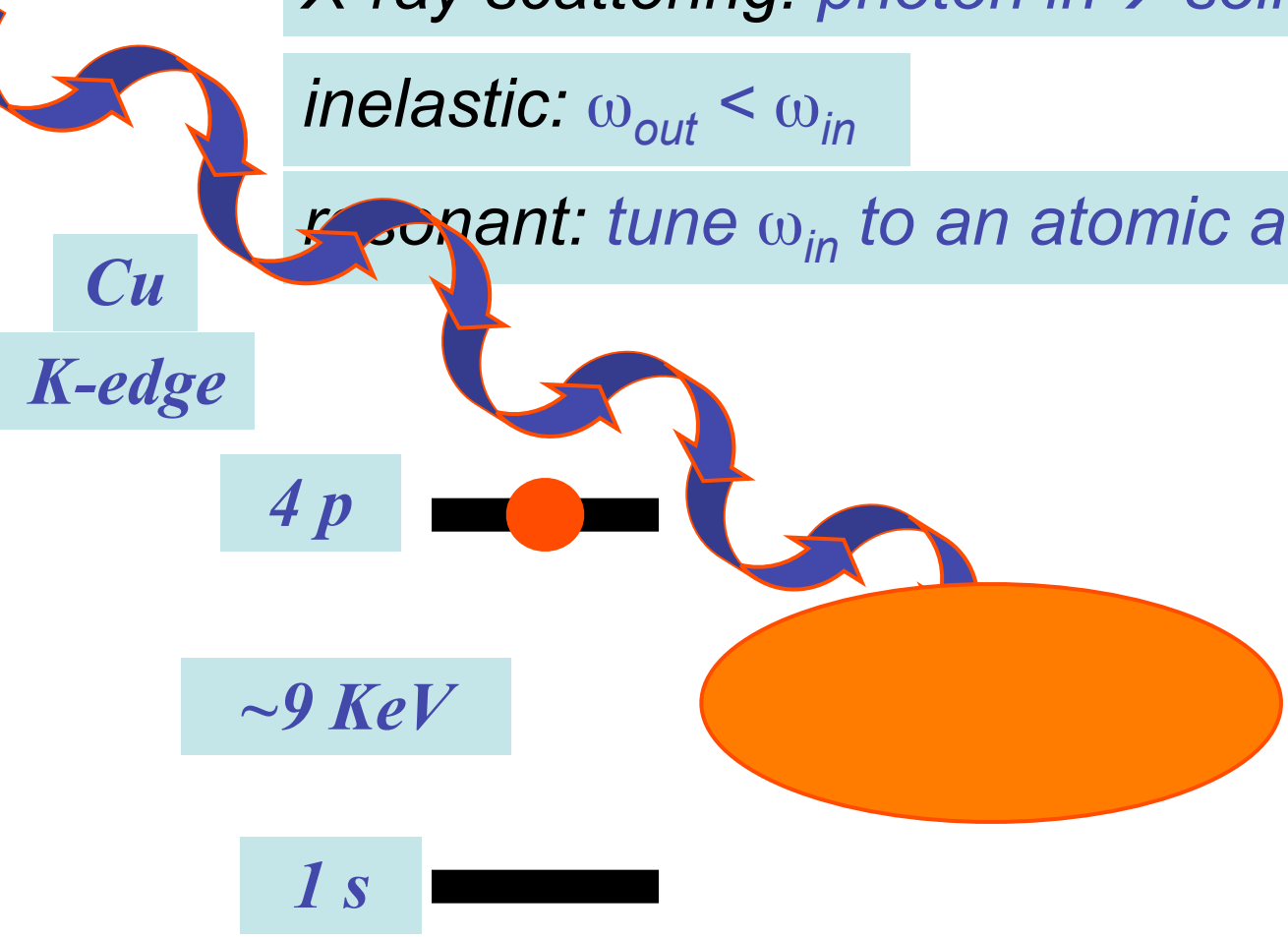

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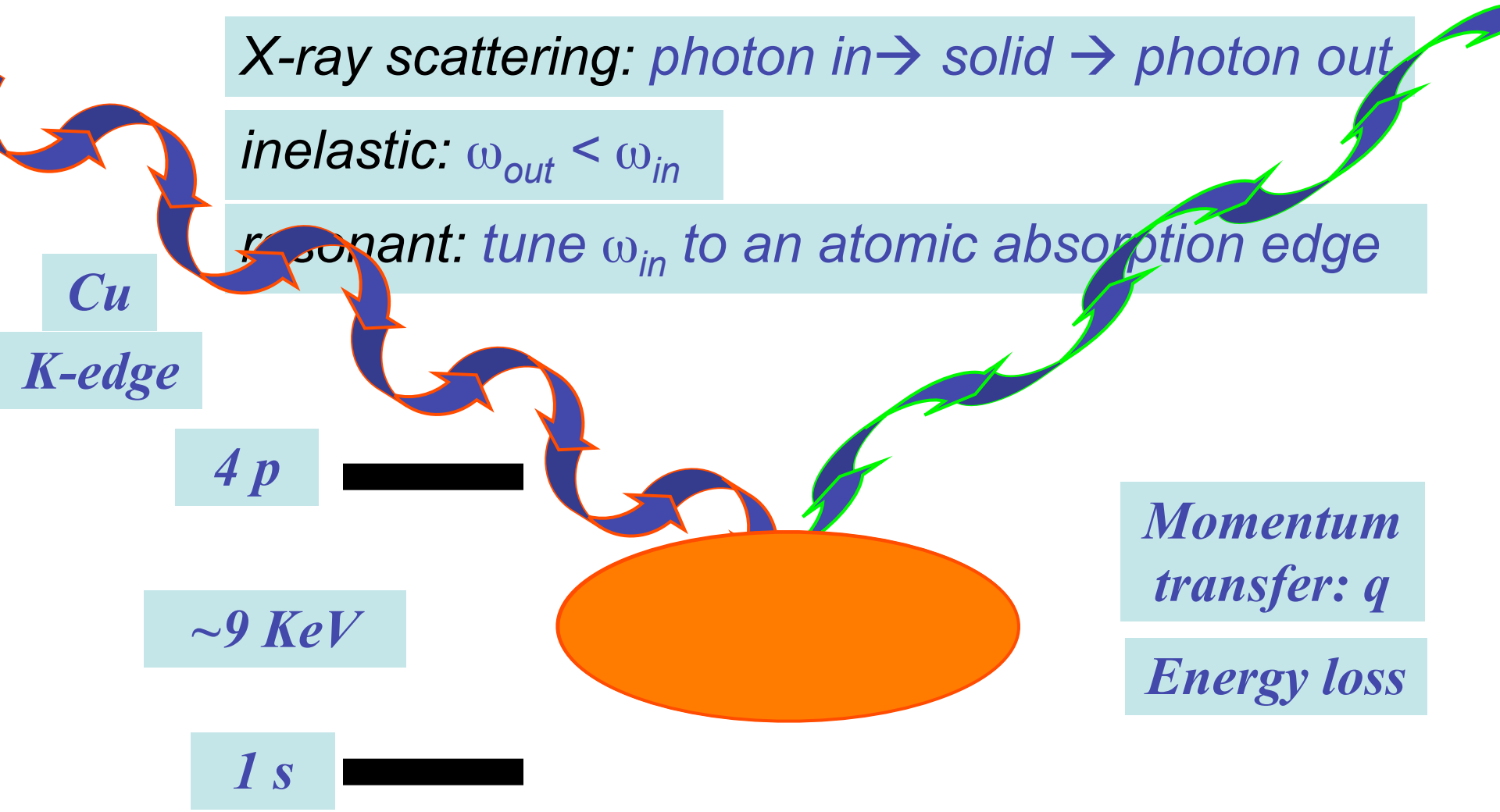

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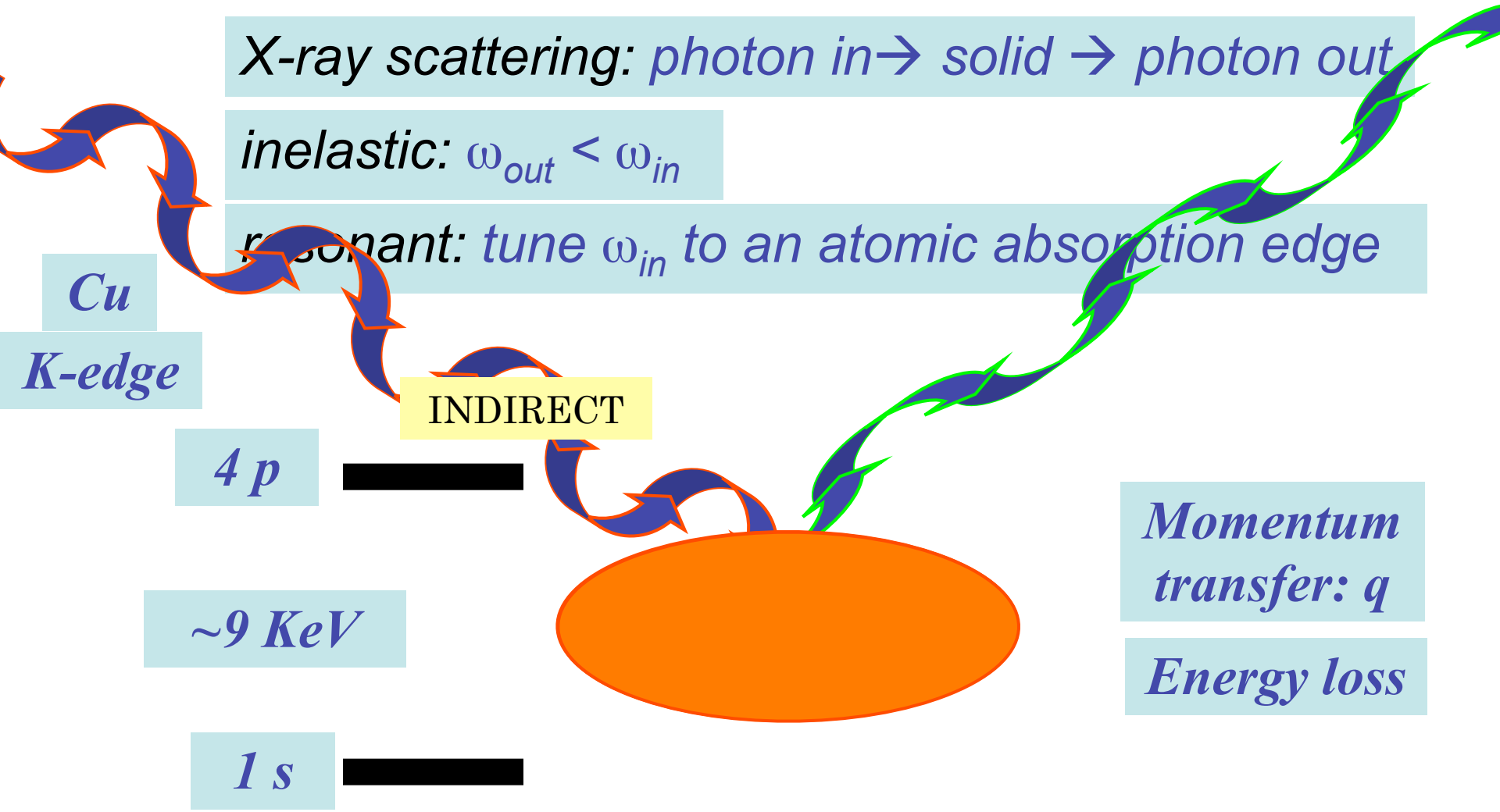

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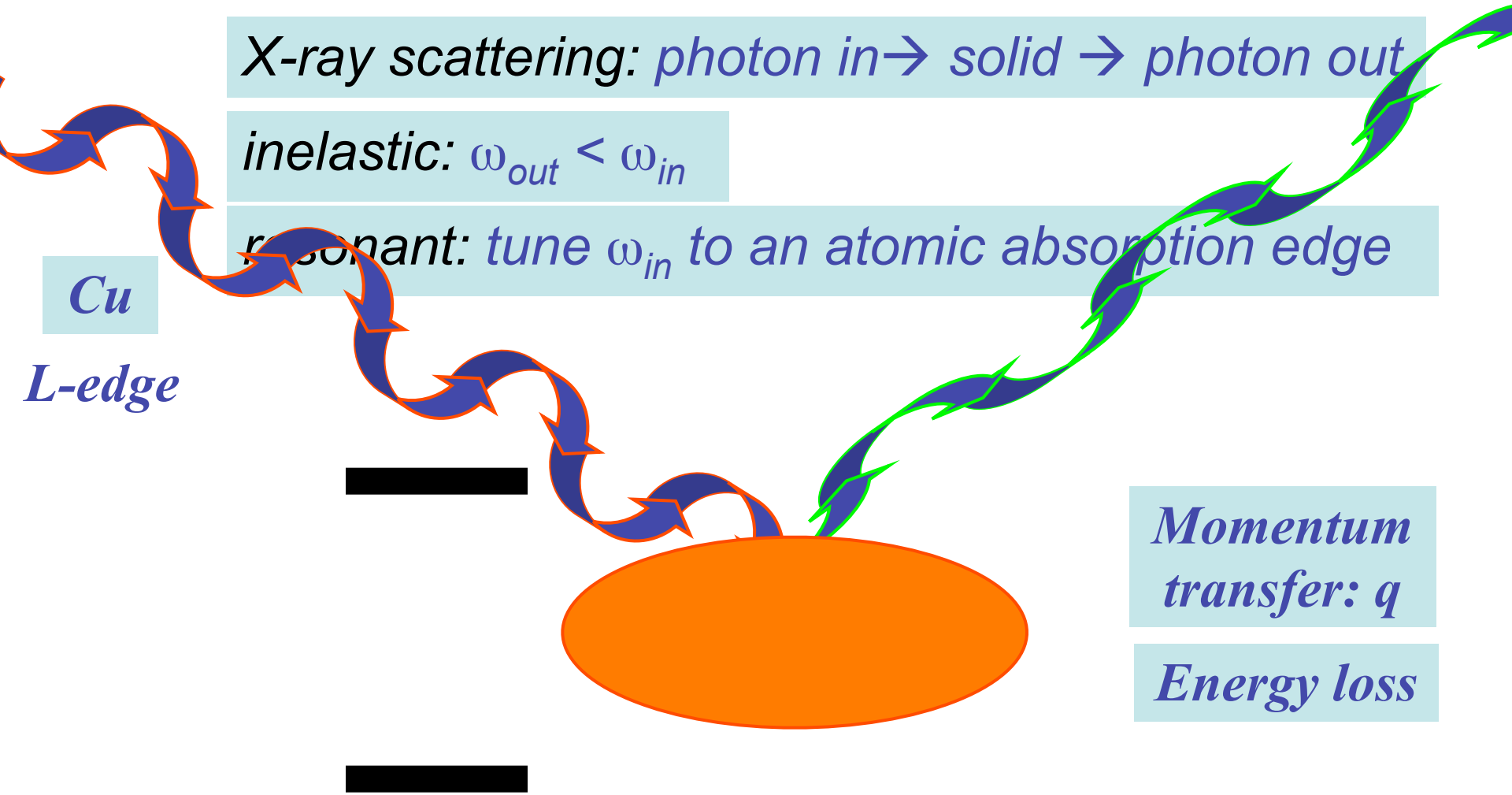
L-edge



Momentum transfer: q

Energy loss

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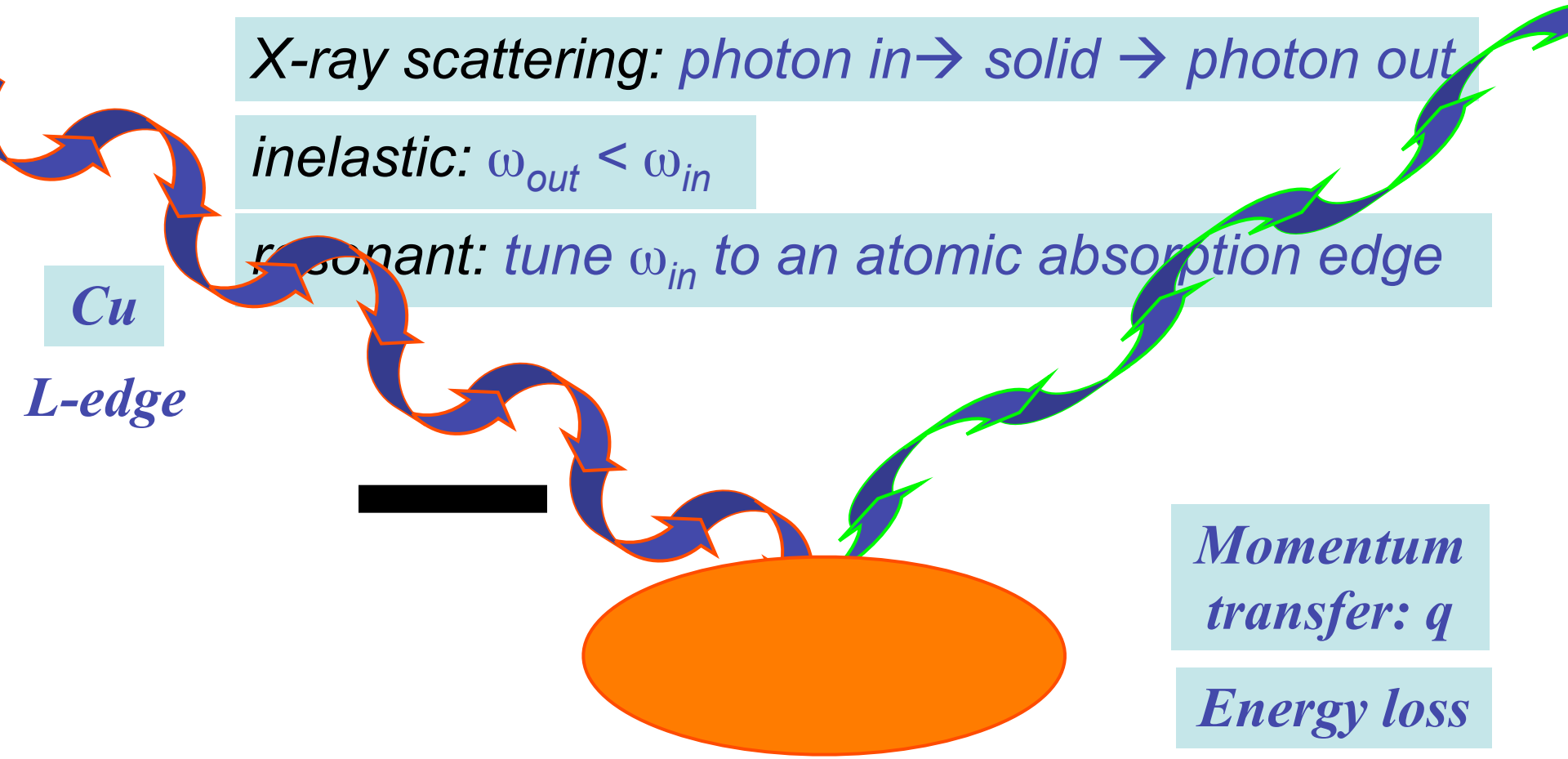

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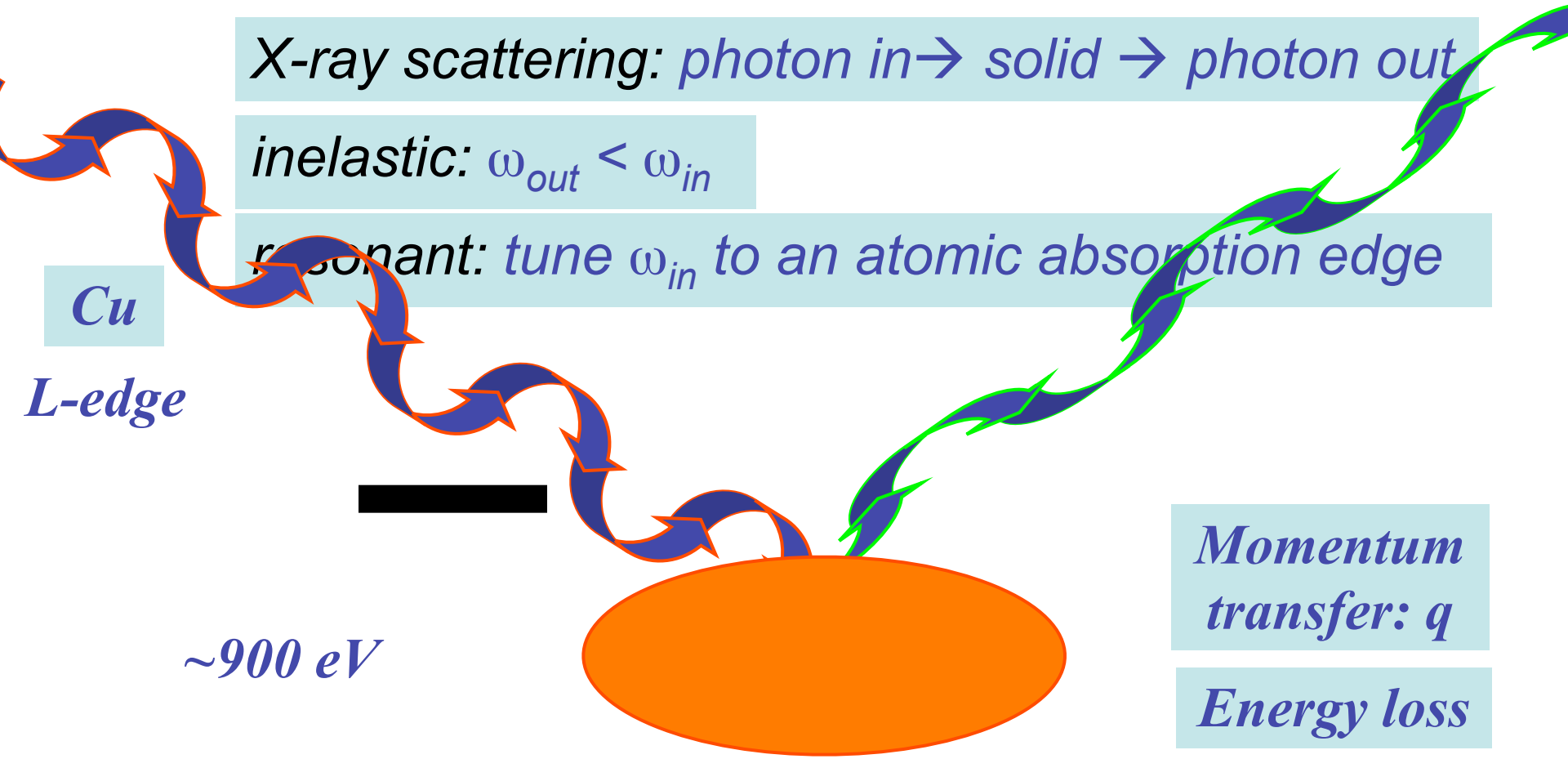

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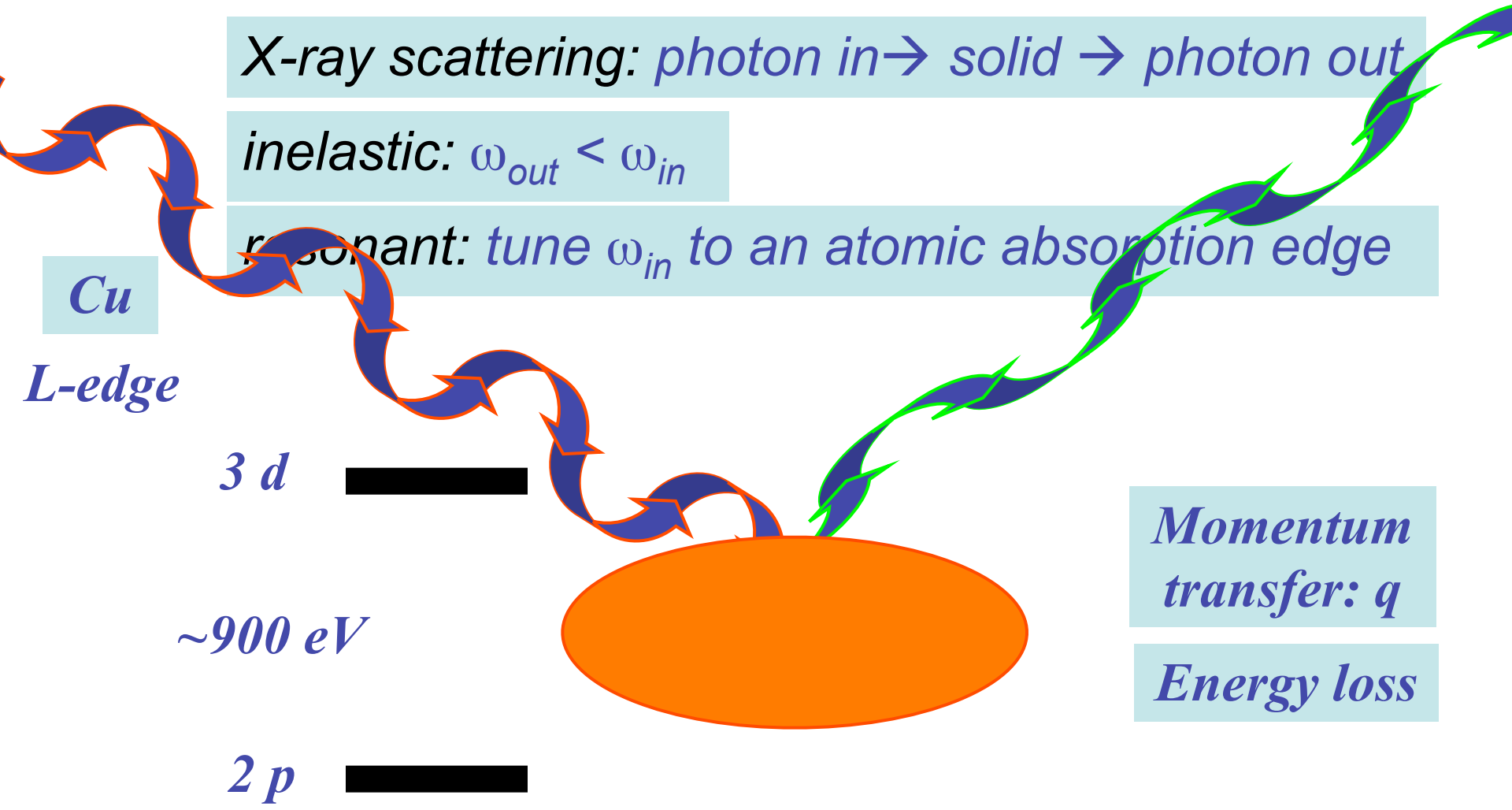

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Cu

L-edge

DIRECT

3 d

~900 eV

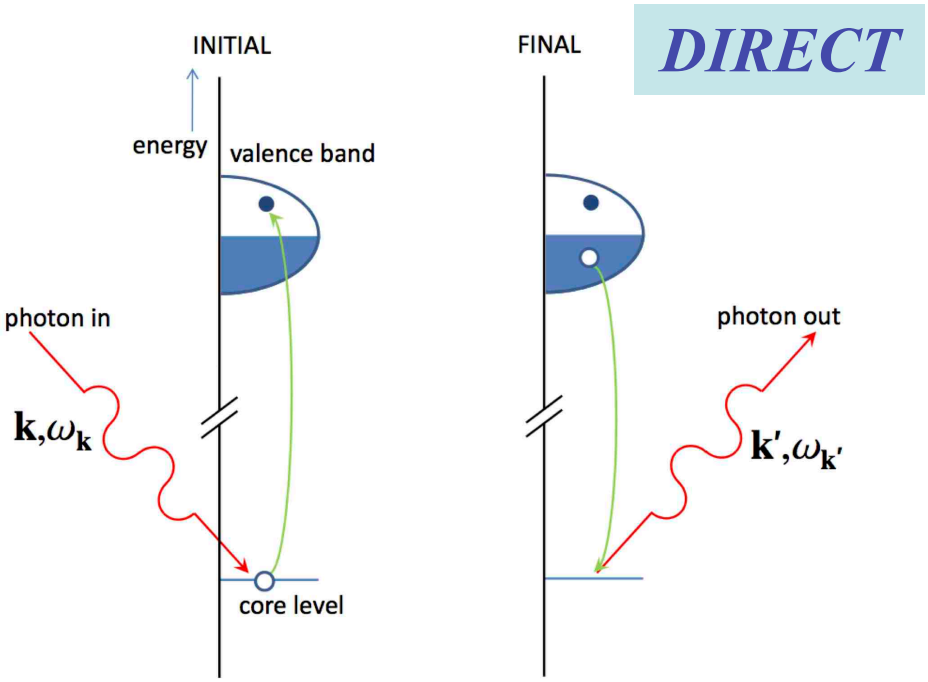
2 p

Momentum transfer: q

Energy loss

resolution < 100 meV

Direct and Indirect RIXS



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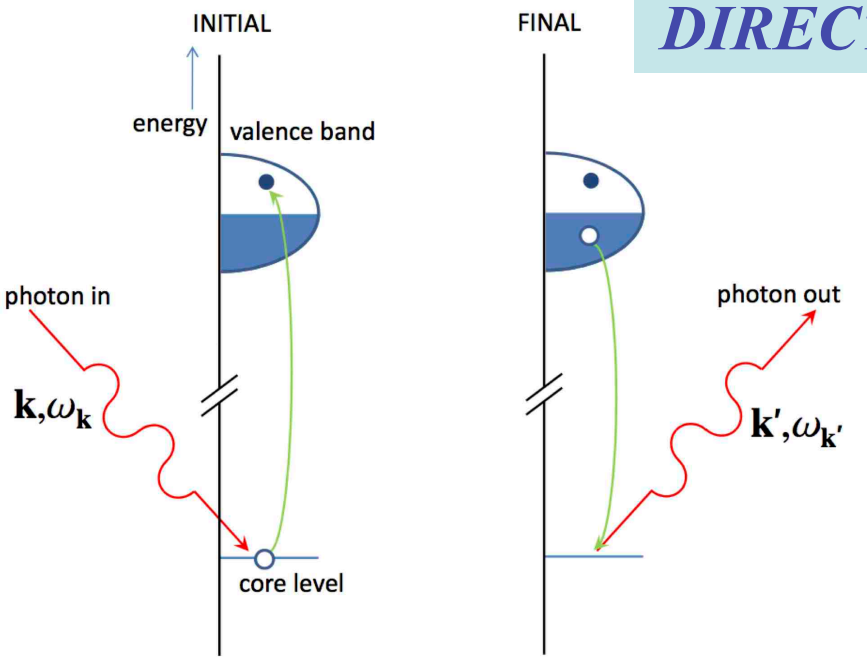
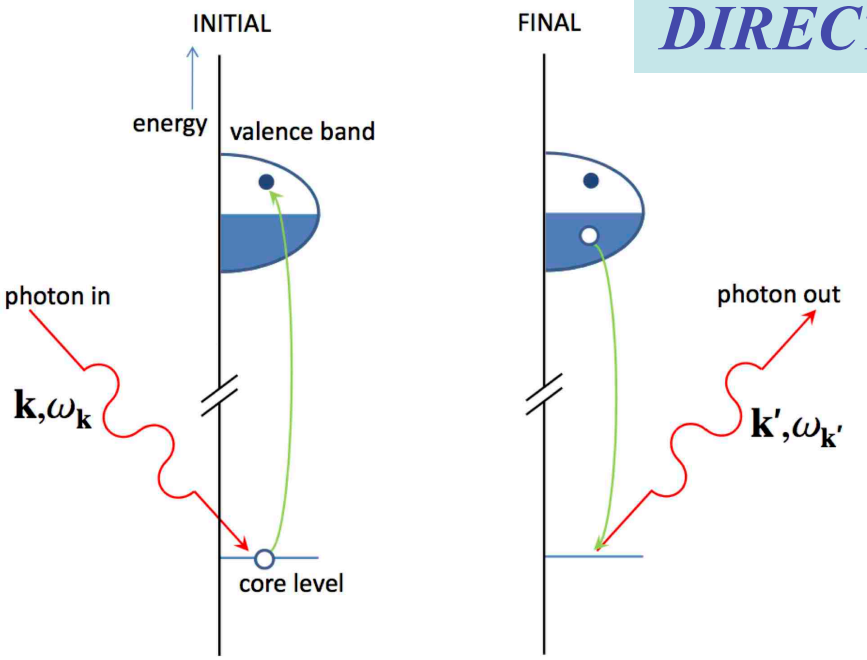


DIRECT

scattering via absorption-emission matrix elements

Direct and Indirect RIXS



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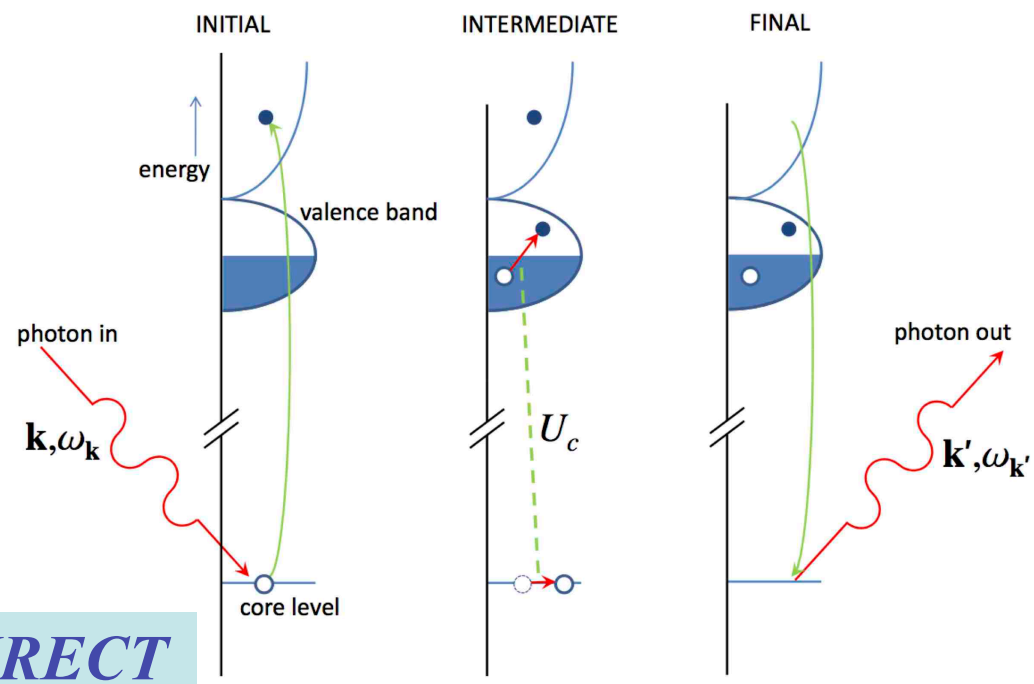

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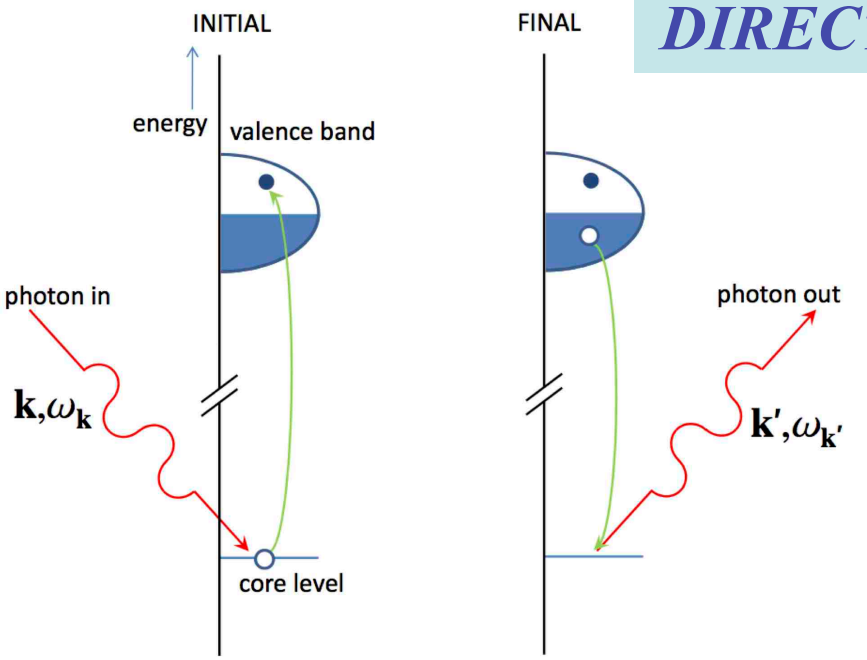

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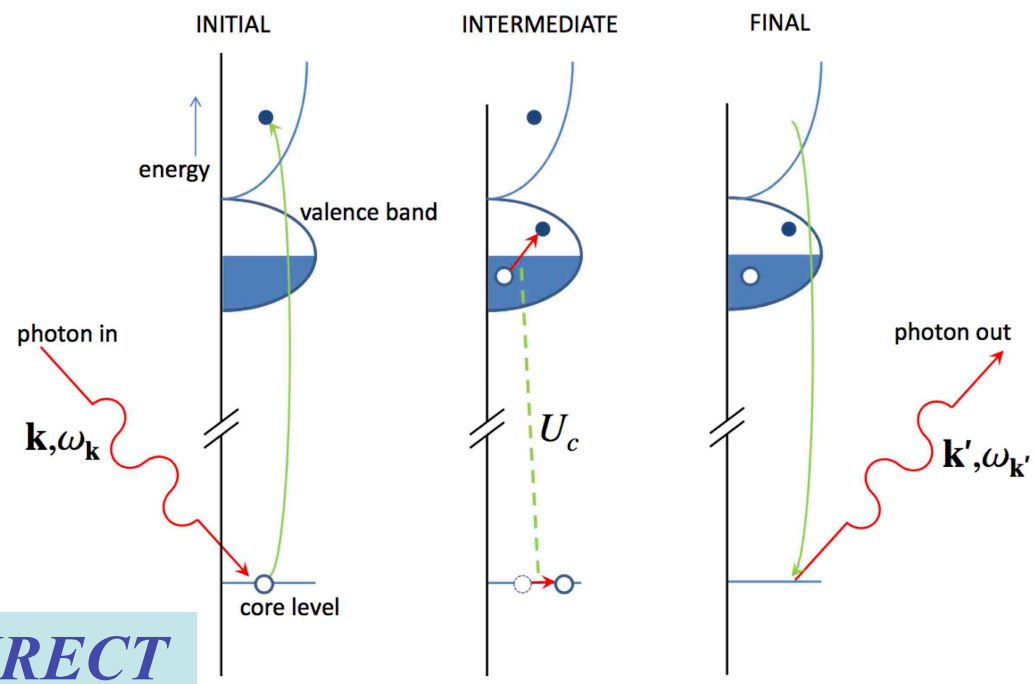
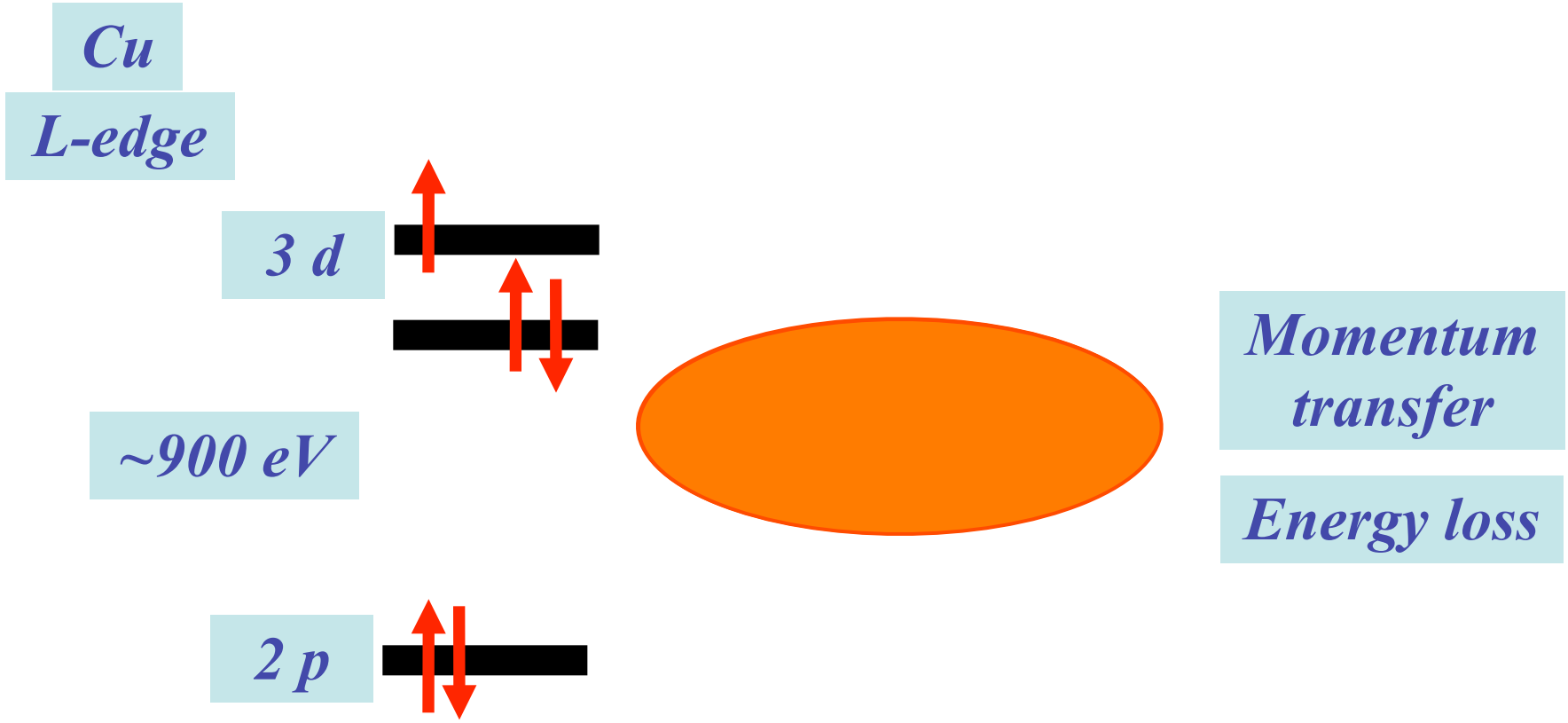


scattering via intermediate state core-hole shake-up

INDIRECT

Direct RIXS @ TM L-edges



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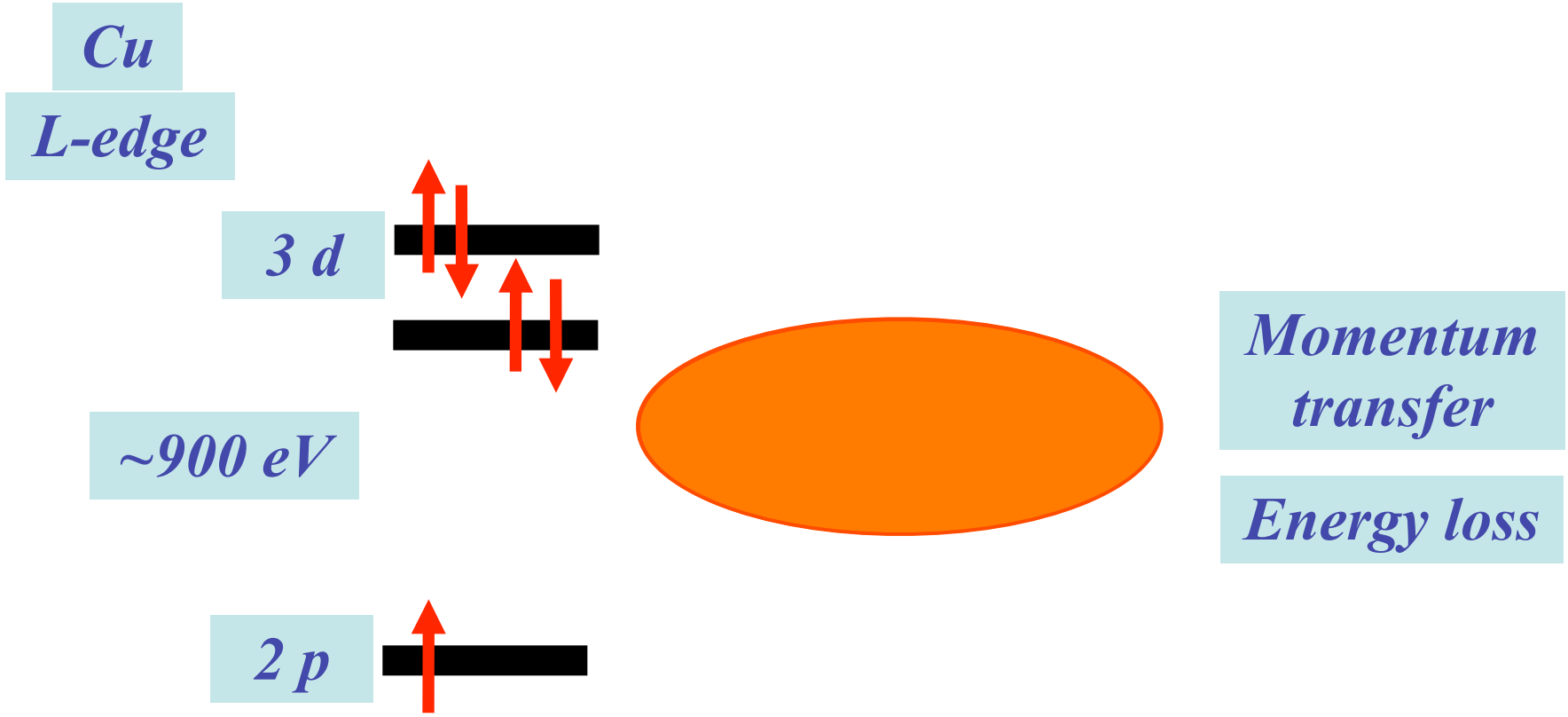

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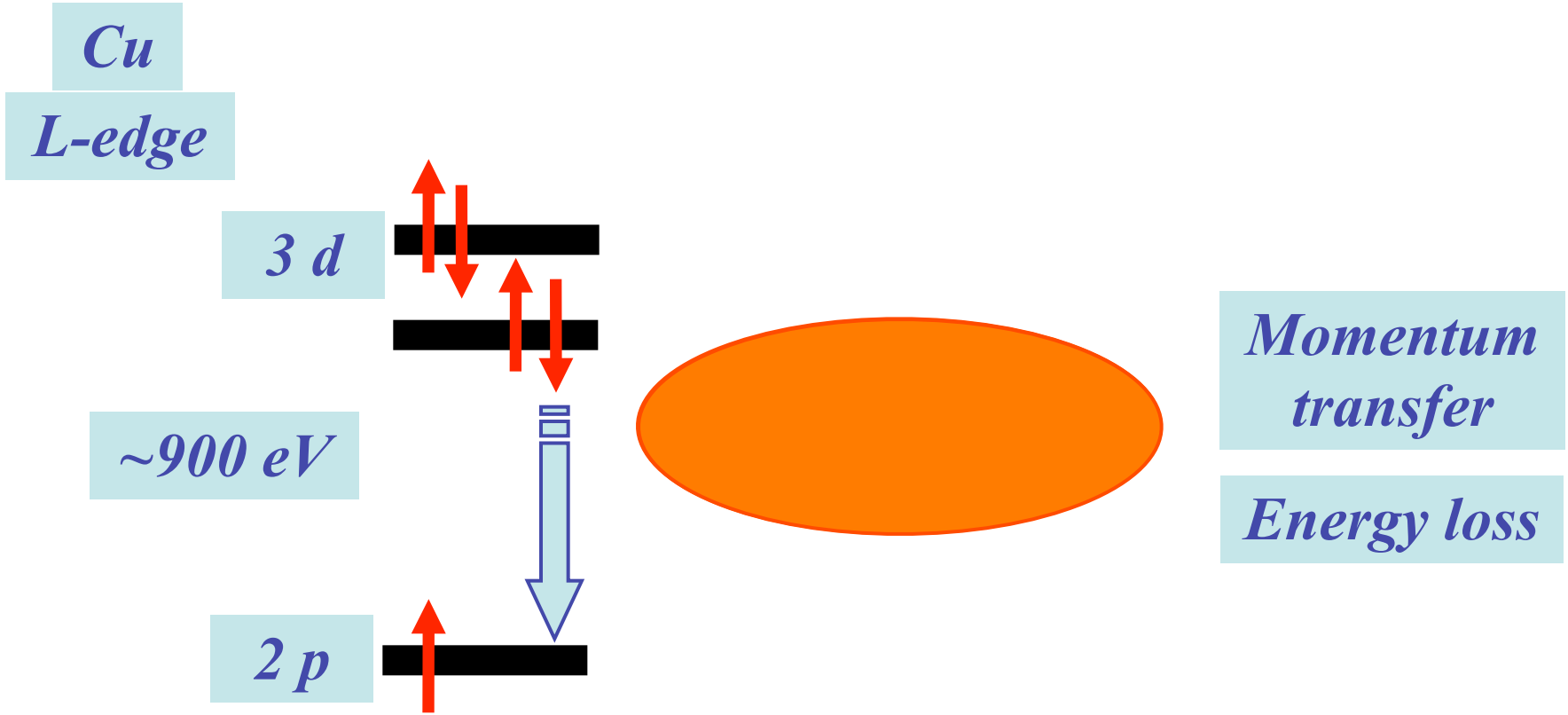

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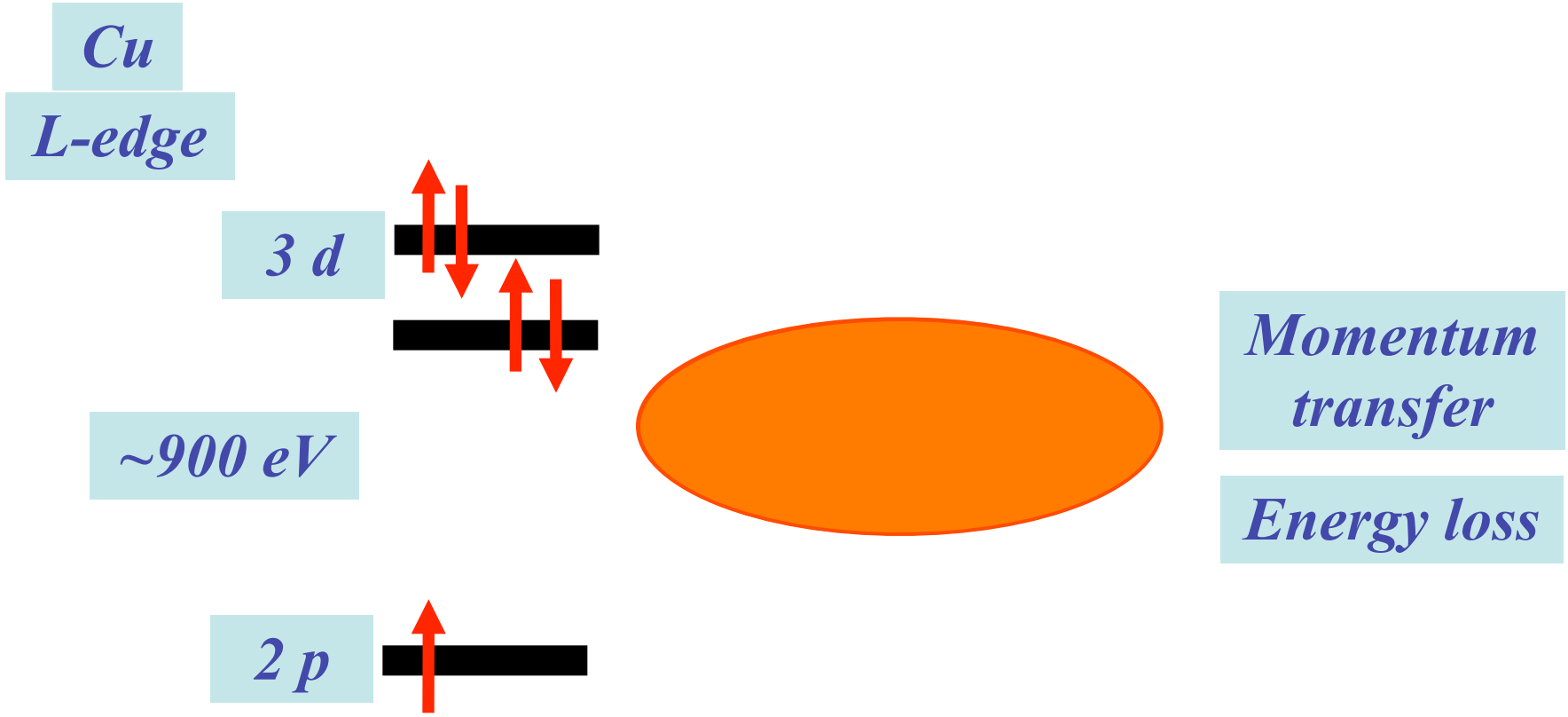

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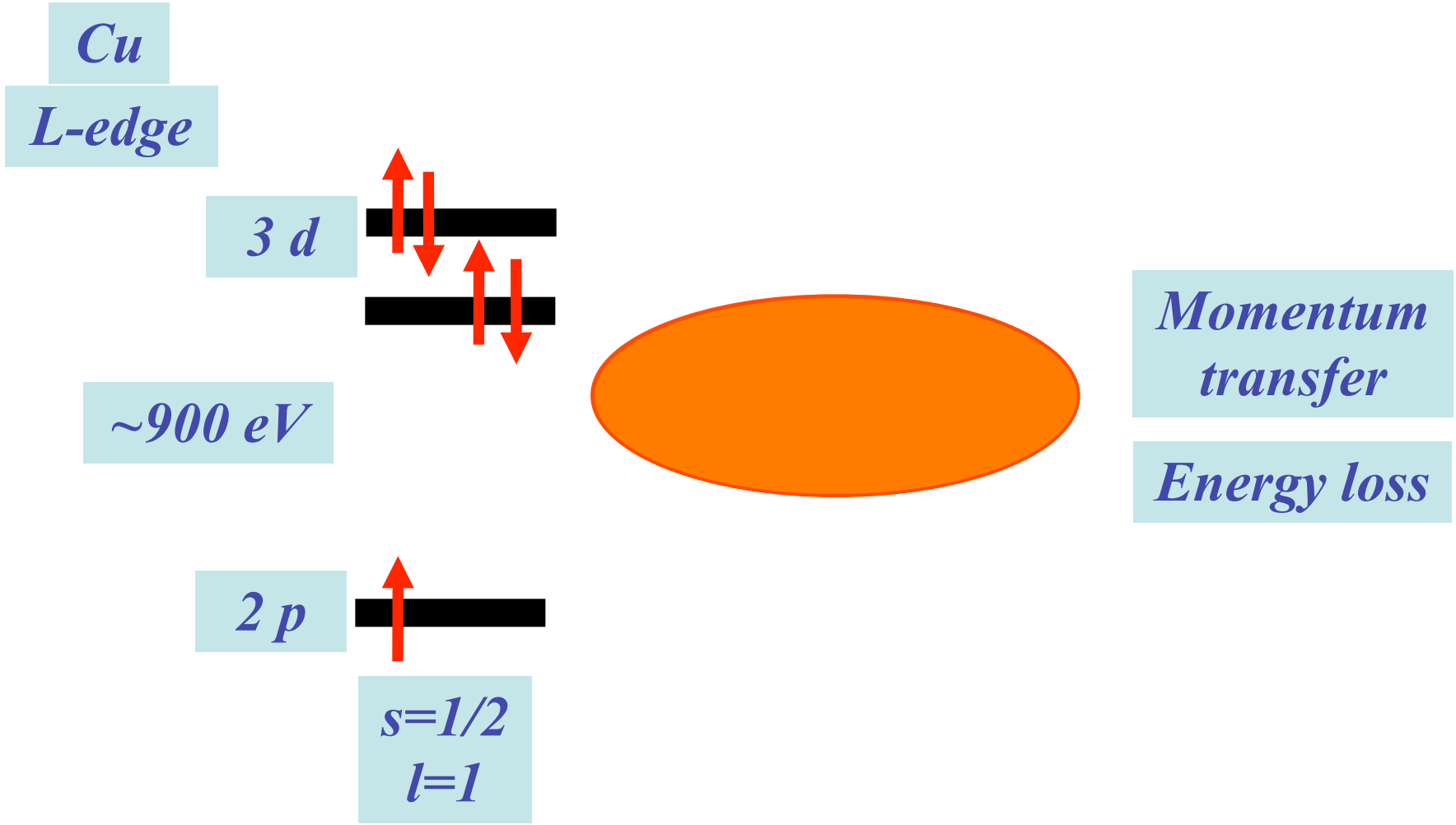

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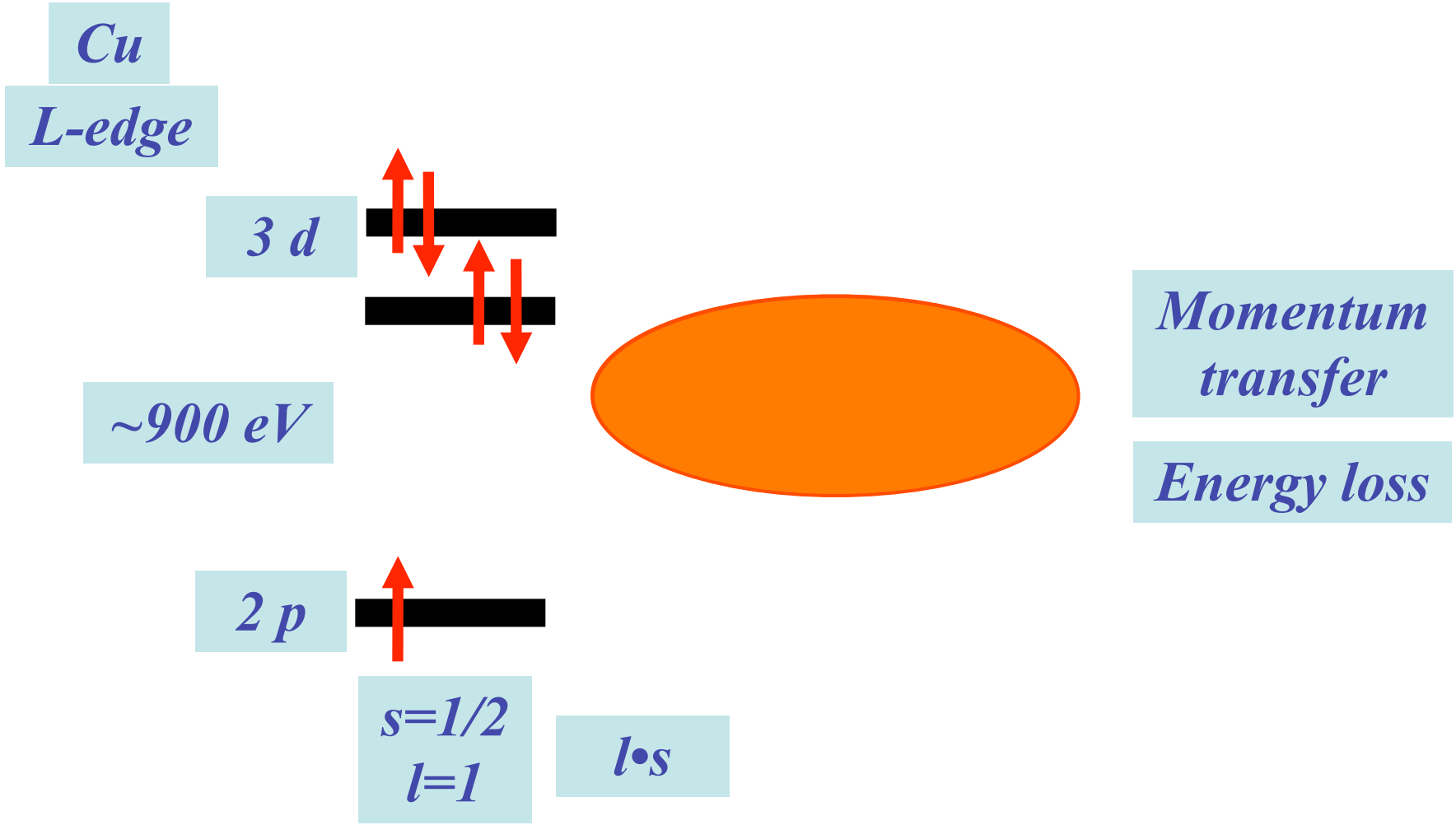

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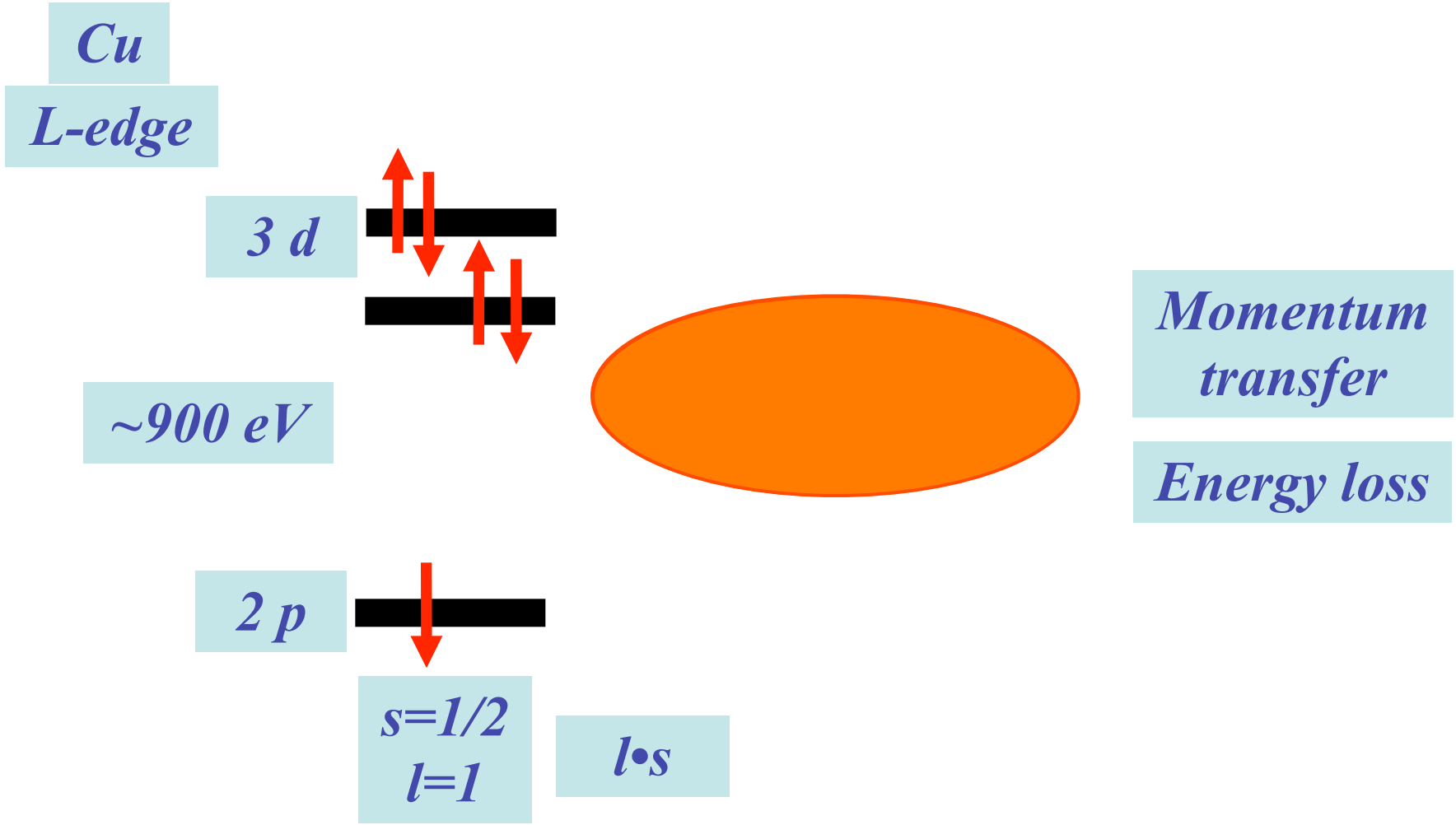

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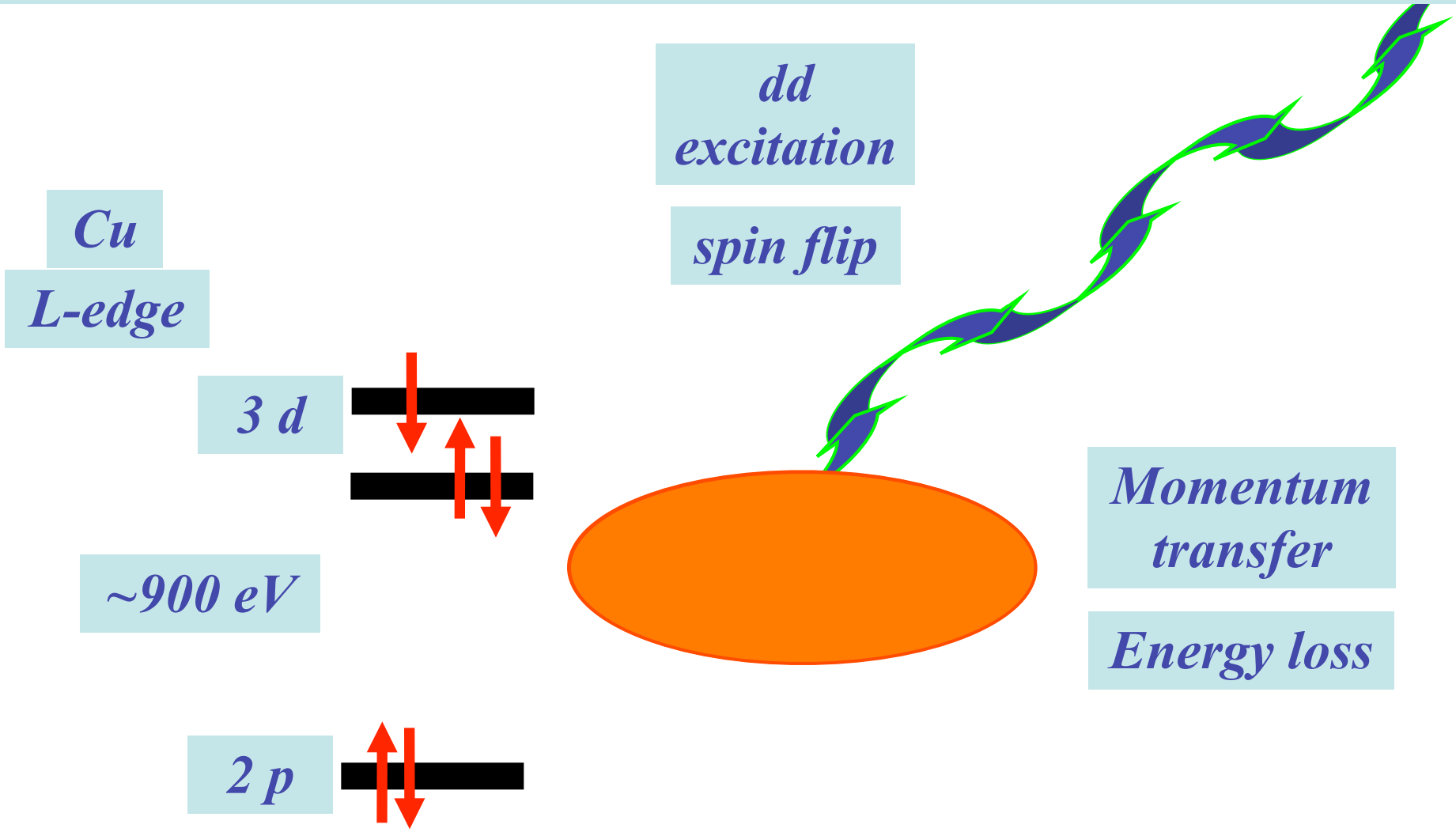

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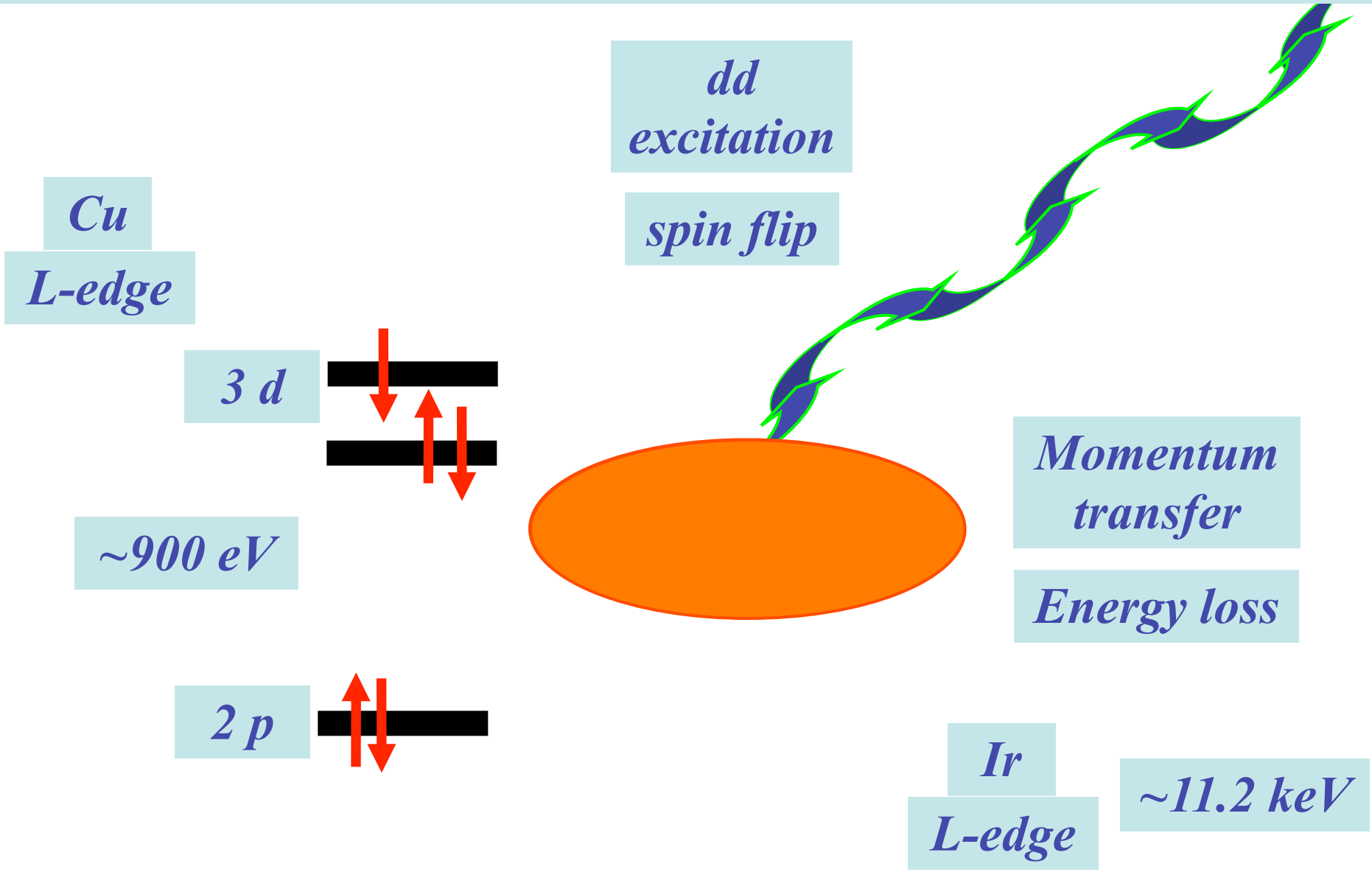

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Local atomic transition

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Carries low energy, long wavelength, elementary excitations

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But: $RIXS = |GS\rangle \rightarrow .... \rightarrow |FS\rangle$

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Universal effective low energy behavior

5 distinguishing features of RIXS

Why ***Inelastic Scattering*** { ***with X-rays*** / ***at a resonance*** }

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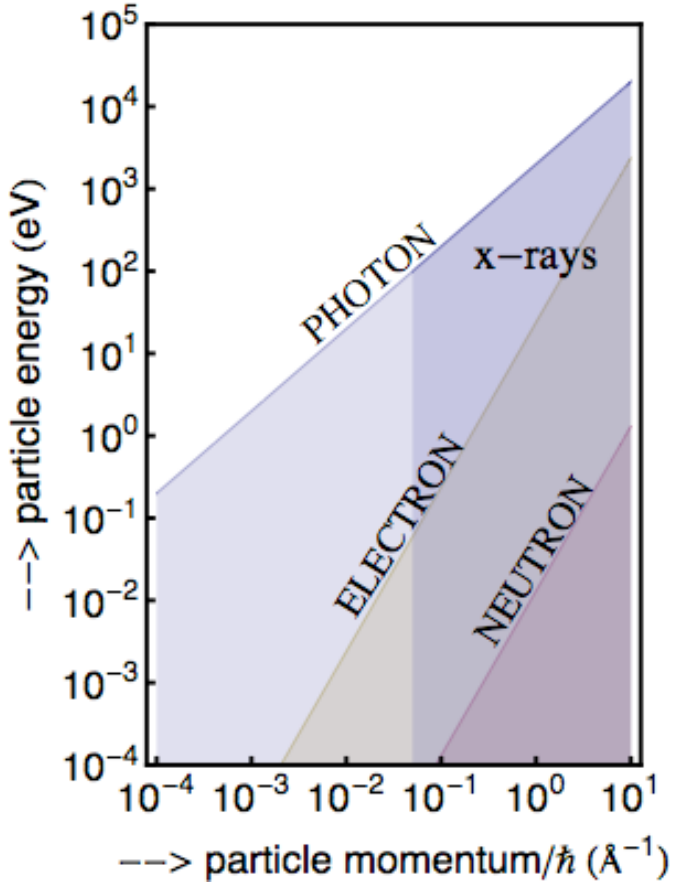
X-rays: ***momentum ~ Å^{-1}***



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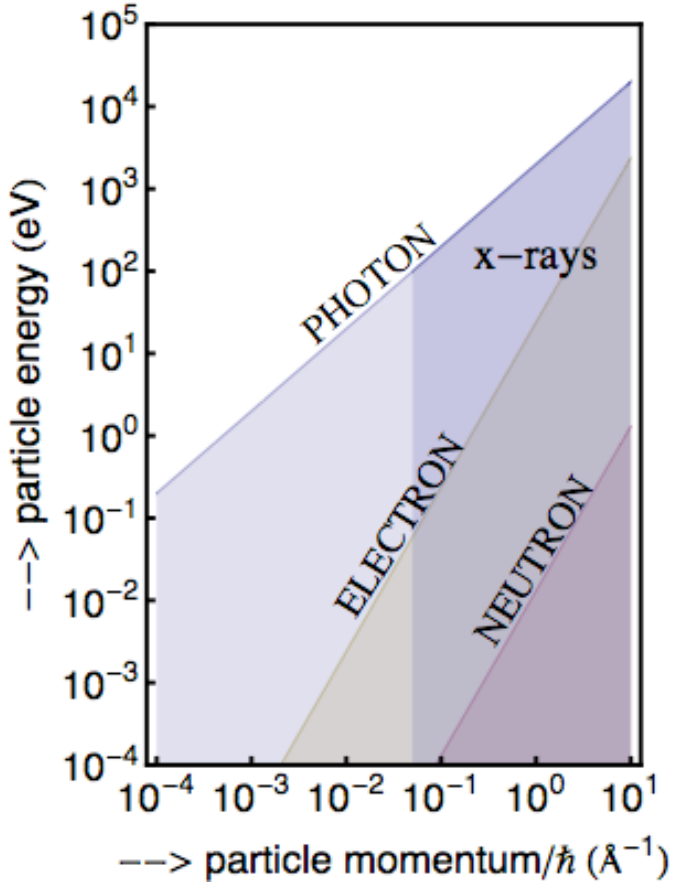

Solid: **Lattice spacings ~ Å**

Brioullin zone ~ Å^{-1}

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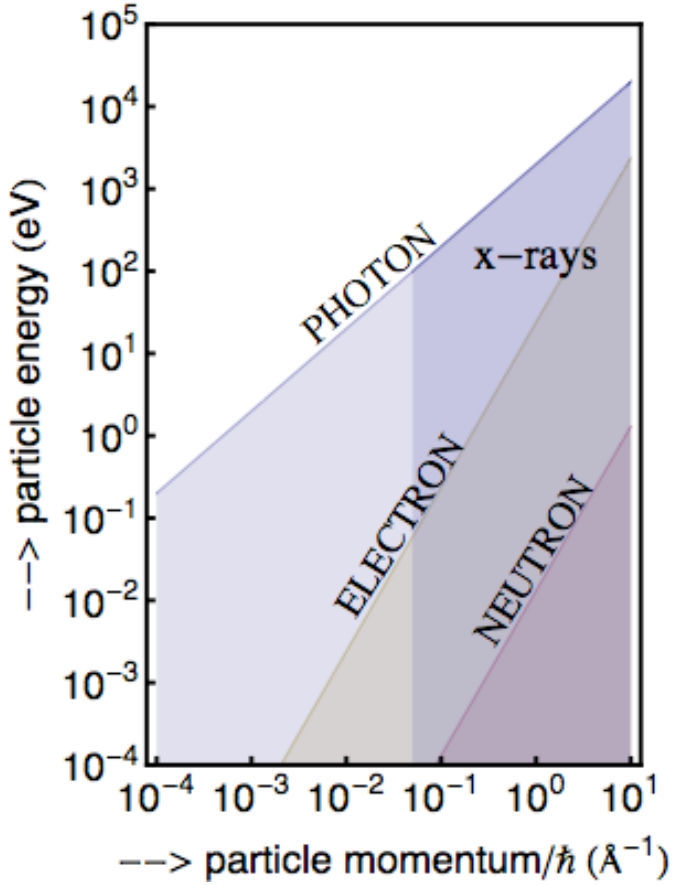

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Visible Photons: **momentum ~ 10^{-3} Å^{-1}**

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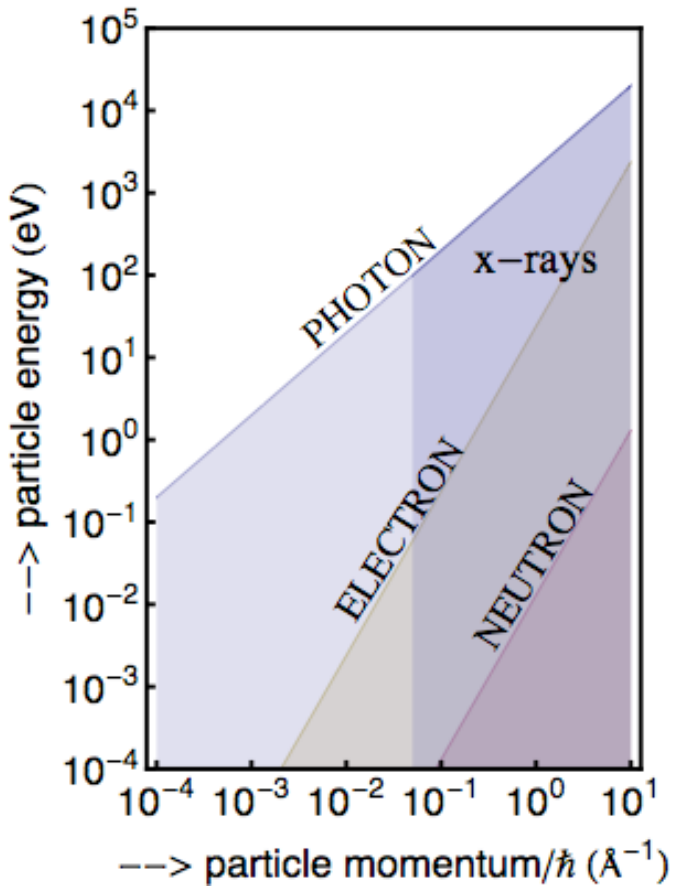

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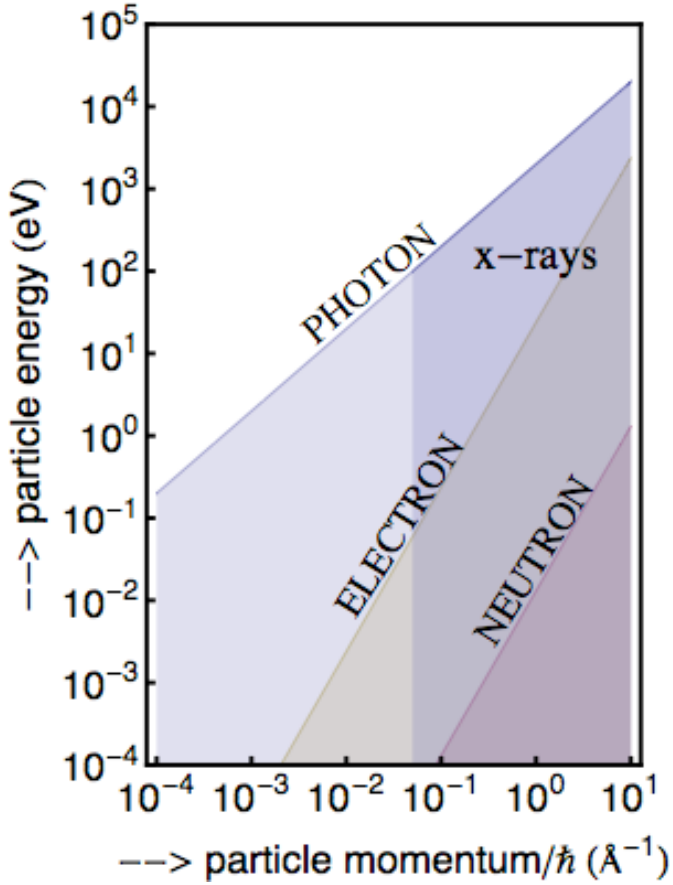
X-rays at 10 keV | **momentum ~ 5 Å^{-1}** / **several BZ's**

Why | **Inelastic Scattering** | **with X-rays** / **at a resonance**

probe charged excitations

X-rays: | **momentum ~ Å^{-1}**



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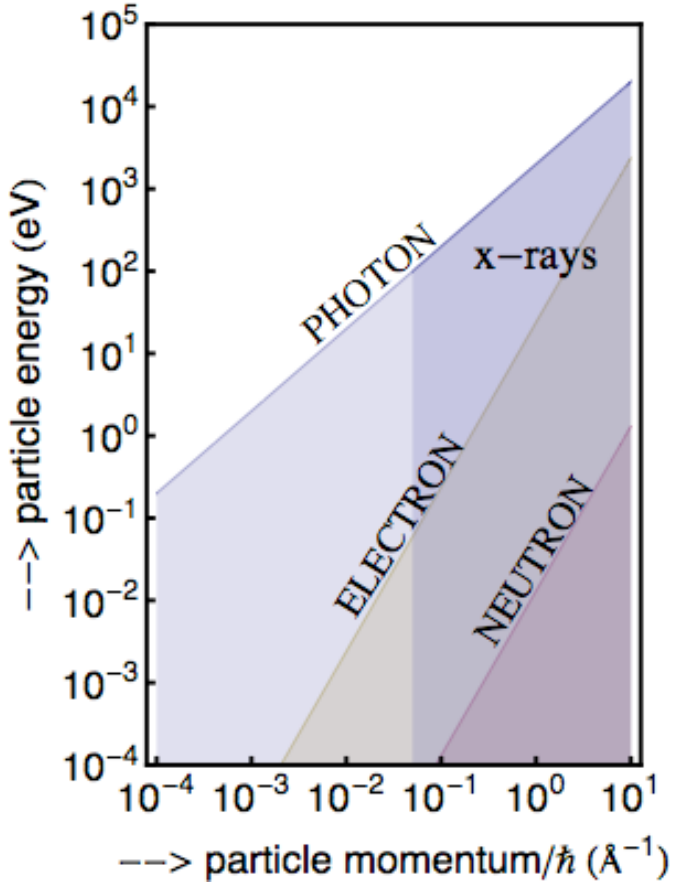

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polarization dependence

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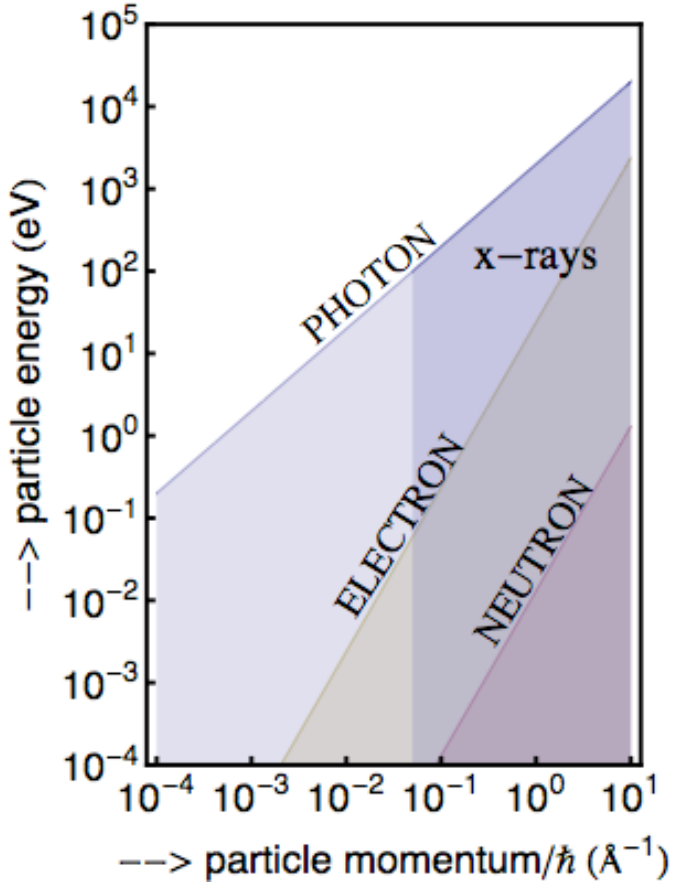

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1. RIXS exploits both the *energy and momentum* dependence of the photon scattering cross-section. Comparing the energies of a neutron, electron, and photon, each with a wavelength on the order of the relevant length scale in a solid, *i.e.* the interatomic lattice spacing, which is on the order of a few Angstroms, it is obvious that an x-ray photon has much more energy than an equivalent neutron or electron.

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The scattering phase space (the range of energies and momenta that can be transferred in a scattering event) available to x-rays is therefore correspondingly larger and is in fact without equal. For instance, unlike photon scattering experiments with visible or infrared light, RIXS can probe the full dispersion of low energy excitations in solids.

2. RIXS can utilize the *polarization* of the photon: the nature of the excitations created in the material can be disentangled through polarization analysis of the incident and scattered photons, which allows one, through the use of various selection rules, to characterize the symmetry and nature of the excitations. To date, no experimental facility allows the polarization of the scattered photon to be measured, though the incident photon polarization is frequently varied.

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- ***at a resonance***

Why ***Inelastic Scattering*** { ***with X-rays*** / ***at a resonance*** }

At resonance:

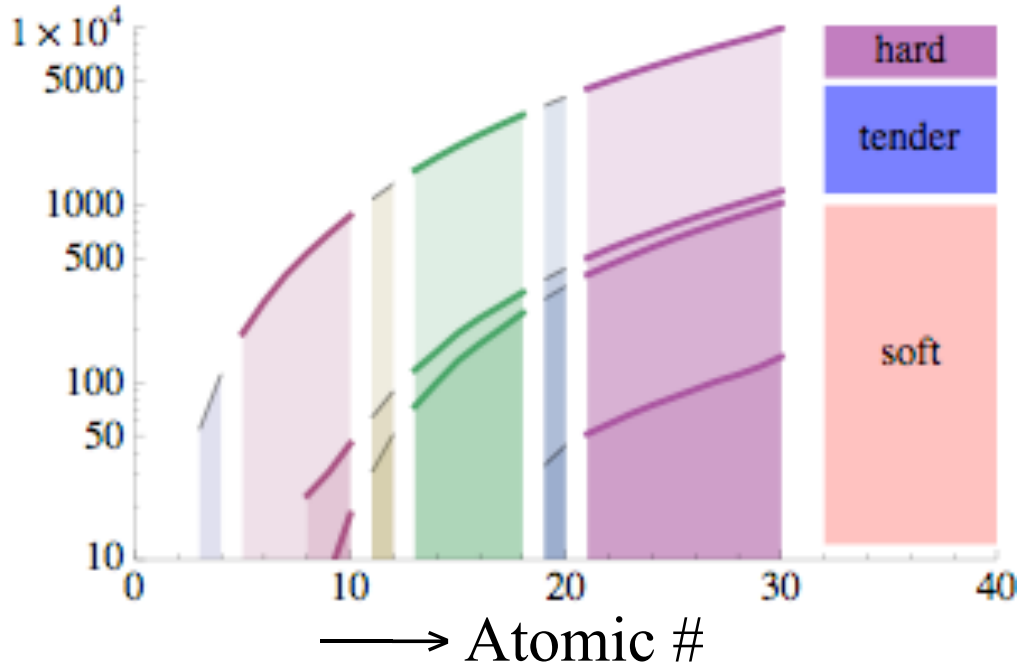
enhanced loss features

Why *Inelastic Scattering* { *with X-rays* / *at a resonance* }

At resonance:

enhanced loss features *choose element & electronic shell*

X-ray Absorption Edges



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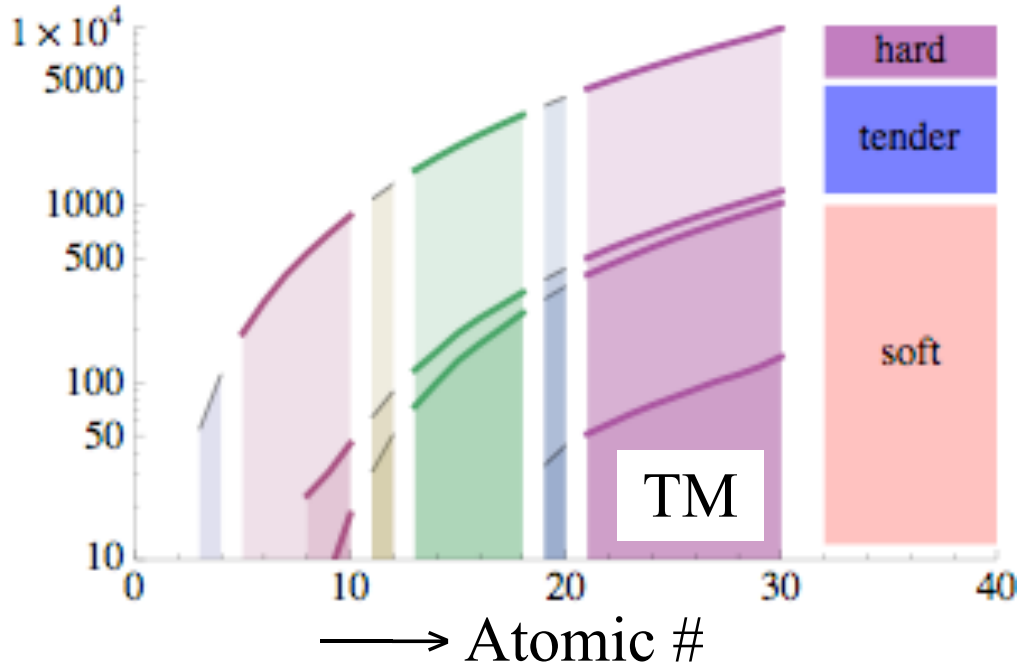

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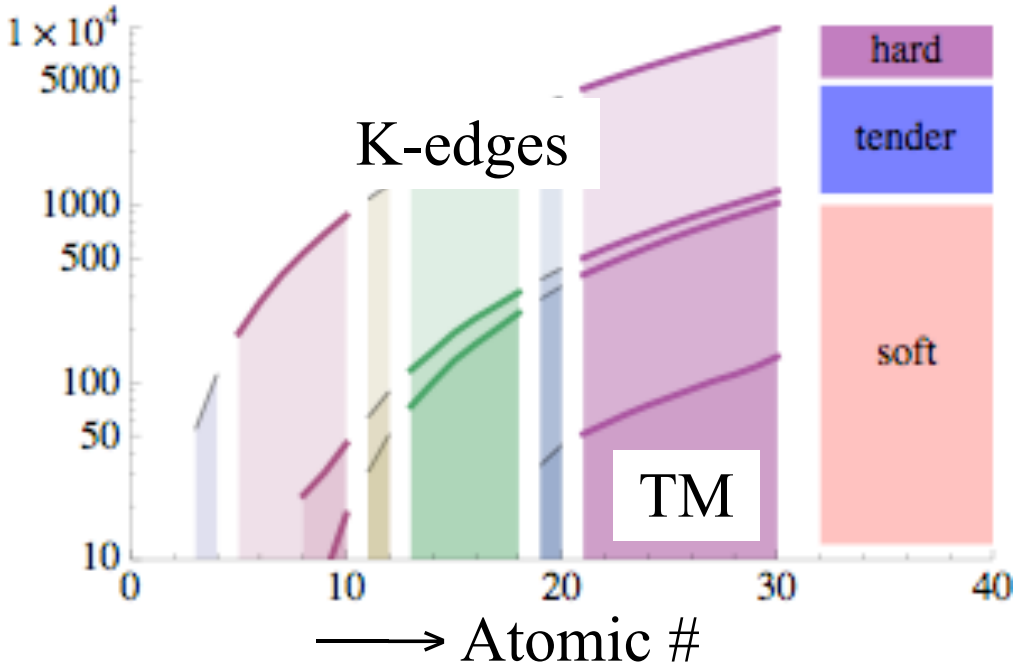

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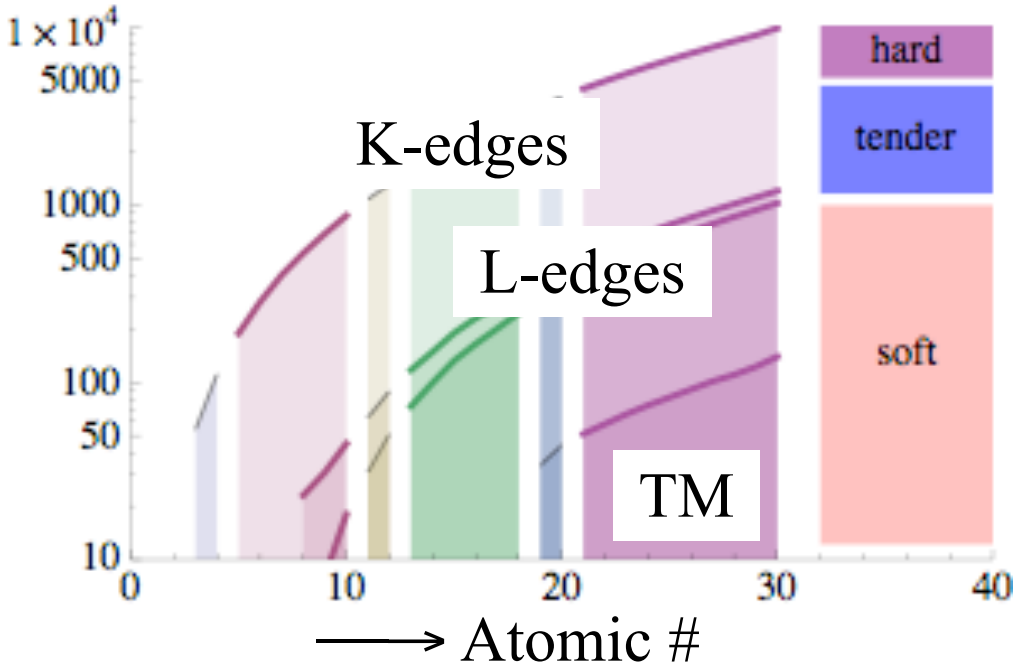

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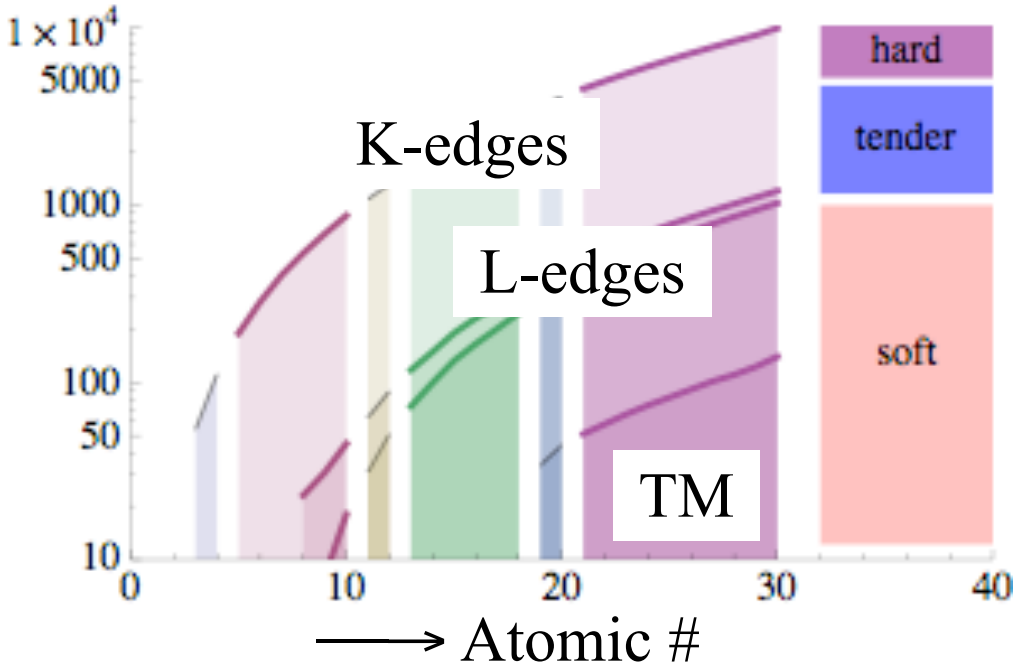

X-ray penetration depth: ~microns

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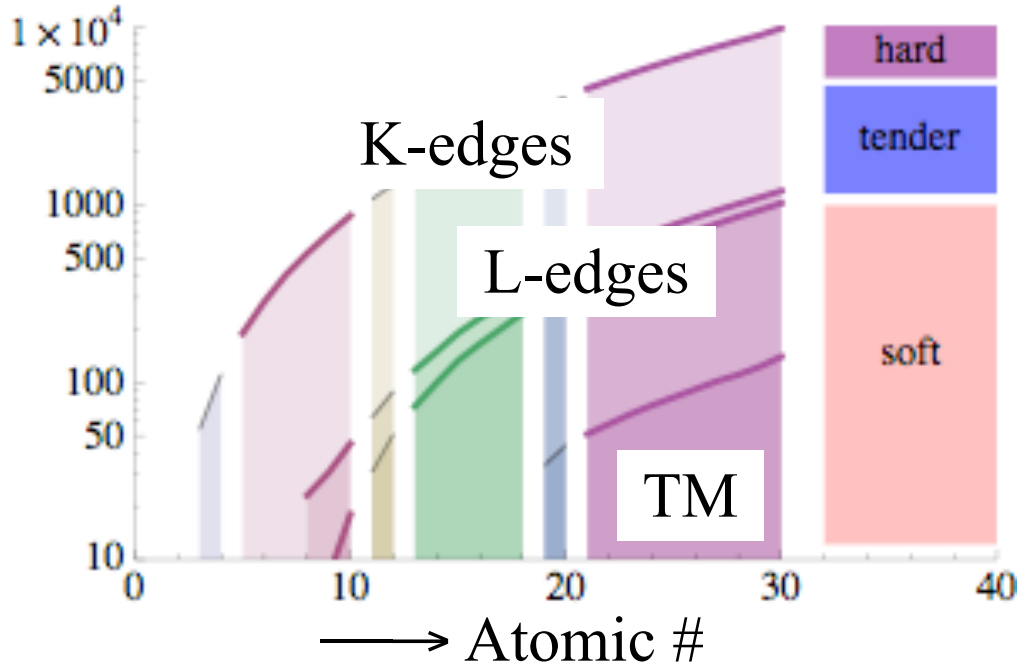
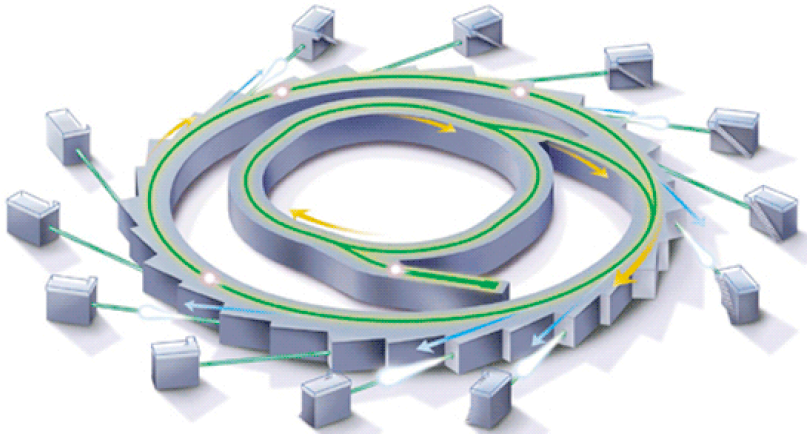


X-ray penetration depth: ~microns

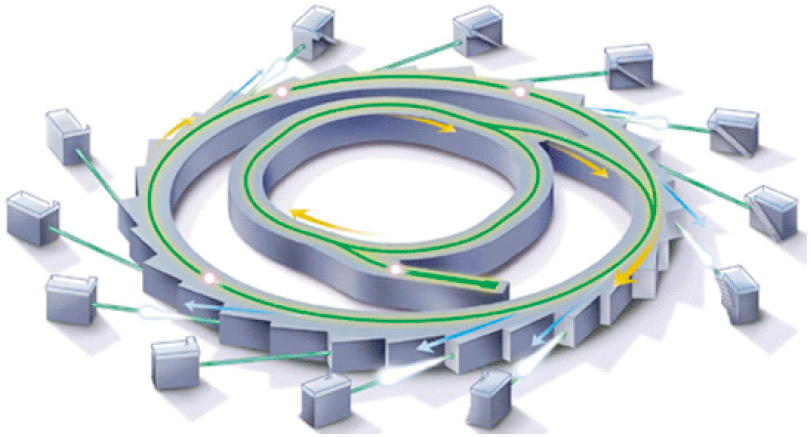
RIXS is bulk sensitive

Tunable X-ray sources



Tunable X-ray sources

synchrotron



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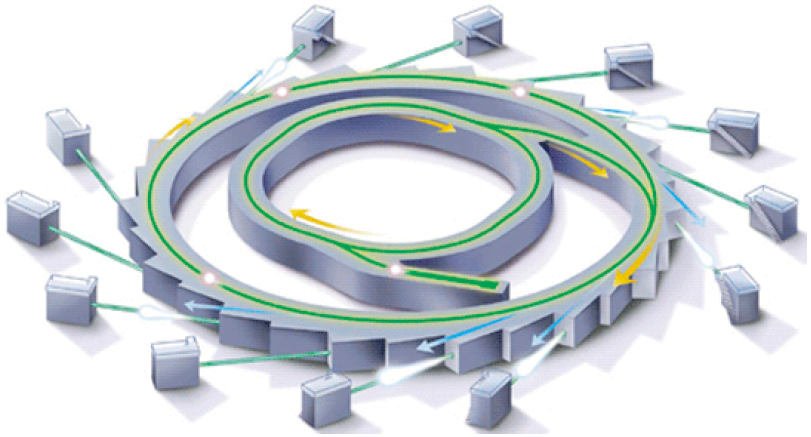
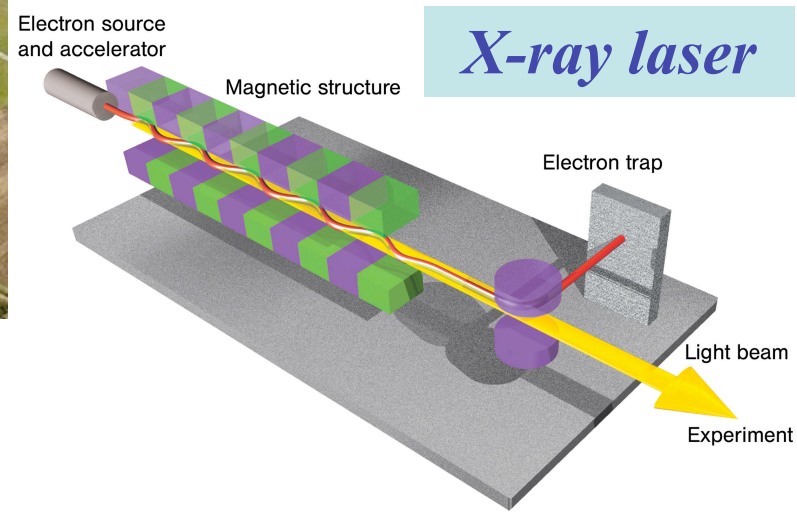


X-ray laser



LCLS, Stanford

3. RIXS is *element and orbital specific*: Chemical sensitivity arises by tuning the incident photon energy to specific atomic transitions of the different types of atoms in a material. Such transitions are called absorption edges. RIXS can even differentiate between the same chemical element at sites with inequivalent chemical bondings, with different valencies or at inequivalent crystallographic positions if the absorption edges in these cases are distinguishable.

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4. RIXS is *bulk sensitive*: the penetration depth of resonant x-ray photons is material and scattering geometry-specific, but typically is on the order of a few μm in the hard x-ray regime (for example at transition metal K-edges) and on the order of 0.1 μm in the soft x-ray regime (e.g transition metal L-edges).

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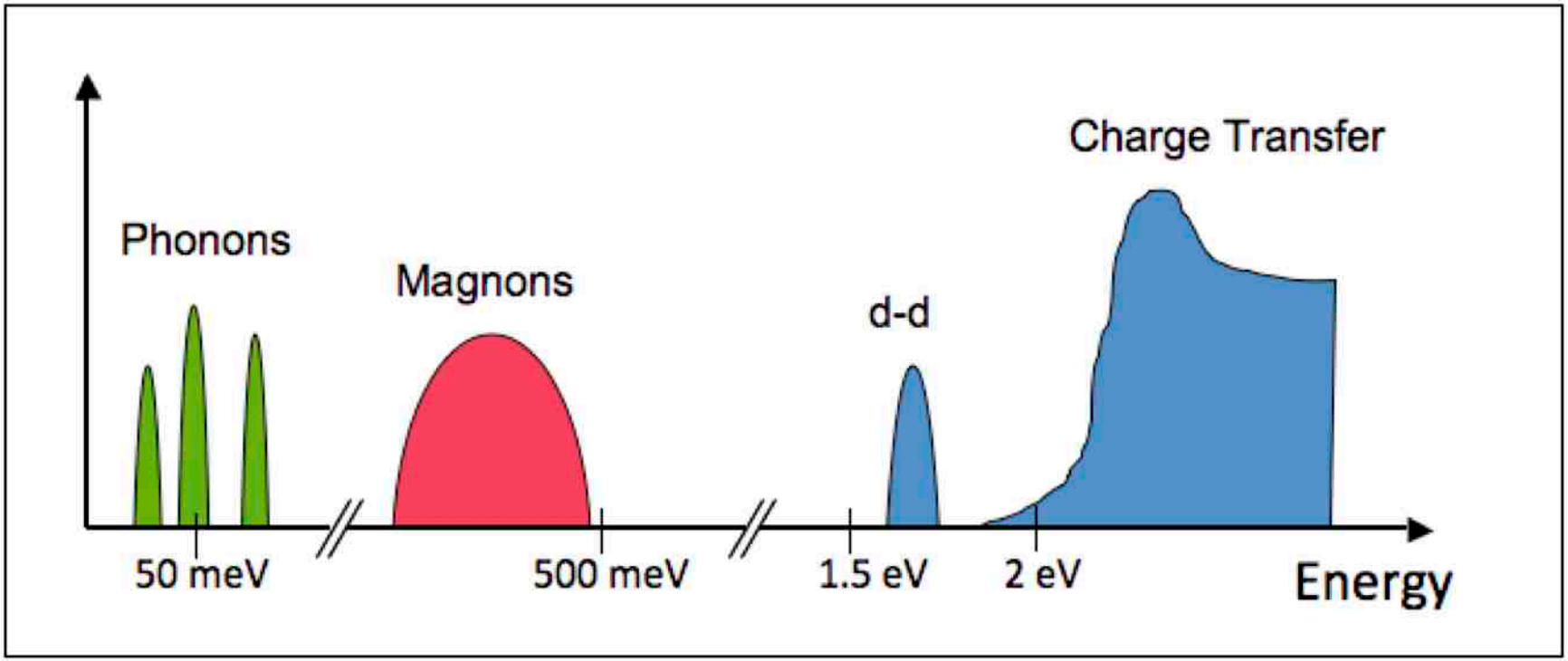
5. RIXS needs only *small sample volumes*: the photon-matter interaction is relatively strong, compared to for instance the neutron-matter interaction strength. In addition, photon sources deliver many orders of magnitude more particles per second, in a much smaller spot, than do neutron sources. These facts make RIXS possible on very small volume samples, thin films, surfaces and nano-objects, in addition to bulk single crystal or powder samples.

Elementary Excitations

accessible to RIXS

Elementary Excitations in TMO: Schematic



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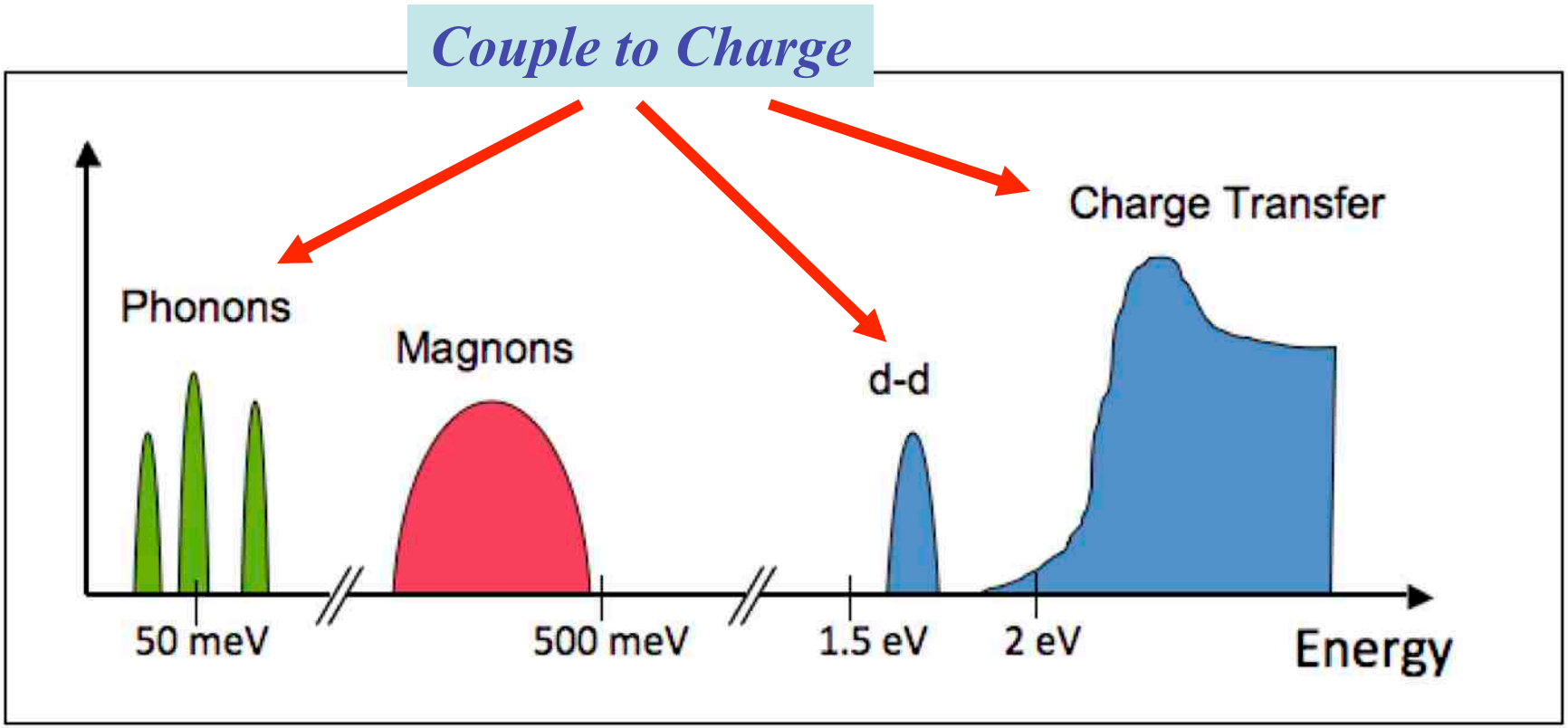

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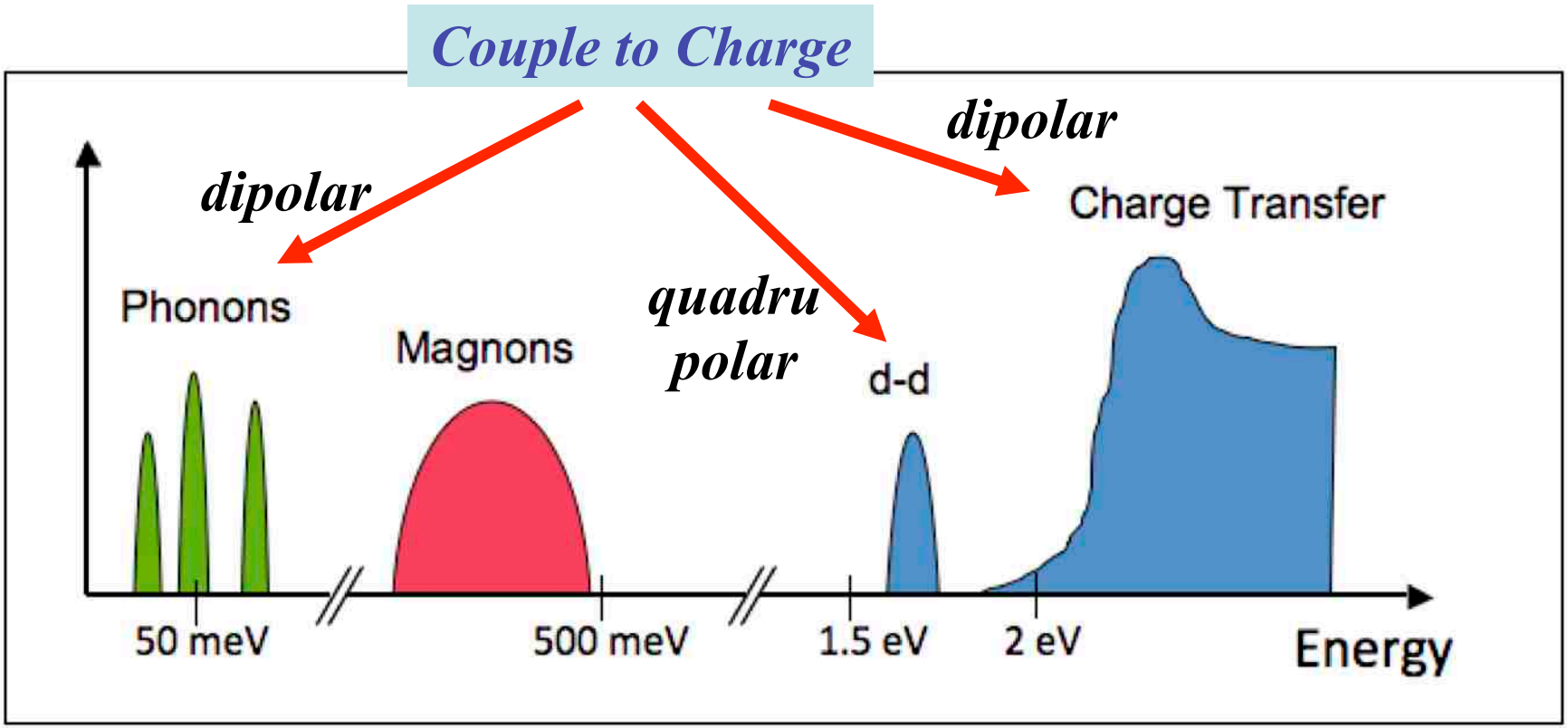

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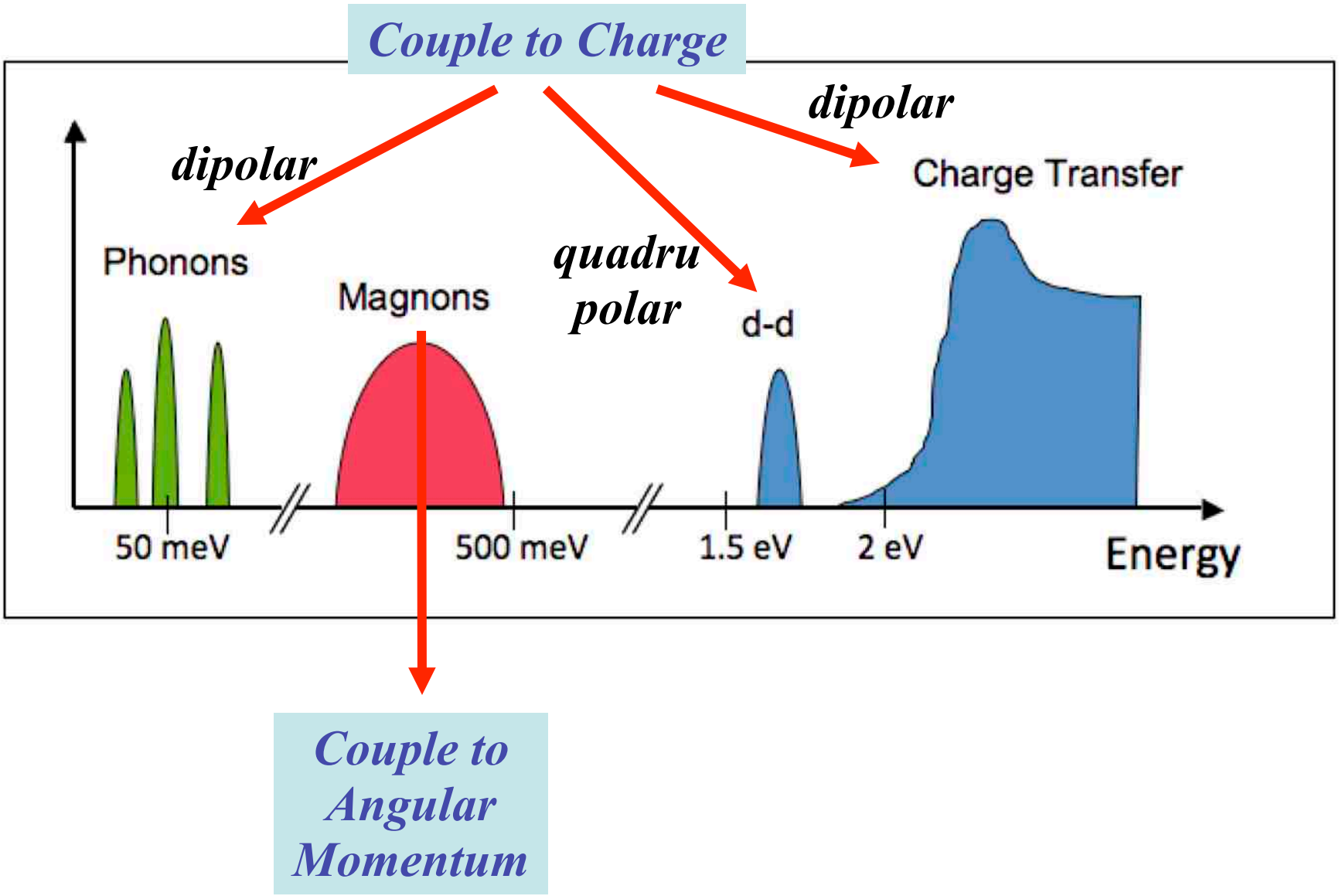

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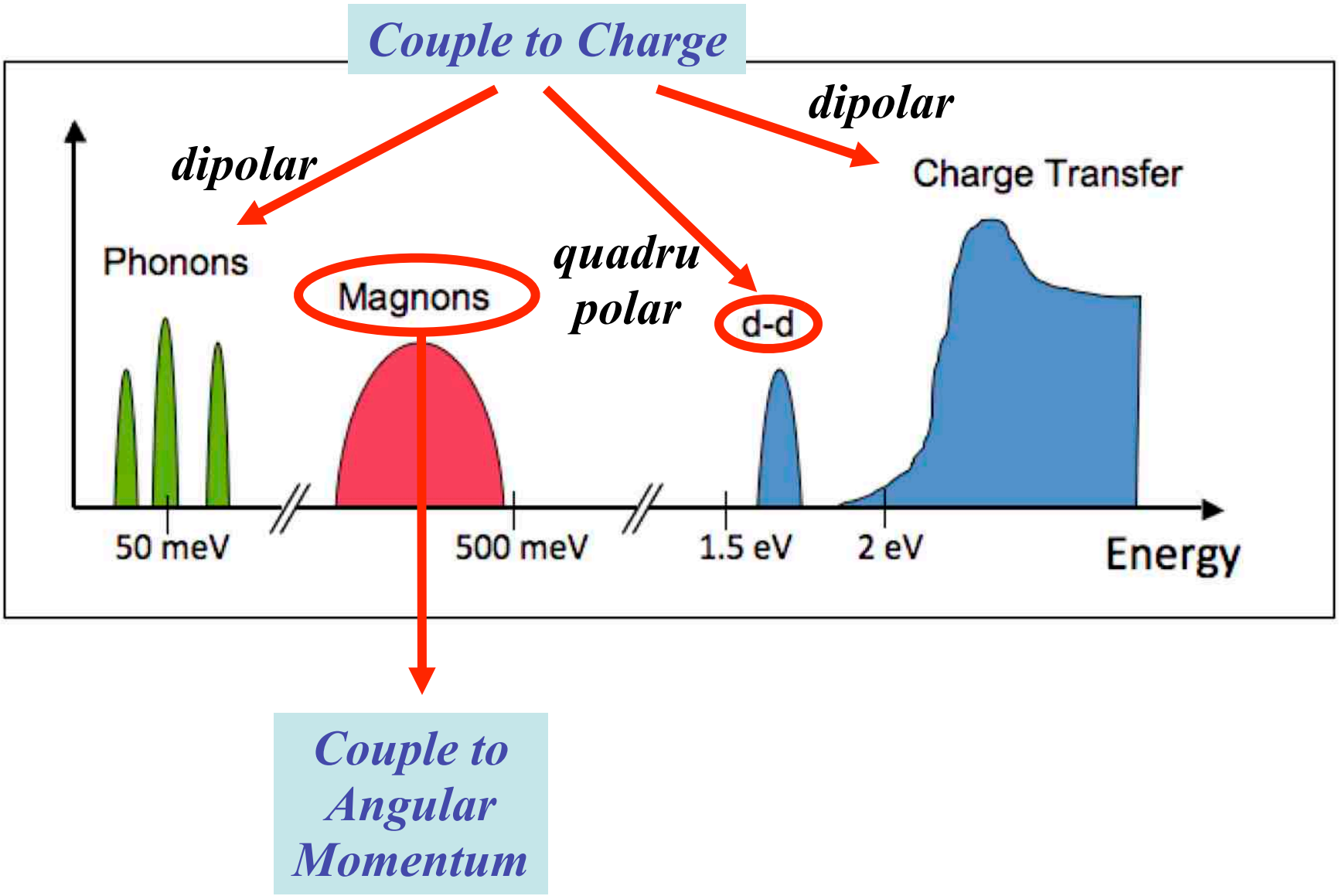

In principle RIXS can probe a very broad class of intrinsic excitations of the system under study – as long as these excitations are overall charge neutral. This constraint arises from the fact that in RIXS the scattered photons do not add or remove charge from the system under study.

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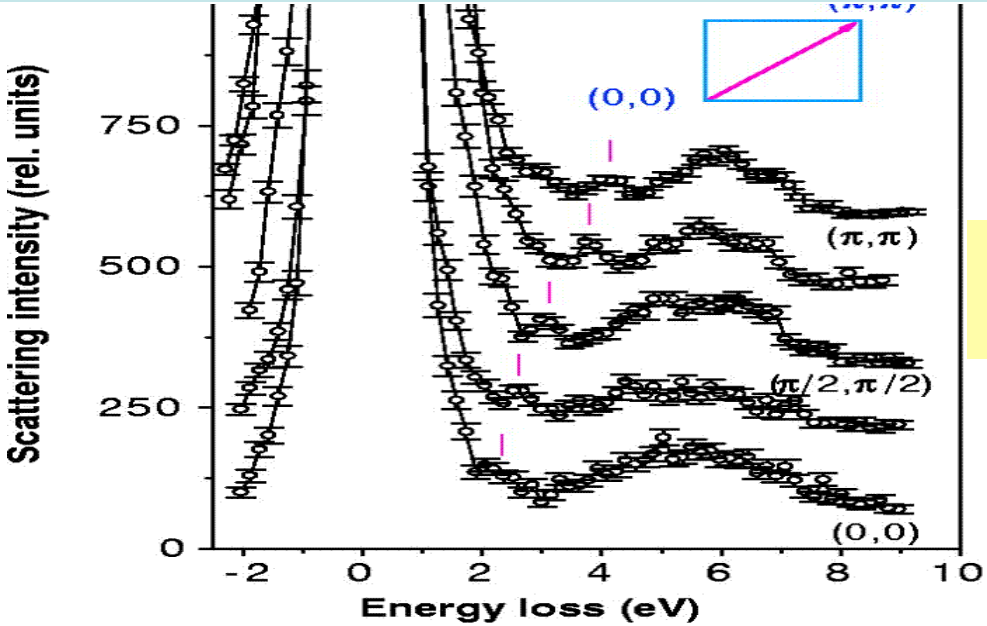
Progress in the Past Decades

Progress @ Cu K-edge resolution



Zahid Hasan et al., (2000)

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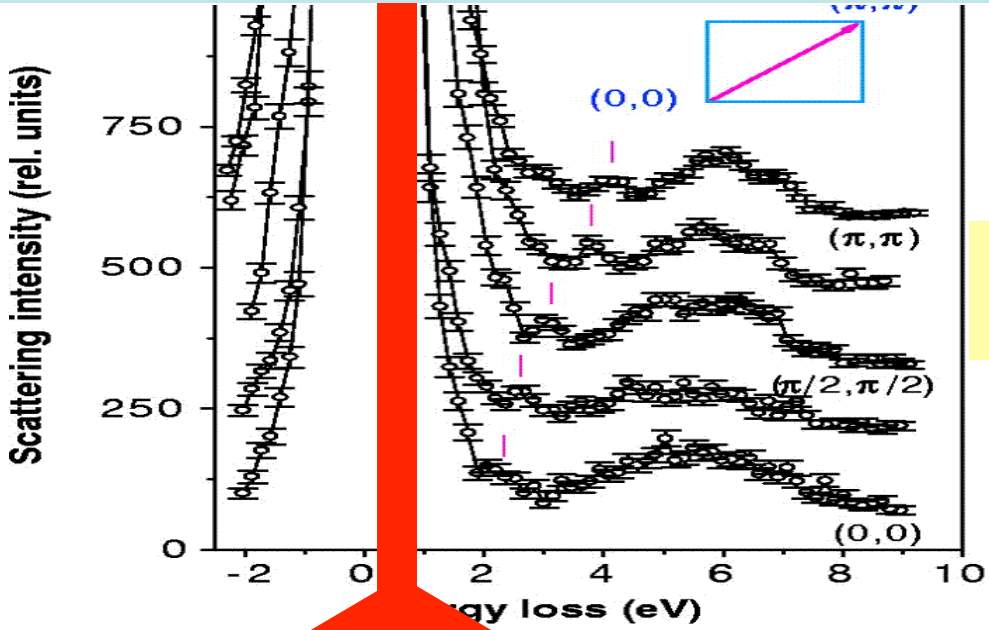

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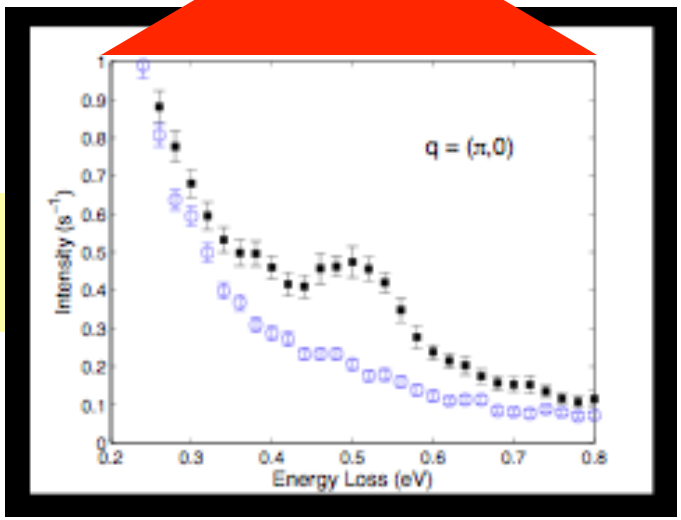
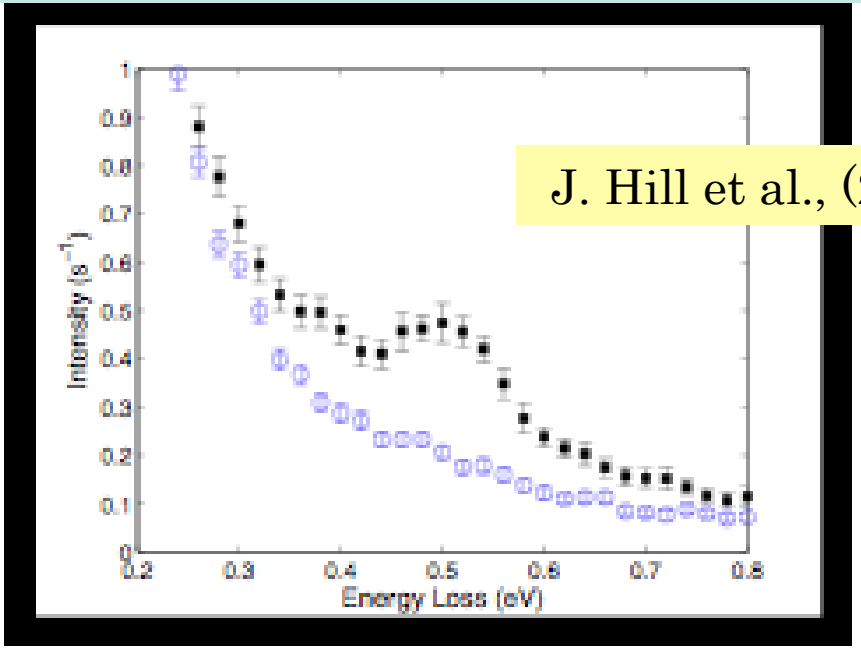


J. Hill et al., PRL 100, 097001 (2008)

Cu K-edge on La_2CuO_4

Progress @ Cu K-edge resolution II

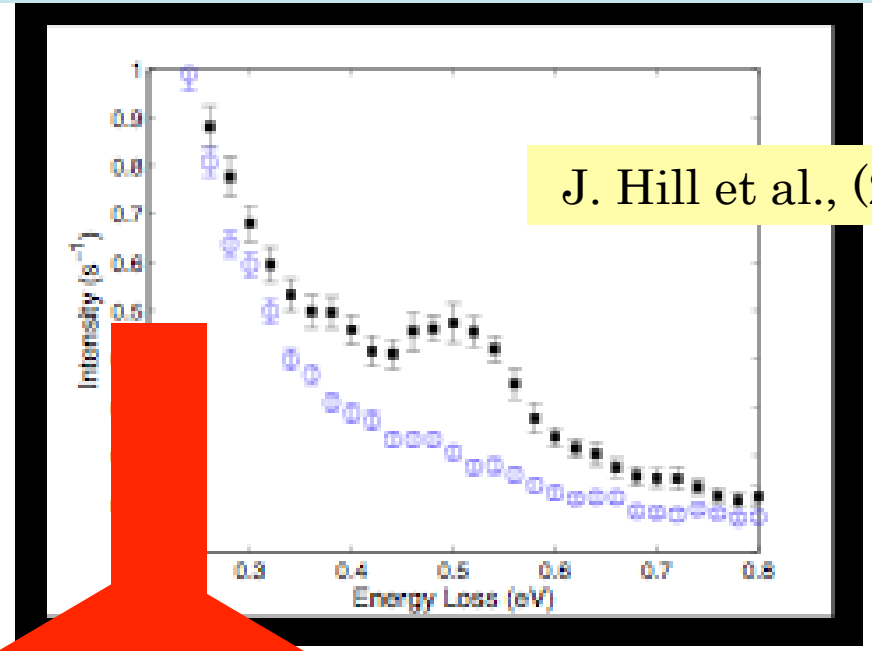
Cu K-edge



J. Hill et al., (2008)

Progress @ Cu K-edge resolution II

Cu K-edge



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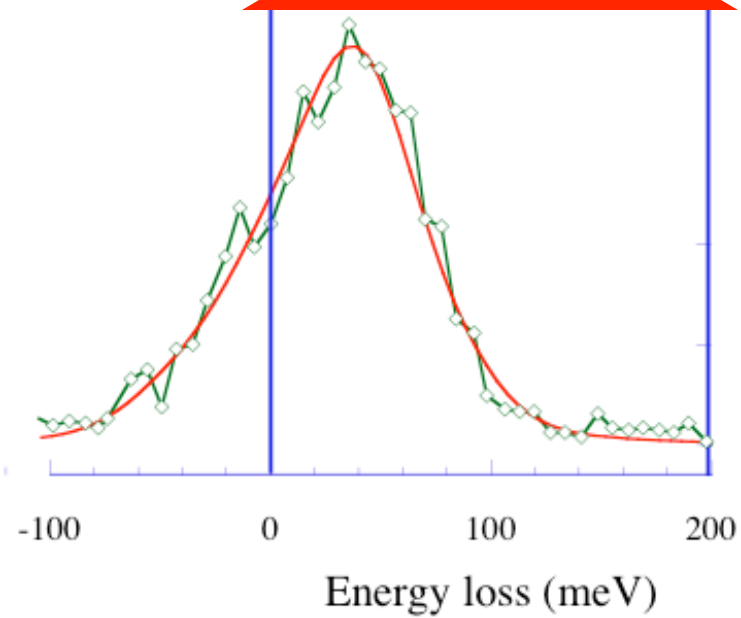
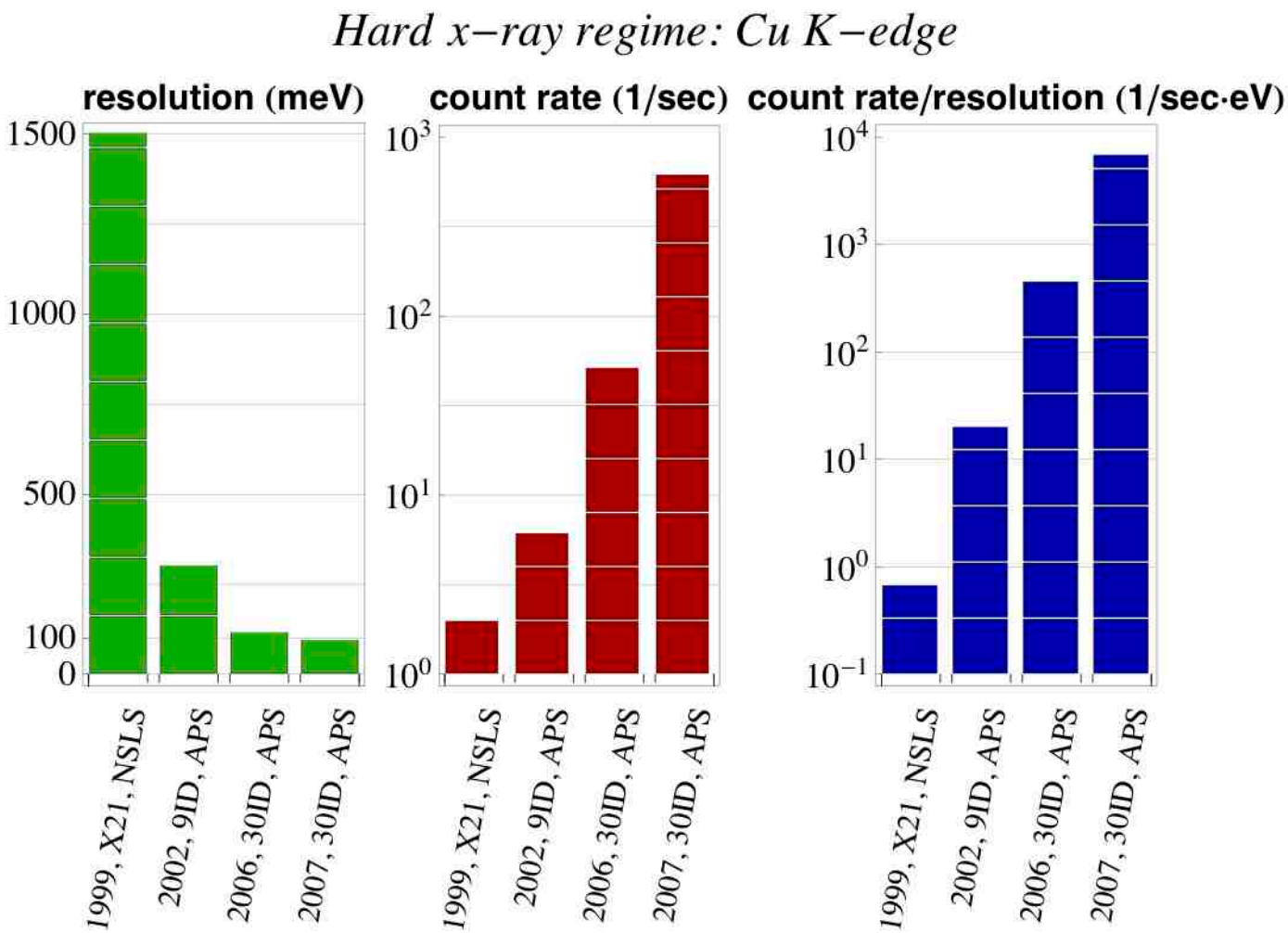
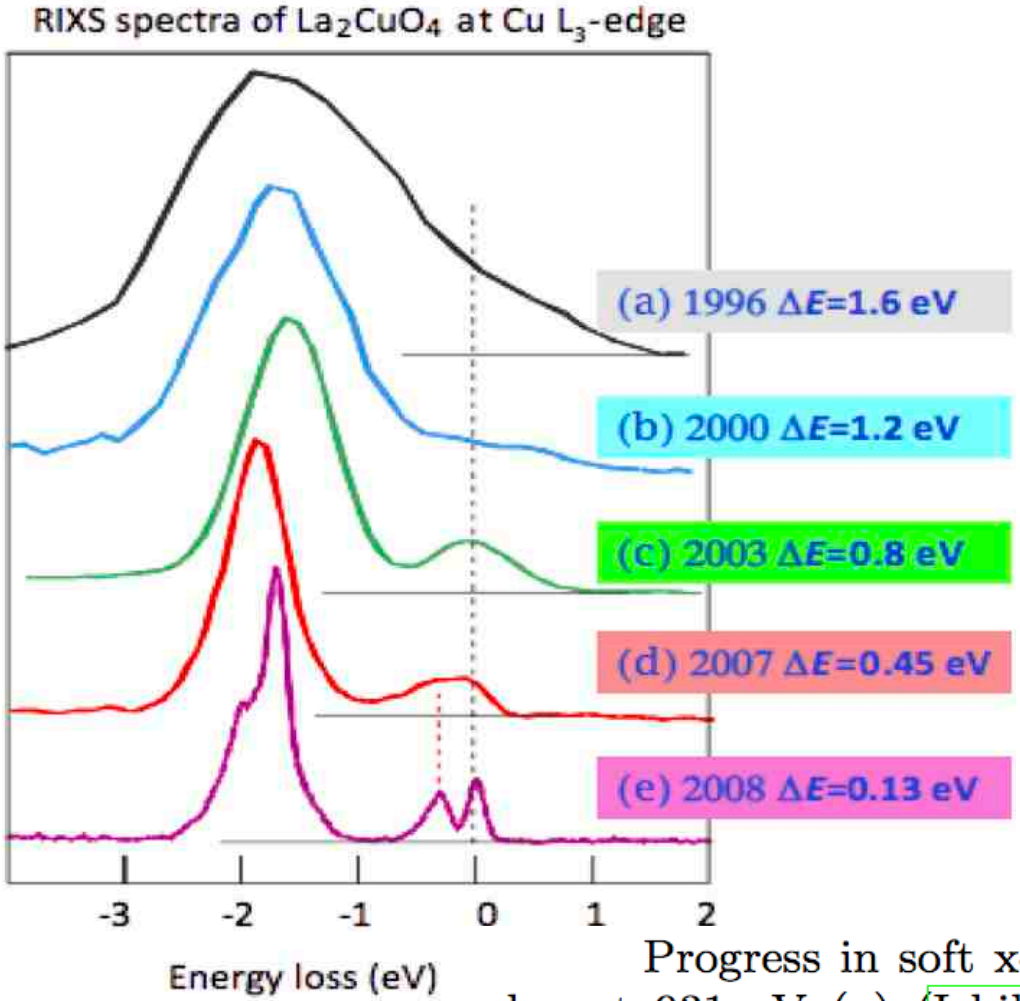


Yavas, et al., JPCM 22, 485601 (2010)

Progress @ Cu K-edge resolution III

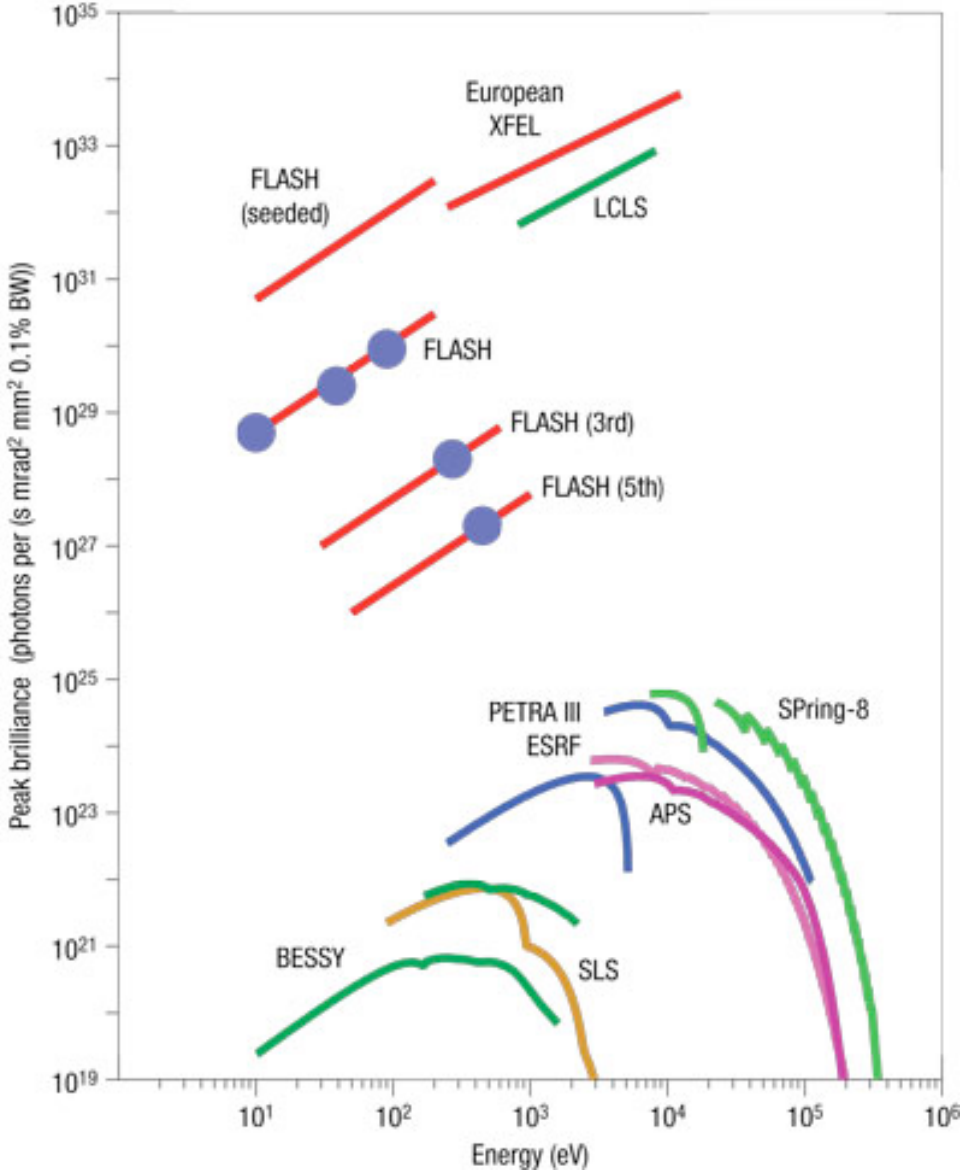


Progress @ Cu L-edge resolution

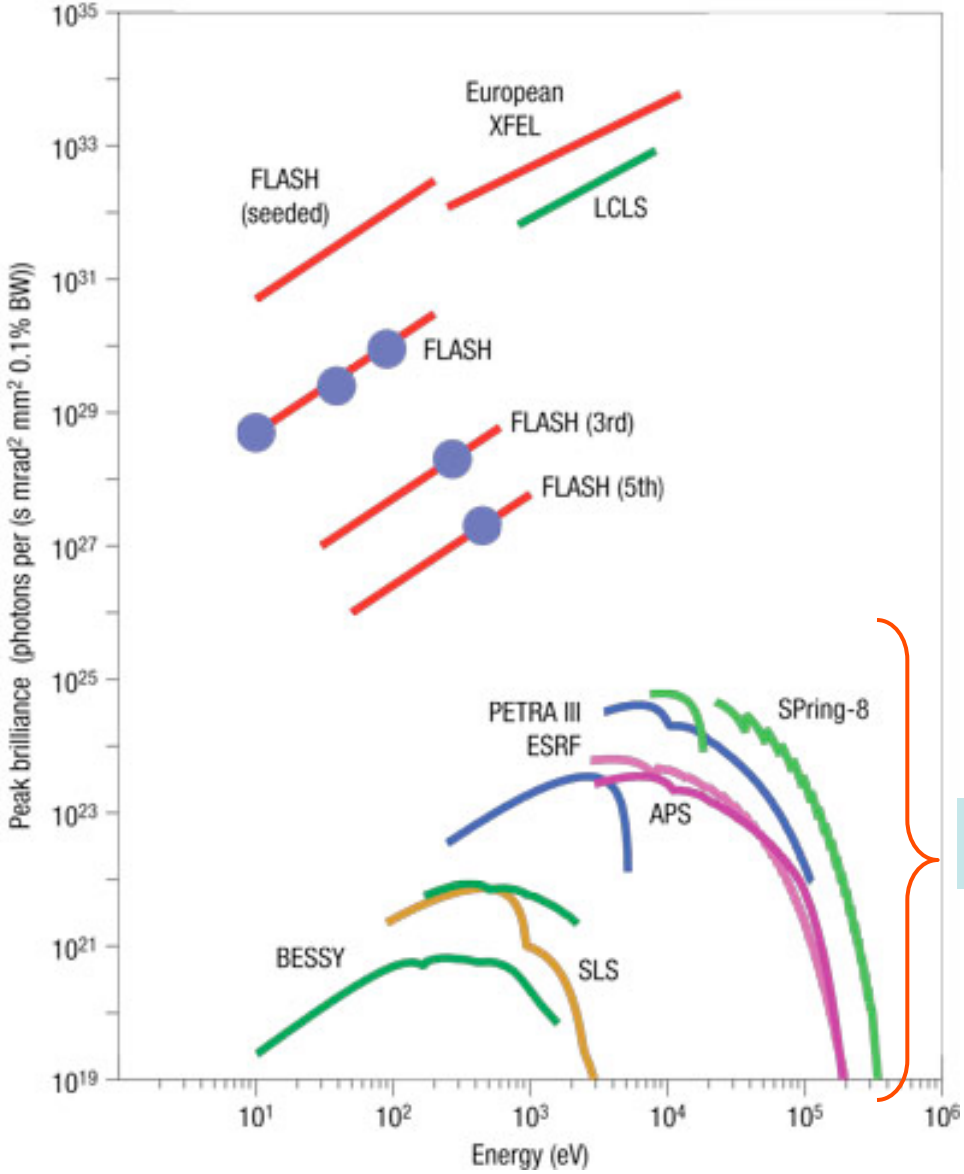


Progress in soft x-ray RIXS resolution at the Cu L-edge at 931 eV (a) (Ichikawa *et al.*, 1996), BLBB @ Photon Factory (b) I511-3 @ MAX II (Duda *et al.*, 2000b), (c) AXES @ ID08, ESRF(Ghiringhelli *et al.*, 2004) (d) AXES @ ID08, ESRF(Braicovich *et al.*, 2009), (e) SAXES @ SLS (Ghiringhelli *et al.*, 2010). Courtesy of G. Ghiringhelli and L. Braicovich.

Progress in X-ray sources...

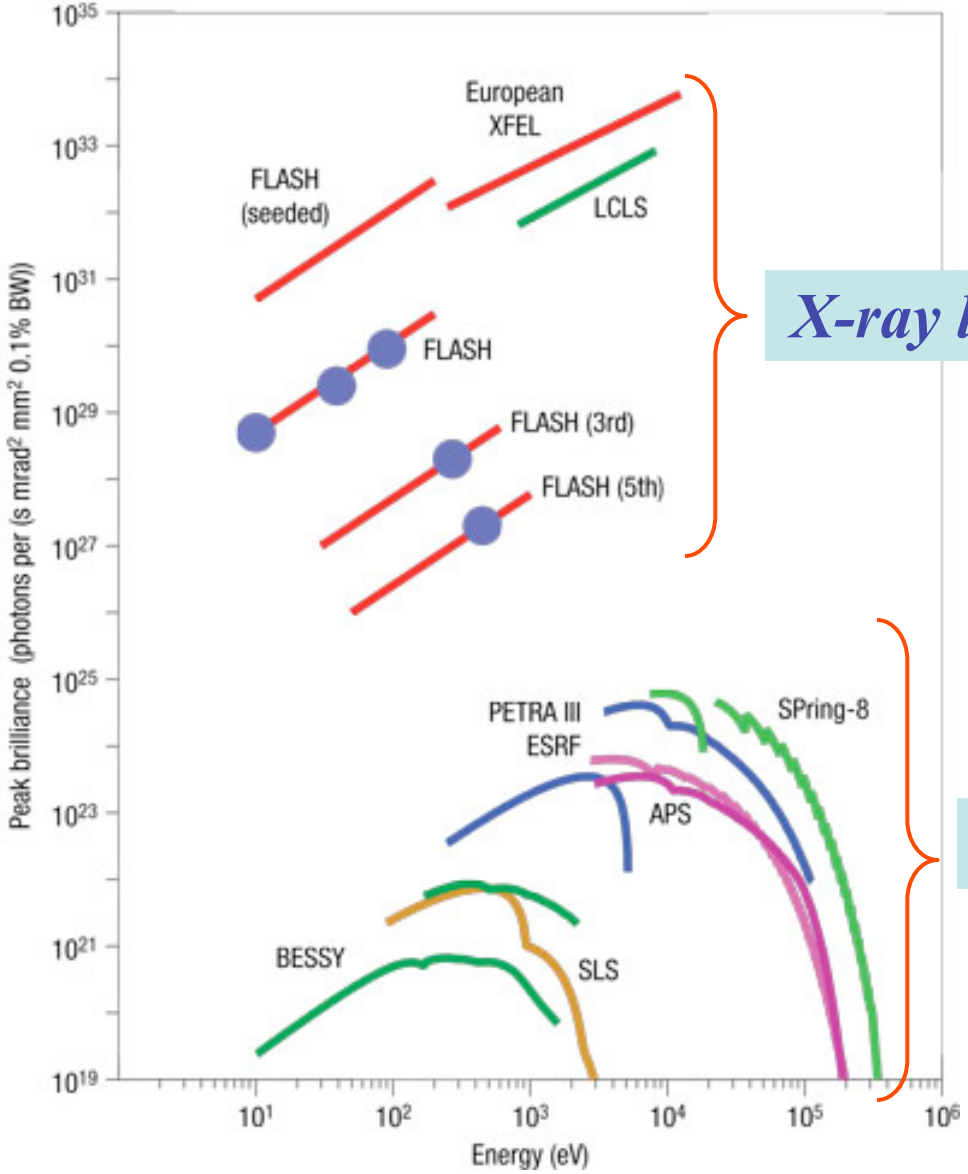


Progress in X-ray sources...



synchrotrons

Progress in X-ray sources...



X-ray lasers

synchrotrons

Summary part I

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  spin, orbital, lattice, charge excitons
- Great progress in resolution in the past decade

2. Magnetic RIXS on low dimensional magnets

Quasi 2D cuprates

Quasi 1D cuprates

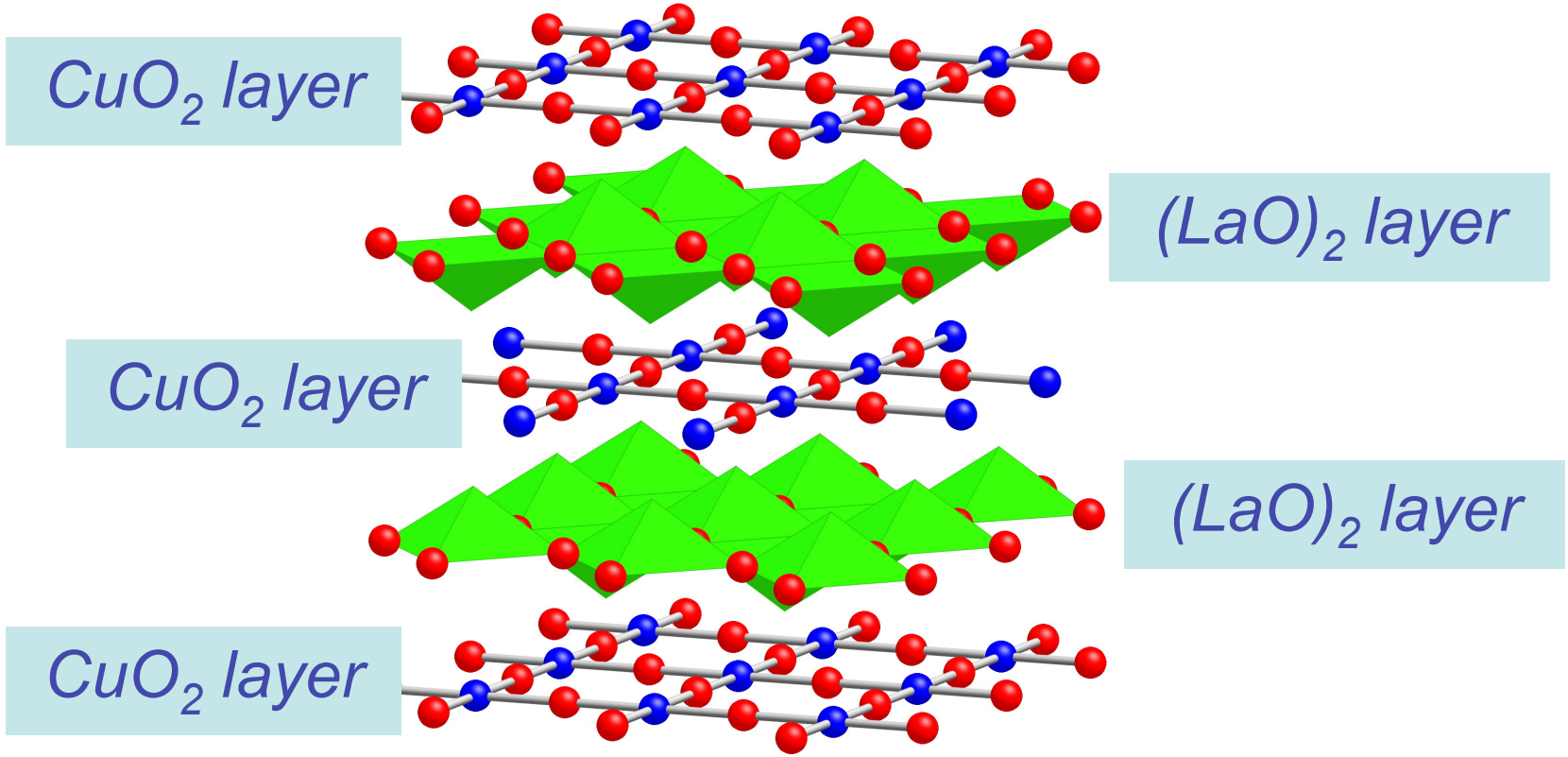
Quasi 2D iron pnictide

Quasi 2D iridate

Doped Cu & Fe systems

Quasi 2D cuprates

La_2CuO_4 crystal structure

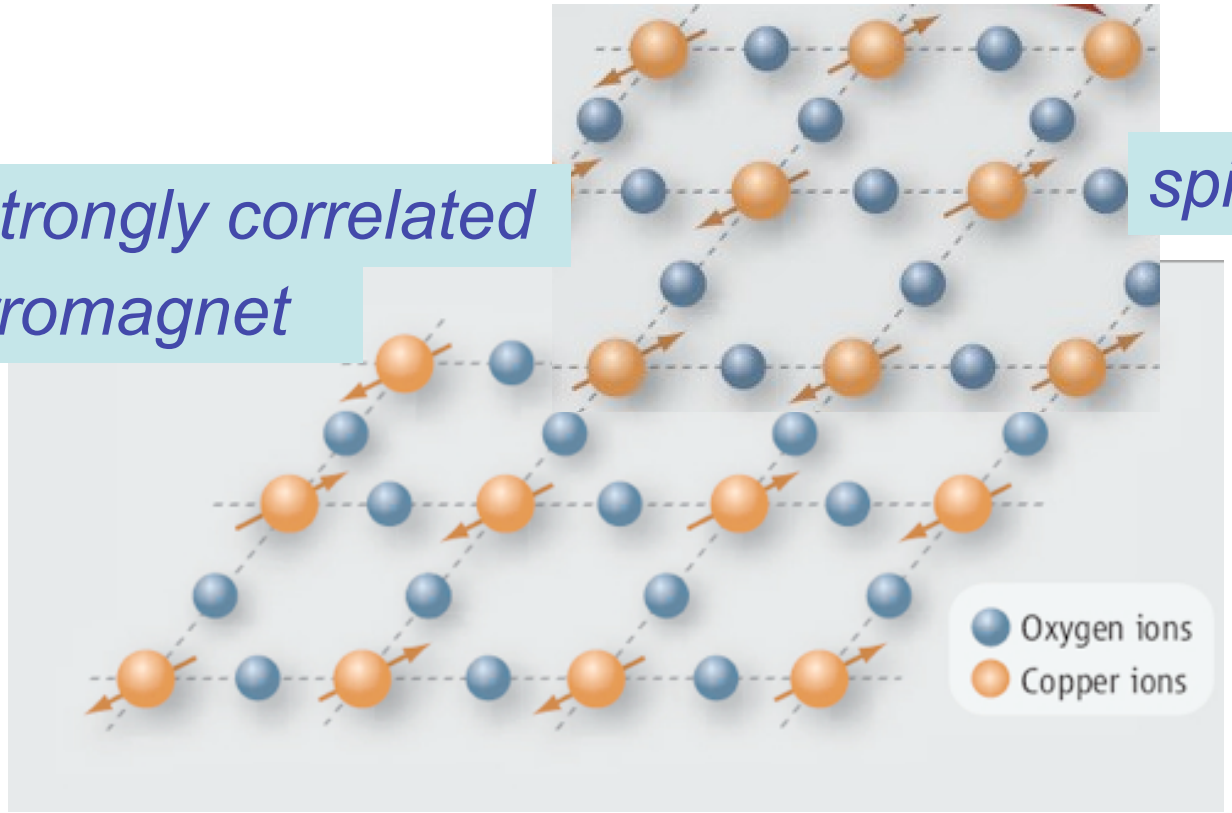


La_2CuO_4 magnetic structure

strongly correlated

antiferromagnet

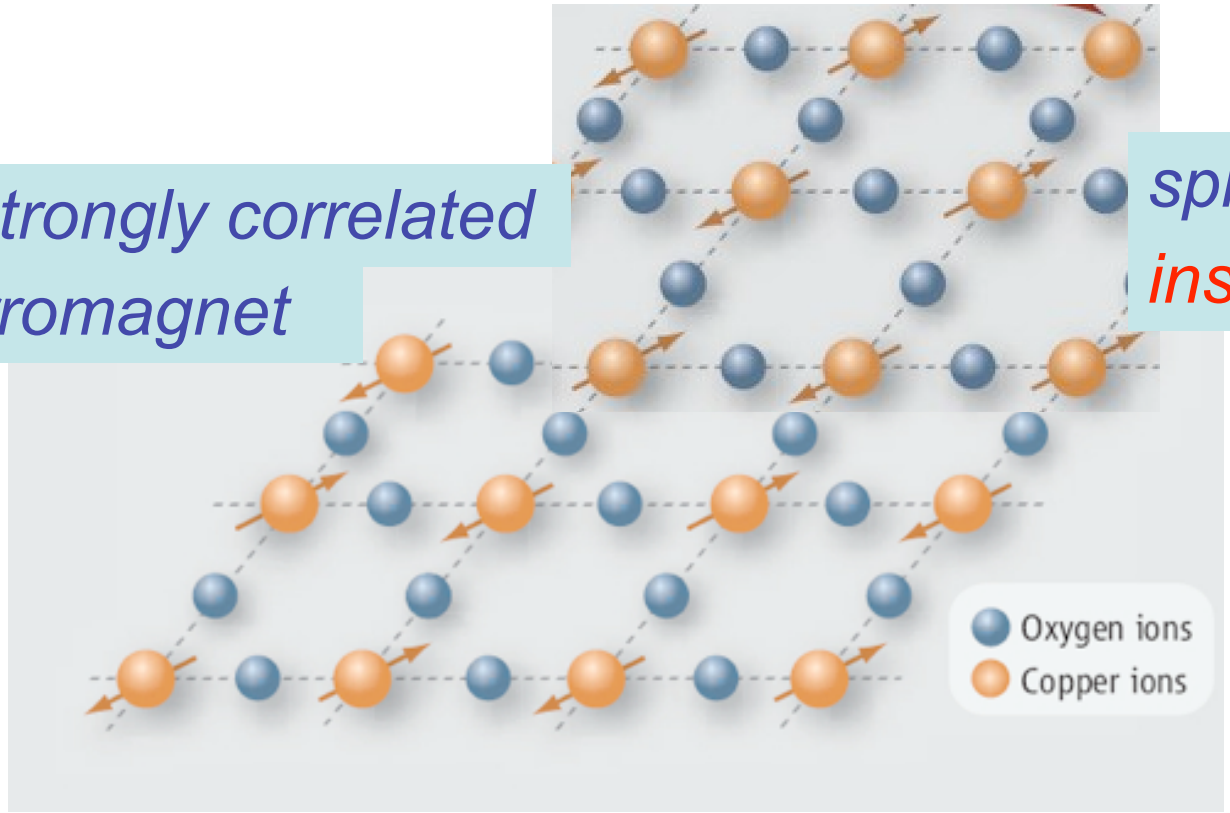
spin 1/2



La_2CuO_4 magnetic structure

strongly correlated antiferromagnet

spin 1/2 insulator



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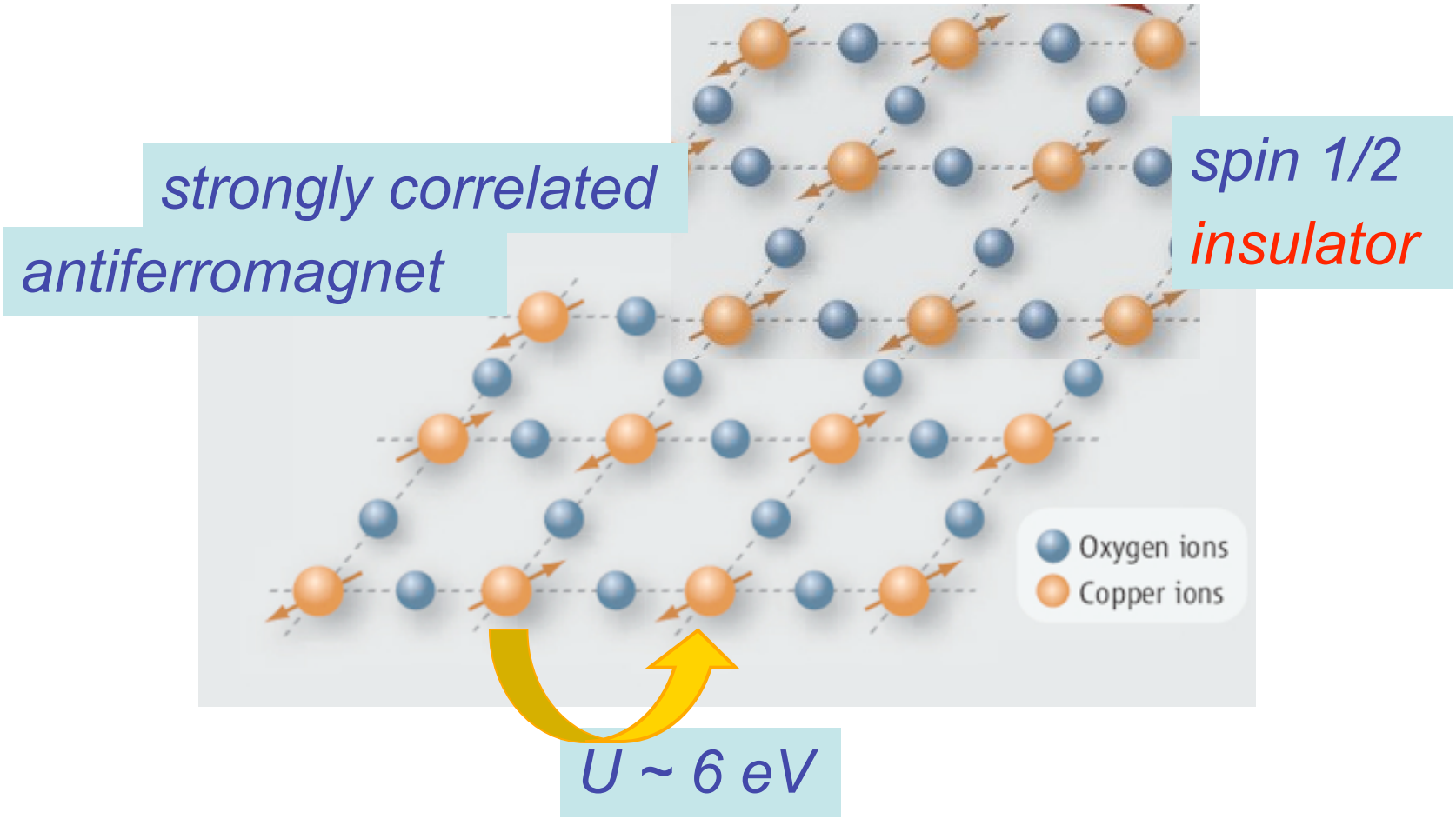

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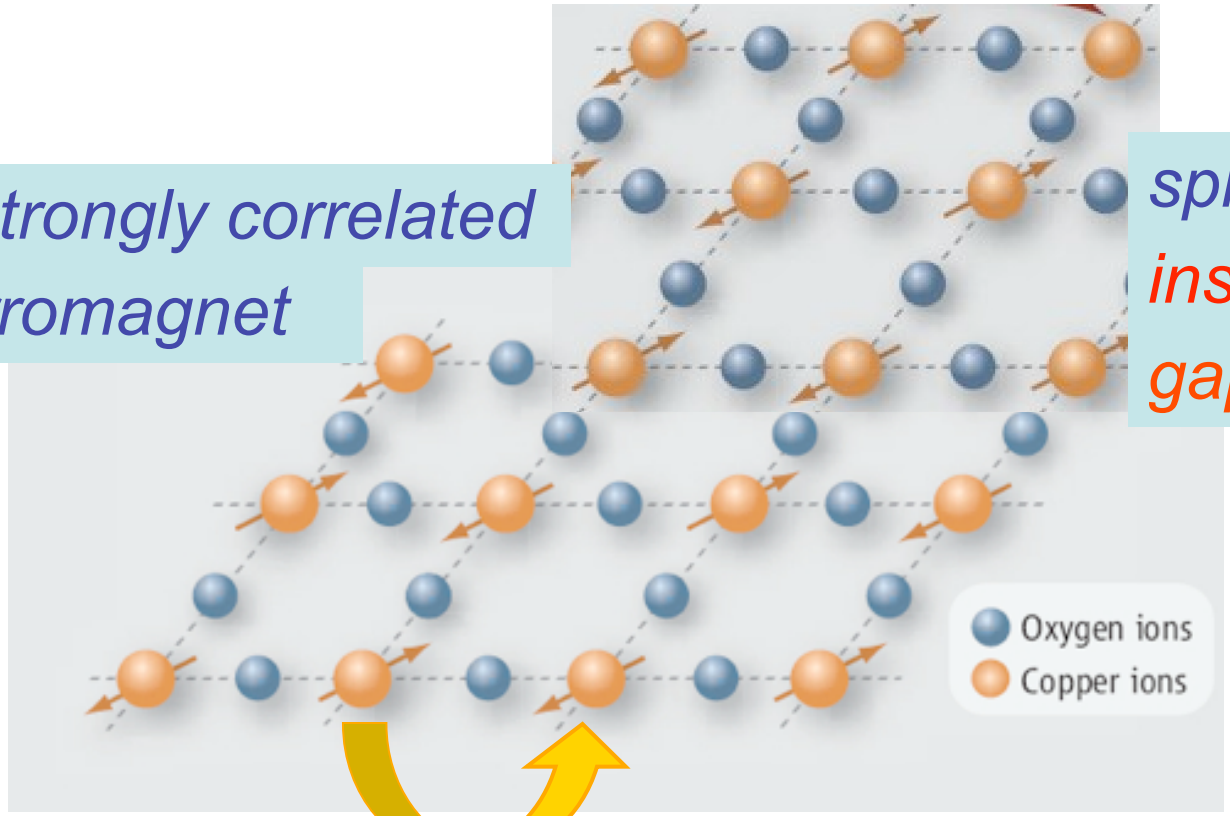


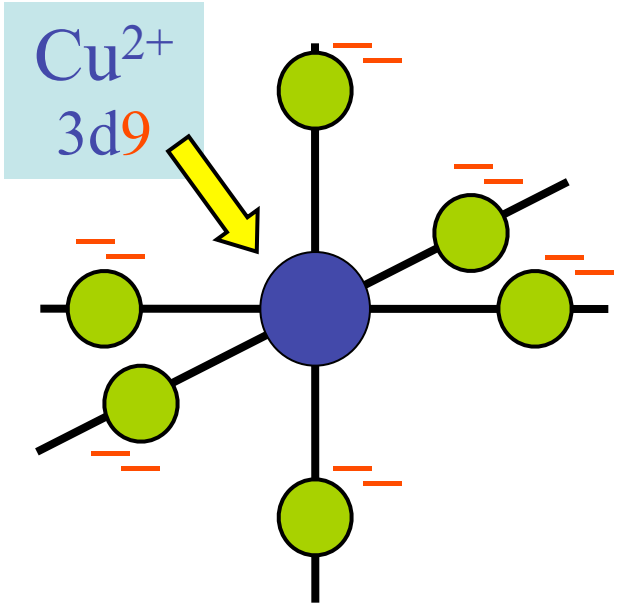
strongly correlated antiferromagnet

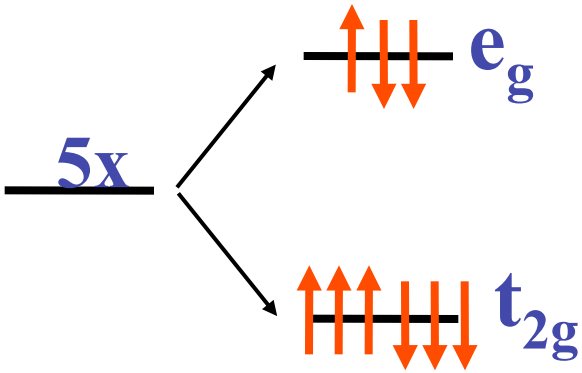
spin 1/2 insulator gap ~2 eV

U ~ 6 eV

Atomic Model: Local d-d orbital splitting: Cu^{2+}

Cubic Crystal field splitting





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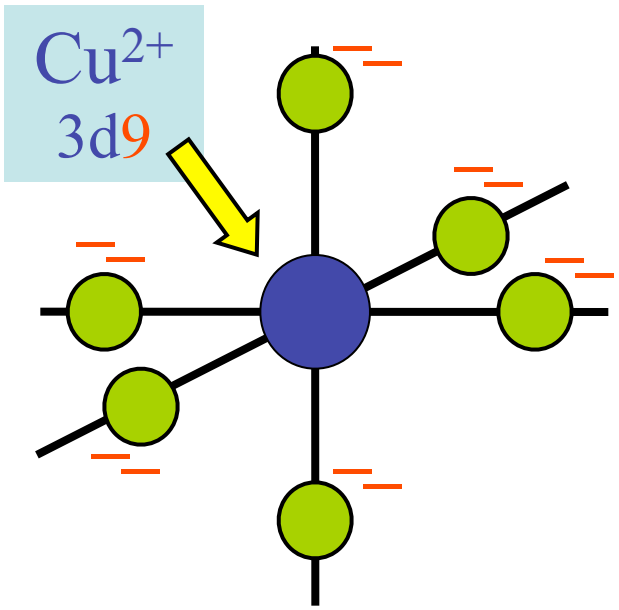
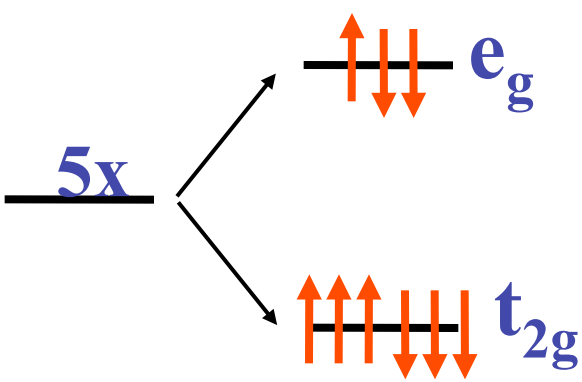
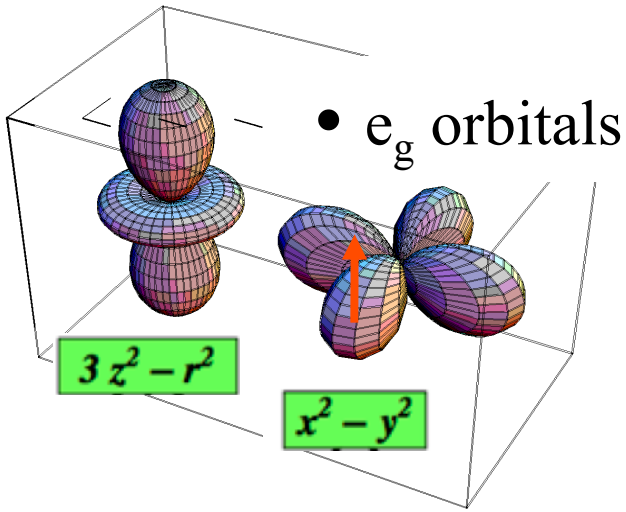
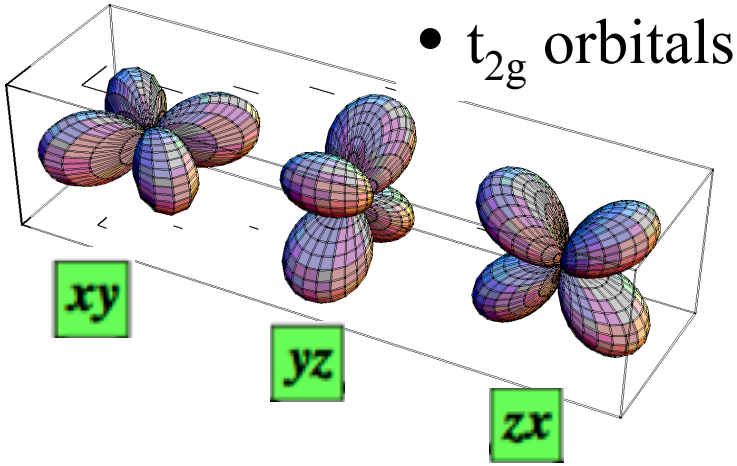






- e_g orbitals



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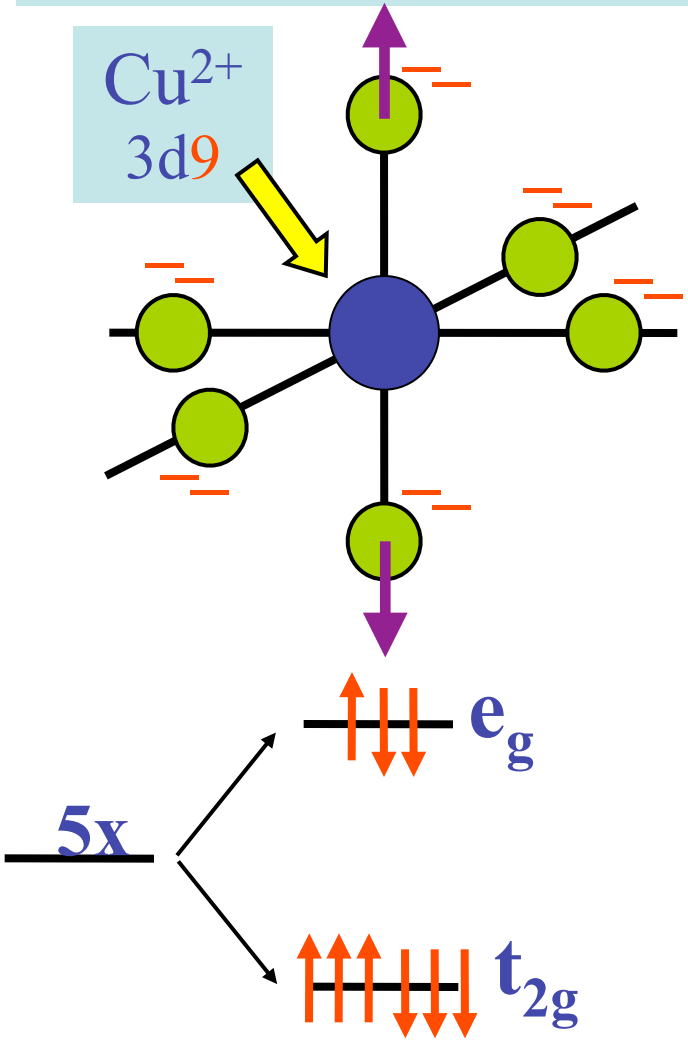

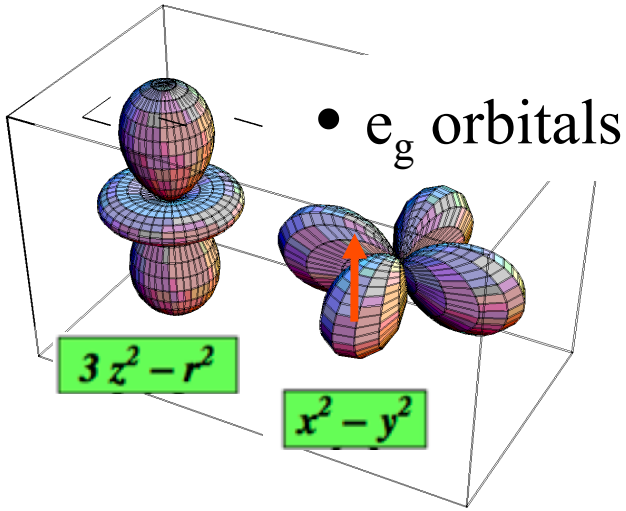

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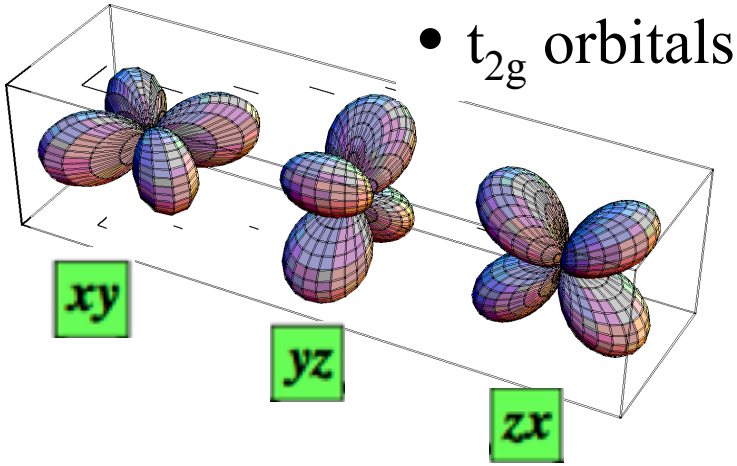

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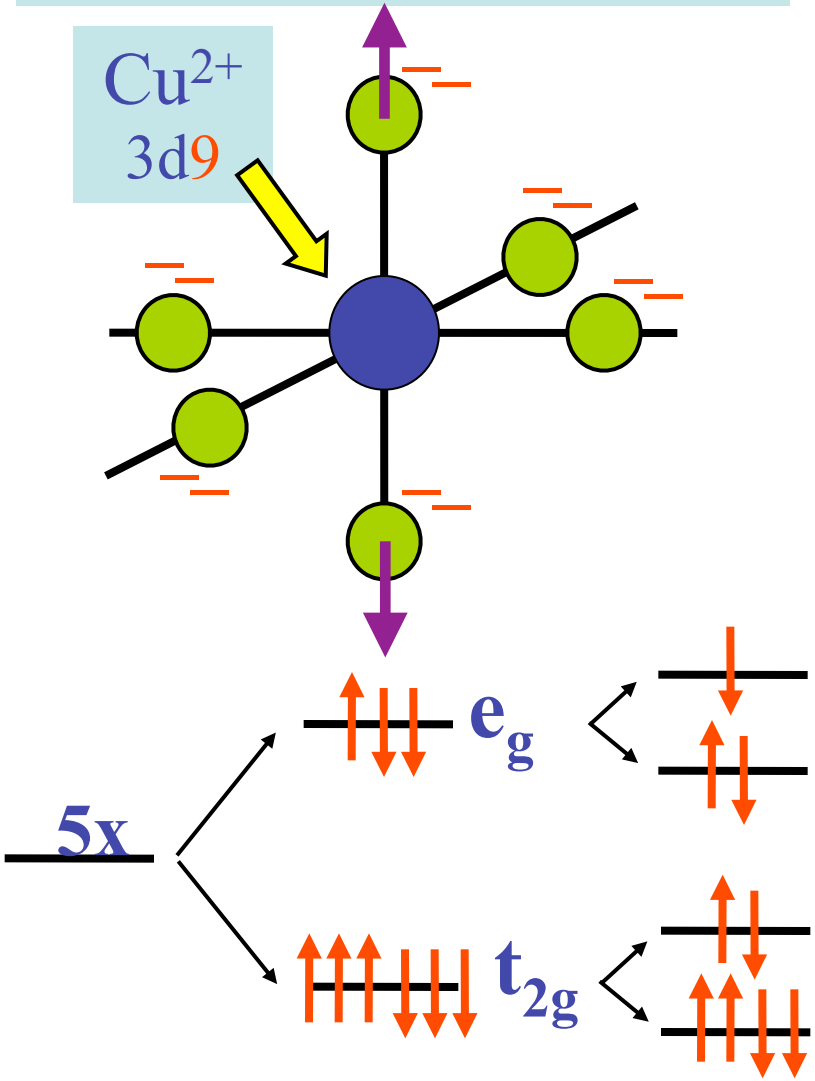

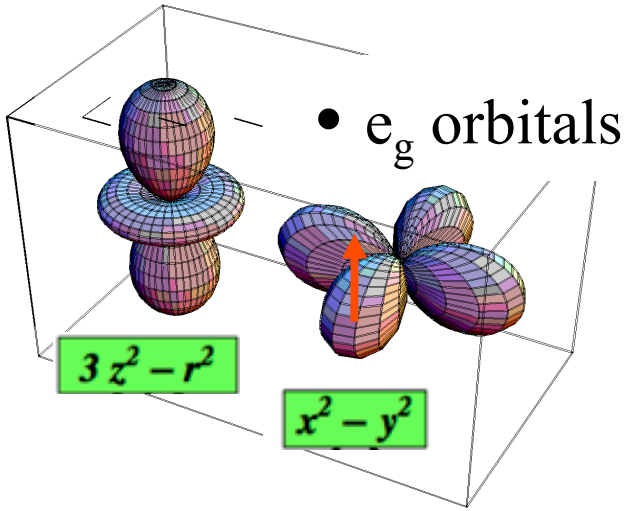

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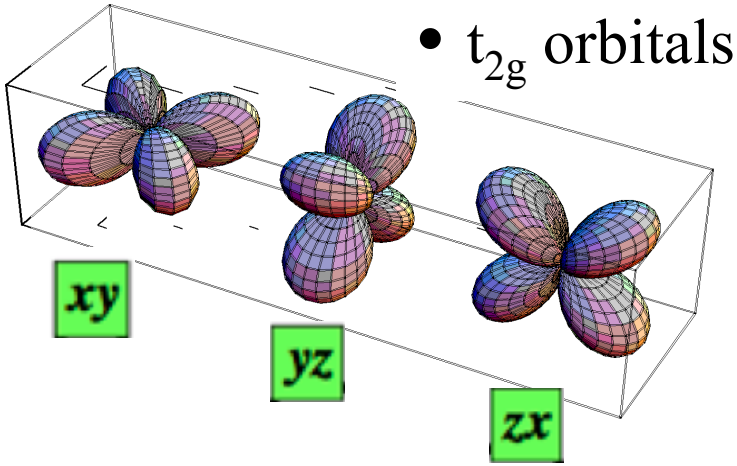

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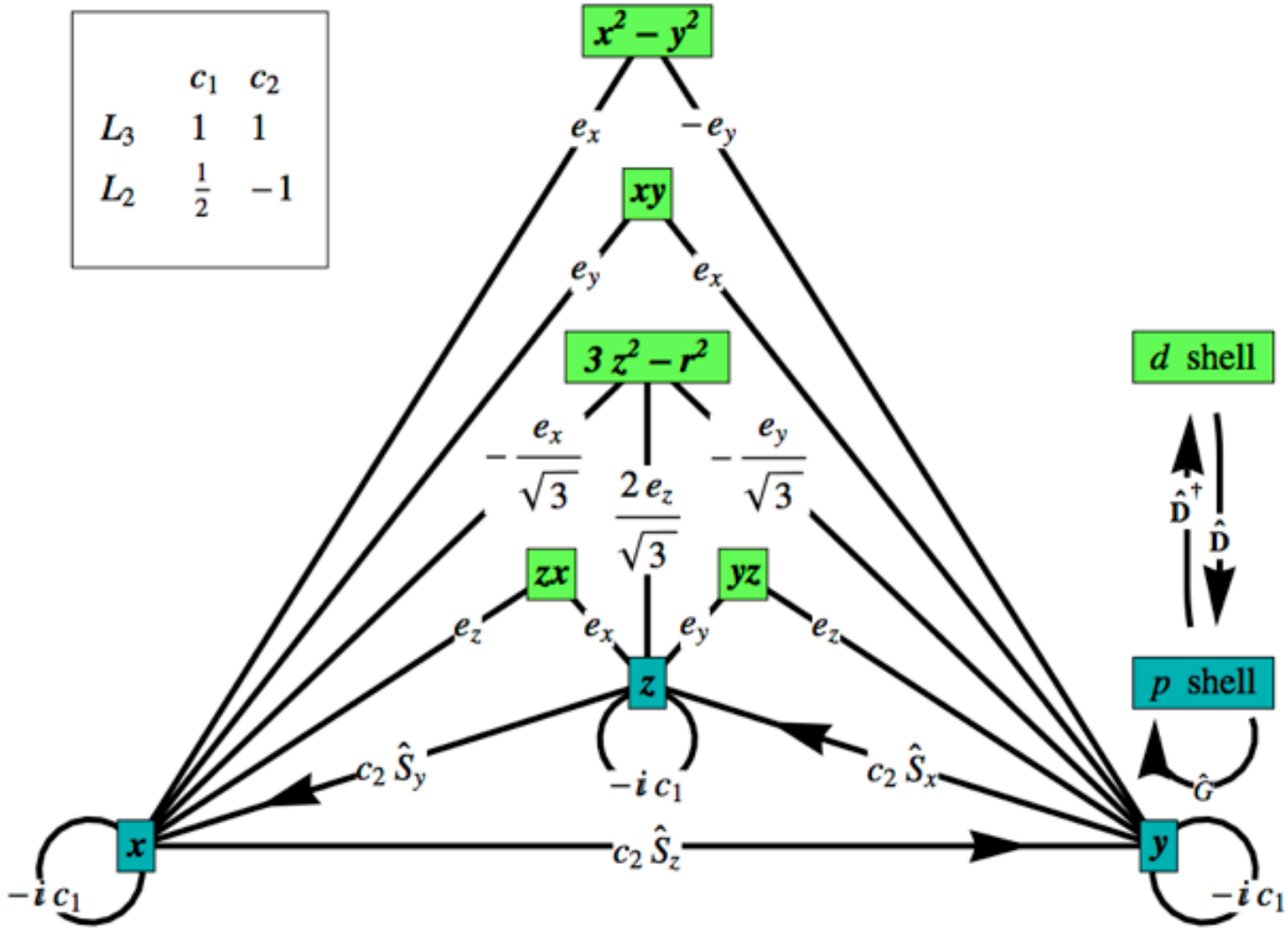
RIXS amplitude @ transition metal L-edge



Ament, Ghiringhelli, Moretti, Braicovich & JvdB, PRL 103, 117003 (2009)

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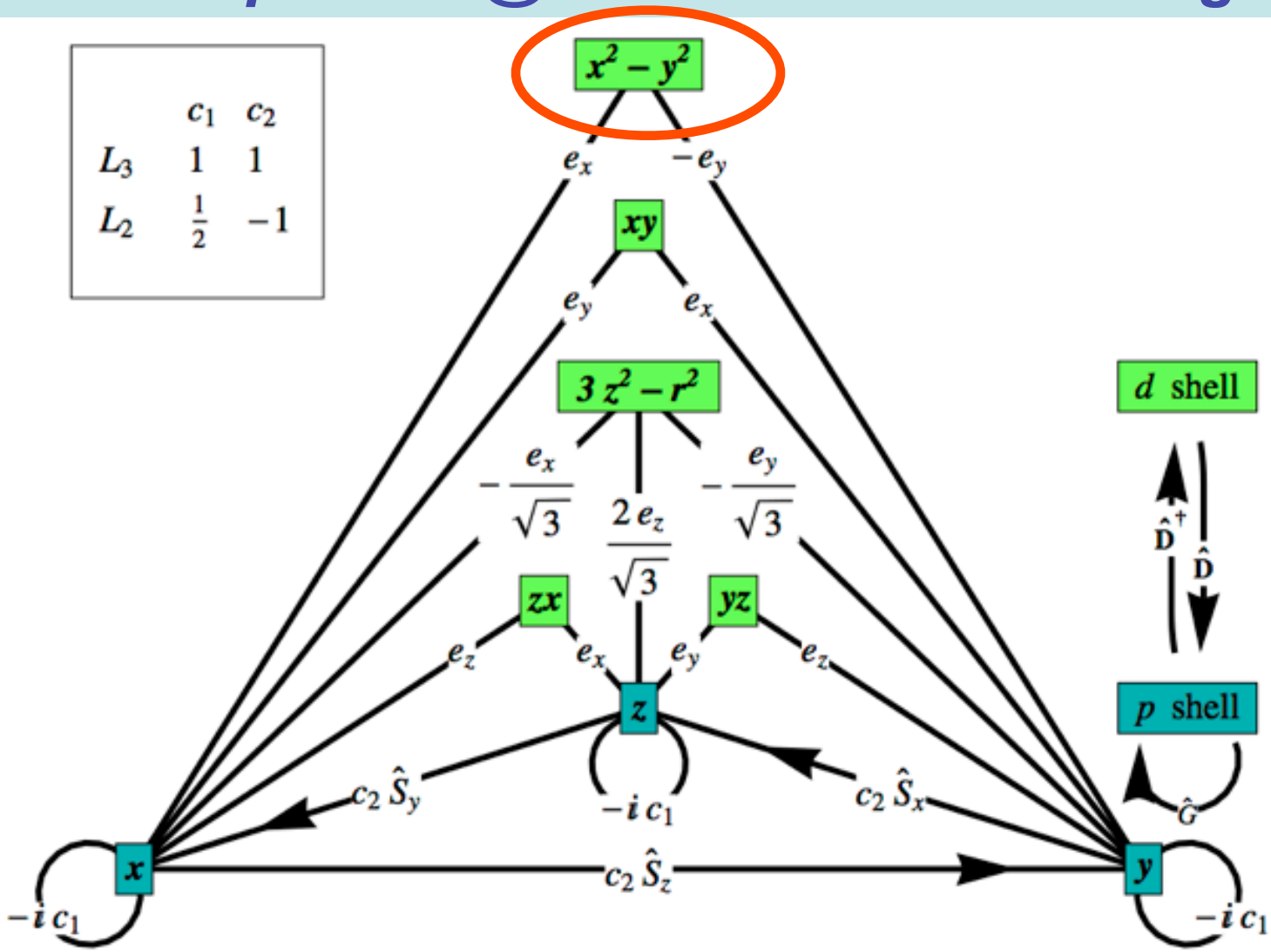

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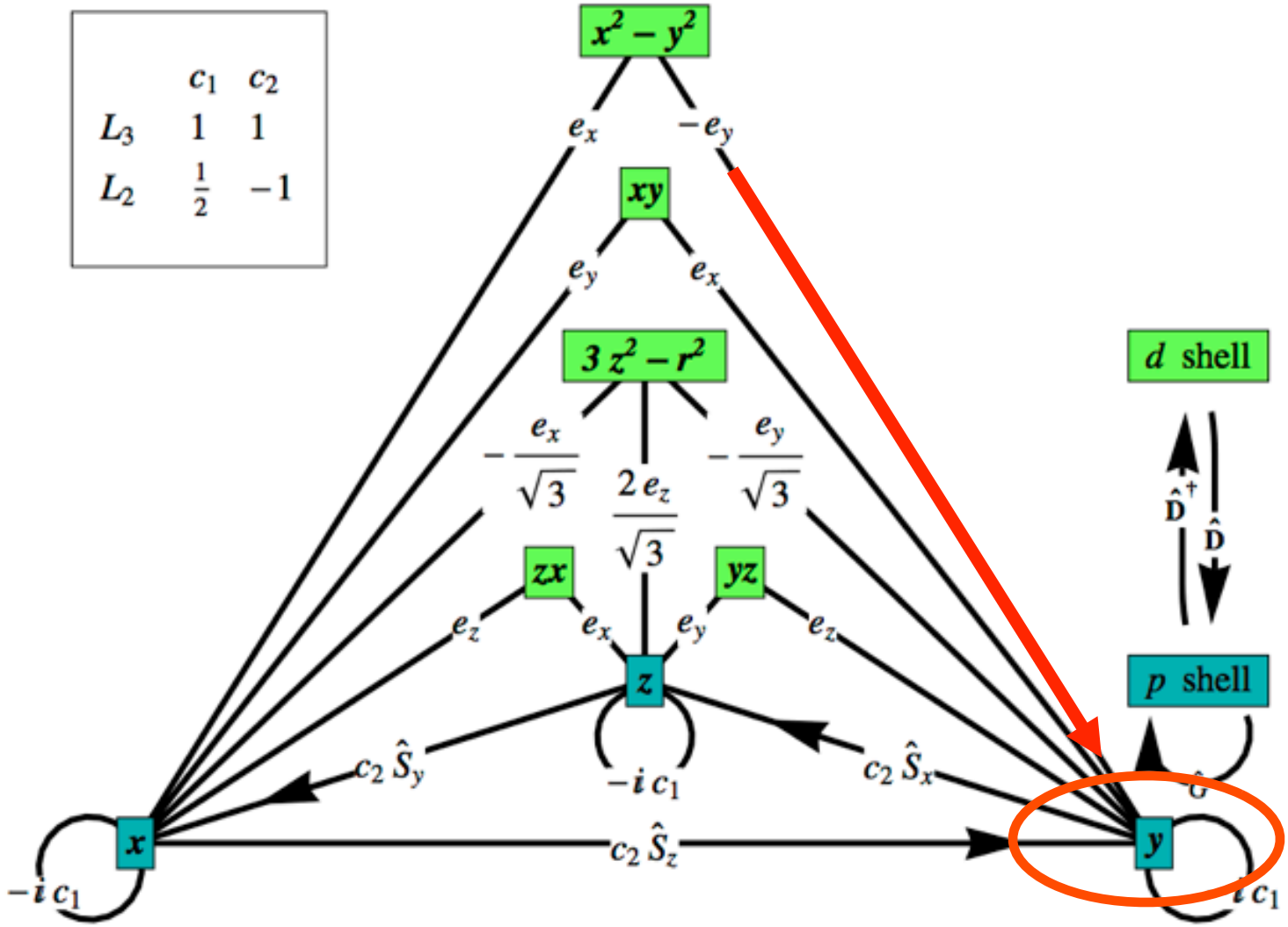

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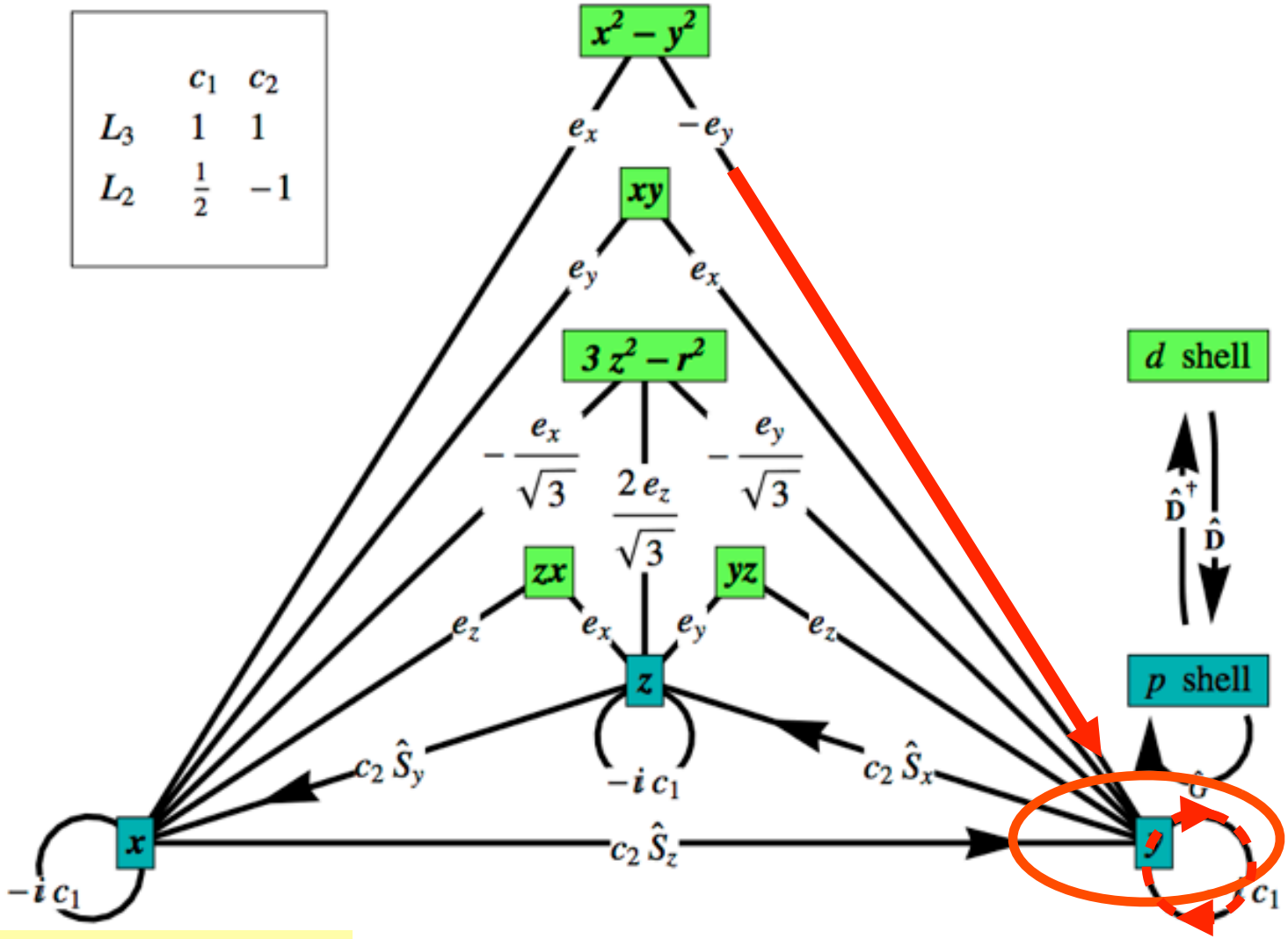

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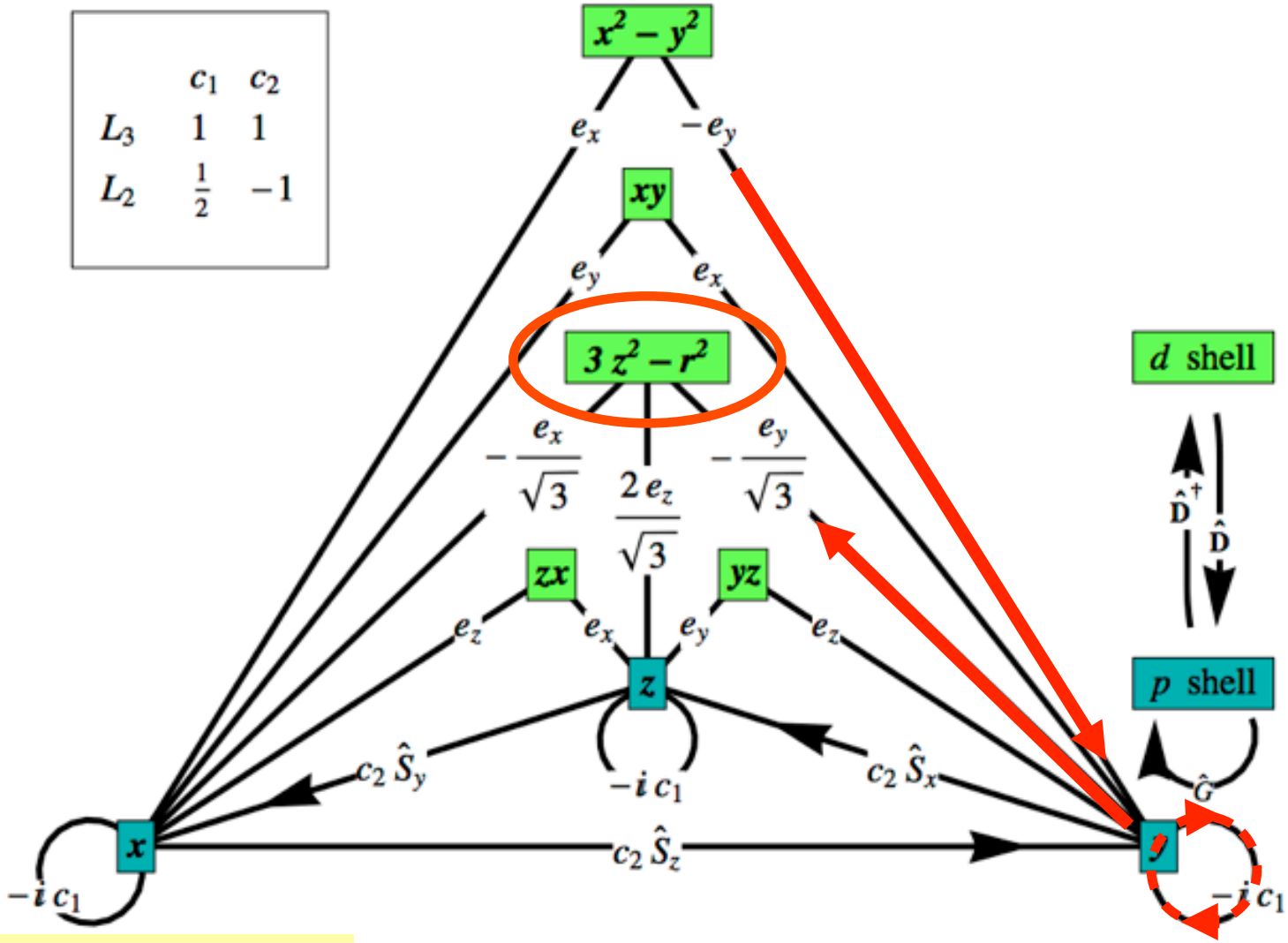

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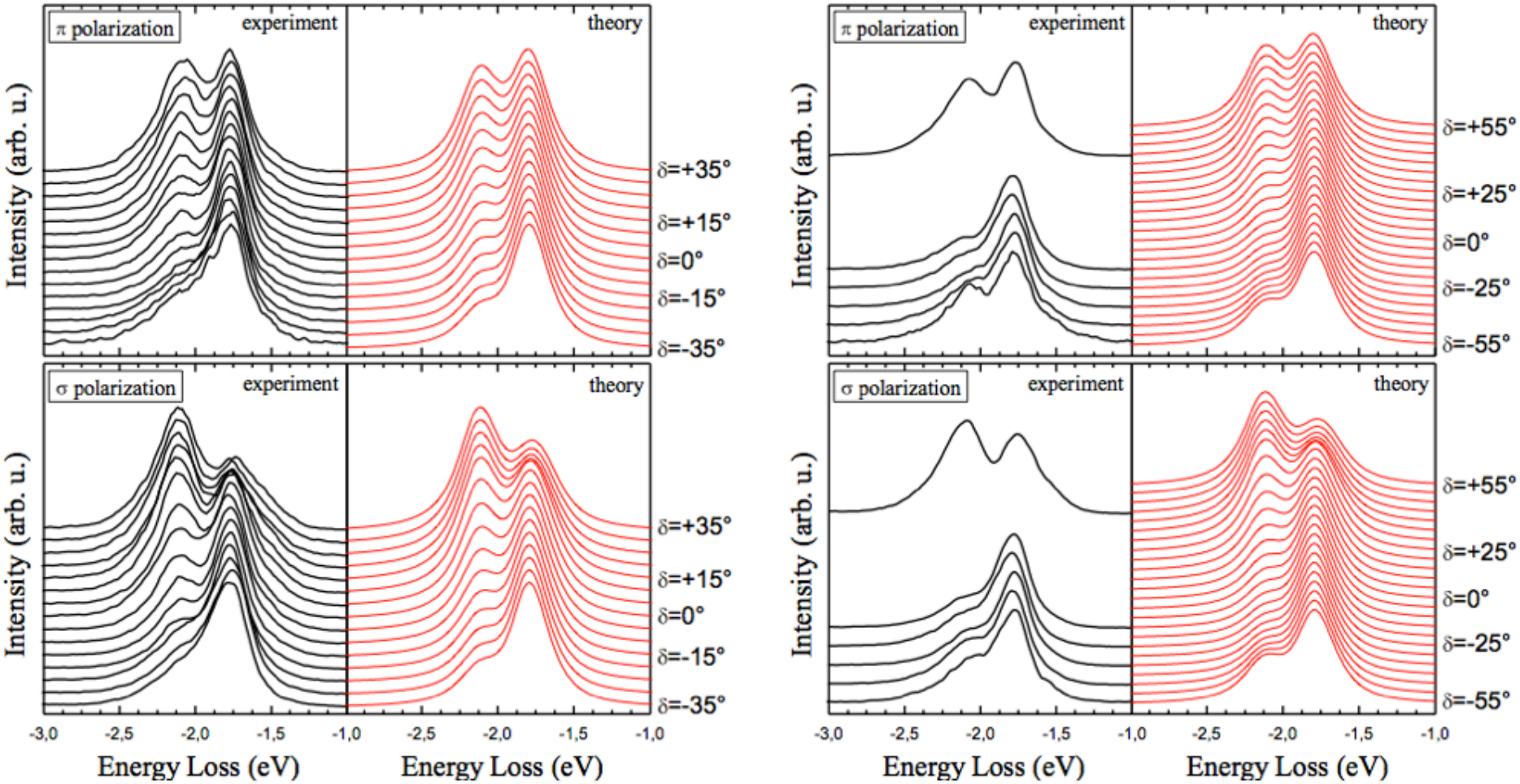
Orbital excitations by direct RIXS on La_2CuO_4



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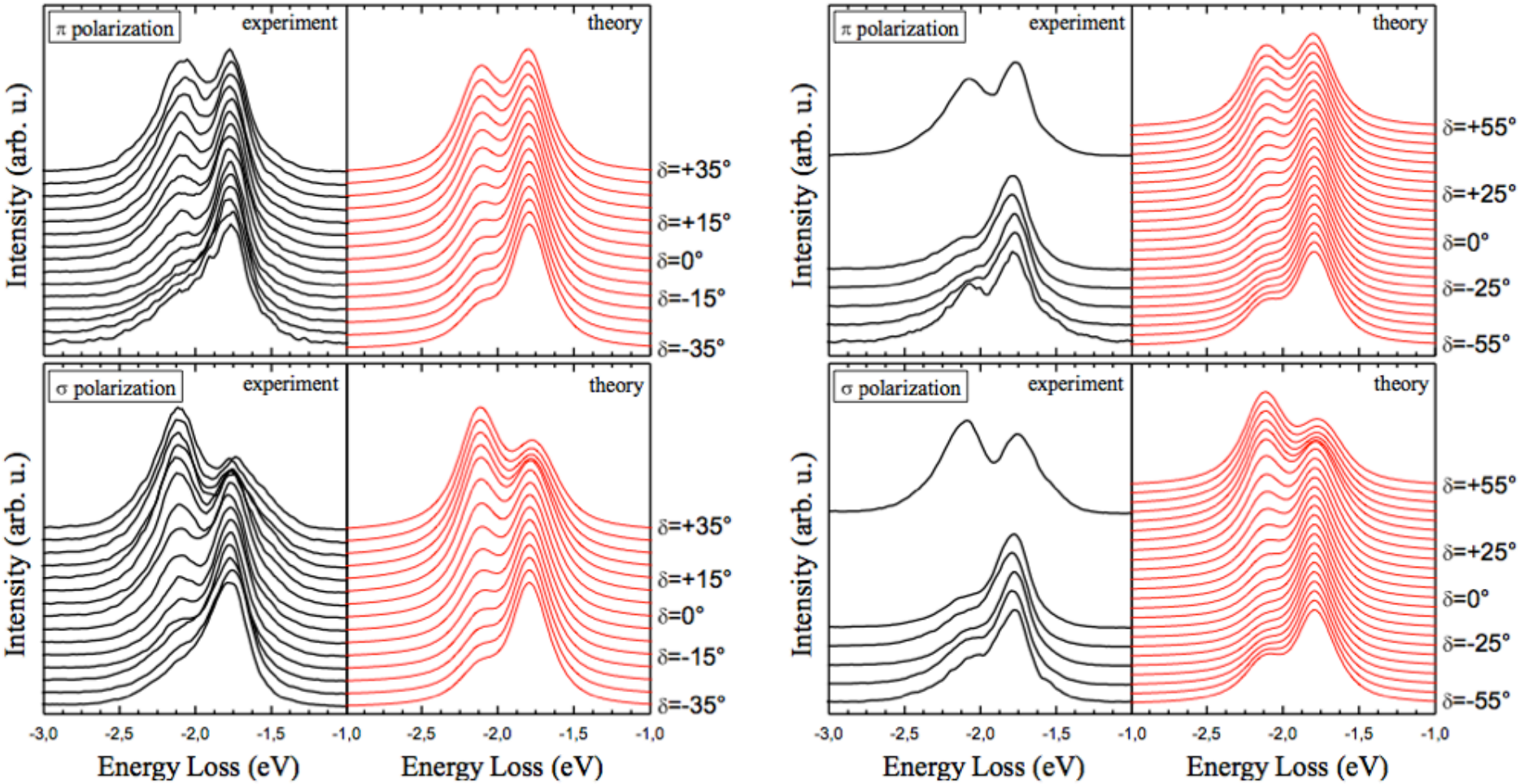
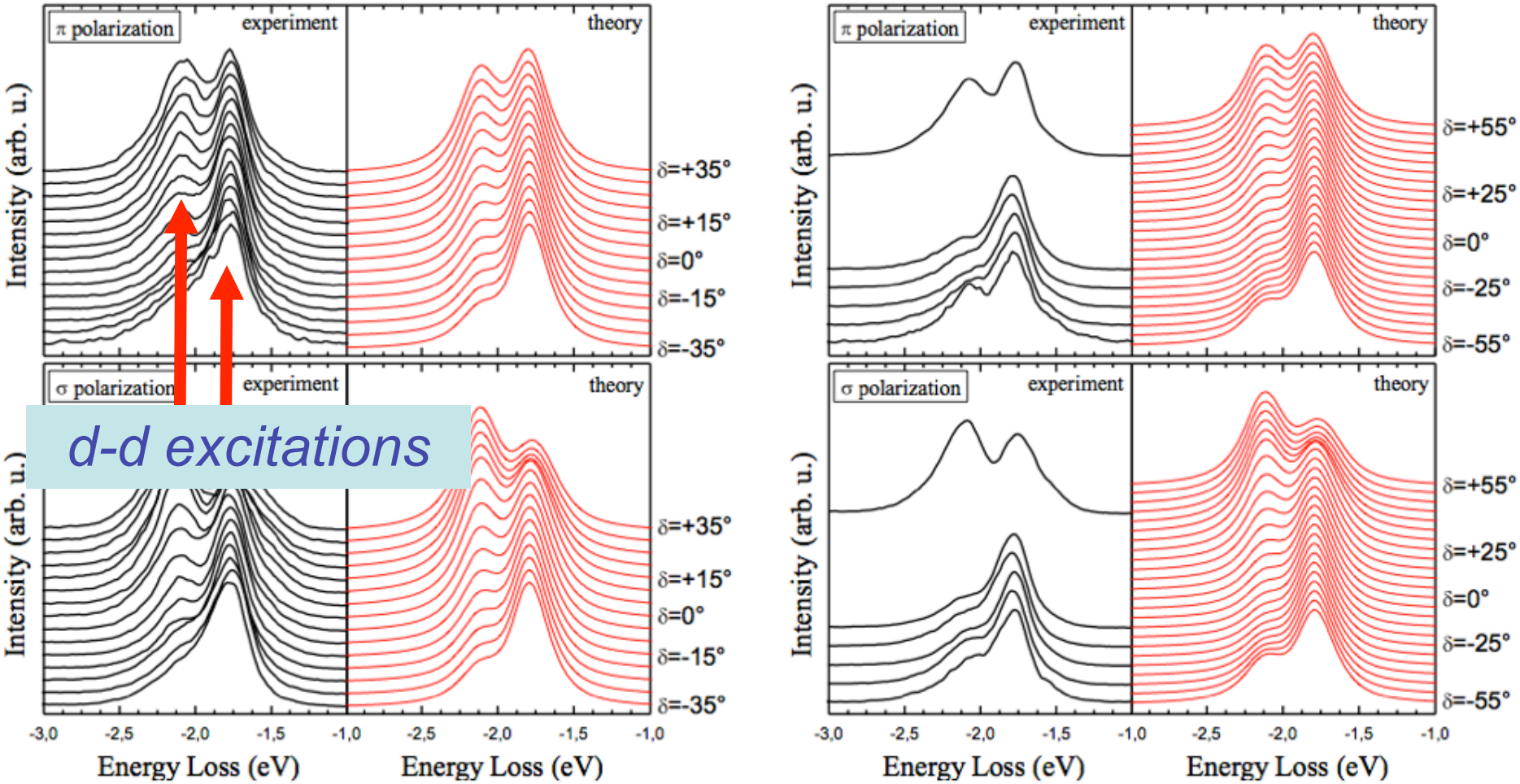


Moretti, Bisogni, Aruta, Balestrino, Berger, Brookes, Luca, Castro, Grioni, Guarise, Medaglia, Miletto, Minola, Perna, Radovic, Salluzzo, Schmitt, Zhou, Braicovich & Ghiringhelli, NJP 13, 043026 (2011)

Orbital excitations by direct RIXS on La_2CuO_4



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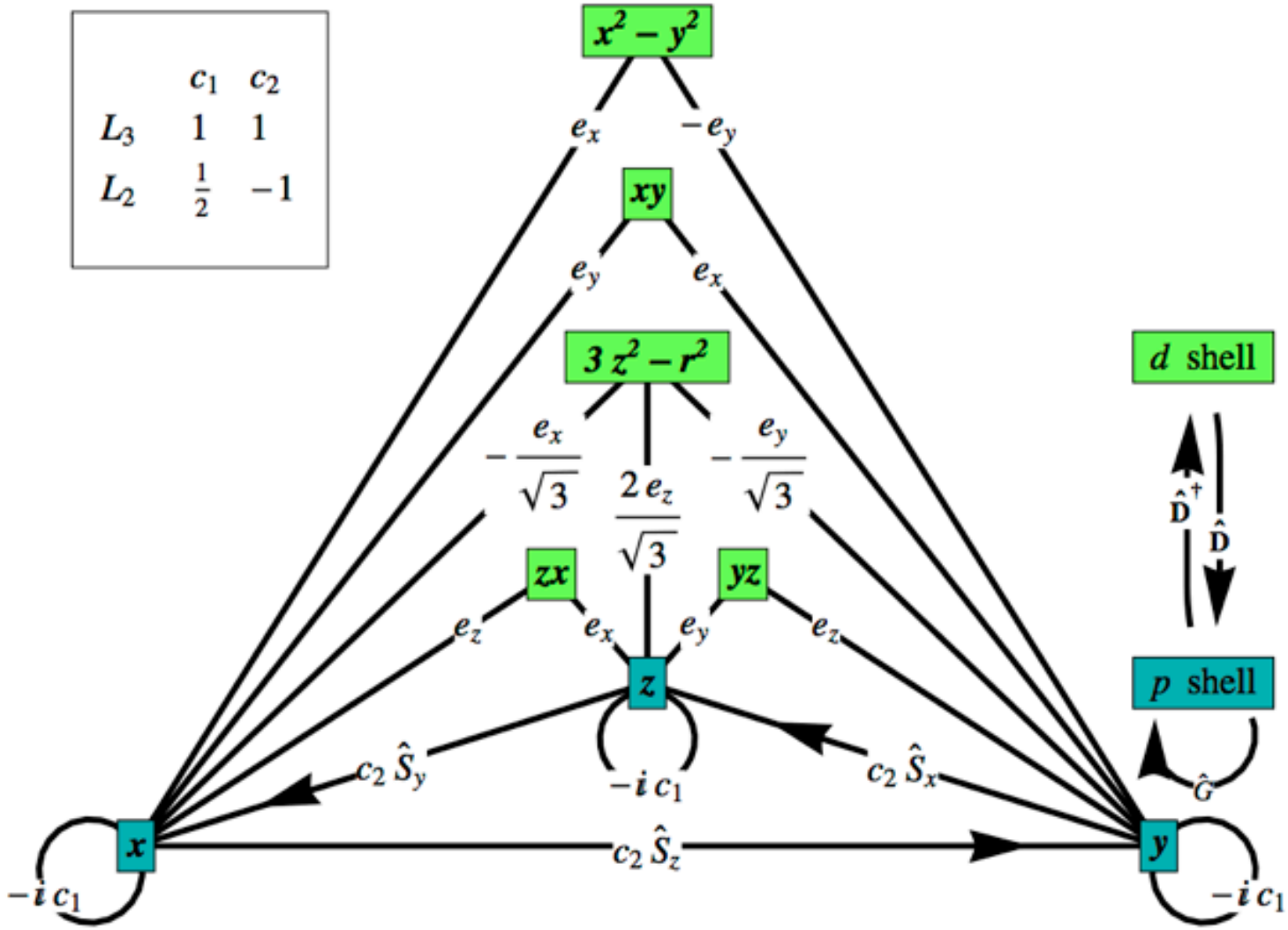
RIXS spin-flip amplitude @ transition metal L-edge



Ament, Ghiringhelli, Moretti, Braicovich & JvdB, PRL 103, 117003 (2009)

Marra, Wohlfeld & JvdB, PRL 109, 117401 (2012)

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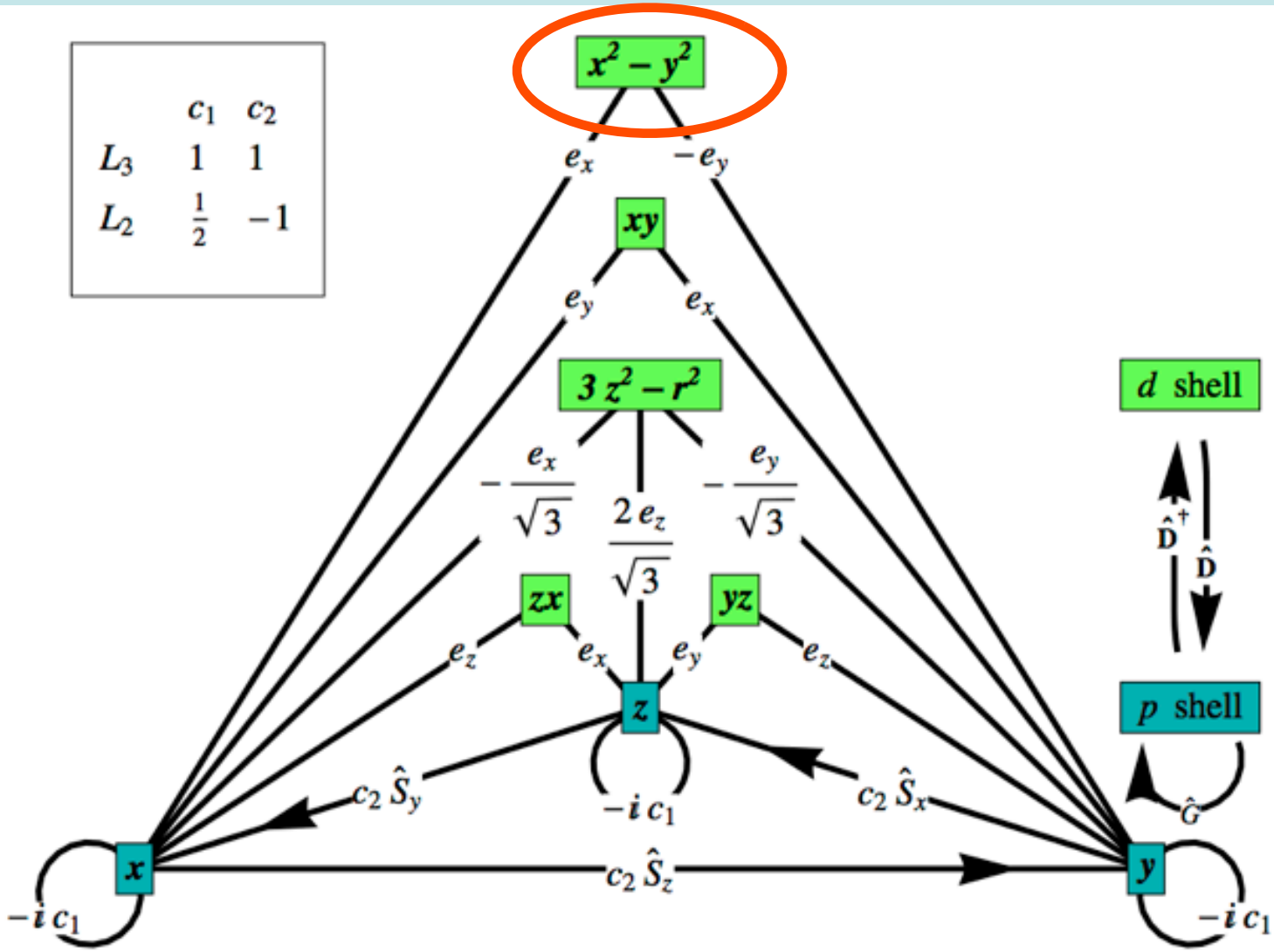

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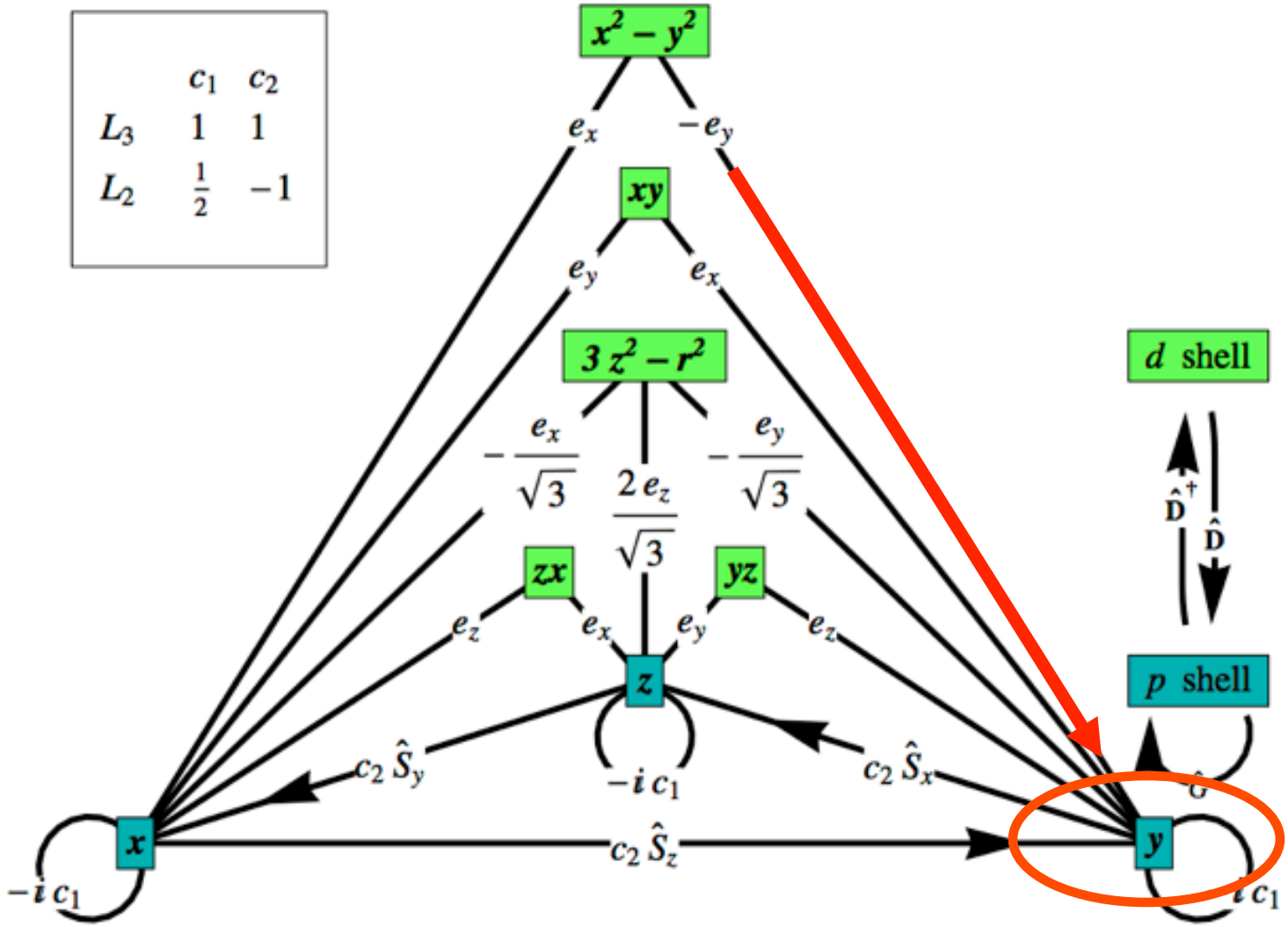

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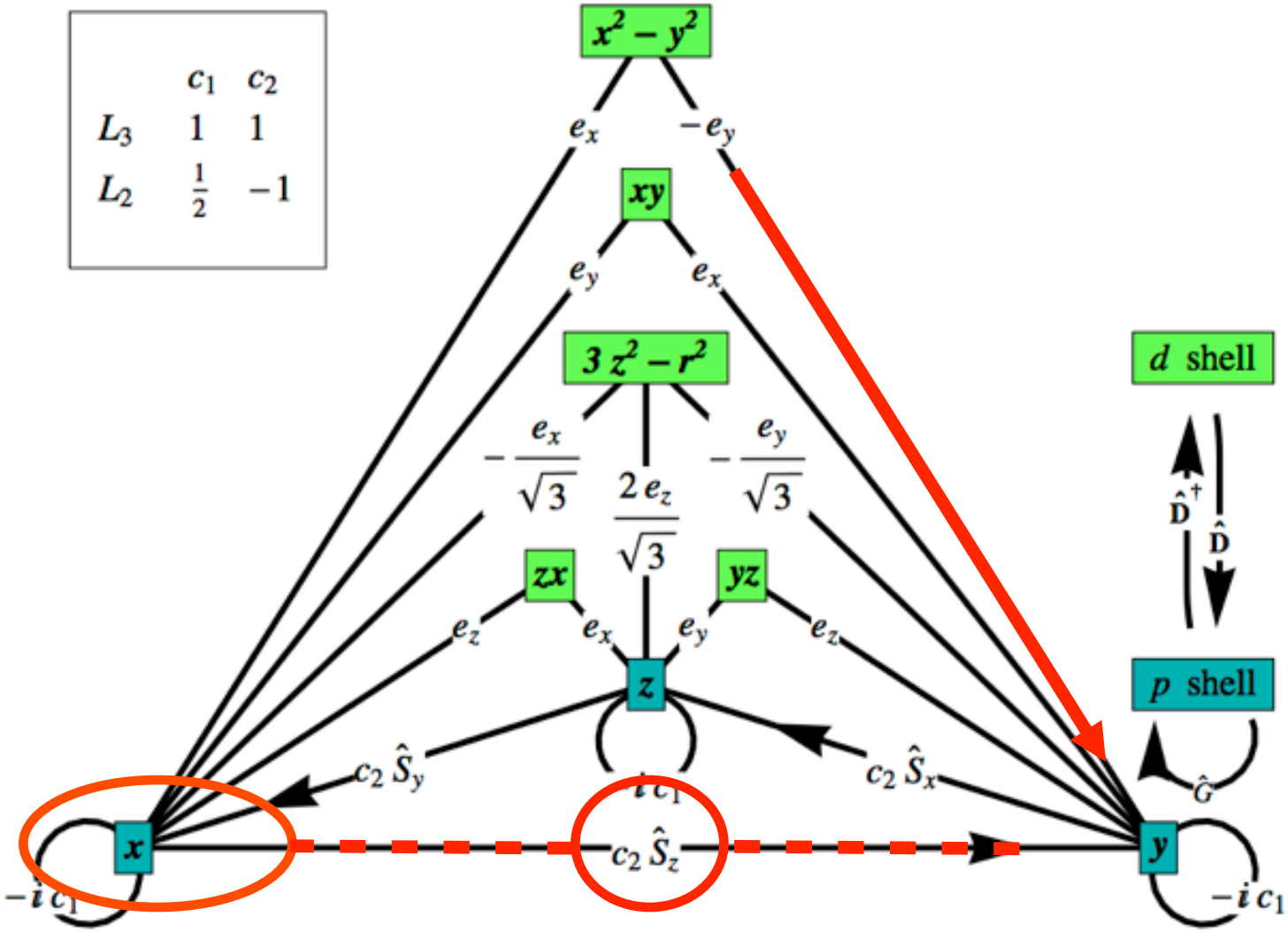

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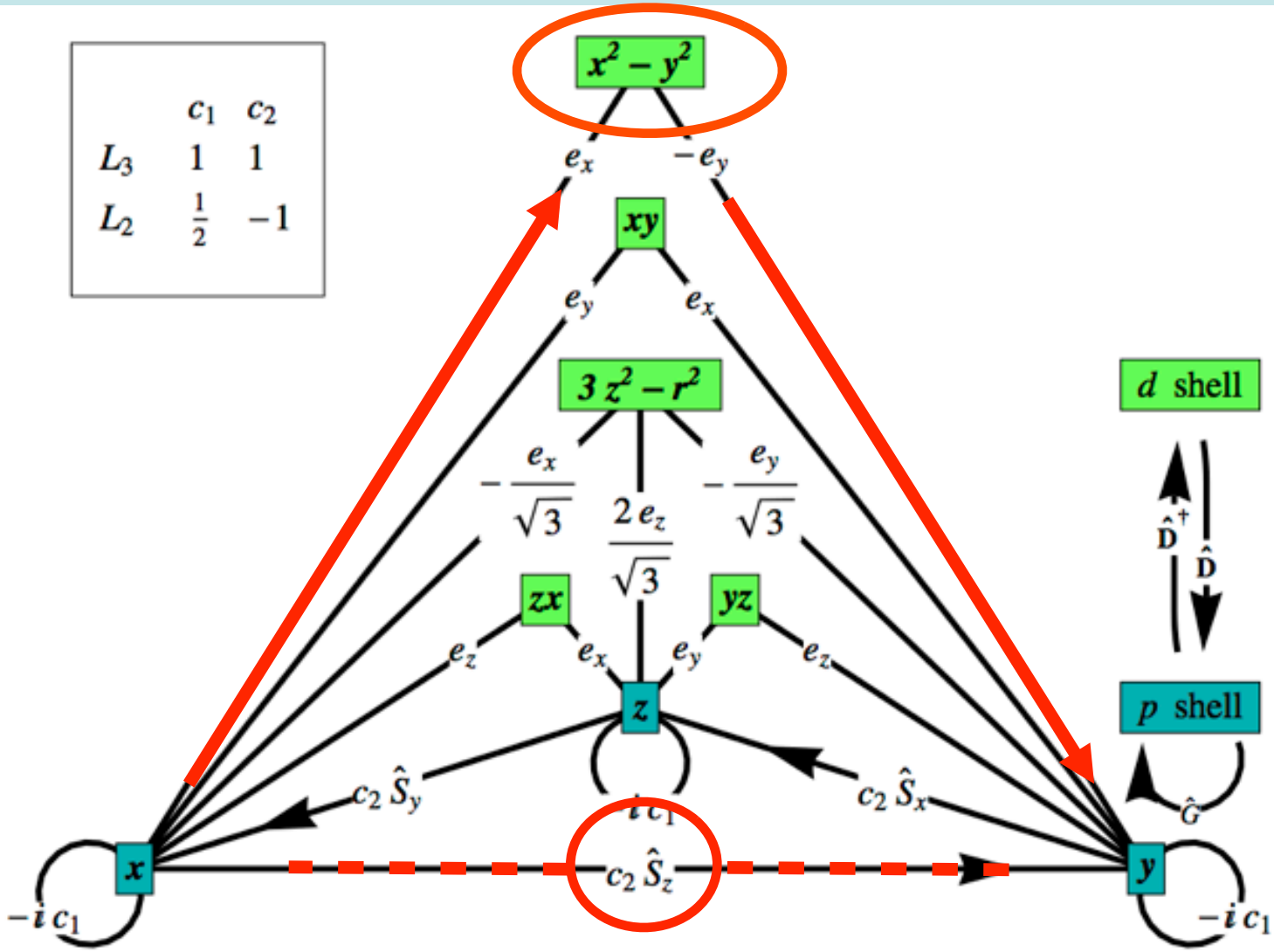

Ament, Ghiringhelli, Moretti, Braicovich & JvdB, PRL 103, 117003 (2009)

x^2-y^2 spin *NOT* // z:
pure spin flip

Marra, Wohlfeld & JvdB, PRL 109, 117401 (2012)

RIXS amplitude/intensity

Interaction light & matter

RIXS amplitude F and intensity I

$$I(\omega, \mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}') = \sum_f |\mathcal{F}_{fg}(\mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}})|^2 \times \delta(E_f + \hbar\omega_{\mathbf{k}'} - E_g - \hbar\omega_{\mathbf{k}})$$

RIXS amplitude F and intensity I

Intensity

Amplitude

$$I(\omega, \mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}') = \sum_f |\mathcal{F}_{fg}(\mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}})|^2 \times \delta(E_f + \hbar\omega_{\mathbf{k}'} - E_g - \hbar\omega_{\mathbf{k}})$$

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ω_{loss}

momentum in

out

RIXS amplitude F and intensity I

Intensity

Amplitude

$$I(\omega, \mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}') = \sum_f |\mathcal{F}_{fg}(\mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}})|^2 \times \delta(E_f + \hbar\omega_{\mathbf{k}'} - E_g - \hbar\omega_{\mathbf{k}})$$

ω_{loss}

momentum in

out

q_{loss}=k'-k

RIXS amplitude F and intensity I

polarization in

out

Intensity

Amplitude

$$I(\omega, \mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}') = \sum_f |\mathcal{F}_{fg}(\mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}})|^2 \times \delta(E_f + \hbar\omega_{\mathbf{k}'} - E_g - \hbar\omega_{\mathbf{k}})$$

ω_{loss}

momentum in

out

RIXS amplitude F and intensity I

polarization in

out

Intensity

Amplitude

$$I(\omega, \mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}') = \sum_f |\mathcal{F}_{fg}(\mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}})|^2 \times \delta(E_f + \hbar\omega_{\mathbf{k}'} - E_g - \hbar\omega_{\mathbf{k}})$$

ω_{loss}

energy conservation

momentum in

out

RIXS amplitude F and intensity I

polarization in

out

Intensity

Amplitude

$$I(\omega, \mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}') = \sum_f |\mathcal{F}_{fg}(\mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}})|^2 \times \delta(E_f + \hbar\omega_{\mathbf{k}'} - E_g - \hbar\omega_{\mathbf{k}})$$

ω_{loss}

energy conservation

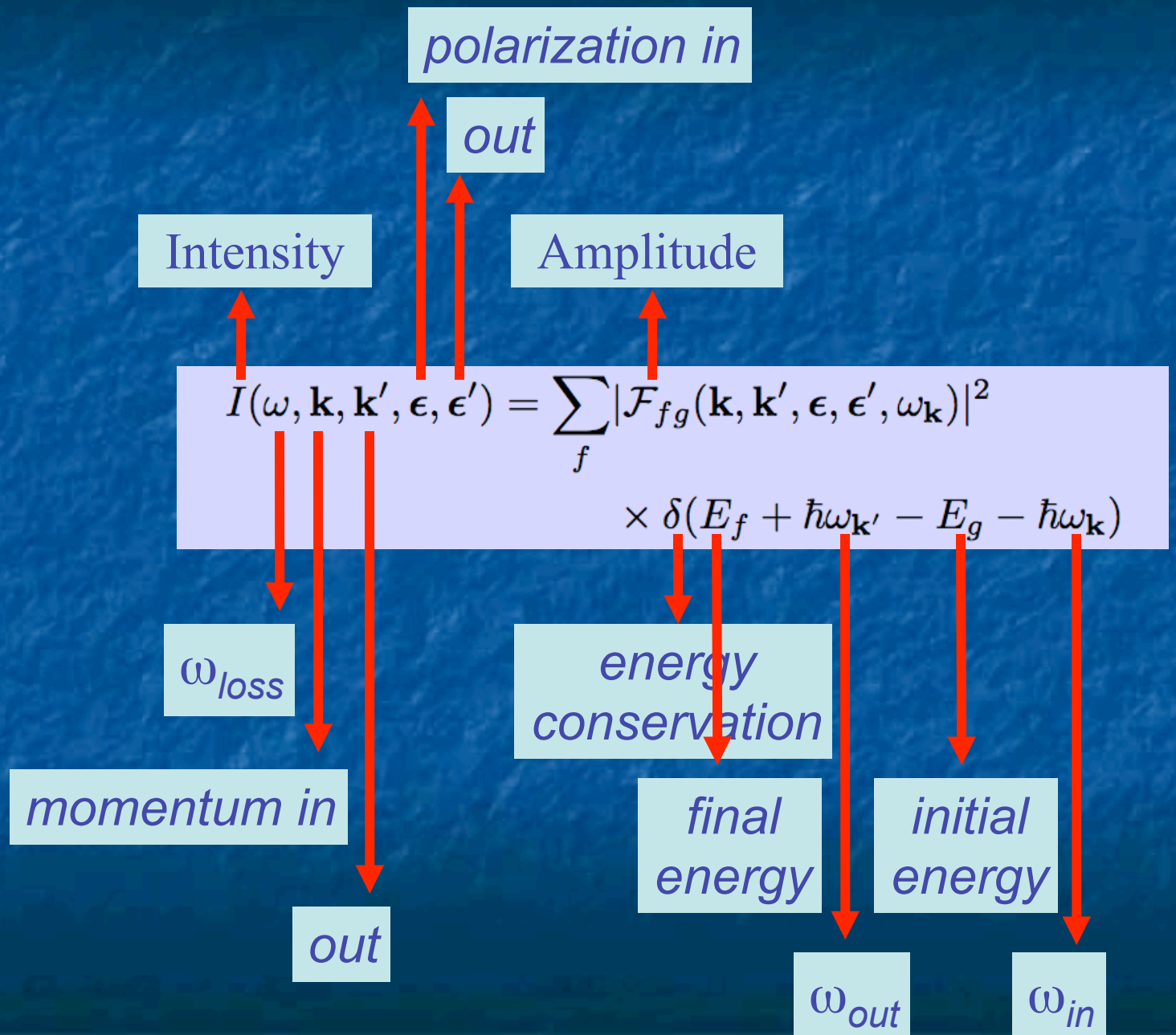
momentum in

out

ω_{out}

ω_{in}

RIXS amplitude F and intensity I



Interaction of light and matter: Hamiltonian

$$H = \sum_{i=1}^{N} \Bigg[\frac{(\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i))^2}{2m} + \frac{e\hbar}{2m} \boldsymbol{\sigma}_i \cdot \mathbf{B}(\mathbf{r}_i) + \frac{e\hbar}{2(2mc)^2} \times$$

$$\boldsymbol{\sigma}_i \cdot \Big(\mathbf{E}(\mathbf{r}_i) \times (\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i)) - (\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i)) \times \mathbf{E}(\mathbf{r}_i) \Big) \Bigg]$$

$$+ \frac{e\hbar^2 \rho(\mathbf{r}_i)}{8(mc)^2 \epsilon_0} + H_{\text{Coulomb}} + \sum_{\boldsymbol{\kappa}, \boldsymbol{\varepsilon}} \hbar\omega_{\boldsymbol{\kappa}} \left(a^\dagger_{\boldsymbol{\kappa}\boldsymbol{\varepsilon}} a_{\boldsymbol{\kappa}\boldsymbol{\varepsilon}} + \frac{1}{2} \right)$$

Interaction of light and matter: Hamiltonian

kinetic

Zeeman

$$H = \sum_{i=1}^{N} \Bigg[\frac{(\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i))^2}{2m} + \frac{e\hbar}{2m} \boldsymbol{\sigma}_i \cdot \mathbf{B}(\mathbf{r}_i) + \frac{e\hbar}{2(2mc)^2} \times$$

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Interaction of light and matter: Hamiltonian

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spin-orbit coupling

Interaction of light and matter: Hamiltonian

kinetic

Zeeman

$$H = \sum_{i=1}^{N} \Bigg[\frac{(\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i))^2}{2m} + \frac{e\hbar}{2m} \boldsymbol{\sigma}_i \cdot \mathbf{B}(\mathbf{r}_i) + \frac{e\hbar}{2(2mc)^2} \times$$

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spin-orbit coupling

Darwin

free photons

electron-nucleus
electron-electron

Interaction of light and matter: Hamiltonian

kinetic

Zeeman

$$H = \sum_{i=1}^{N} \Bigg[\frac{(\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i))^2}{2m} + \frac{e\hbar}{2m} \boldsymbol{\sigma}_i \cdot \mathbf{B}(\mathbf{r}_i) + \frac{e\hbar}{2(2mc)^2} \times$$

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spin-orbit coupling

Darwin

free photons

electron-nucleus
electron-electron

vector potential

plane wave

$$\mathbf{A}(\mathbf{r}) = \sum_{\boldsymbol{\kappa},\boldsymbol{\varepsilon}} \sqrt{\frac{\hbar}{2\mathcal{V}\epsilon_0\omega_{\boldsymbol{\kappa}}}} \left(\boldsymbol{\varepsilon}\, a_{\boldsymbol{\kappa}\boldsymbol{\varepsilon}} e^{i\boldsymbol{\kappa}\cdot\mathbf{r}} + \boldsymbol{\varepsilon}^* a^\dagger_{\boldsymbol{\kappa}\boldsymbol{\varepsilon}} e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}} \right)$$

Lowest order perturbing Hamiltonian: small A

$$H' = \sum_{i=1}^{N} \left[\frac{e}{m} \mathbf{A}(\mathbf{r}_i) \cdot \mathbf{p}_i + \frac{e^2}{2m} \mathbf{A}^2(\mathbf{r}_i) + \frac{e\hbar}{2m} \boldsymbol{\sigma}_i \cdot \nabla \times \mathbf{A}(\mathbf{r}_i) \right.$$
$$\left. - \frac{e^2\hbar}{(2mc)^2} \boldsymbol{\sigma}_i \cdot \frac{\partial \mathbf{A}(\mathbf{r}_i)}{\partial t} \times \mathbf{A}(\mathbf{r}_i) \right],$$

Lowest order perturbing Hamiltonian: small A

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small

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small

Fermi Golden Rule, to second order:

transition rate

$$w = \frac{2\pi}{\hbar} \sum_{\mathtt{f}} \left| \langle \mathtt{f} | H' | \mathtt{g} \rangle + \sum_{n} \frac{\langle \mathtt{f} | H' | n \rangle \langle n | H' | \mathtt{g} \rangle}{E_{\mathtt{g}} - E_n} \right|^2 \delta(E_{\mathtt{f}} - E_{\mathtt{g}})$$

1st Order: Thompson Scattering

$$\frac{e^2}{2m}\langle \mathbf{f}|\sum_i \mathbf{A}^2(\mathbf{r}_i)|\mathbf{g}\rangle = \frac{\hbar e^2}{2m\mathcal{V}\epsilon_0}\frac{\boldsymbol{\epsilon}'^* \cdot \boldsymbol{\epsilon}}{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\langle f|\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}|g\rangle$$

1st Order: Thompson Scattering

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Fourier transform of charge density

Elastic part: causes Bragg scattering & diffraction

1st Order: Thompson Scattering

$$\frac{e^2}{2m}\langle \mathbf{f}|\sum_i \mathbf{A}^2(\mathbf{r}_i)|\mathbf{g}\rangle = \frac{\hbar e^2}{2m\mathcal{V}\epsilon_0}\frac{\boldsymbol{\epsilon}'^* \cdot \boldsymbol{\epsilon}}{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\langle f|\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}|g\rangle$$

Fourier transform of charge density

Elastic part: causes Bragg scattering & diffraction

Inelastic part: causes Inelastic X-ray Scattering (IXS)

= Non-Resonant Inelastic X-ray Scattering (NIXS)

1st Order: Thompson Scattering

$$\frac{e^2}{2m}\langle \mathbf{f}|\sum_i \mathbf{A}^2(\mathbf{r}_i)|\mathbf{g}\rangle = \frac{\hbar e^2}{2m\mathcal{V}\epsilon_0}\frac{\boldsymbol{\epsilon}'^* \cdot \boldsymbol{\epsilon}}{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\langle f|\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}|g\rangle$$

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transition operator

$$e^{iqr} \approx 1 + iqr - \frac{1}{2}(qr)^2 + \ldots.$$

1st Order: Thompson Scattering

$$\frac{e^2}{2m}\langle \mathbf{f}|\sum_i \mathbf{A}^2(\mathbf{r}_i)|\mathbf{g}\rangle = \frac{\hbar e^2}{2m\mathcal{V}\epsilon_0}\frac{\boldsymbol{\epsilon}'^* \cdot \boldsymbol{\epsilon}}{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\langle f|\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}|g\rangle$$

Fourier transform of charge density

Elastic part: causes Bragg scattering & diffraction

Inelastic part: causes Inelastic X-ray Scattering (IXS)

= Non-Resonant Inelastic X-ray Scattering (NIXS)

quadrupole

transition operator

$$e^{iqr} \approx 1 + iqr - \frac{1}{2}(qr)^2 + \ldots.$$

dipole

1st order: X-ray Absorption

$$\langle f | A \cdot p | g \rangle$$

1st order: X-ray Absorption

$$\langle f | A \cdot p | g \rangle \propto \langle f | e^{ikr} \varepsilon \cdot p | g \rangle$$

1st order: X-ray Absorption

$$\langle f | A \cdot p | g \rangle \propto \langle f | e^{ikr} \varepsilon \cdot p | g \rangle \approx \langle f | \varepsilon \cdot p | g \rangle$$

when expanding

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when expanding

$$e^{iqr} \approx 1 + iqr - \frac{1}{2}(qr)^2 + \ldots.$$

dipole:

transitions caused by momentum operator p

2nd Order...

$$H' = \sum_{i=1}^{N} \frac{e}{m}\mathbf{A}(\mathbf{r}_i)\cdot\mathbf{p}_i + \frac{e^2}{2m}\mathbf{A}^2(\mathbf{r}_i) + \frac{e\hbar}{2m}\boldsymbol{\sigma}_i\cdot\nabla\times\mathbf{A}(\mathbf{r}_i)$$

Fermi Golden Rule, to second order:

transition rate

$$w = \frac{2\pi}{\hbar}\sum_{\mathtt{f}}\left|\langle\mathtt{f}|\,H'\,|\mathtt{g}\rangle + \sum_{n}\frac{\langle\mathtt{f}|\,H'\,|n\rangle\,\langle n|\,H'\,|\mathtt{g}\rangle}{E_{\mathtt{g}}-E_n}\right|^2\delta(E_{\mathtt{f}}-E_{\mathtt{g}})$$

2nd Order...

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2nd Order: Resonant Scattering I

RIXS amplitude

$$\frac{e^2\hbar}{2m^2\mathcal{V}\epsilon_0\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\sum_n\sum_{i,j=1}^{N}$$

$$\times\frac{\langle f|\,e^{-i\mathbf{k}'\cdot\mathbf{r}_i}\left(\boldsymbol{\epsilon}'^*\cdot\mathbf{p}_i-\frac{i\hbar}{2}\boldsymbol{\sigma}_i\cdot\mathbf{k}'\times\boldsymbol{\epsilon}'^*\right)|n\rangle}{E_g+\hbar\omega_{\mathbf{k}}-E_n+i\Gamma_n}$$

$$\times\langle n|\,e^{i\mathbf{k}\cdot\mathbf{r}_j}\left(\boldsymbol{\epsilon}\cdot\mathbf{p}_j+\frac{i\hbar}{2}\boldsymbol{\sigma}_j\cdot\mathbf{k}\times\boldsymbol{\epsilon}\right)|g\rangle$$

H.A. Kramers and W. Heisenberg, Z. Phys. 31, 681 (1925)

2nd Order: Resonant Scattering I

RIXS amplitude

$$\frac{e^2\hbar}{2m^2\mathcal{V}\epsilon_0\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\sum_n\sum_{i,j=1}^{N}$$

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small

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small

RIXS transition operator

$$\mathcal{D}=\frac{1}{im\omega_{\mathbf{k}}}\sum_{i=1}^{N}e^{i\mathbf{k}\cdot\mathbf{r}_i}\boldsymbol{\epsilon}\cdot\mathbf{p}_i,$$

H.A. Kramers and W. Heisenberg, Z. Phys. 31, 681 (1925)

2nd Order: Resonant Scattering I

RIXS amplitude

$$\frac{e^2\hbar}{2m^2\mathcal{V}\epsilon_0\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\sum_n\sum_{i,j=1}^{N}$$
$$\times\frac{\langle f|\,e^{-i\mathbf{k}'\cdot\mathbf{r}_i}\left(\boldsymbol{\epsilon}'^*\cdot\mathbf{p}_i-\frac{i\hbar}{2}\boldsymbol{\sigma}_i\cdot\mathbf{k}'\times\boldsymbol{\epsilon}'^*\right)|n\rangle}{E_g+\hbar\omega_{\mathbf{k}}-E_n+i\Gamma_n}$$
$$\times\langle n|\,e^{i\mathbf{k}\cdot\mathbf{r}_j}\left(\boldsymbol{\epsilon}\cdot\mathbf{p}_j+\frac{i\hbar}{2}\boldsymbol{\sigma}_j\cdot\mathbf{k}\times\boldsymbol{\epsilon}\right)|g\rangle$$

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RIXS amplitude

$$\mathcal{F}_{fg}(\mathbf{k},\mathbf{k}',\boldsymbol{\epsilon},\boldsymbol{\epsilon}',\omega_{\mathbf{k}},\omega_{\mathbf{k}'})=\sum_n\frac{\langle f|\,\mathcal{D}'^{\dagger}\,|n\rangle\,\langle n|\,\mathcal{D}\,|g\rangle}{E_g+\hbar\omega_{\mathbf{k}}-E_n+i\Gamma_n}$$

H.A. Kramers and W. Heisenberg, Z. Phys. 31, 681 (1925)

2nd Order: Resonant Scattering I

RIXS amplitude

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small

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RIXS amplitude

$$\mathcal{F}_{fg}(\mathbf{k},\mathbf{k}',\boldsymbol{\epsilon},\boldsymbol{\epsilon}',\omega_{\mathbf{k}},\omega_{\mathbf{k}'})=\sum_n\frac{\langle f|\,\mathcal{D}'^{\dagger}\,|n\rangle\,\langle n|\,\mathcal{D}\,|g\rangle}{E_g+\hbar\omega_{\mathbf{k}}-E_n+i\Gamma_n}$$

Kramers-Heisenberg expression

H.A. Kramers and W. Heisenberg, Z. Phys. 31, 681 (1925)

2nd Order: Resonant Scattering II

RIXS amplitude

$$\mathcal{F}_{fg}(\mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}}, \omega_{\mathbf{k}'}) = \sum_n \frac{\langle f | \mathcal{D}'^{\dagger} | n \rangle \langle n | \mathcal{D} | g \rangle}{E_g + \hbar\omega_{\mathbf{k}} - E_n + i\Gamma_n}$$

2nd Order: Resonant Scattering II

RIXS amplitude

$$\mathcal{F}_{fg}(\mathbf{k},\mathbf{k}',\boldsymbol{\epsilon},\boldsymbol{\epsilon}',\omega_{\mathbf{k}},\omega_{\mathbf{k}'}) = \sum_n \frac{\langle f|\,\mathcal{D}'^{\dagger}\,|n\rangle\,\langle n|\,\mathcal{D}\,|g\rangle}{E_g + \hbar\omega_{\mathbf{k}} - E_n + i\Gamma_n}$$

RIXS intensity:

$$I(\omega,\mathbf{k},\mathbf{k}',\boldsymbol{\epsilon},\boldsymbol{\epsilon}') = r_e^2 m^2 \omega_{\mathbf{k}'}^3 \omega_{\mathbf{k}} \sum_{\mathtt{f}} |\mathcal{F}_{fg}(\mathbf{k},\mathbf{k}',\boldsymbol{\epsilon},\boldsymbol{\epsilon}',\omega_{\mathbf{k}},\omega_{\mathbf{k}'})|^2 \times \delta(E_g - E_f + \hbar\omega),$$

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This expression is essentially exact (non-relativistic limit)

Resonant ELASTIC Scattering (REXS or RXS)

RIXS amplitude

$$\mathcal{F}_{fg}(\mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}}, \omega_{\mathbf{k}'}) = \sum_n \frac{\langle f | \mathcal{D}'^{\dagger} | n \rangle \langle n | \mathcal{D} | g \rangle}{E_g + \hbar\omega_{\mathbf{k}} - E_n + i\Gamma_n}$$

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REXS amplitude

$$\mathcal{F}_{\hat{g}g}(\mathbf{k},\mathbf{k}',\boldsymbol{\epsilon},\boldsymbol{\epsilon}',\omega_{\mathbf{k}},\omega_{\mathbf{k}'}) = \sum_n \frac{\langle \hat{g}|\,\mathcal{D}'^{\dagger}\,|n\rangle\,\langle n|\,\mathcal{D}\,|g\rangle}{E_g + \hbar\omega_{\mathbf{k}} - E_n + i\Gamma_n}$$

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Greens function expression for *F*

RIXS amplitude

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Greens function

$$G(z_{\mathbf{k}}) = \frac{1}{z_{\mathbf{k}} - H} = \sum_n \frac{|n\rangle\langle n|}{z_{\mathbf{k}} - E_n}$$

Greens function expression for *F*

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=intermediate state propagator

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Greens function expression for F

RIXS amplitude

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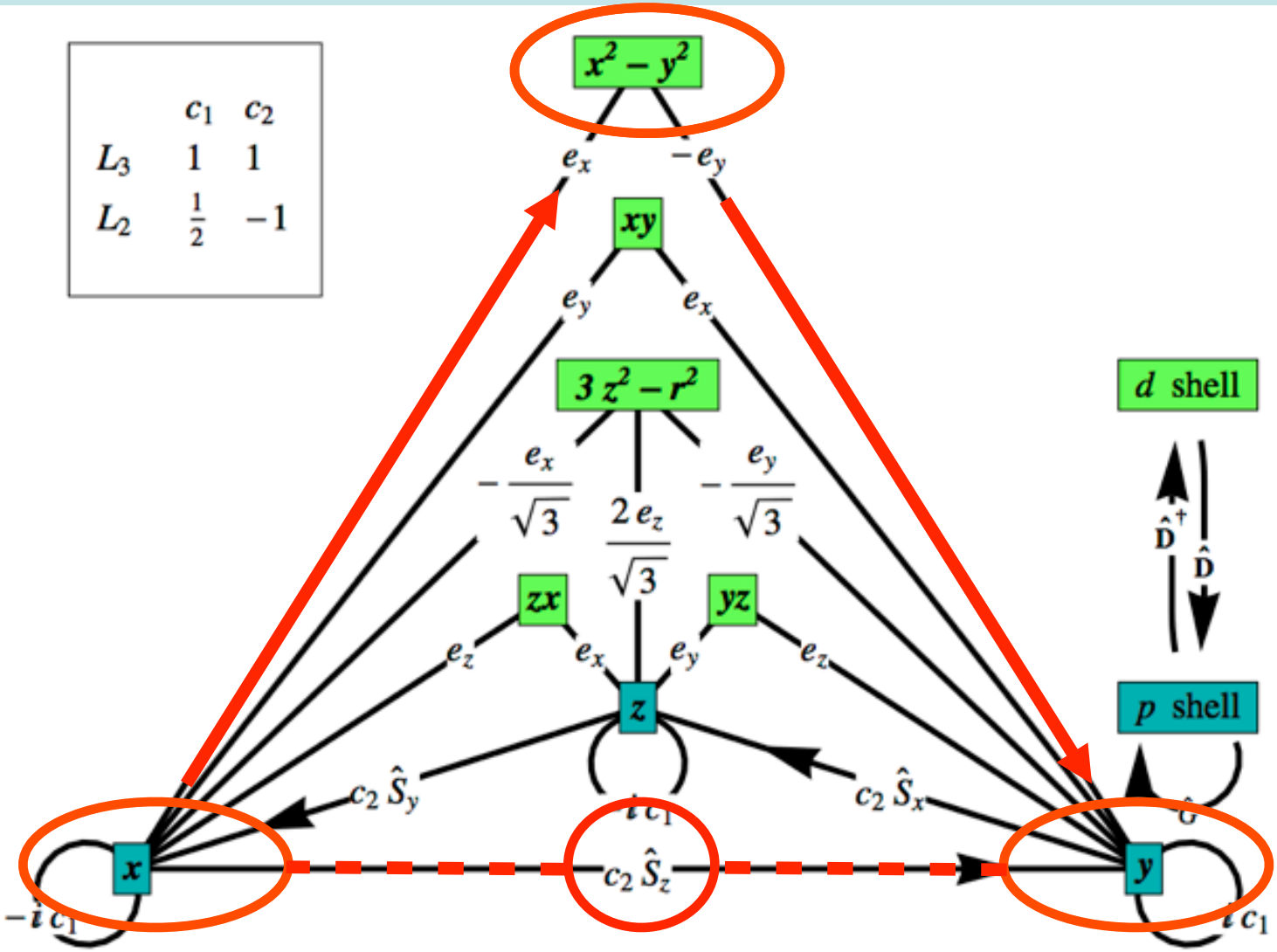
=intermediate state propagator

with $z_{\mathbf{k}} = E_g + \hbar\omega_{\mathbf{k}} + i\Gamma$

so that:

$$\mathcal{F}_{fg} = \langle f|\,\mathcal{D}'^{\dagger} G(z_{\mathbf{k}})\mathcal{D}\,|g\rangle$$

RIXS spin-flip amplitude @ transition metal L-edge



Ament, Ghiringhelli, Moretti, Braicovich & JvdB, PRL 103, 117003 (2009)

x^2-y^2 spin *NOT* // z:
pure spin flip

Marra, Wohlfeld & JvdB, PRL 109, 117401 (2012)

Quasi 2D Cuprates

Magnetic RIXS on La_2CuO_4 @ Cu L-edge

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In special cases direct spin-flip scattering is allowed at Cu L-edge

CuO's are such special cases...

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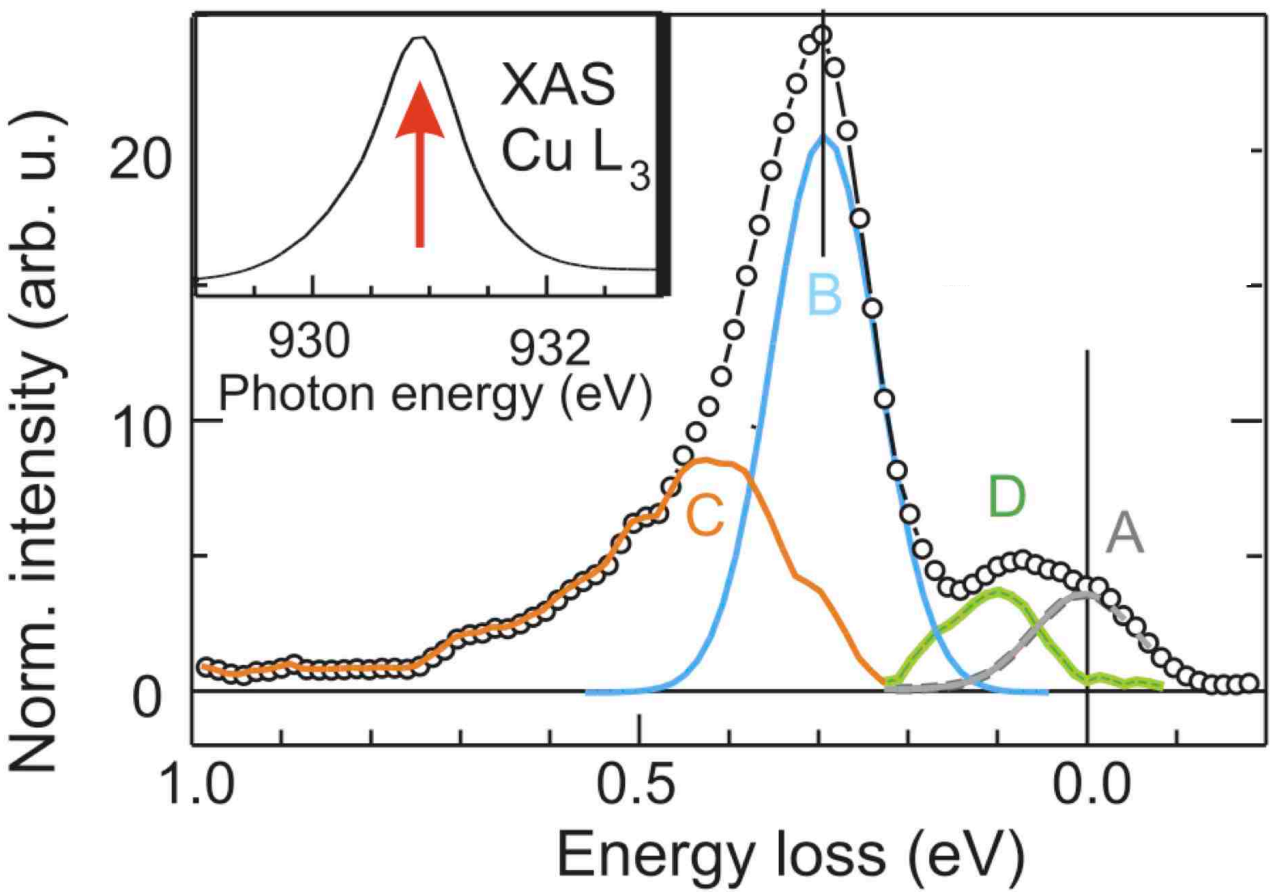

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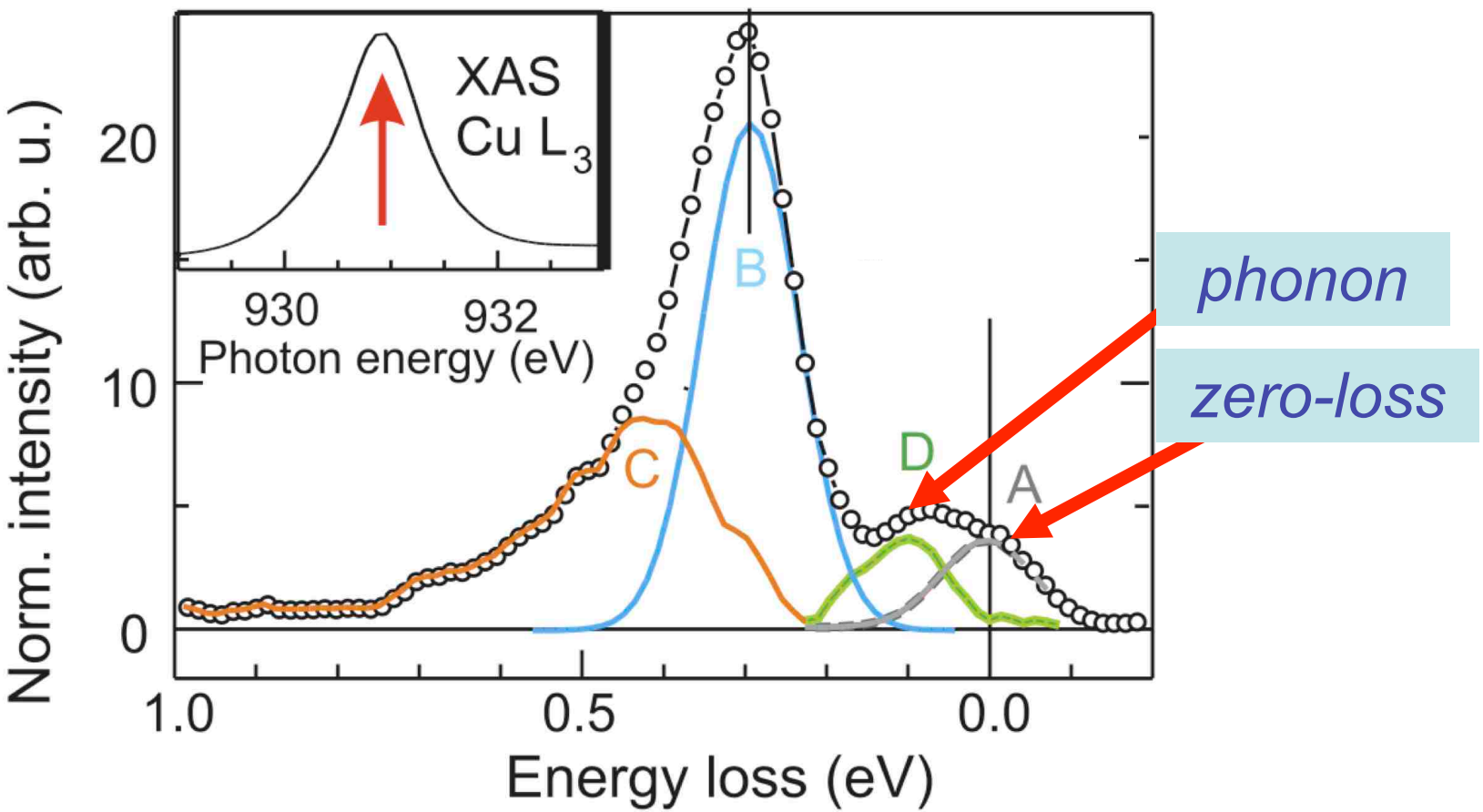

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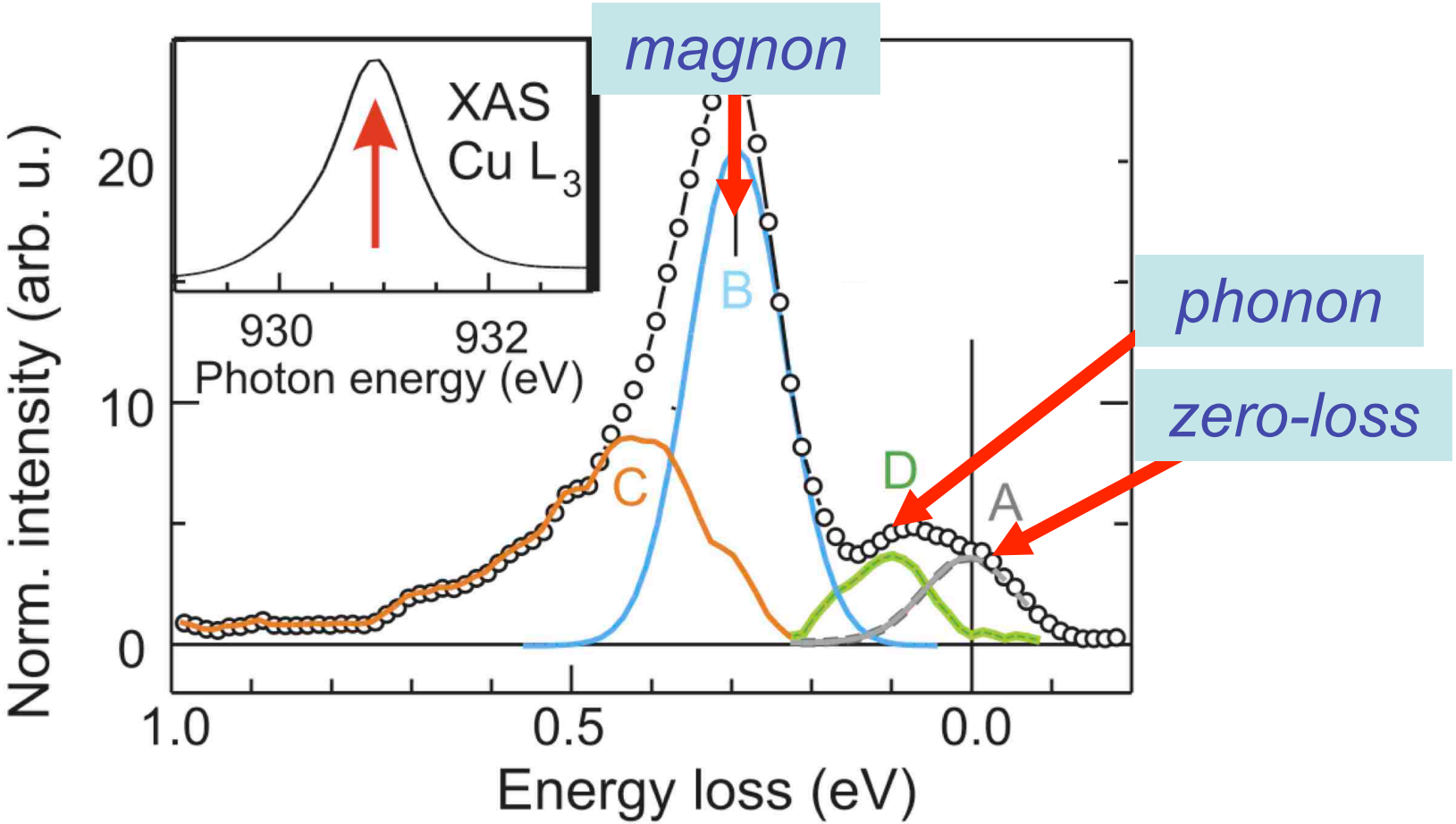

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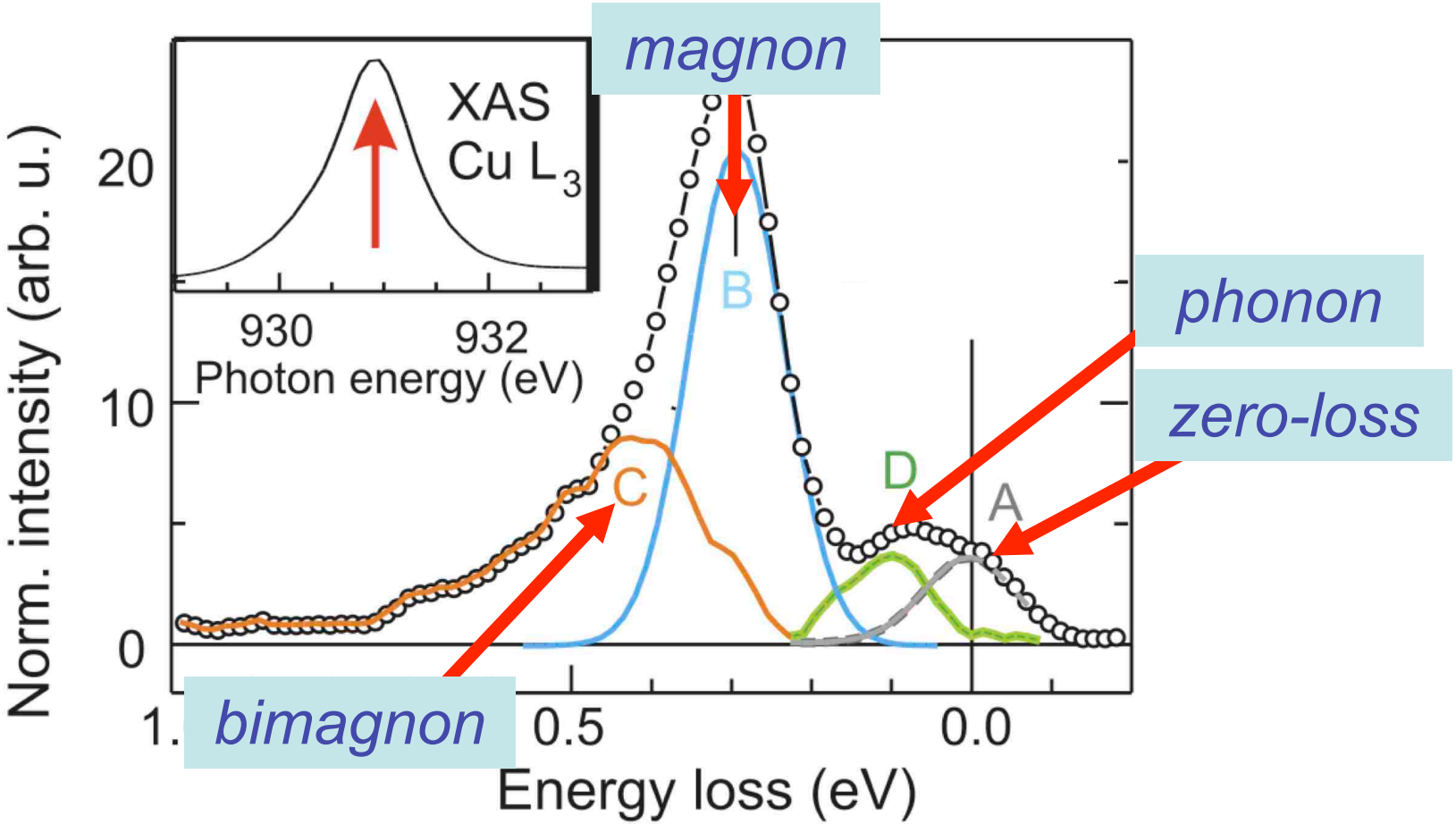

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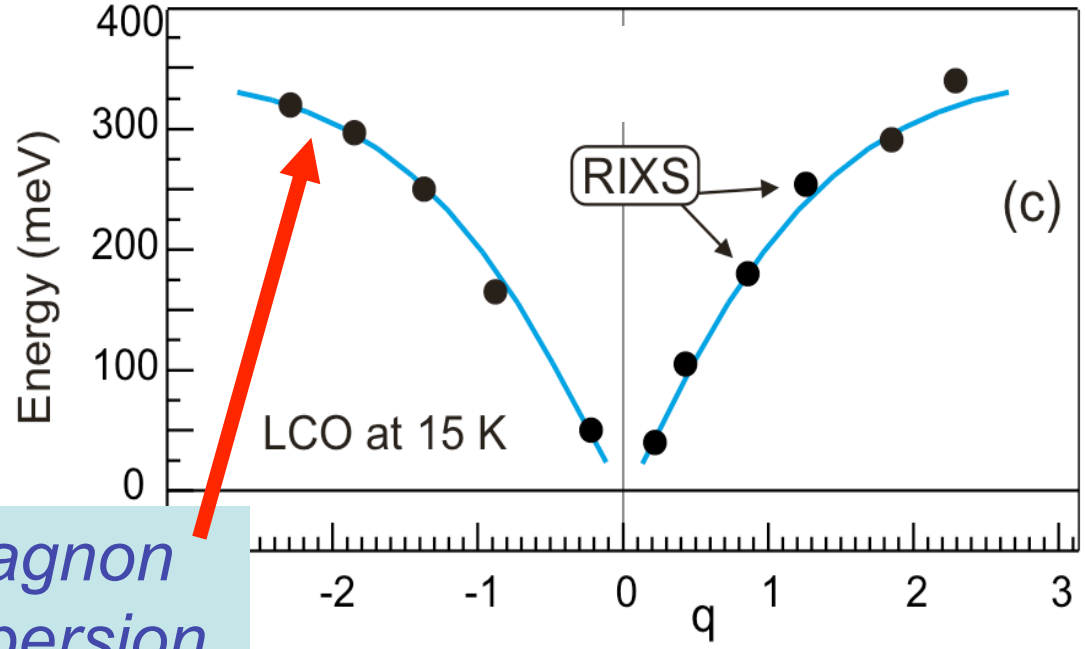

magnon dispersion

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

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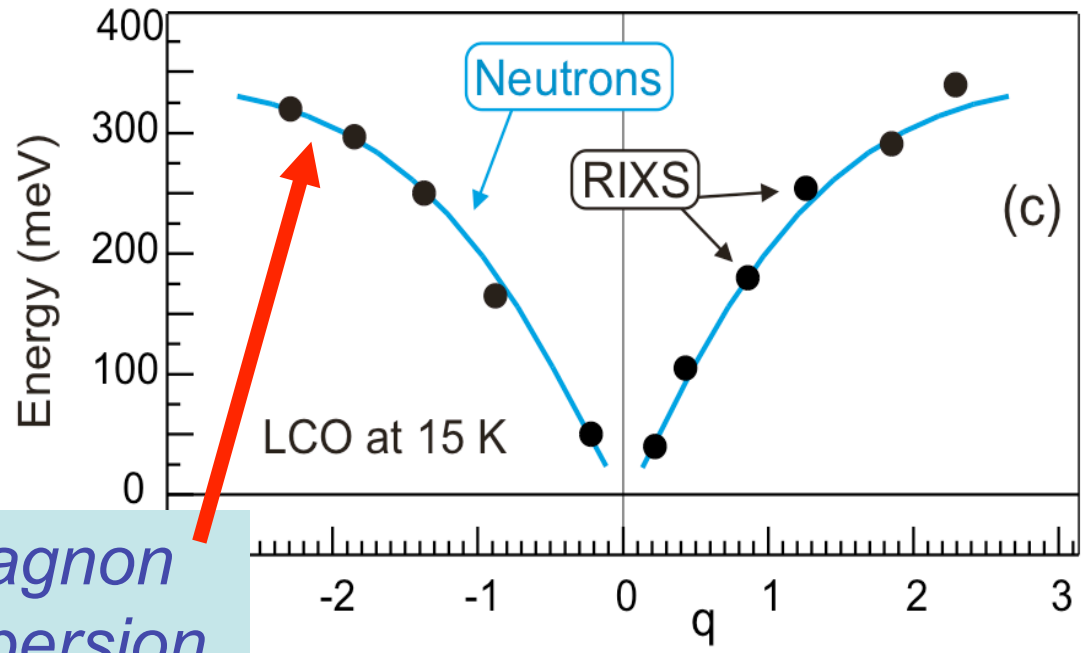

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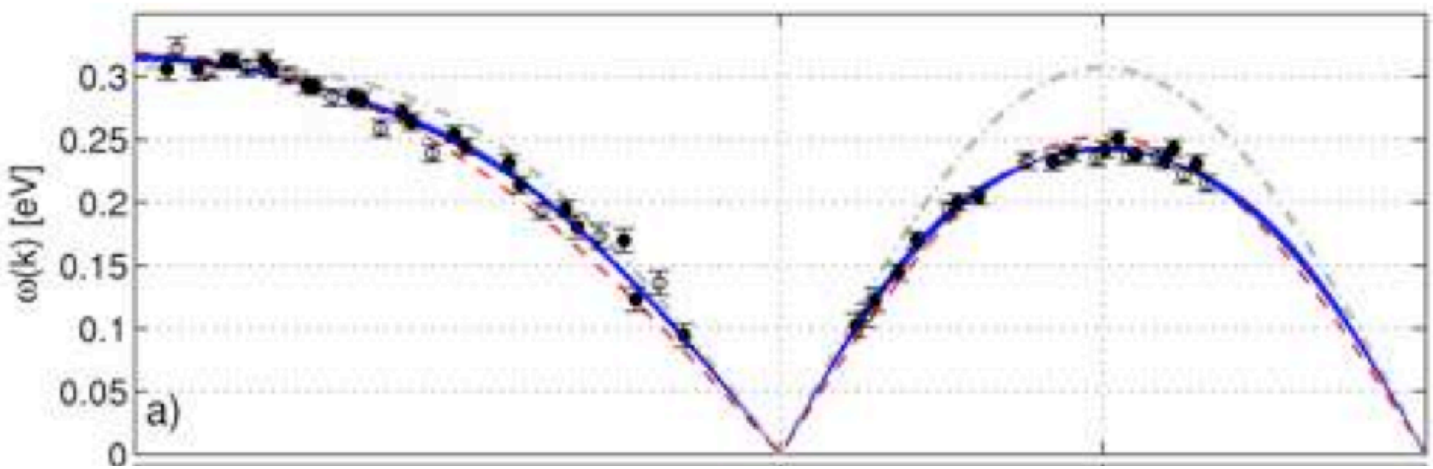
PRL 104, 077002 (2010)

RIXS magnon dispersion of $Sr_2CuO_2Cl_2$

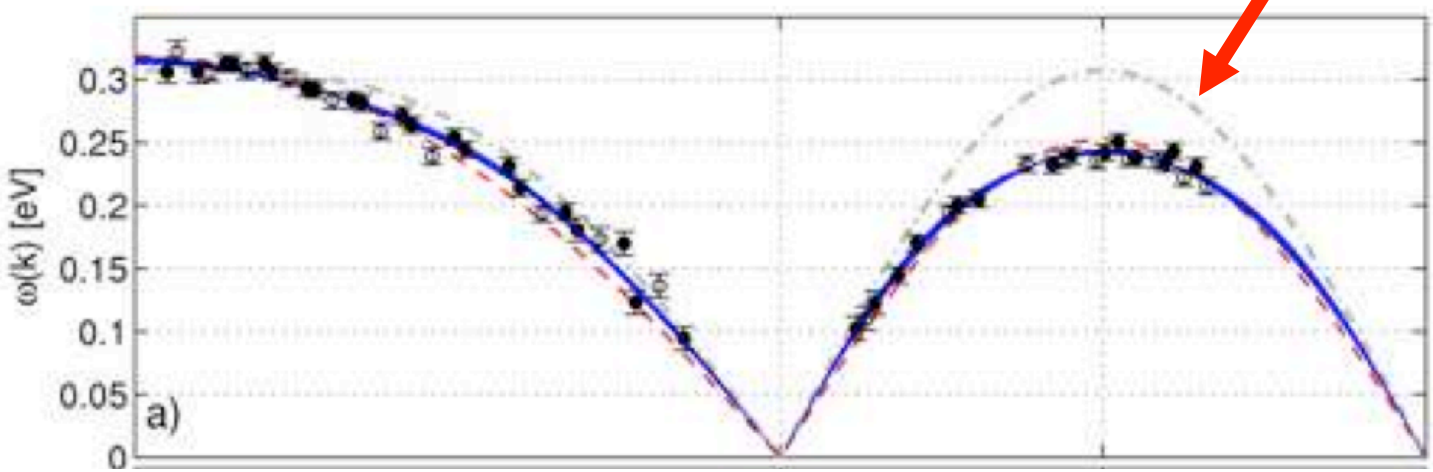


—> transferred momentum q

Guarise *et al.*,
PRL 105, 157006 (2010)

RIXS magnon dispersion of $Sr_2CuO_2Cl_2$

deviation from simple Heisenberg



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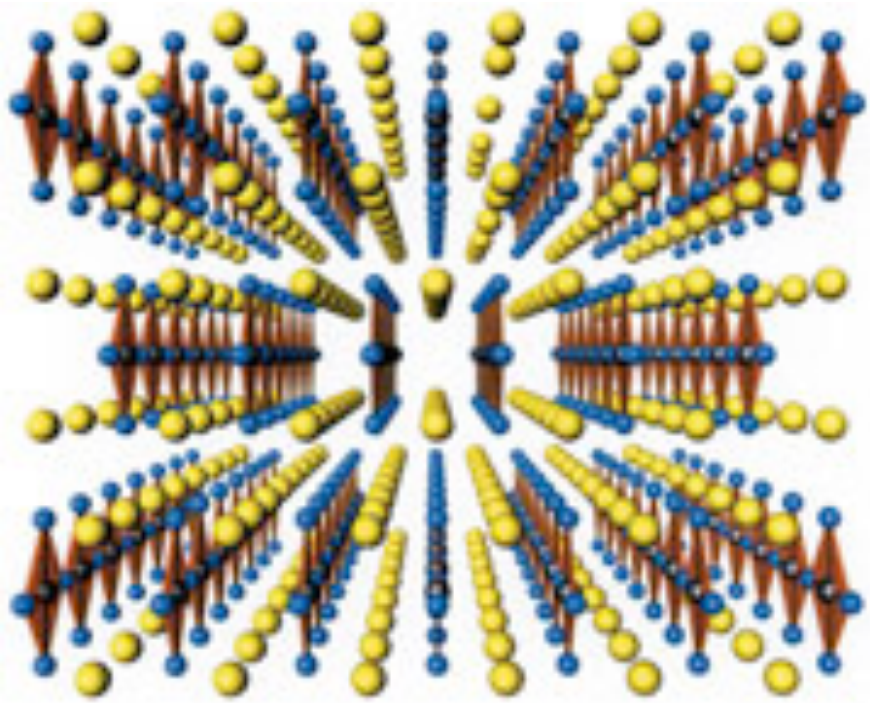
Quasi 1D Cuprate

Cuprate spin chain system Sr_2CuO_3

weakly coupled spin chains



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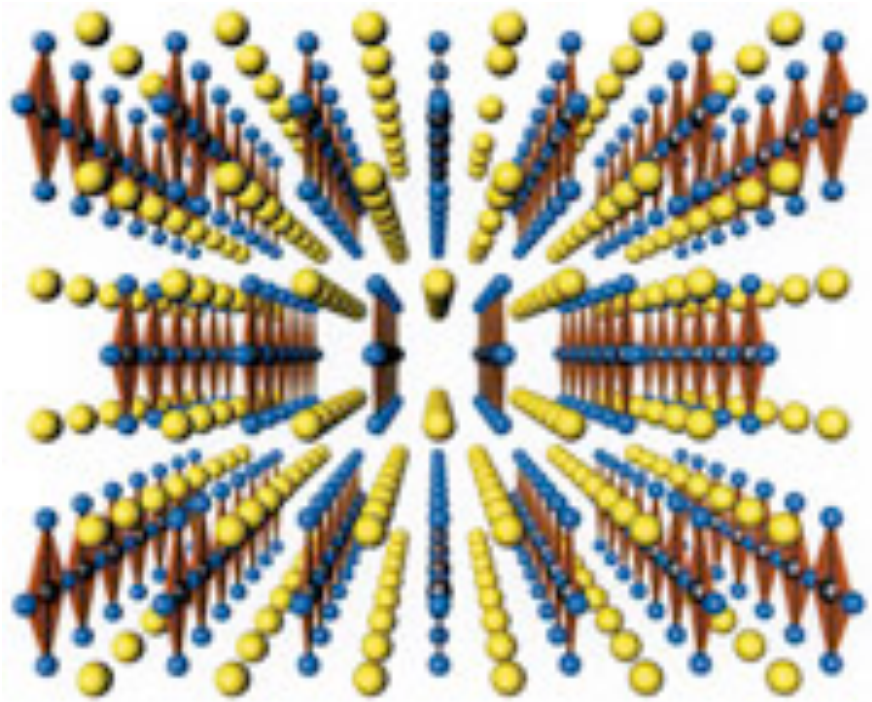

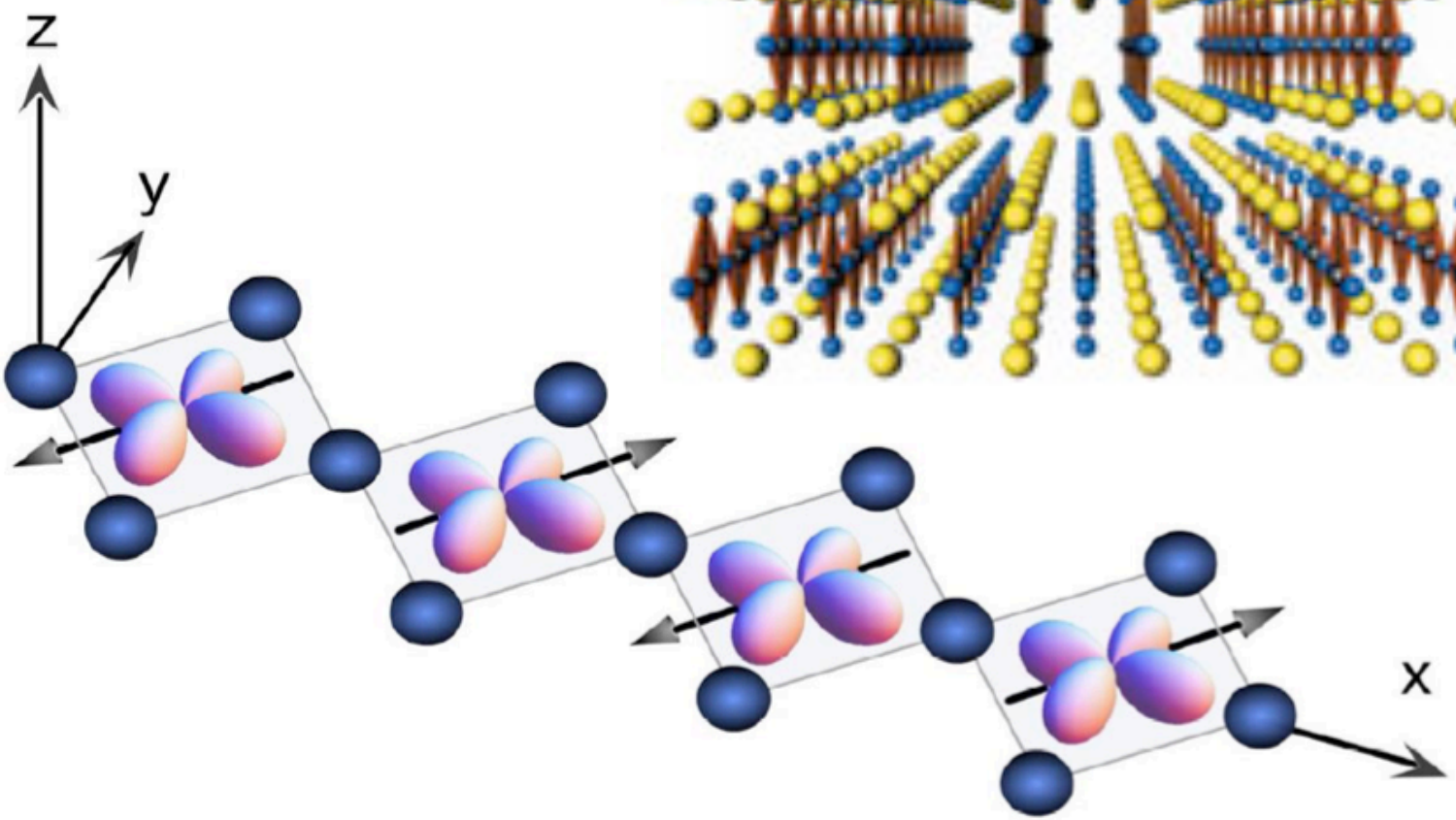

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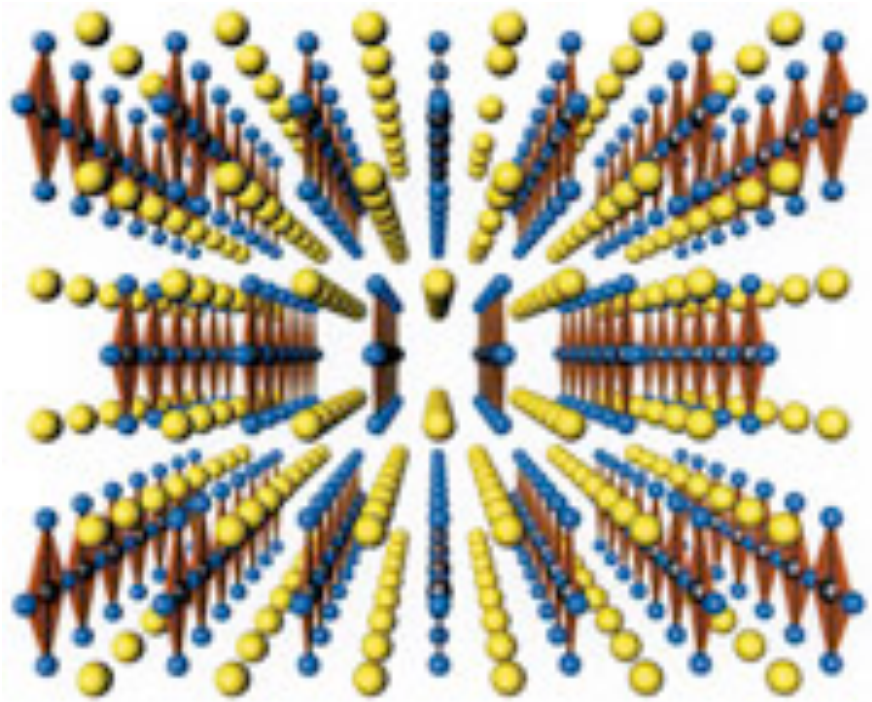

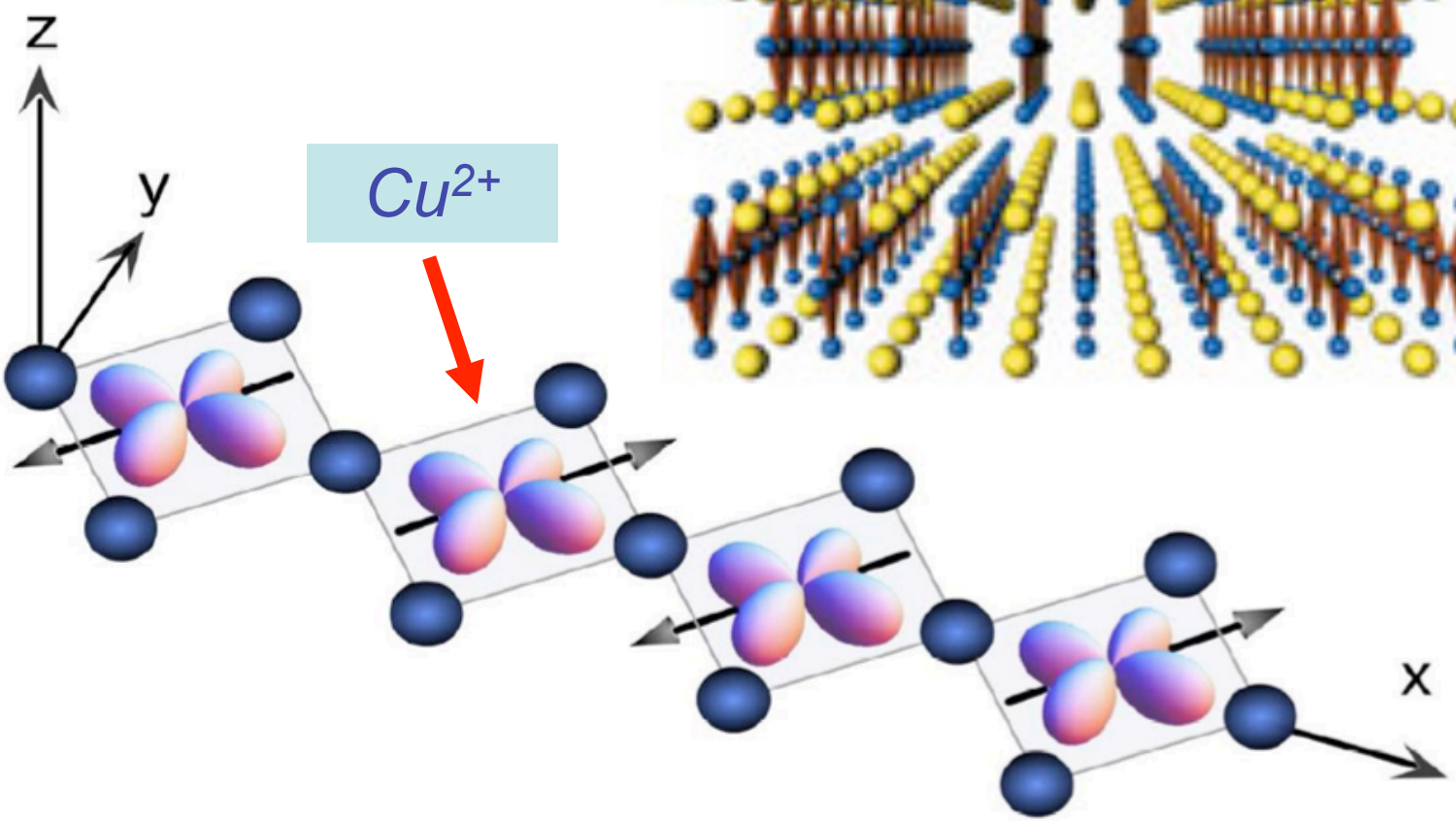

Heisenberg antiferromagnet

$S^z = +\hbar/2$ ↑ $S^z = -\hbar/2$ ↓

$$H = J\, S^z_i\, S^z_{i+1}$$

Allow for spin-exchange

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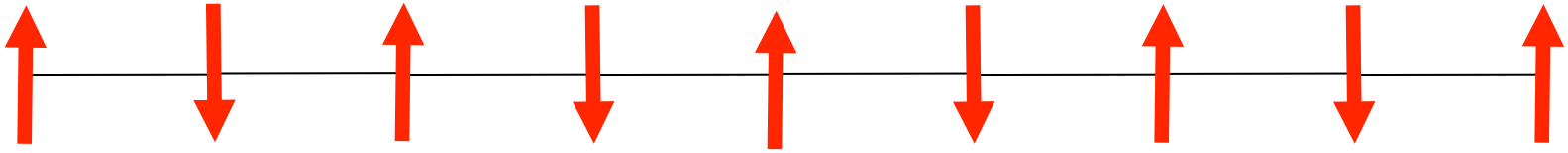
Allow for spin-exchange

ground state



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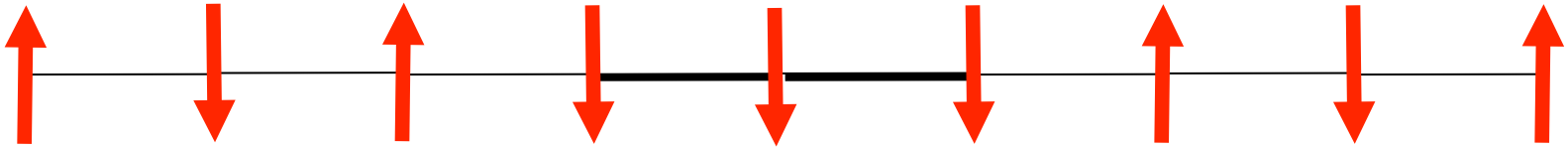
Allow for spin-exchange

spin flip $\Delta S^z = \hbar$ *in d=3: magnon*



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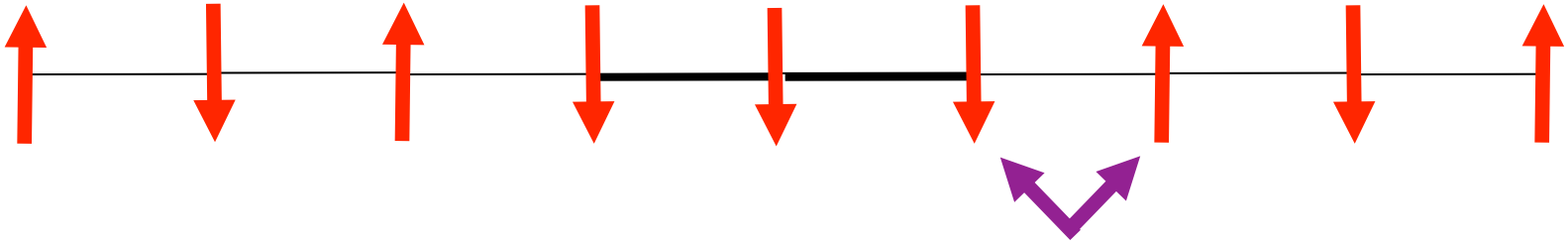

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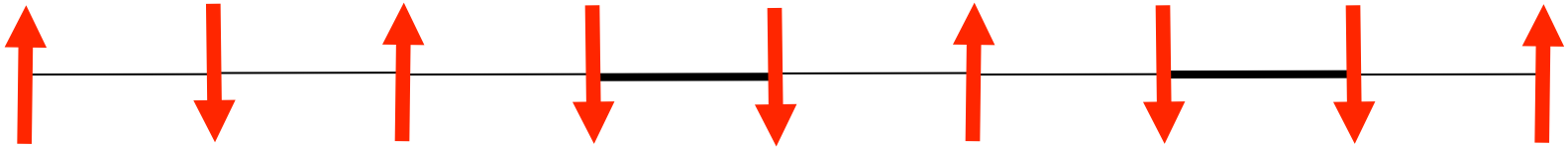

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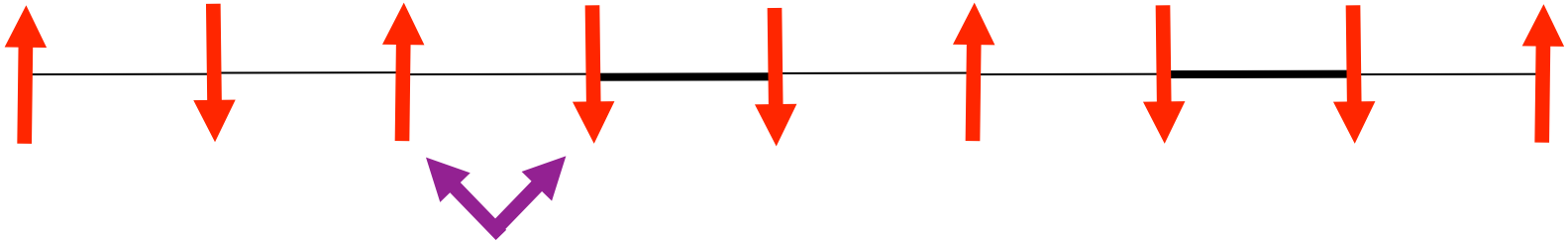

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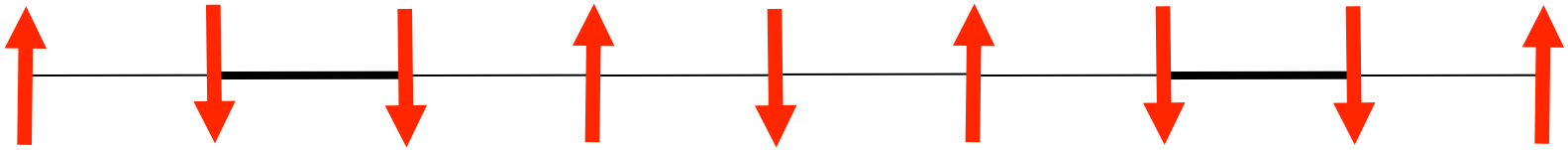

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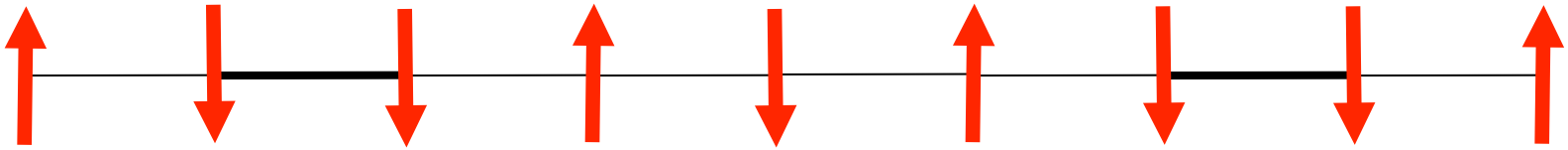
spin flip $\Delta S^z = \hbar$

in d=3: magnon



two domain walls, each with $\Delta S^z = \hbar/2$ → spinon

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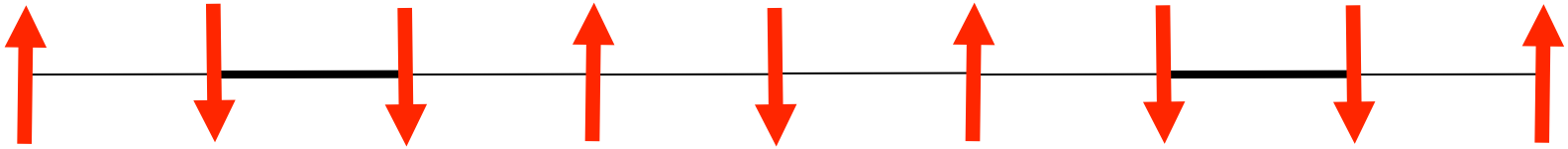
Allow for spin-exchange

spin flip $\Delta S^z = \hbar$

in d=3: magnon



two domain walls, each with $\Delta S^z = \hbar/2$ → spinon

d=1: magnon fractionalizes into spinons

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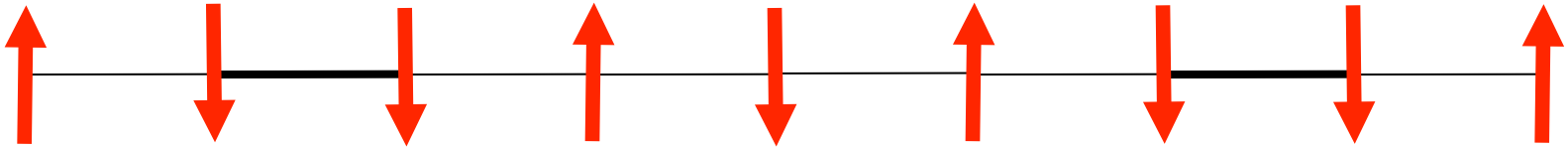
Allow for spin-exchange

spin flip $\Delta S^z = \hbar$ *in d=3: magnon*



two domain walls, each with $\Delta S^z = \hbar/2$ → *spinon*

d=1: magnon fractionalizes into spinons

magnon q, ω → *spinon* k_1, ω_1
spinon k_2, ω_2

Heisenberg antiferromagnet $S^z=+\hbar/2$ ↑ $S^z=-\hbar/2$ ↓

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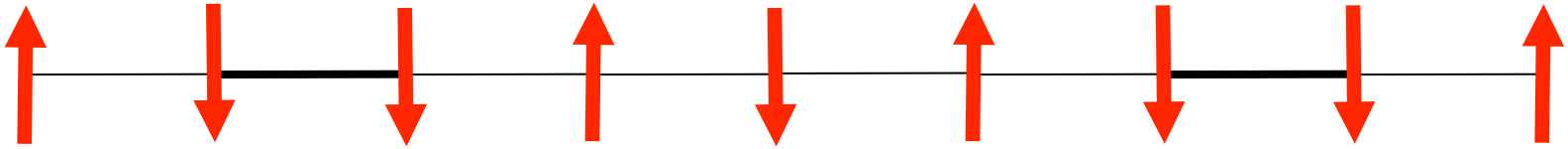

two domain walls, each with $\Delta S^z = \hbar/2$ → *spinon*

d=1: magnon fractionalizes into spinons

magnon q, ω → *spinon* k_1, ω_1 *spinon* k_2, ω_2 $q = k_1 + k_2,\ \omega = \omega_1 + \omega_2$

Spinons in 1d Heisenberg antiferromagnet

magnon q, ω → *spinon* k_1, ω_1 *spinon* k_2, ω_2

$q = k_1 + k_2, \ \omega = \omega_1 + \omega_2$

Spinons in 1d Heisenberg antiferromagnet

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relative momentum of spinons
$p = k_2 - k_1$ *not yet determined*

Spinons in 1d Heisenberg antiferromagnet

magnon q, ω → *spinon* k_1, ω_1 *spinon* k_2, ω_2

$q = k_1 + k_2, \ \omega = \omega_1 + \omega_2$

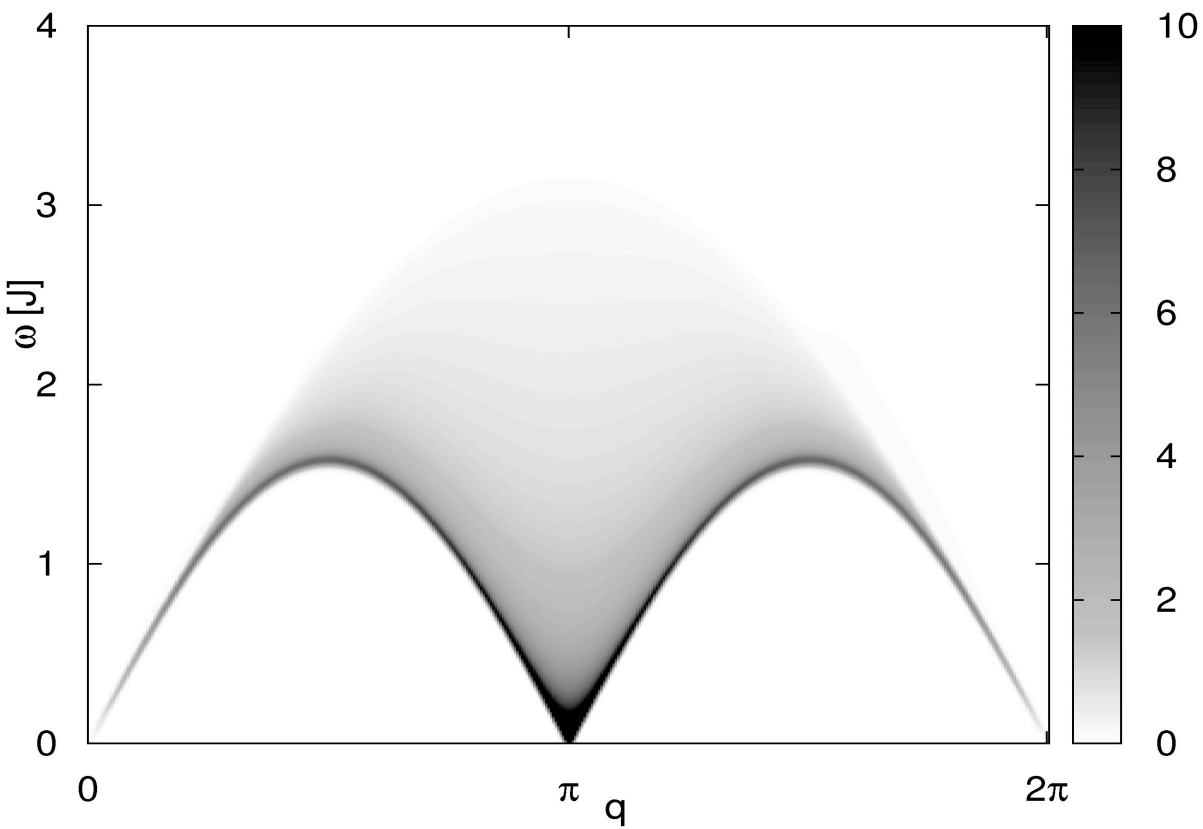
excitation **continuum** q, ω ← *relative momentum of spinons* $p = k_2 - k_1$ *not yet determined*

Spinon excitations in 1d Heisenberg antiferromagnet

excitation
continuum q, ω

relative momentum of spinons
$q = k_2 - k_1$ *not yet determined*

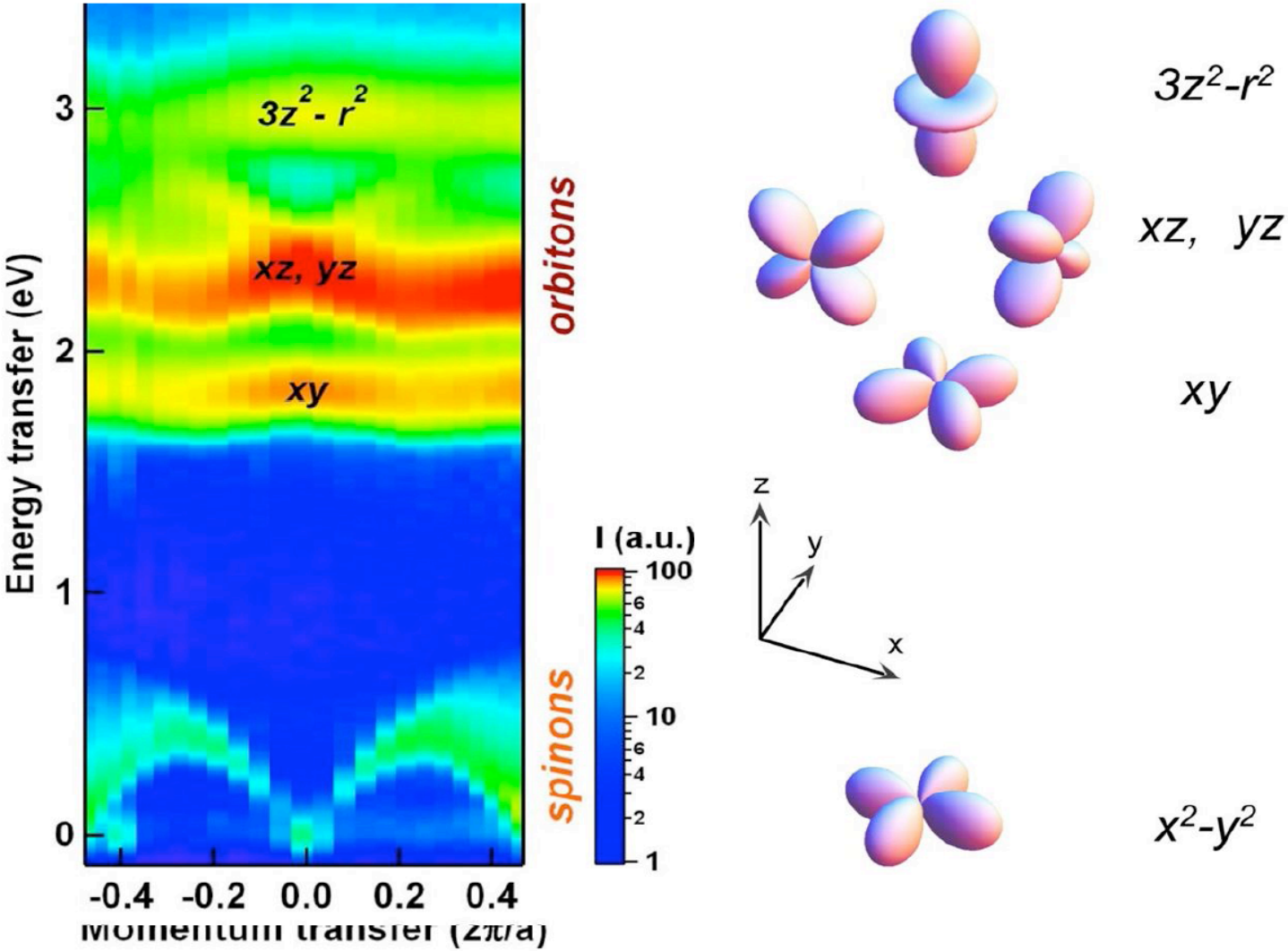
neutron scattering magnetic excitations



Bethe-Ansatz
exact solution

Klauser, Mossel, Caux, JvdB, PRL 106, 157205 (2011)

RIXS spectrum of Sr_2CuO_3 spin chain



Schlappa, Wohlfeld, Zhou, Mourigal, Haverkort, Strocov, Hozoi, Monney, Nishimoto, Singh, Revcolevschi, Caux, Patthey, Ronnow, JvdB, Schmitt, Nature 485, 82 (2012)

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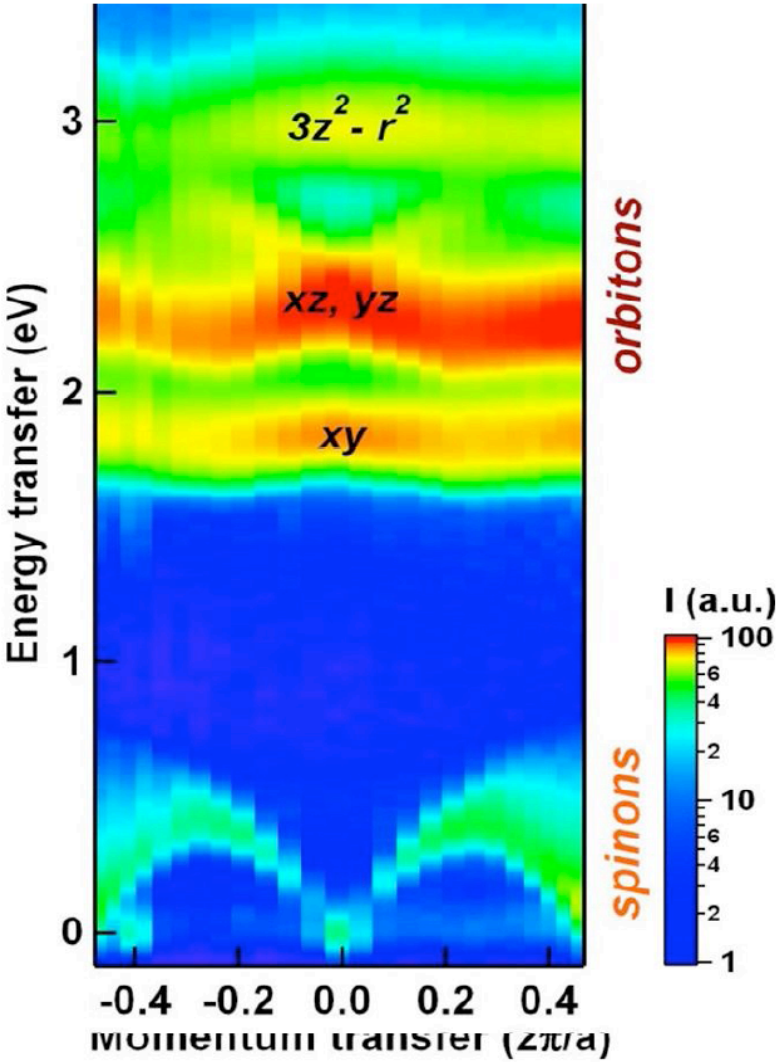

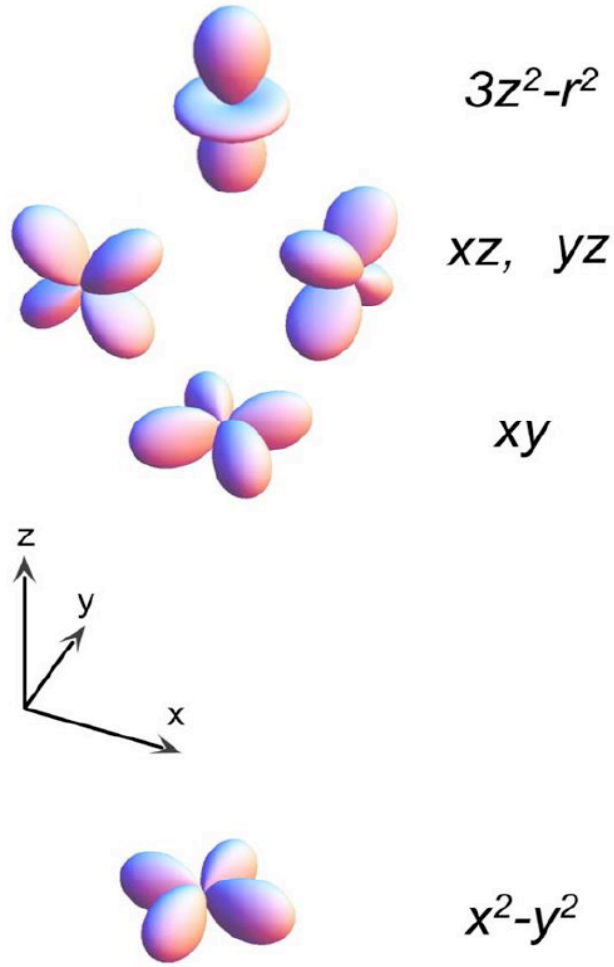

Orbital excitations

Schlappa, Wohlfeld, Zhou, Mourigal, Haverkort, Strocov, Hozoi, Monney, Nishimoto, Singh, Revcolevschi, Caux, Patthey, Ronnow, JvdB, Schmitt, Nature 485, 82 (2012)

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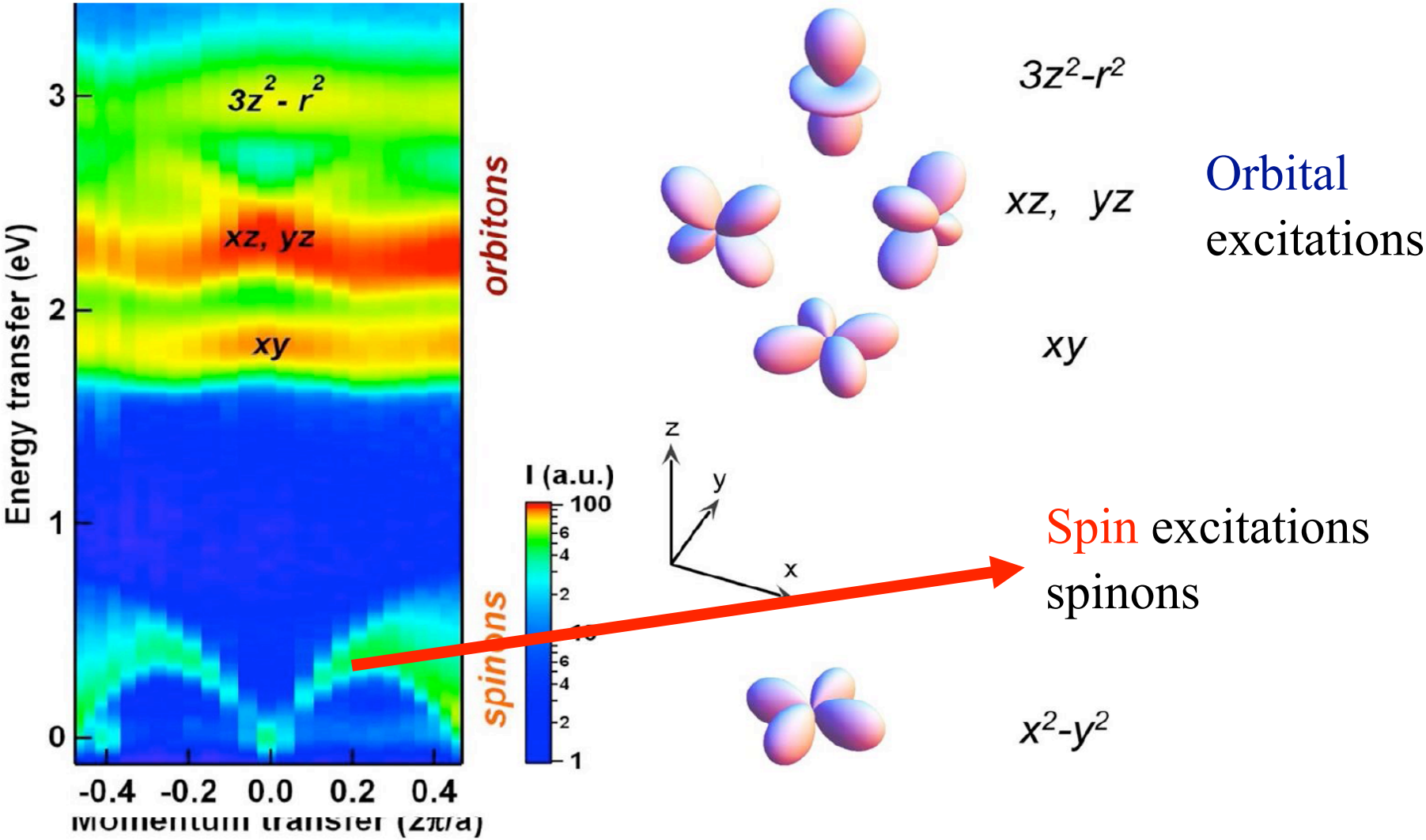
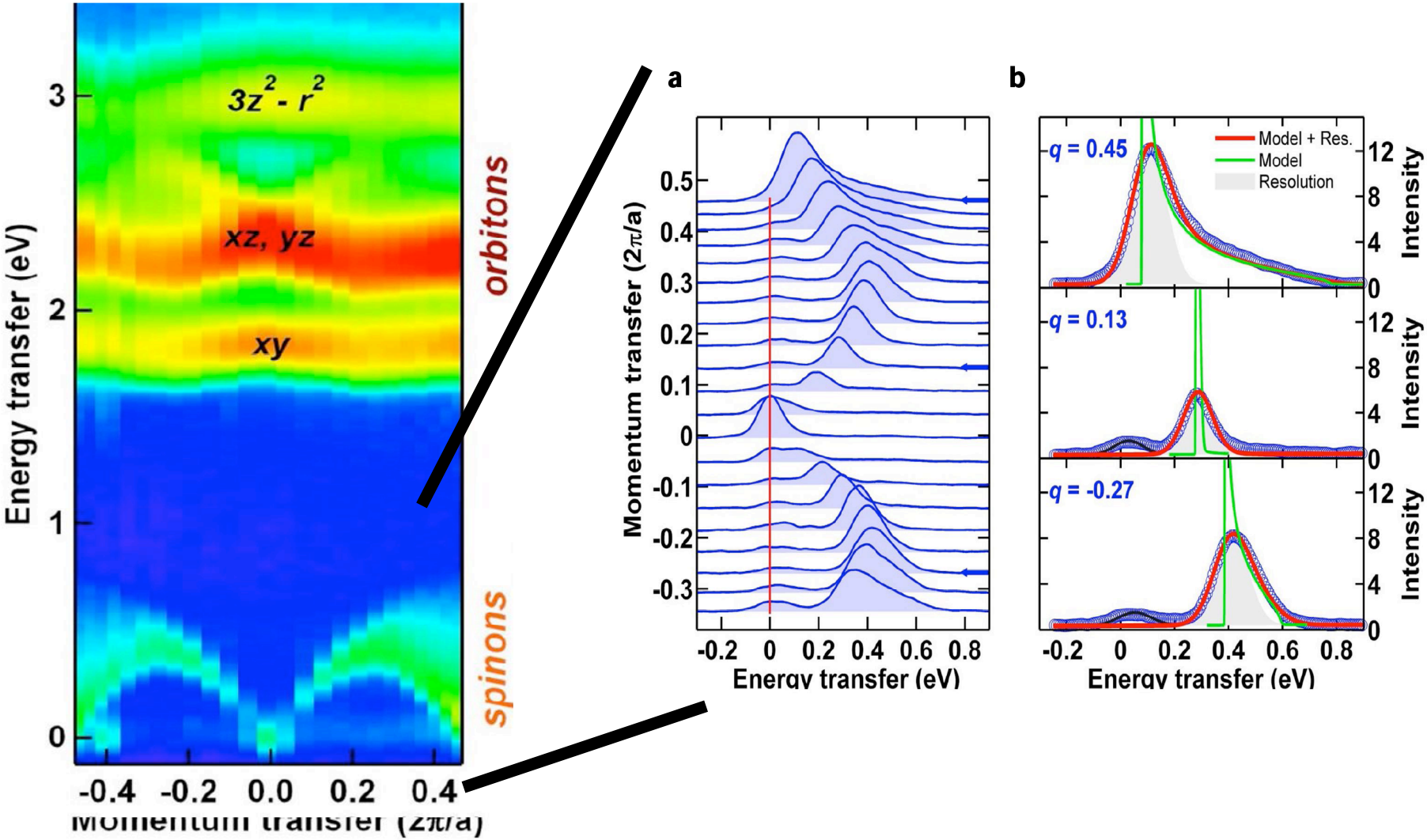


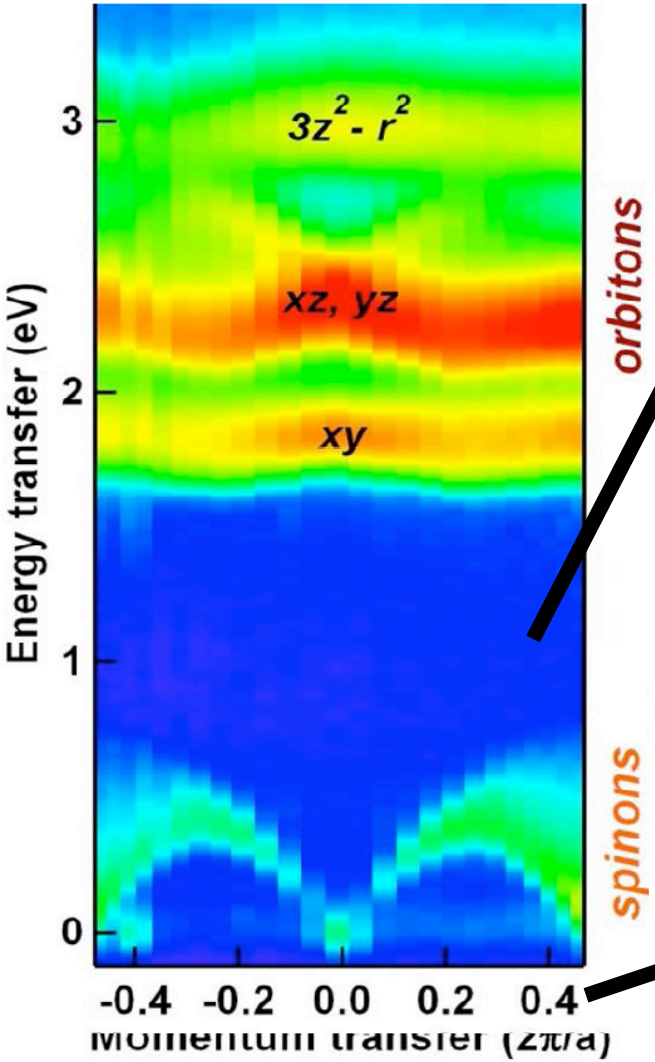
Schlappa, Wohlfeld, Zhou, Mourigal, Haverkort, Strocov, Hozoi, Monney, Nishimoto, Singh, Revcolevschi, Caux, Patthey, Ronnow, JvdB, Schmitt, Nature 485, 82 (2012)

Spinons in Sr_2CuO_3

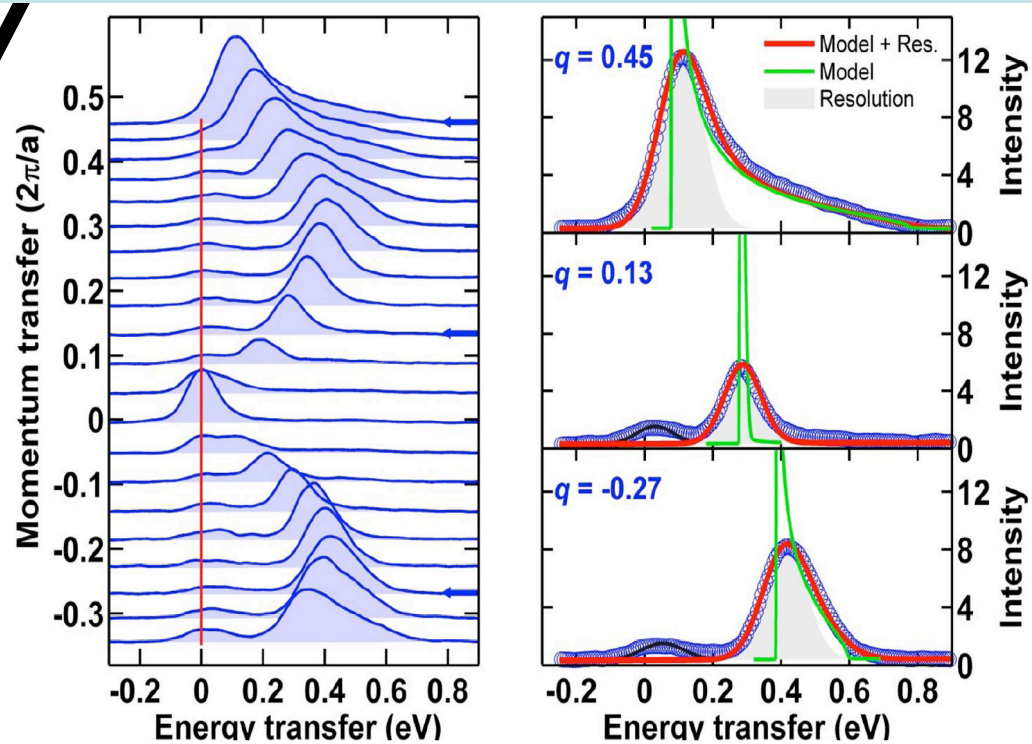


Schlappa, Wohlfeld, Zhou, Mourigal, Haverkort, Strocov, Hozoi, Monney, Nishimoto, Singh, Revcolevschi, Caux, Patthey, Ronnow, JvdB, Schmitt, Nature 485, 82 (2012)

Spinons in Sr_2CuO_3



spinons of Heisenberg spin chain



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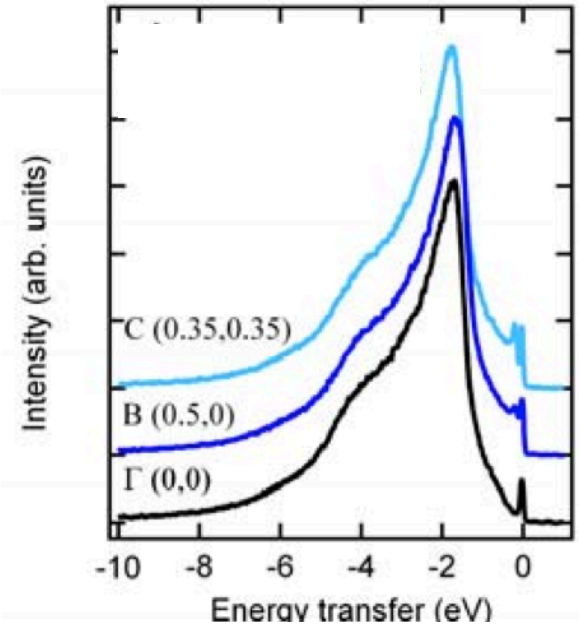
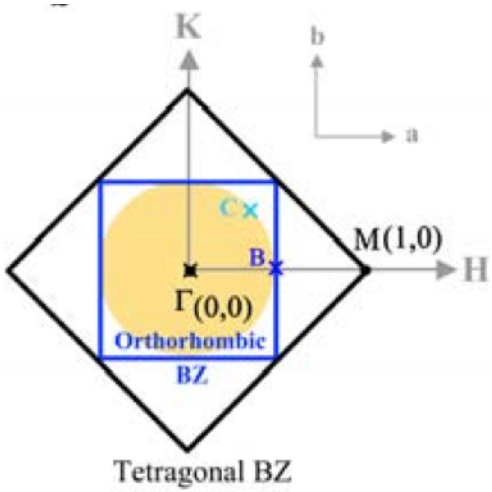
Quasi 2D Iron Pnictide

Magnetic RIXS on $BaFe_2As_2$ @ Fe L-edge





Kejin Zhou, Huang, Monney, Dai, Strocov, Wang, Chen, Zhang, Dai, Patthey, JvdB, Ding & Schmitt, Nat. Comm. 4, 1470 (2013)

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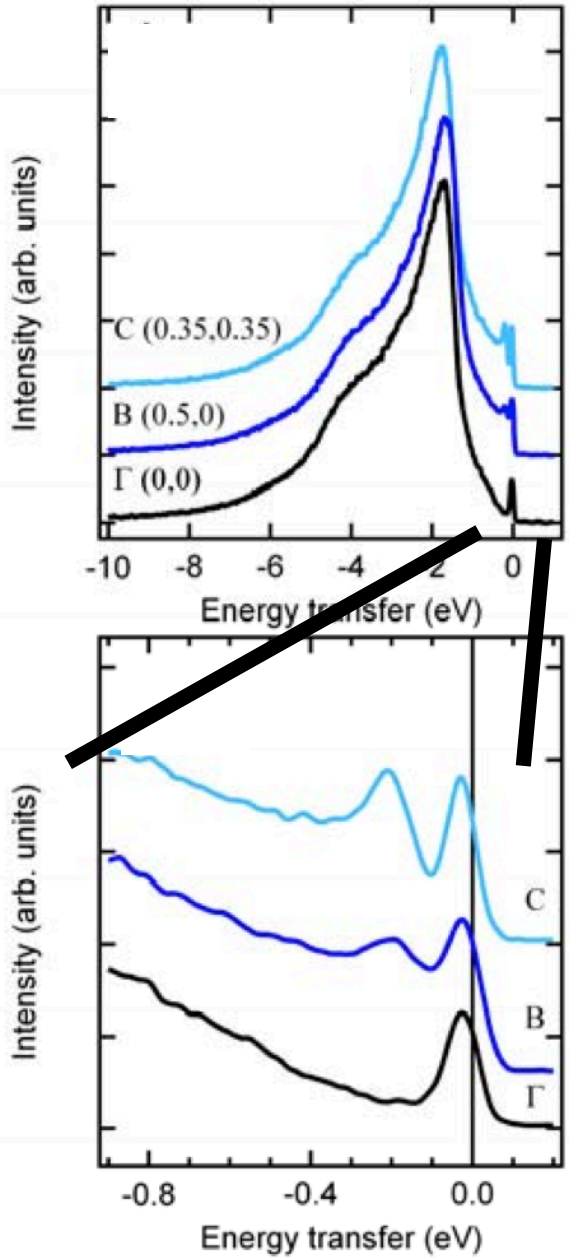

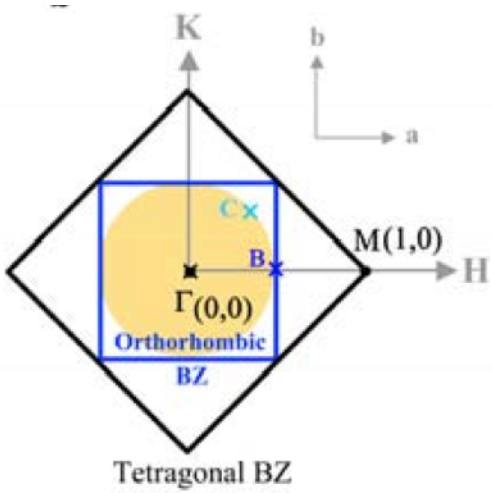

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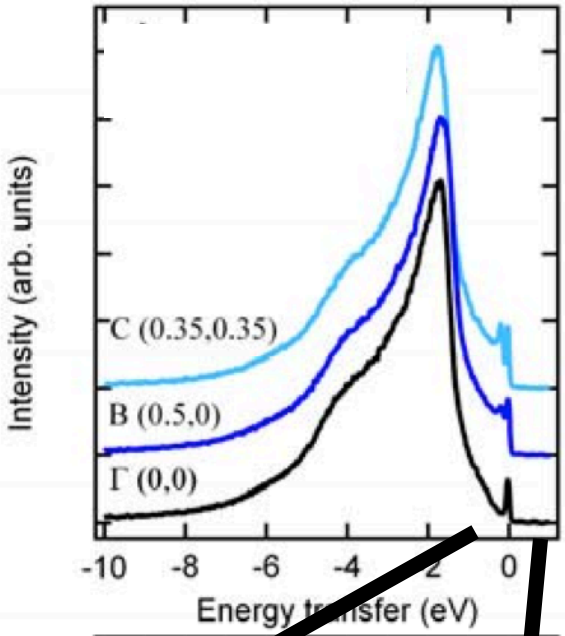
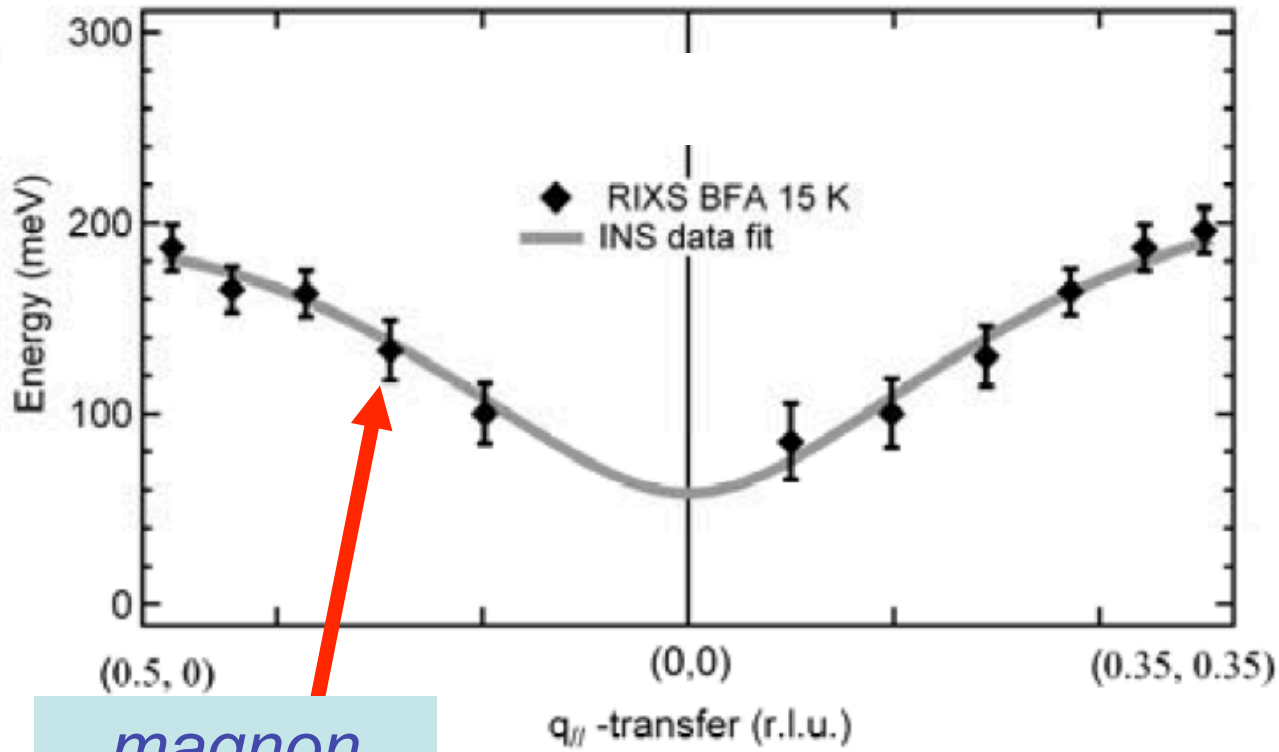
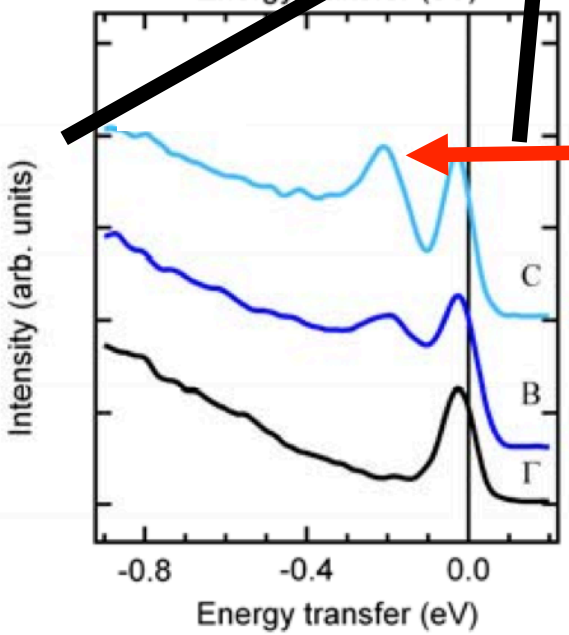
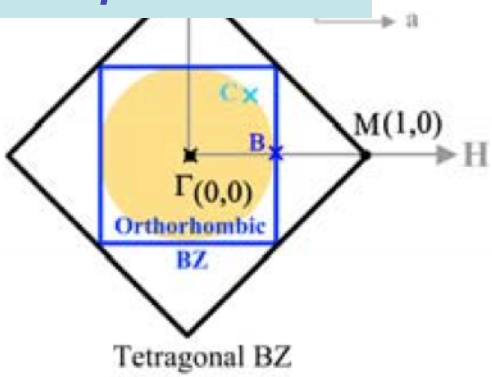






magnon dispersion



Kejin Zhou, Huang, Monney, Dai, Strocov, Wang, Chen, Zhang, Dai, Patthey, JvdB, Ding & Schmitt, Nat. Comm. 4, 1470 (2013)

Magnetic RIXS vs. *Inelastic Neutron Scattering*

	RIXS	*Neutrons*
amount of material needed		
magnon energy accessible		
materials		

Magnetic RIXS vs. *Inelastic Neutron Scattering*

	RIXS	*Neutrons*
amount of material needed	*small*	*large*
magnon energy accessible		
materials		

Magnetic RIXS vs. *Inelastic Neutron Scattering*

	RIXS	*Neutrons*
amount of material needed	*small*	*large*
magnon energy accessible	*high* ($>10^2$ *meV*)	*low* ($<10^2$ *meV*)
materials		

Magnetic RIXS vs. *Inelastic Neutron Scattering*

	RIXS	*Neutrons*
amount of material needed	*small*	*large*
magnon energy accessible	*high* ($>10^2$ *meV*)	*low* ($<10^2$ *meV*)
materials	*Cu, Fe ...*	*non-absorbers*

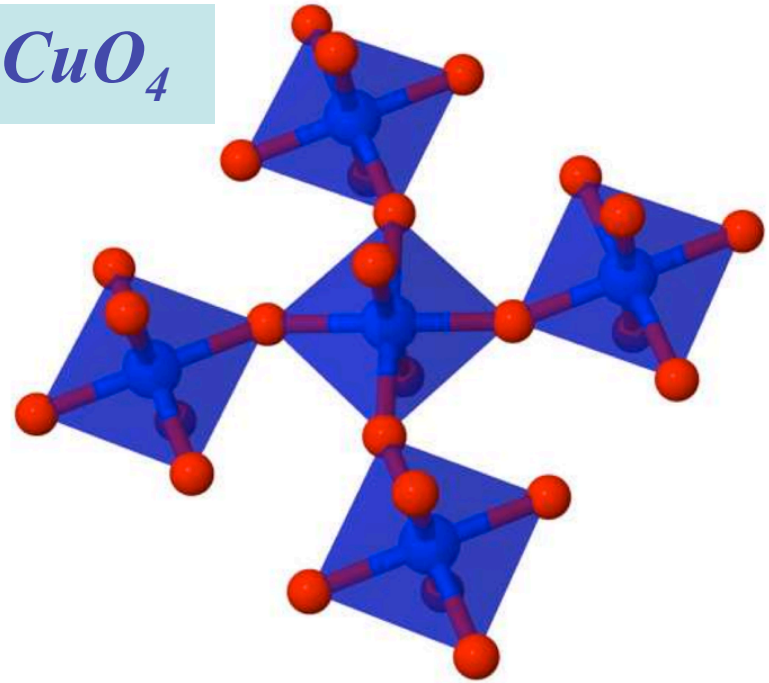
Quasi 2D Iridate

Magnetic Iridium Oxides

Sr_2IrO_4 : equivalent of cuprate La_2CuO_4

Jackeli & Khaliullin, PRL 102,017205 (2009)

B.J. Kim, Ohsumi, Komesu, Sakai, Morita, Takagi, Arima, Science 323, 1329 (2009)



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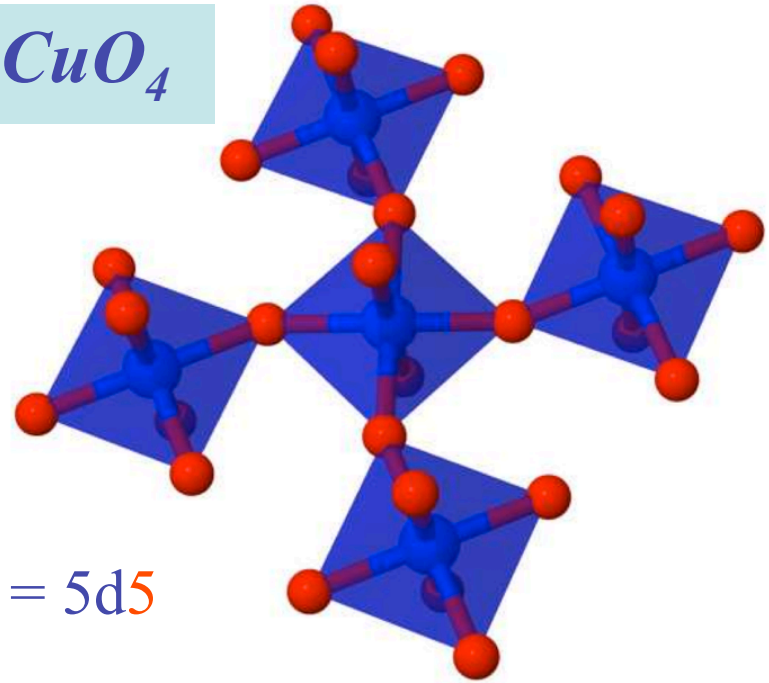
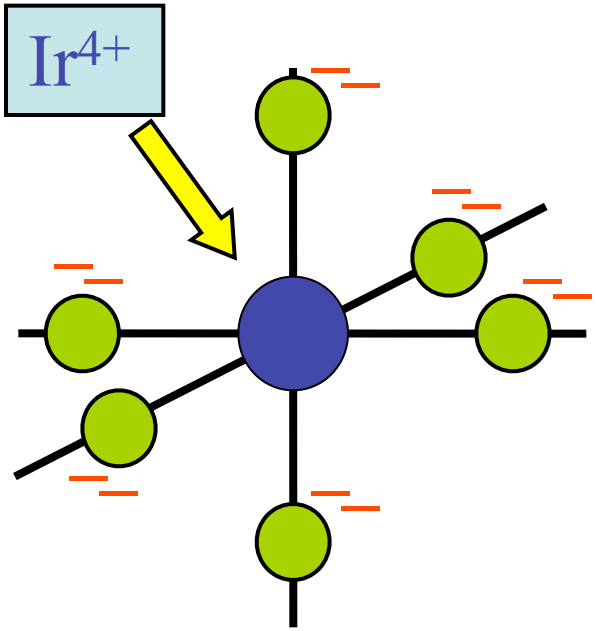
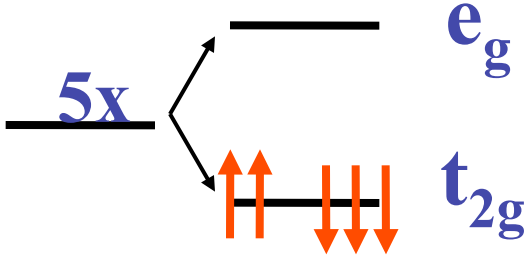




Ir (4+) = 5d5



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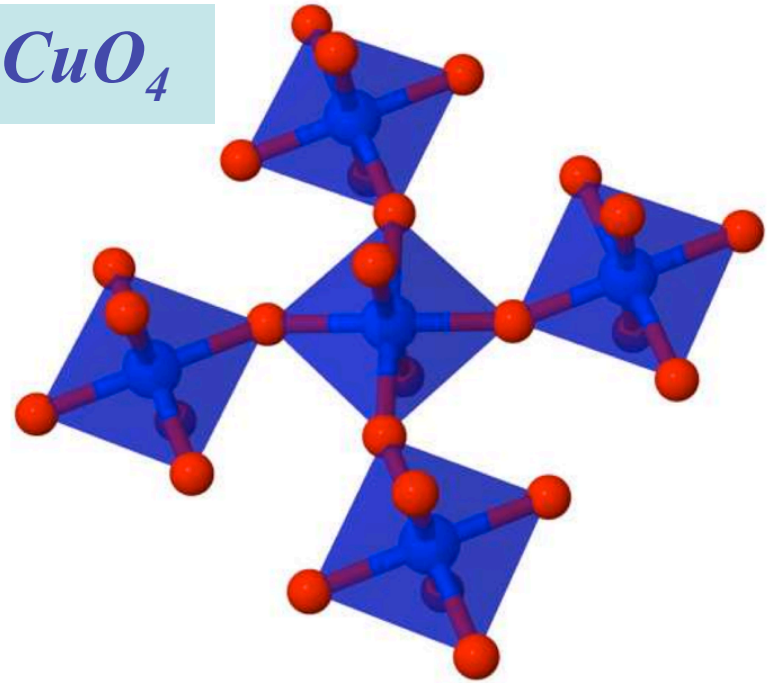
t_{2g}^5: single hole s=1/2 in 3-fold degenerate l=1 state



Magnetic Iridium Oxides

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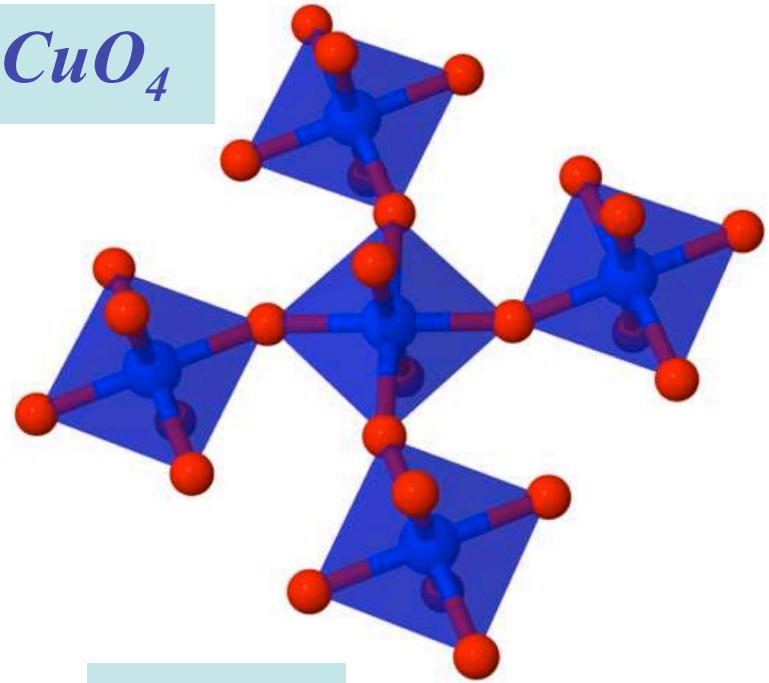
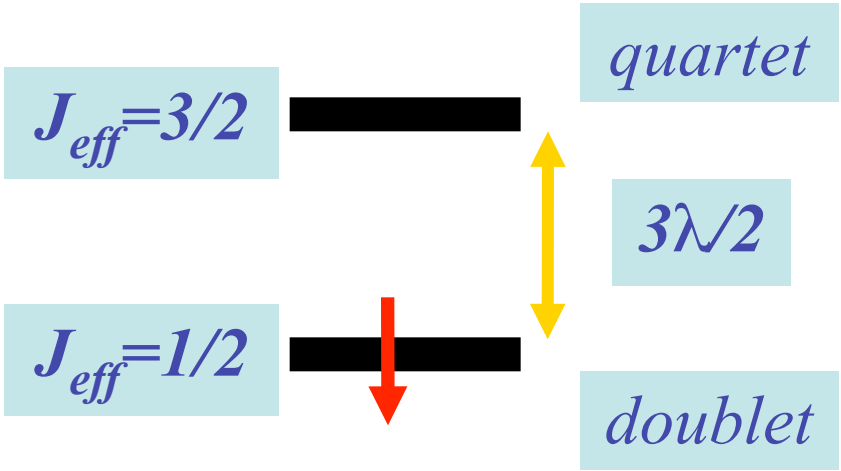
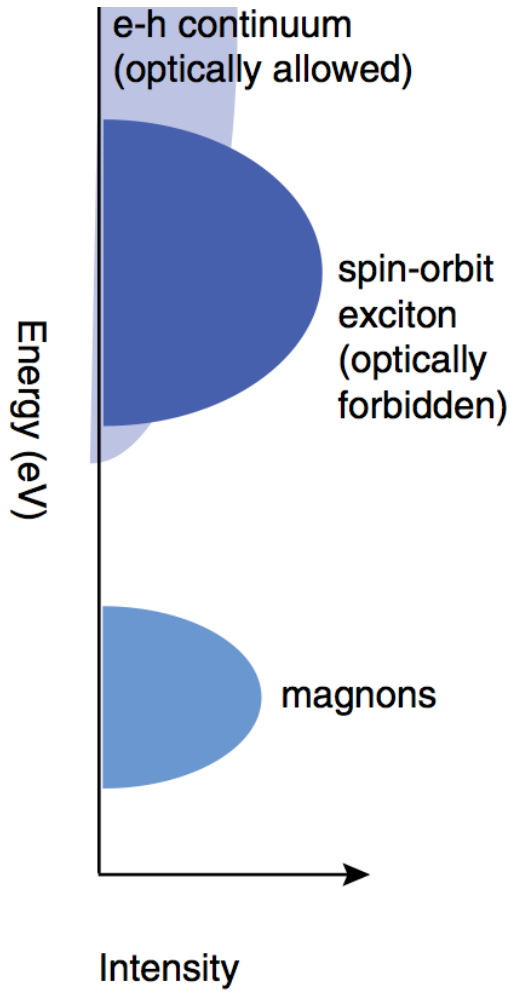


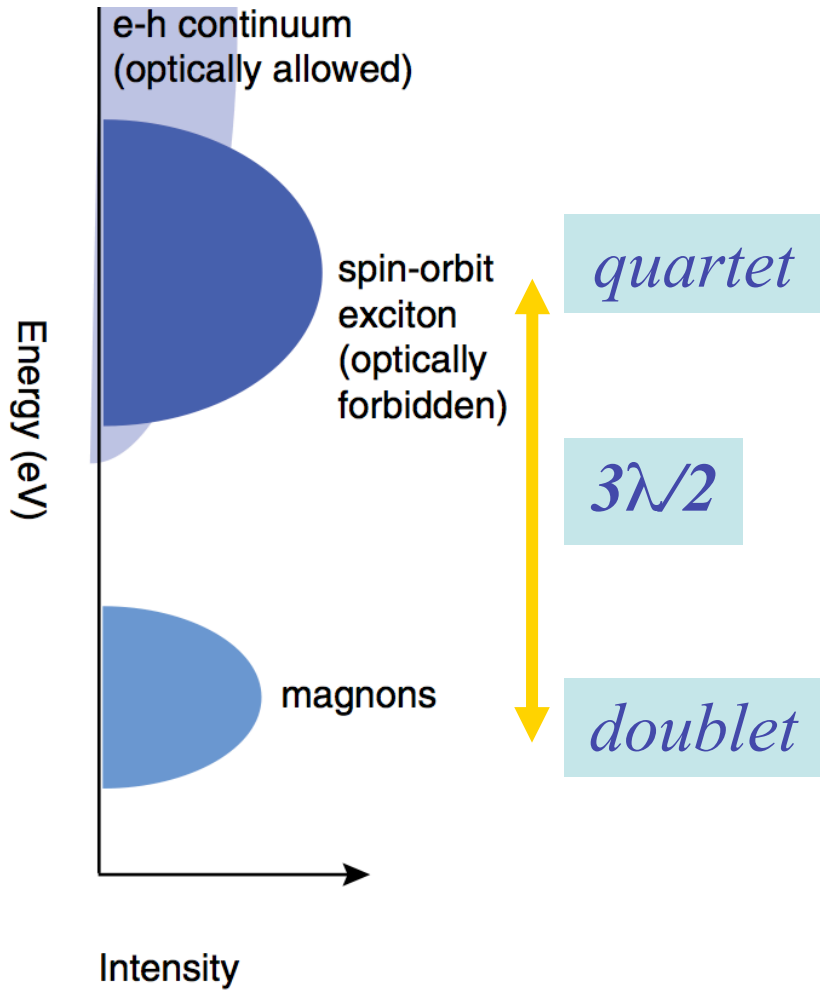
J=L+S



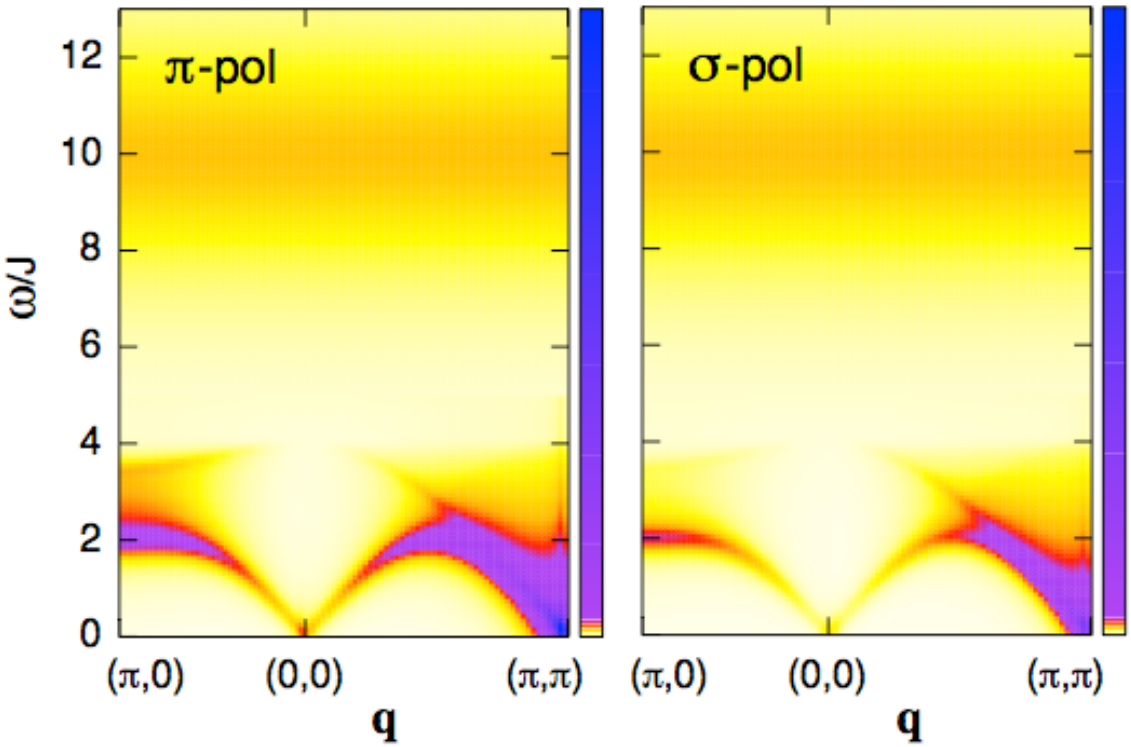
Direct RIXS on Sr_2IrO_4

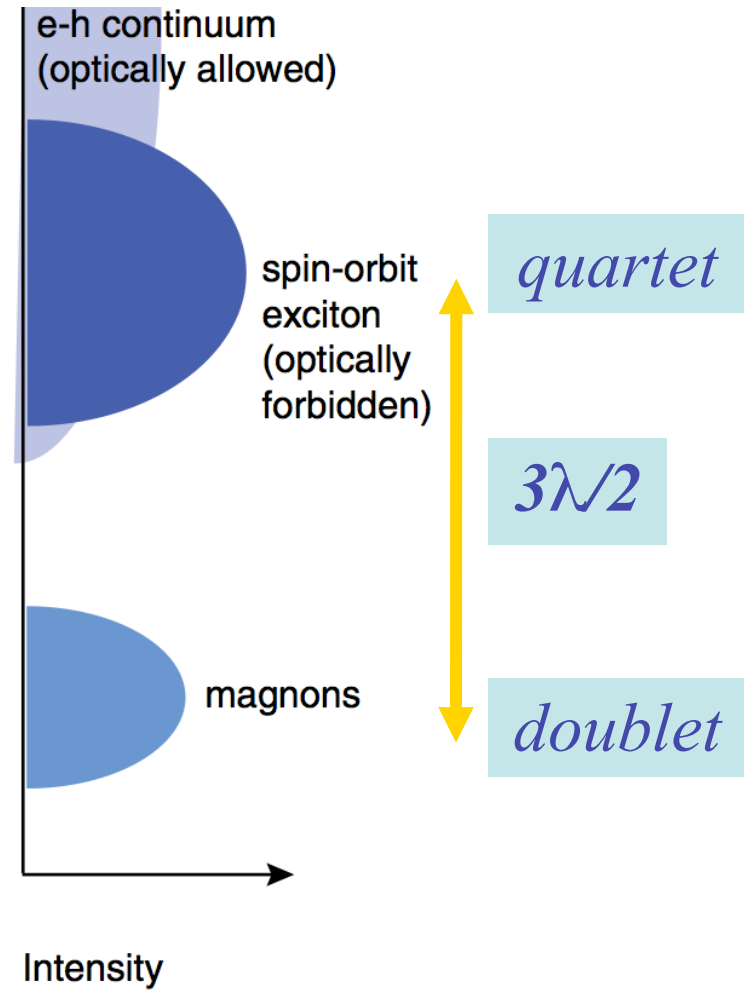


Direct RIXS on Sr_2IrO_4



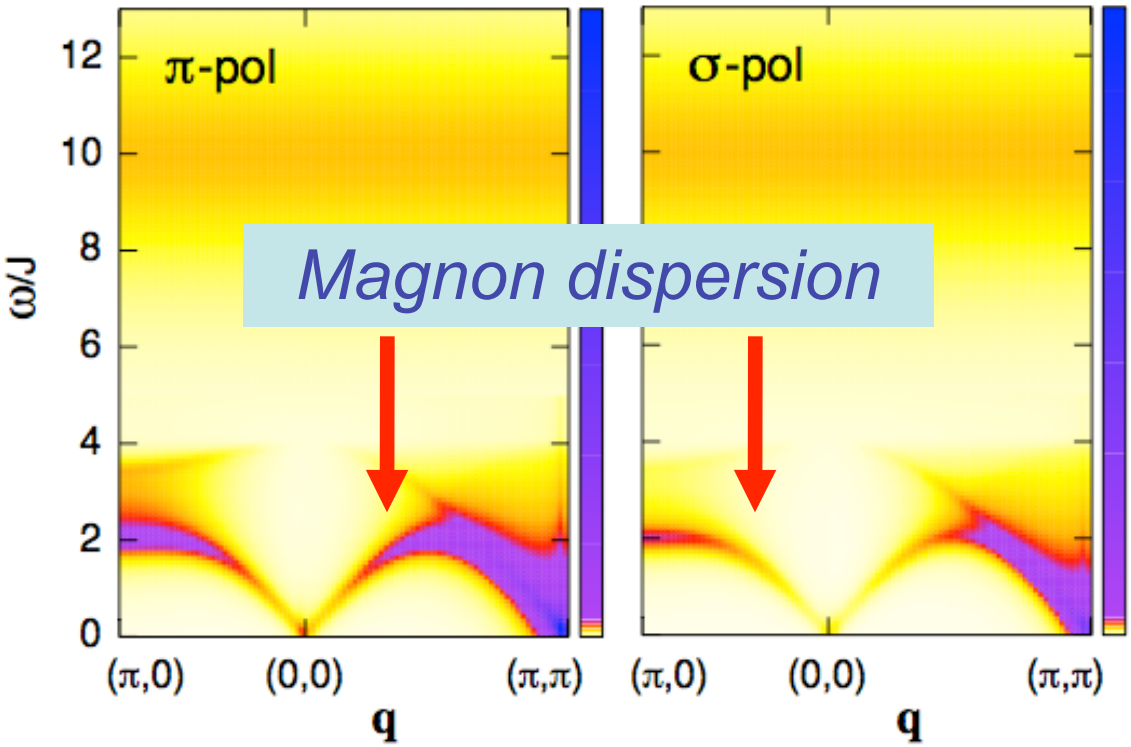
Direct RIXS on Sr_2IrO_4





Ament, Khaliullin & JvdB
PRB 84, 020403 (2011)

Direct RIXS on Sr_2IrO_4



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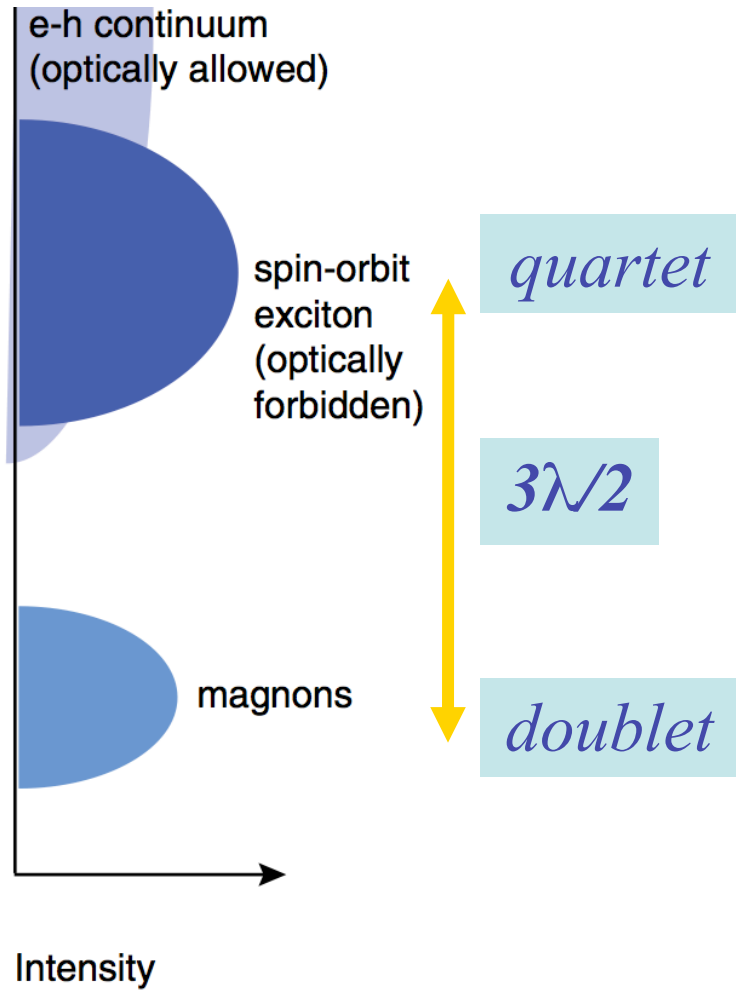

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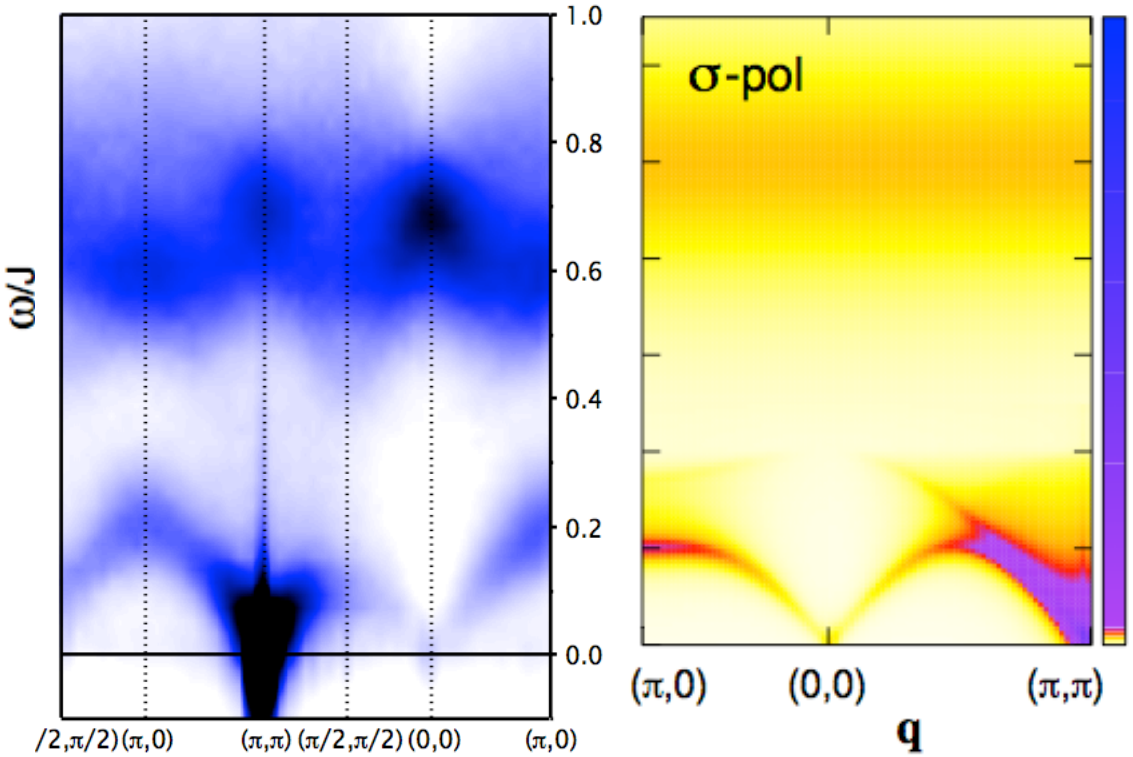
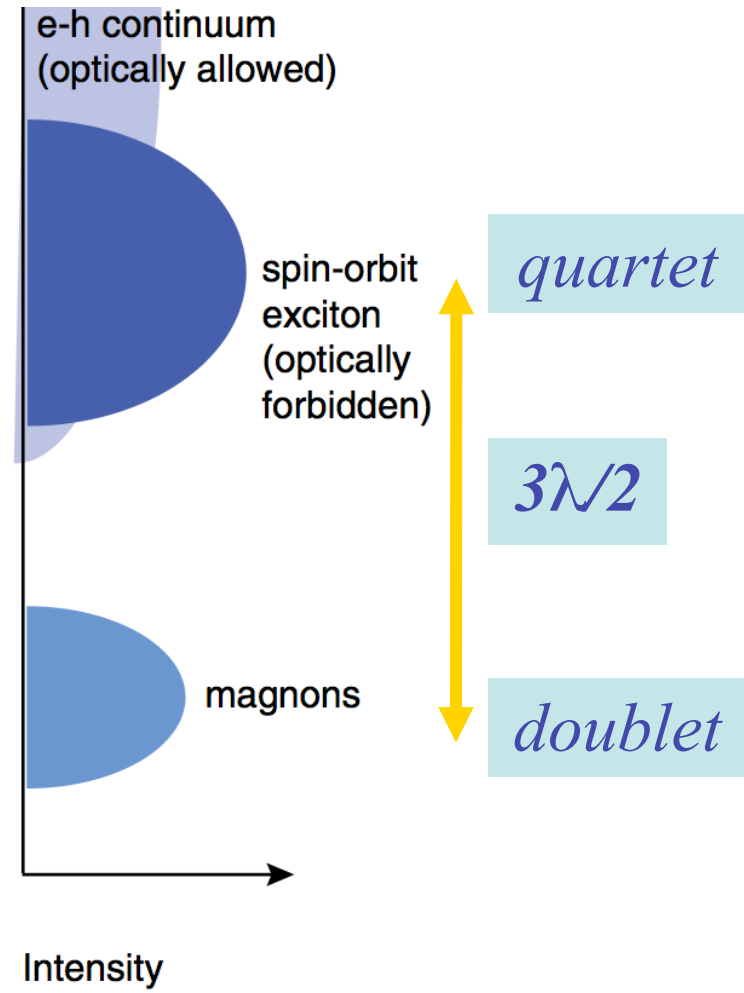




Ament, Khaliullin & JvdB
PRB 84, 020403 (2011)

Jungho Kim,[1] D. Casa,[1] M. H. Upton,[1] T. Gog,[1] Young-June Kim,[2]
J. F. Mitchell,[3] M. van Veenendaal,[1,4] M. Daghofer, [5] J. van den Brink,[5]
G. Khaliullin,[6] B. J. Kim[3,*]

PRL 108, 177003 (2012)

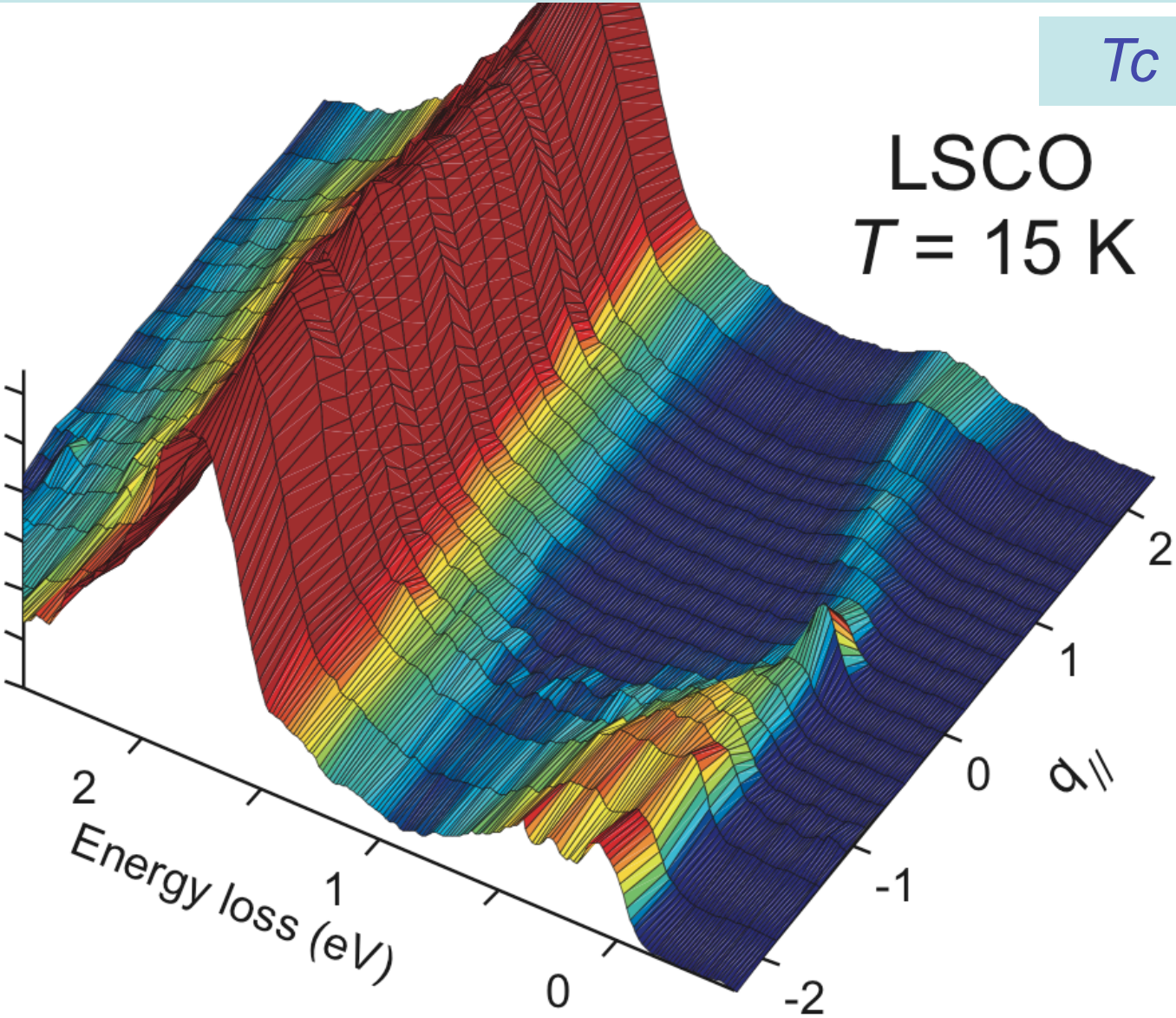
Magnetic RIXS on

doped quasi-2D

Cu-oxides and Fe-pnictides

Magnetic L-edge RIXS on 8% doped $La_{2-x}Sr_xCuO_4$

Tc = 21K



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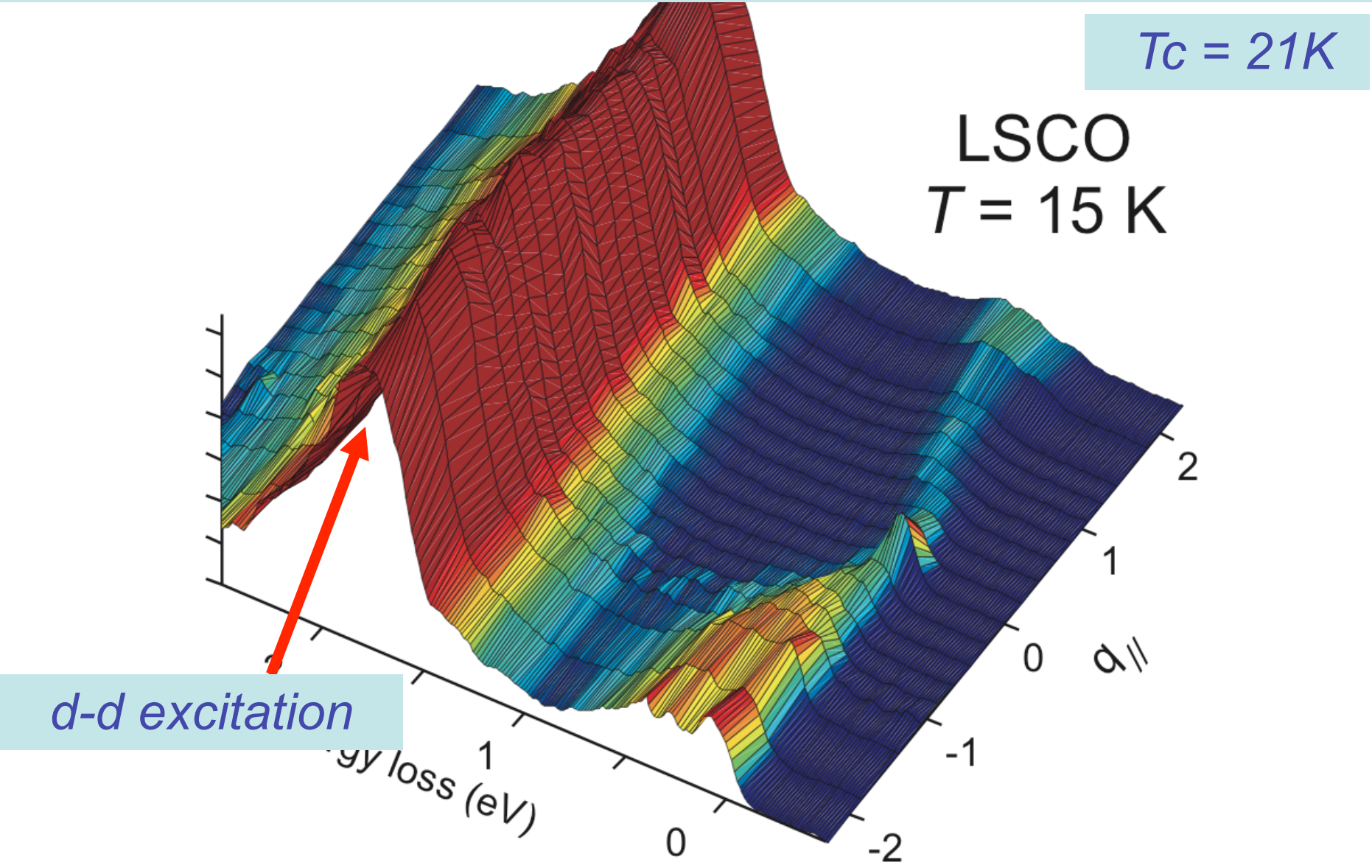

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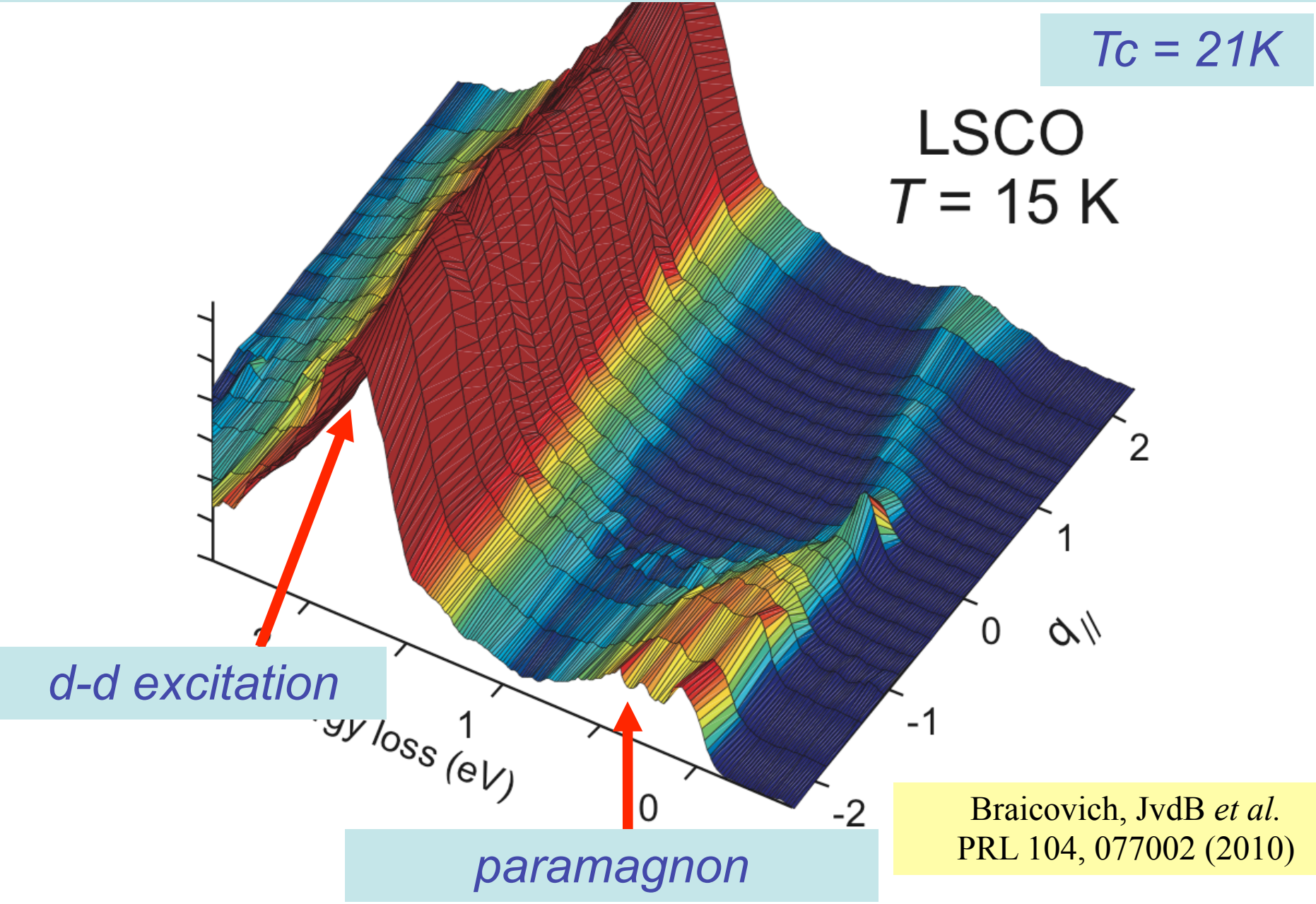

Braicovich, JvdB *et al.*
PRL 104, 077002 (2010)

nature physics

ARTICLES

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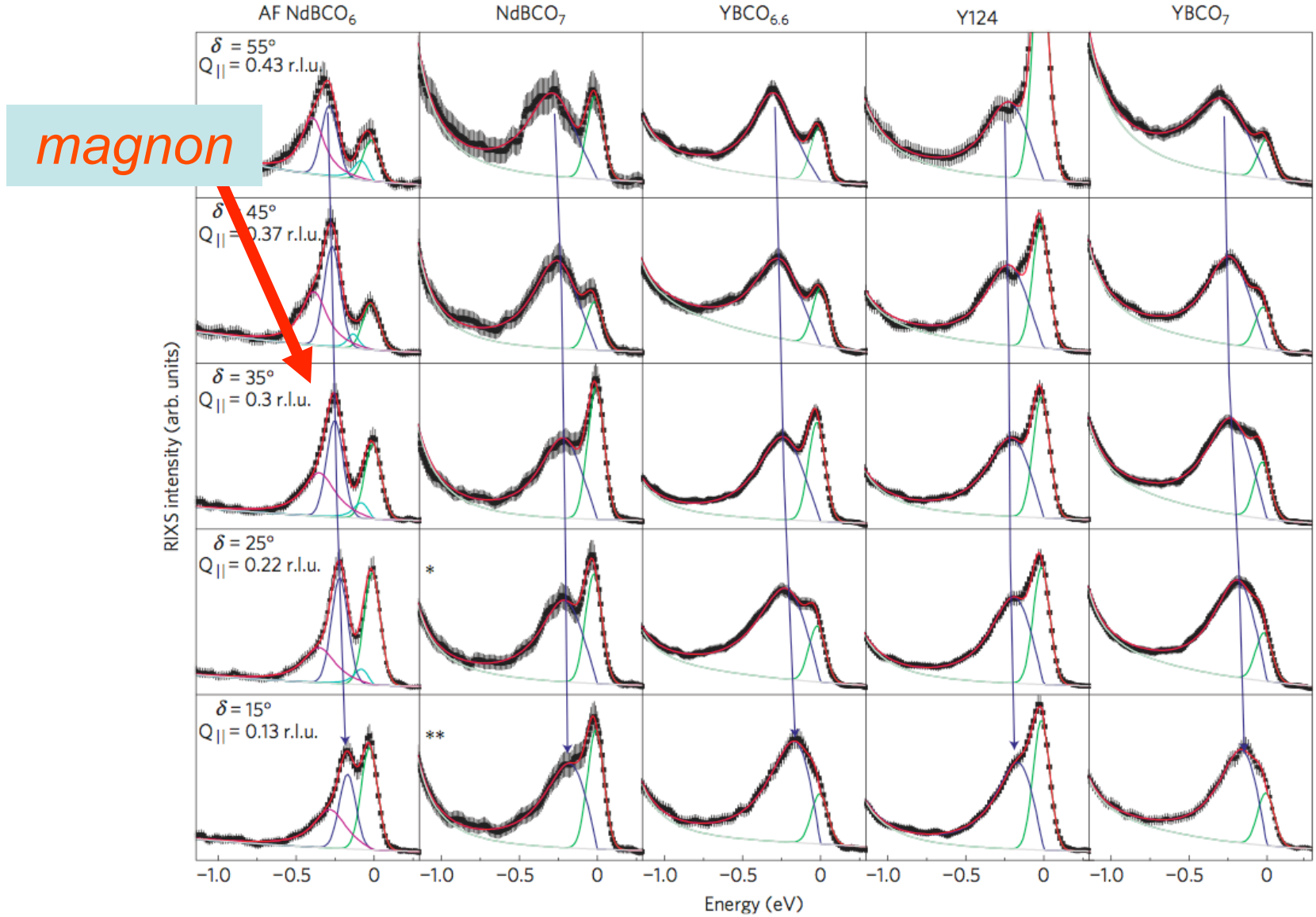
Intense paramagnon excitations in a large family of high-temperature superconductors

M. Le Tacon[1]*, G. Ghiringhelli[2], J. Chaloupka[1], M. Moretti Sala[2], V. Hinkov[1,3], M. W. Haverkort[1], M. Minola[2], M. Bakr[1], K. J. Zhou[4], S. Blanco-Canosa[1], C. Monney[4], Y. T. Song[1], G. L. Sun[1], C. T. Lin[1], G. M. De Luca[5], M. Salluzzo[5], G. Khaliullin[1], T. Schmitt[4], L. Braicovich[2] and B. Keimer[1]*



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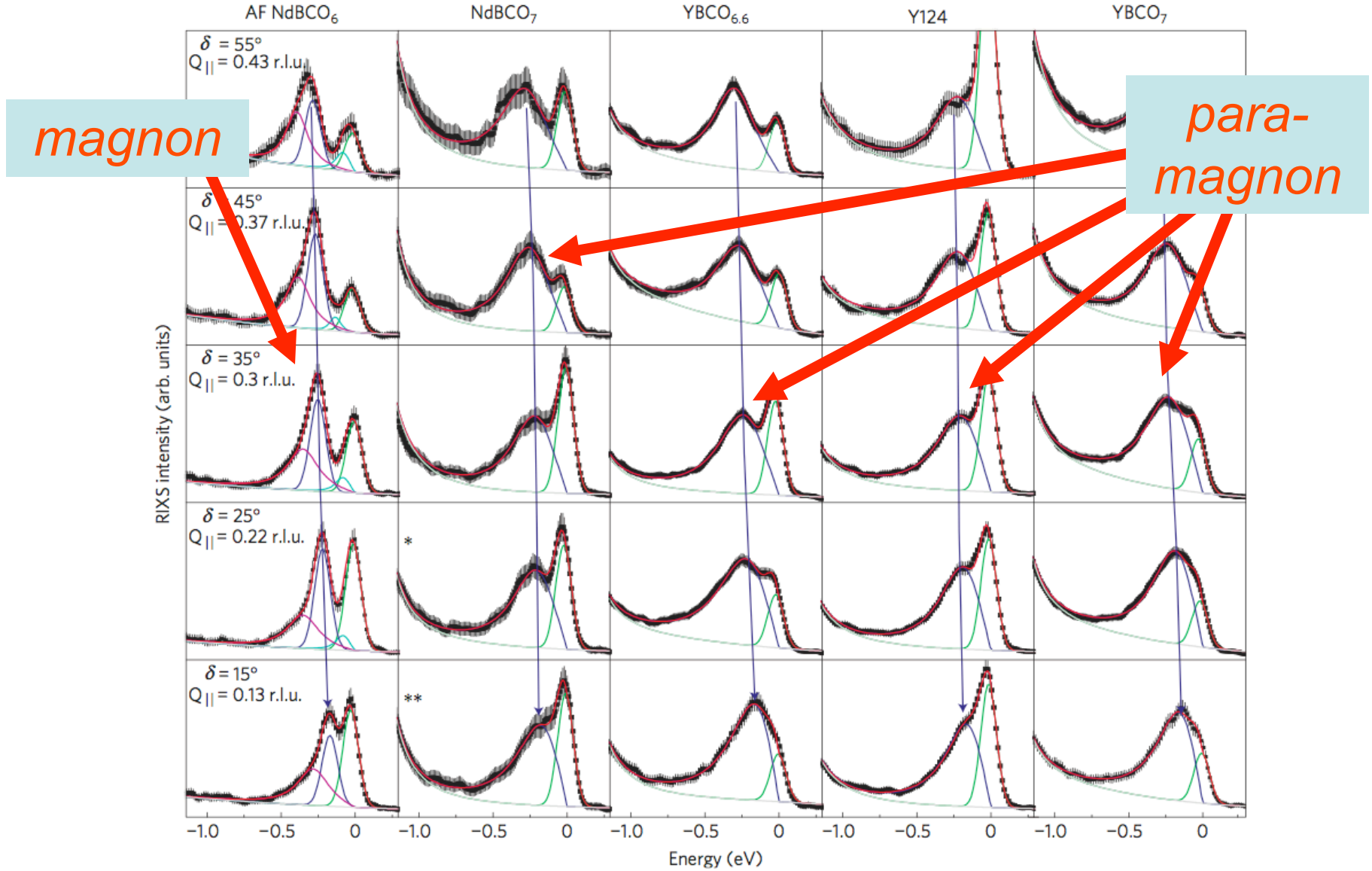

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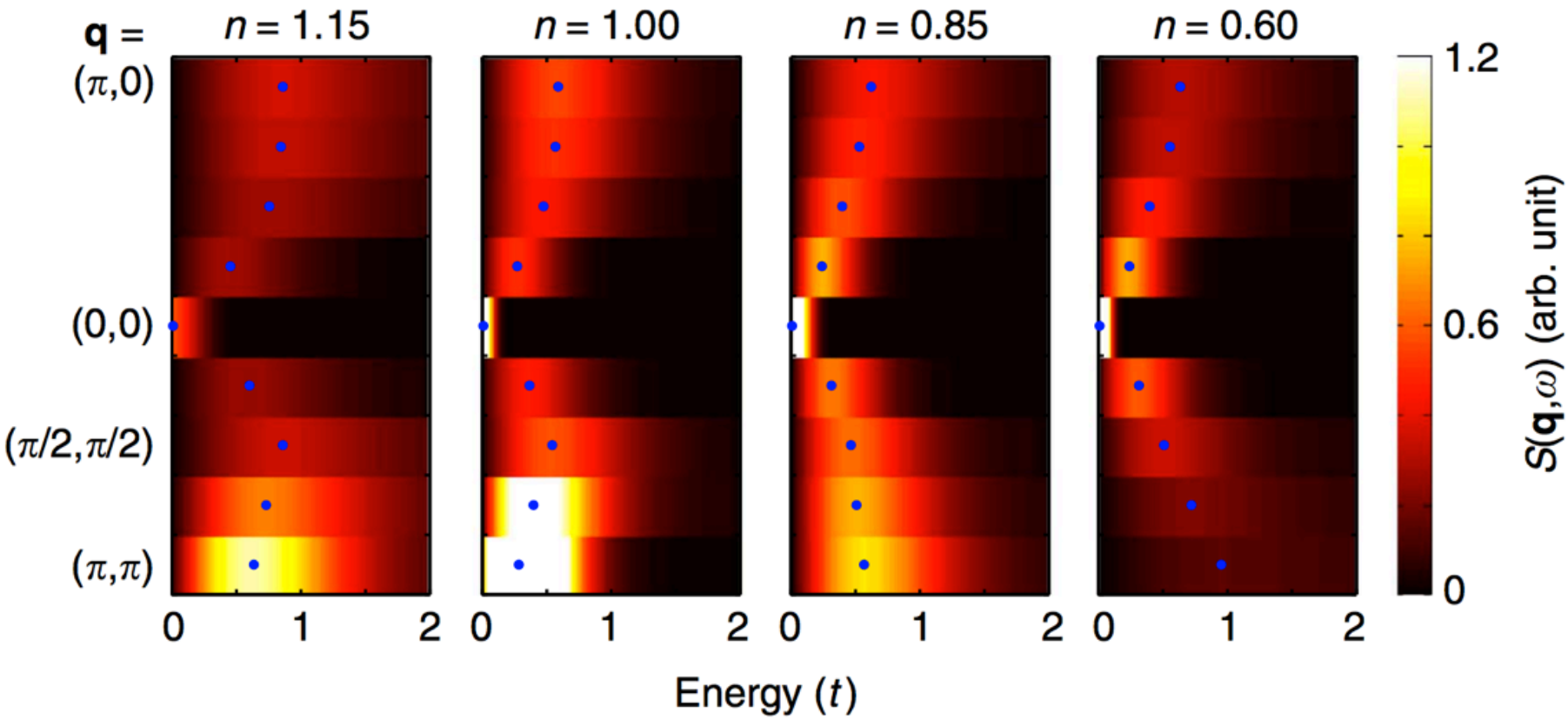
Dynamical structure factor Hubbard model, QMC

U=8t



Jia, Nowadnick, Wohlfeld, Kung, Chen, Johnston, Tohyama, Moritz & Devereaux
Nat. Comm. 5, 3314 (2014)

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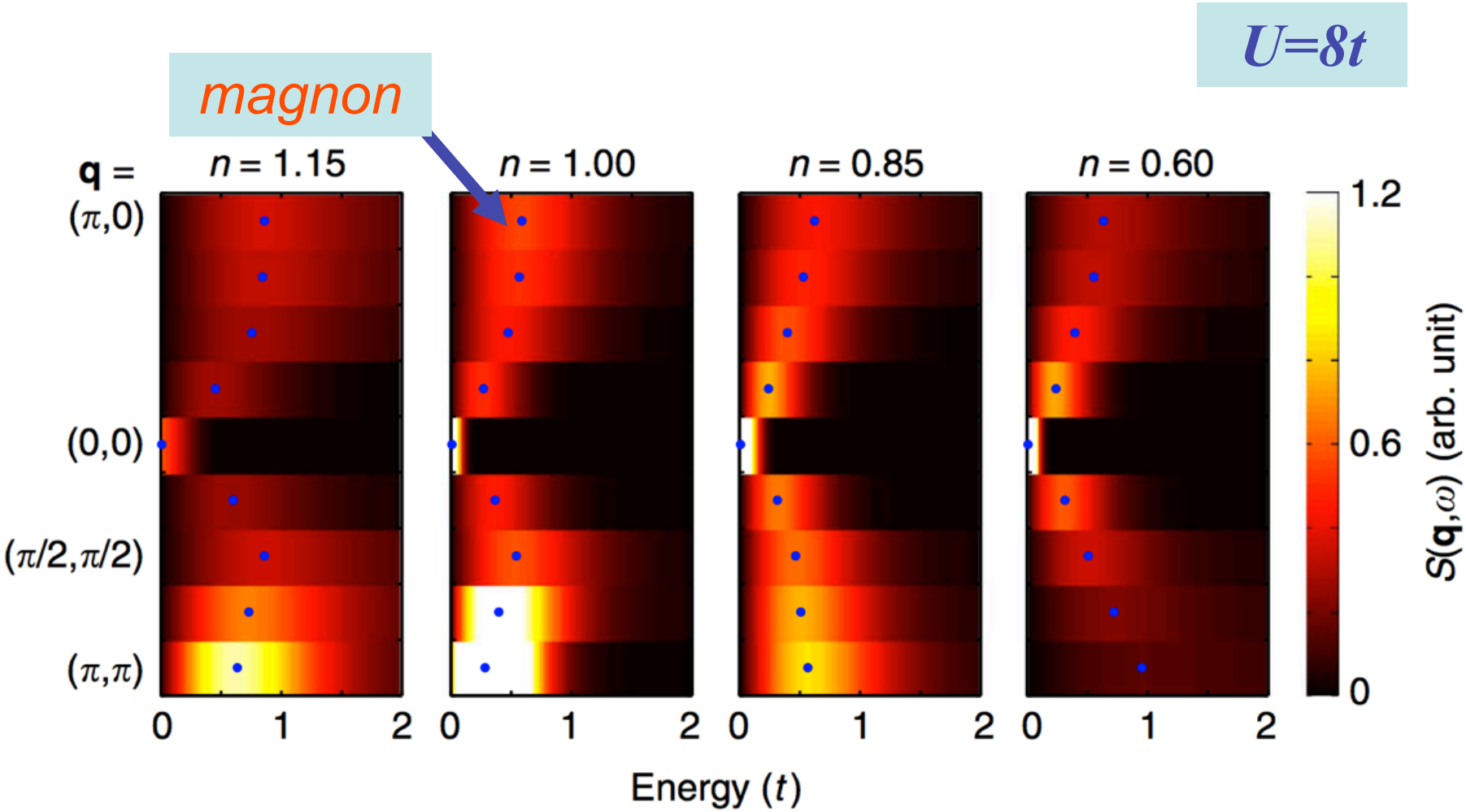

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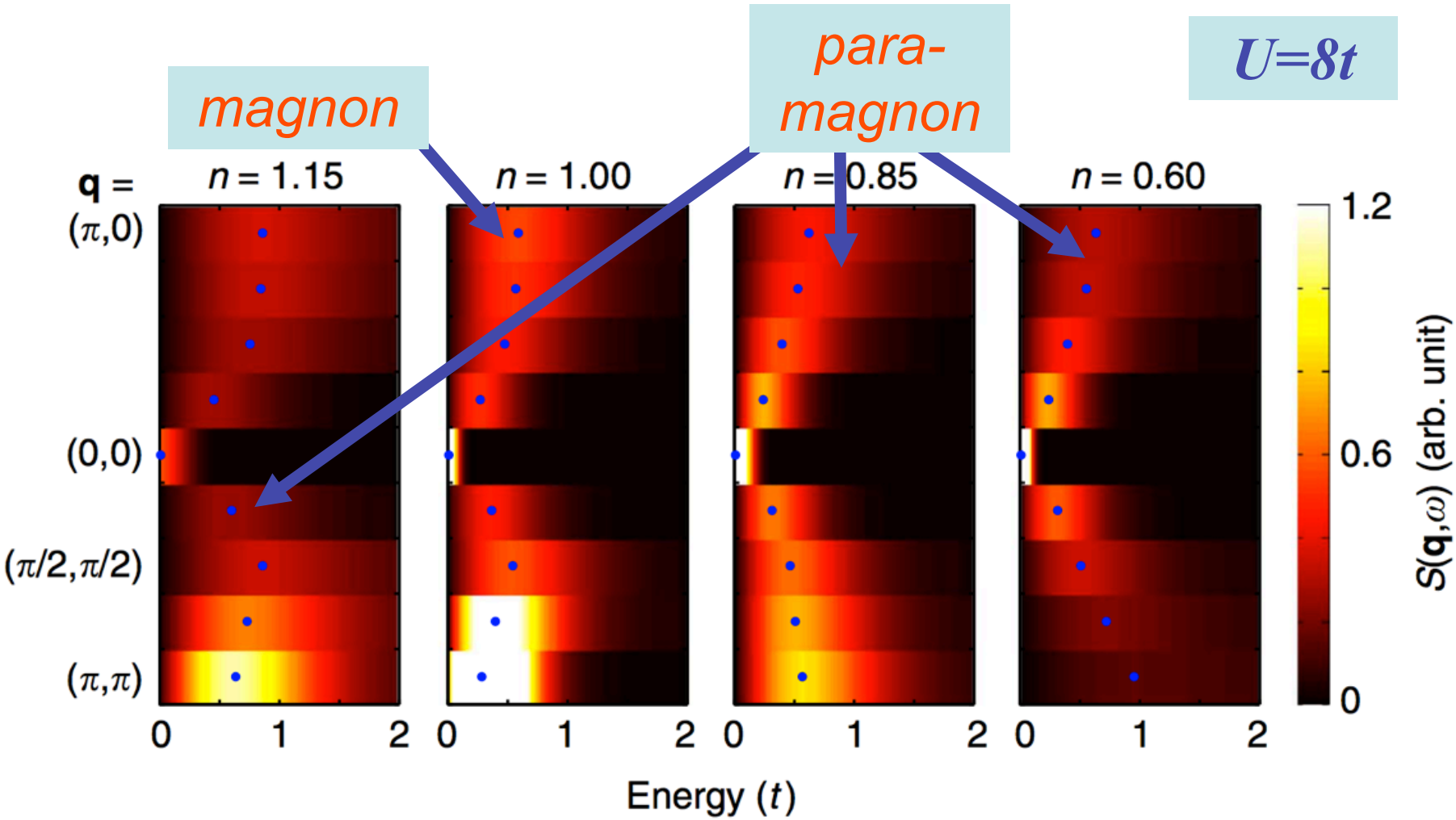

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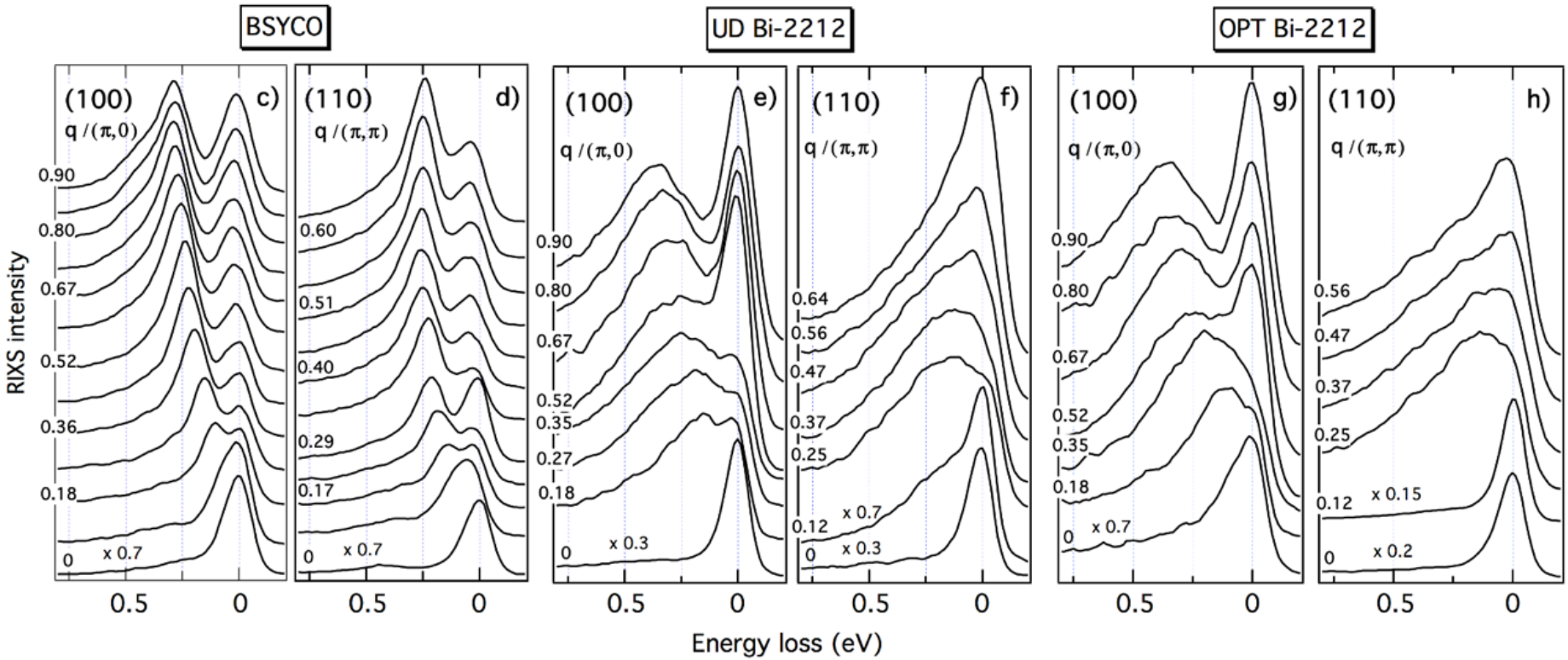
RIXS on Bi-2212 cuprate



Guarise, Piazza, Berger, Giannini, Schmitt, Rønnow, Sawatzky, JvdB, Altenfeld, Eremin & Grioni (2014)

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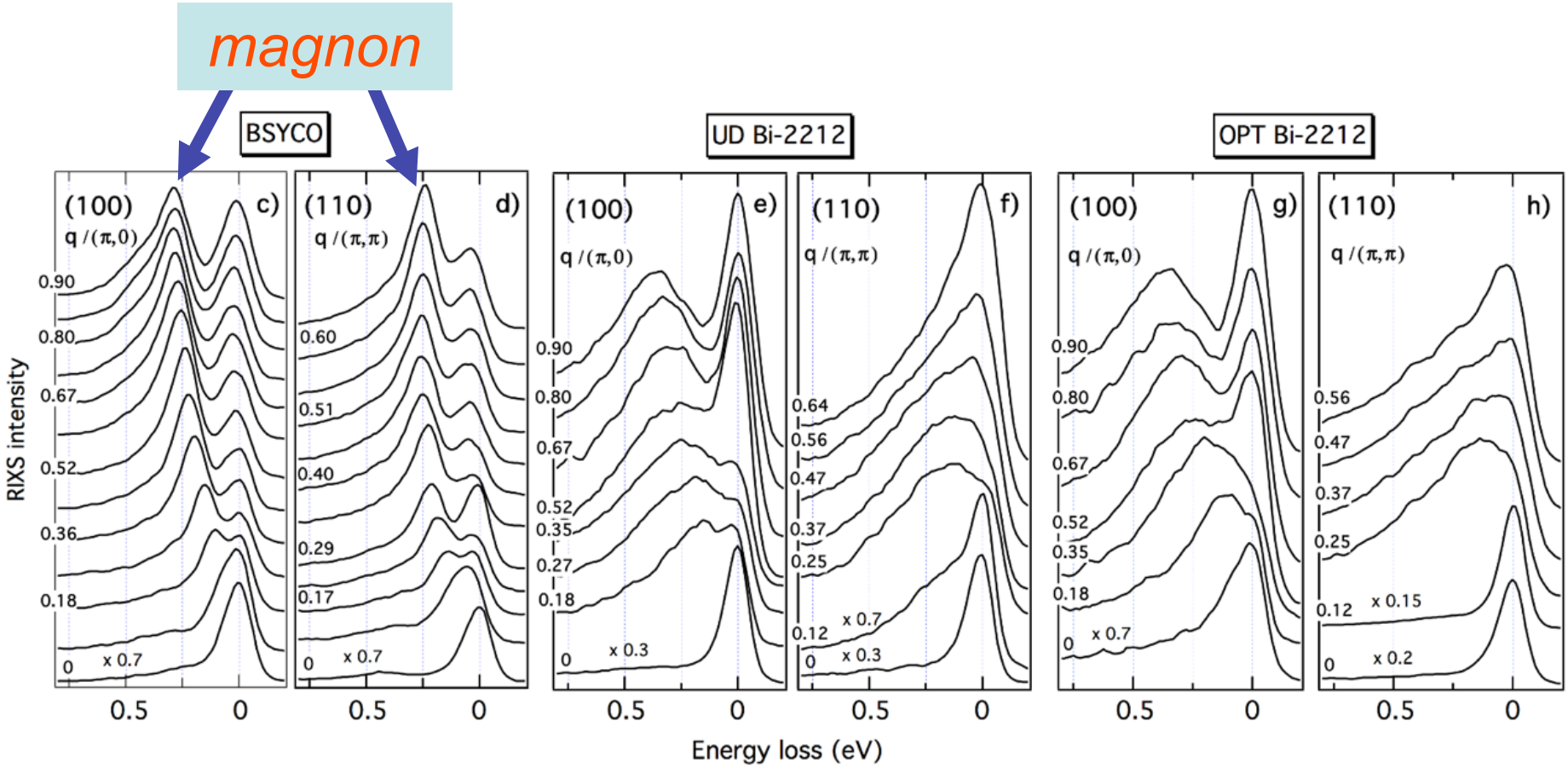

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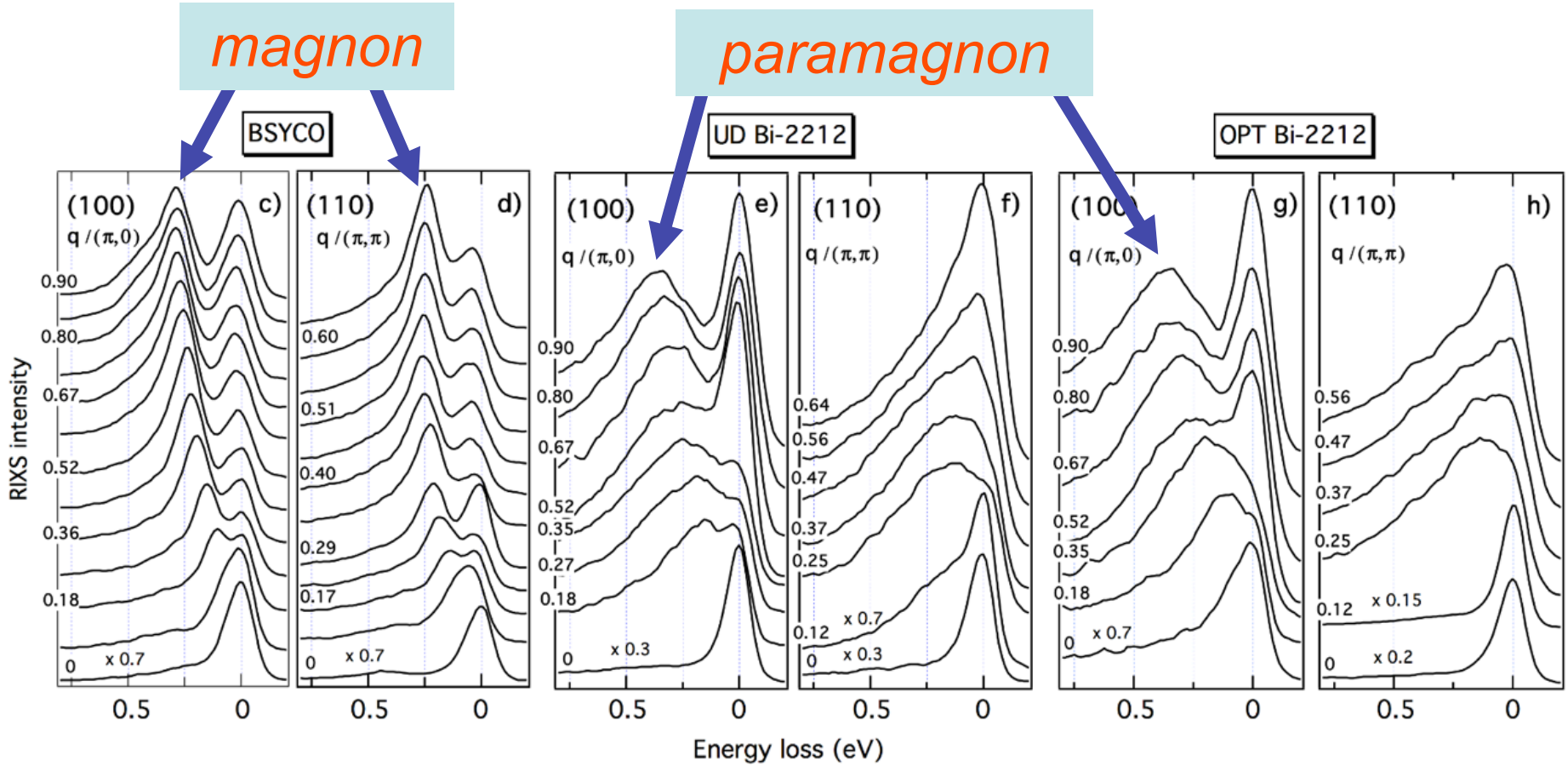
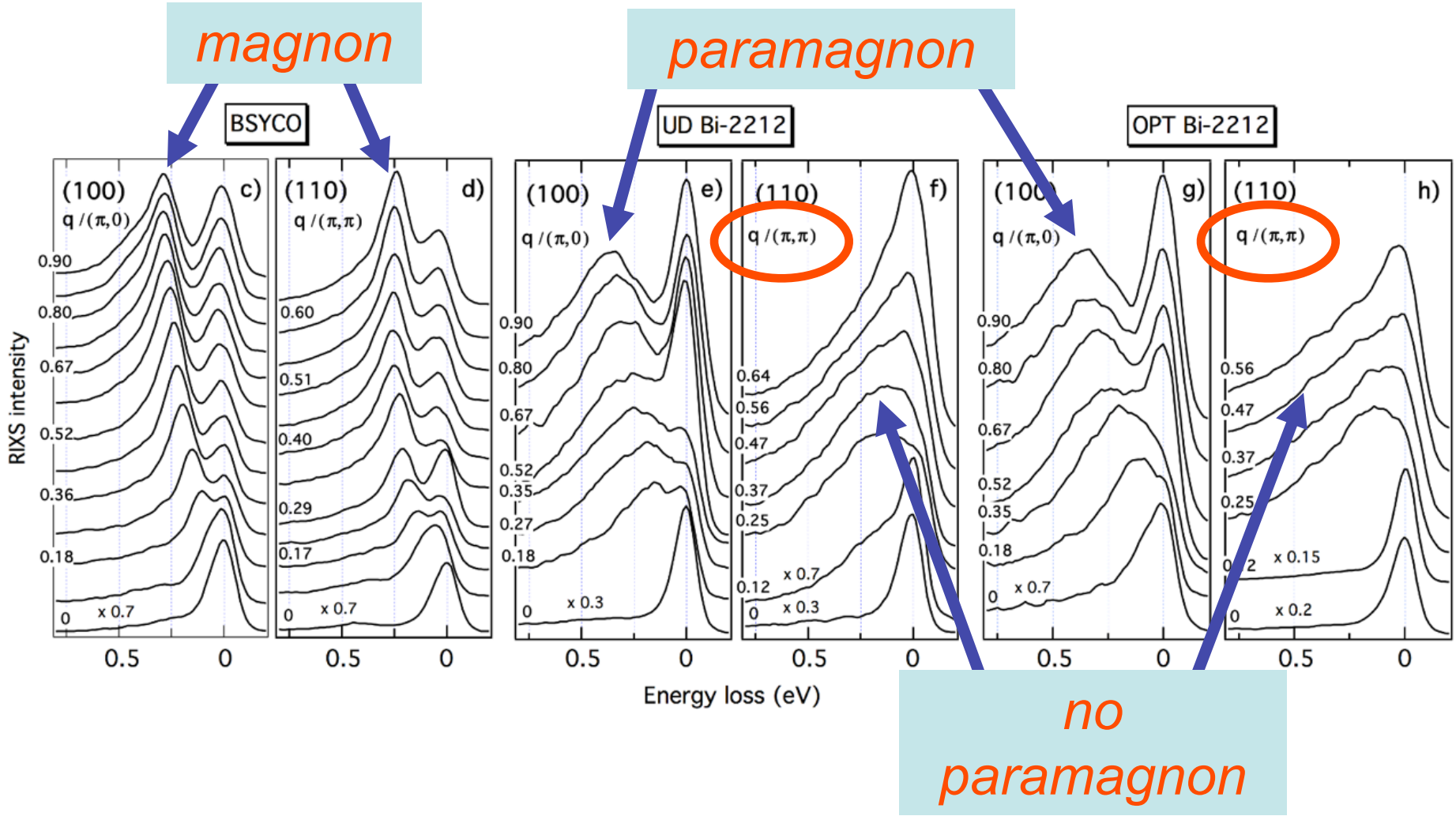


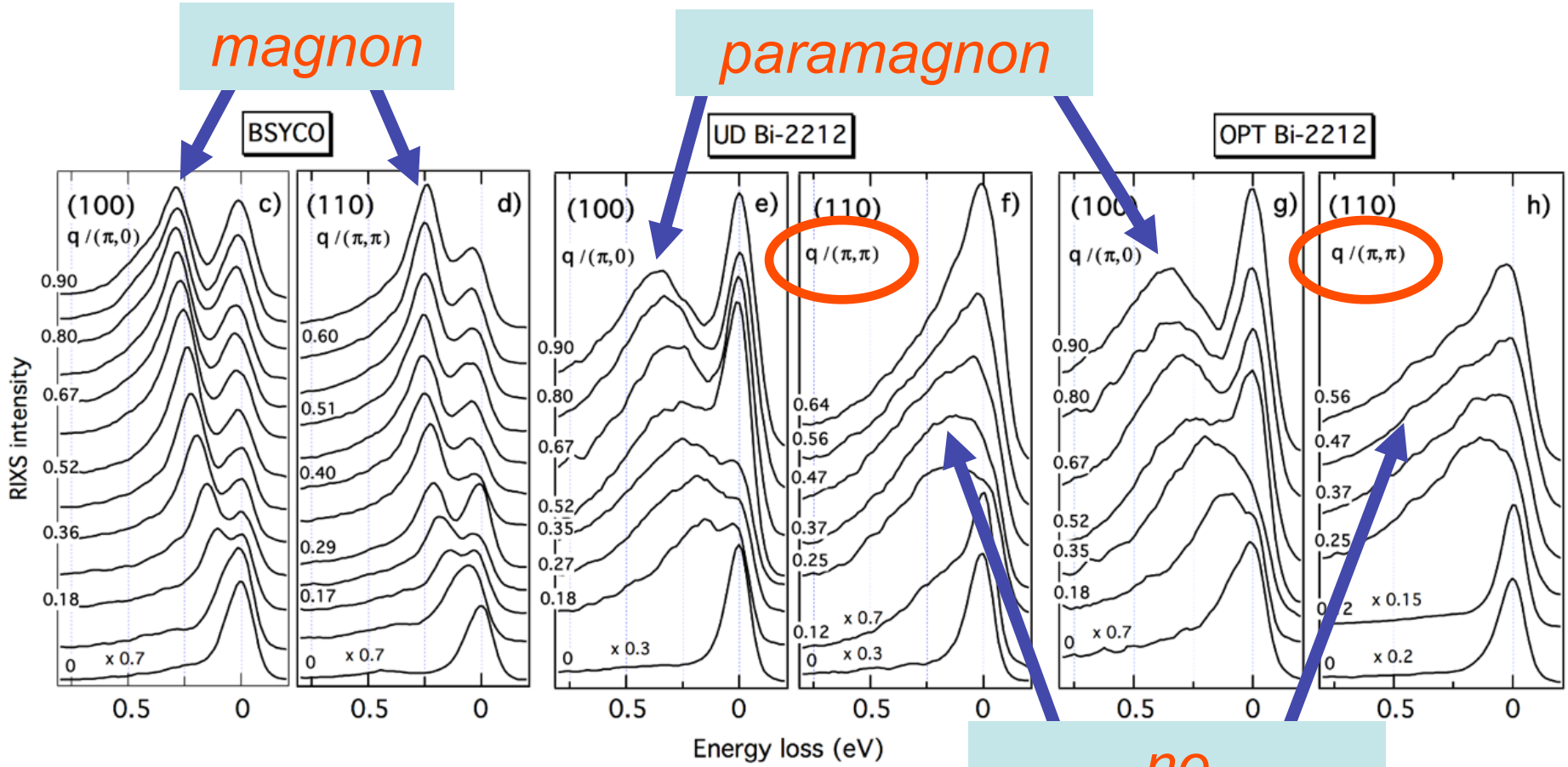
Guarise, Piazza, Berger, Giannini, Schmitt, Rønnow, Sawatzky, JvdB, Altenfeld, Eremin & Grioni (2014)

RIXS on Bi-2212 cuprate



Guarise, Piazza, Berger, Giannini, Schmitt, Rønnow, Sawatzky, JvdB, Altenfeld, Eremin & Grioni (2014)

RIXS on Bi-2212 cuprate



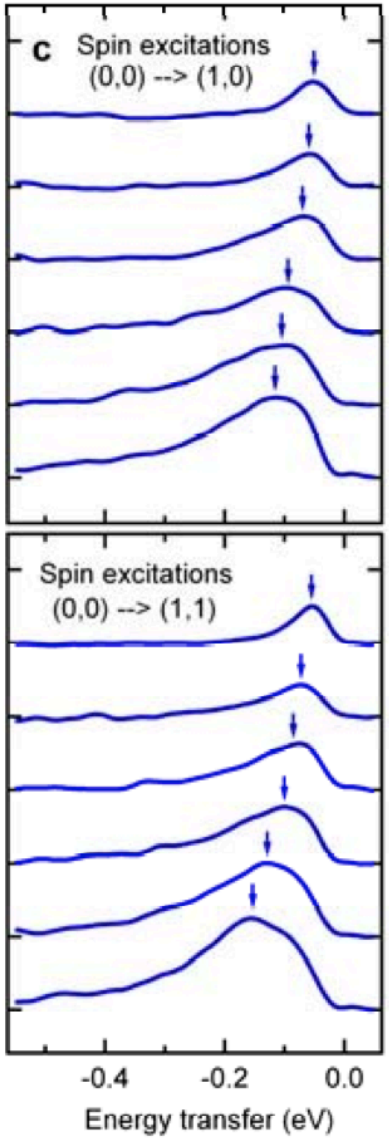
Related to presence of e-h continuum?

no paramagnon

Benjamin, Klich & Demler
PRL 112, 247002 (2014)

Guarise, Piazza, Berger, Giannini, Schmitt, Rønnow, Sawatzky, JvdB, Altenfeld, Eremin & Grioni (2014)

Magnetic RIXS on $Ba_{0.6}K_{0.4}Fe_2As_2$



Zhou, Huang, Monney, Dai, Strocov, Wang, Chen, Zhang, Dai, Patthey, JvdB, Ding & Schmitt, Nat. Comm. 4, 1470 (2013)

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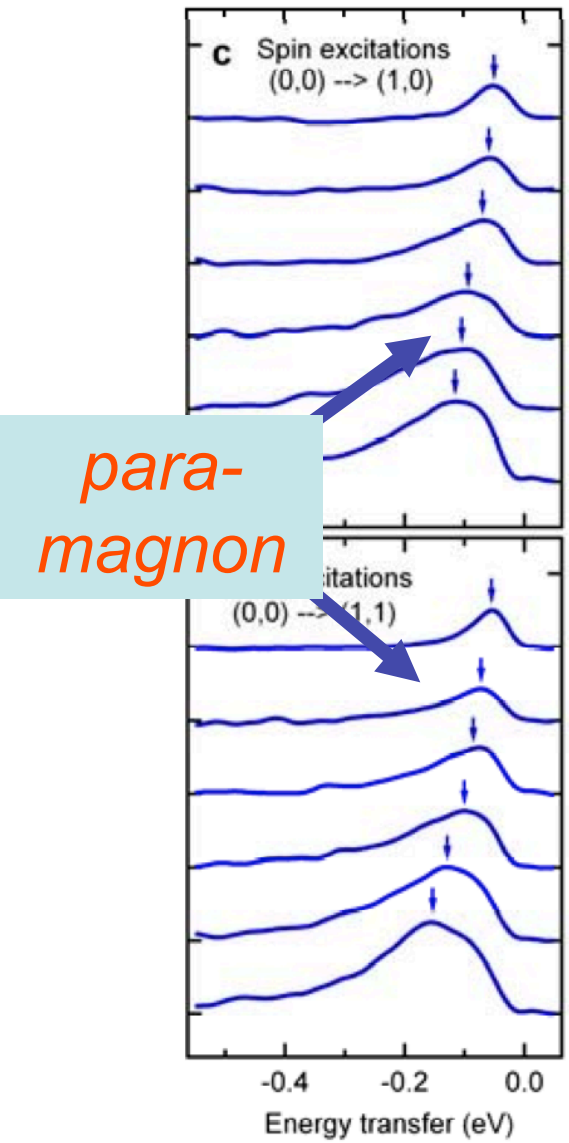

Zhou, Huang, Monney, Dai, Strocov, Wang, Chen, Zhang, Dai, Patthey, JvdB, Ding & Schmitt, Nat. Comm. 4, 1470 (2013)

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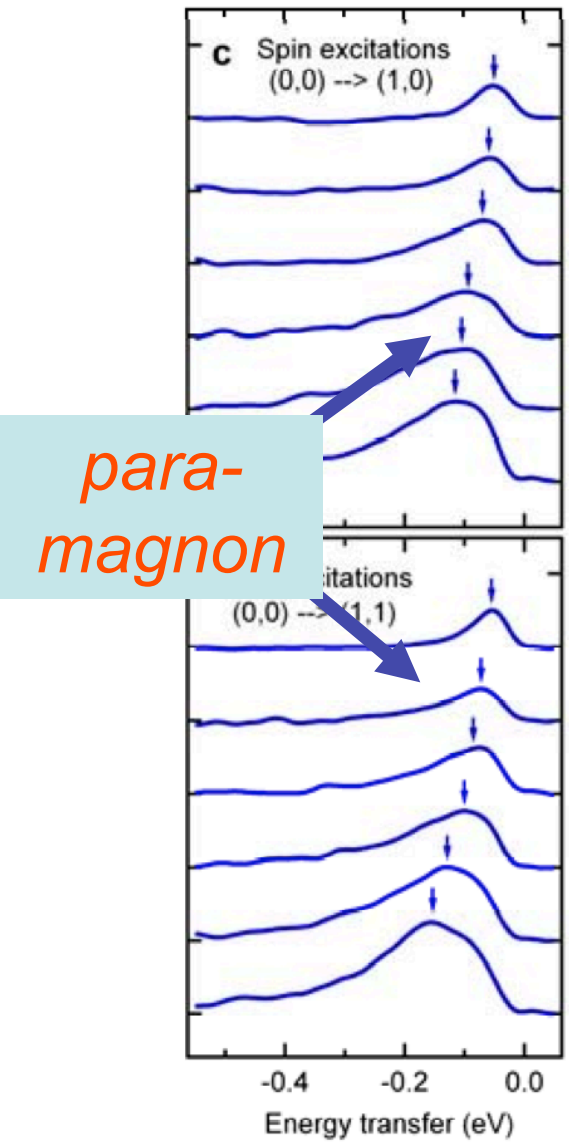
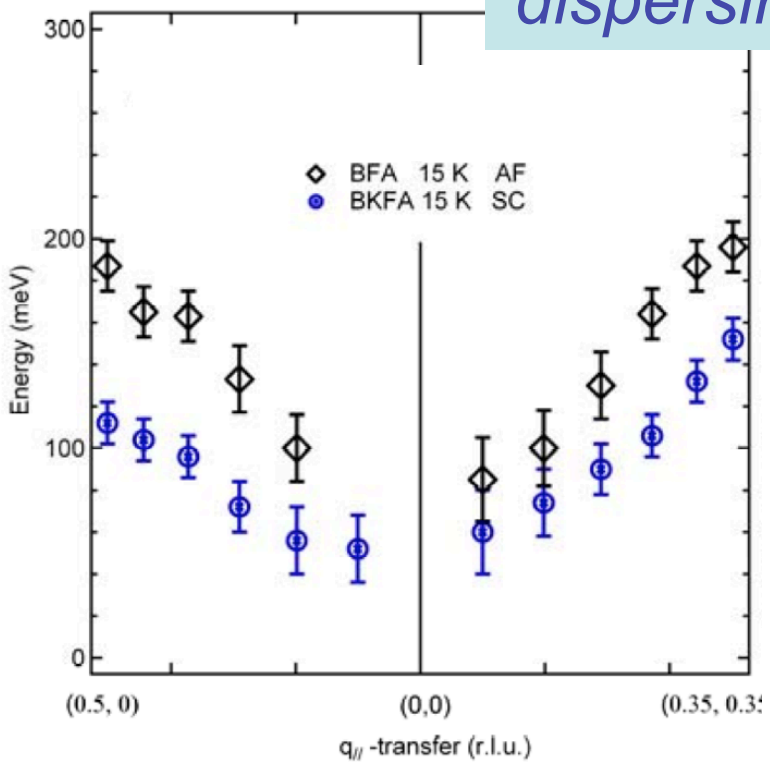


para-magnon



dispersing paramagnon

Significant softening

Zhou, Huang, Monney, Dai, Strocov, Wang, Chen, Zhang, Dai, Patthey, JvdB, Ding & Schmitt, Nat. Comm. 4, 1470 (2013)

Summary part 2

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- More and better beam-lines, experiments, theory