Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3

"Splitting" the electron

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December 7, 2012

The paper

- We describe the following article by J. Schlappa, *et al.*, *Nature* **485**, 82 (2012).

LETTER

doi:10.1038/nature10974

Spin–orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3

J. Schlappa[1,2], K. Wohlfeld[3], K. J. Zhou[1]†, M. Mourigal[4], M. W. Haverkort[5], V. N. Strocov[1], L. Hozoi[3], C. Monney[1], S. Nishimoto[3], S. Singh[6]†, A. Revcolevschi[6], J.-S. Caux[7], L. Patthey[1,8], H. M. Rønnow[4], J. van den Brink[3] & T. Schmitt[1]

When viewed as an elementary particle, the electron has spin and charge. When binding to the atomic nucleus, it also acquires an angular momentum quantum number corresponding to the quantized atomic orbital it occupies. Even if electrons in solids form bands and delocalize from the nuclei, in Mott insulators they retain their three fundamental quantum numbers: spin, charge and orbital[1]. The hallmark of one-dimensional physics is a breaking up of the elementary electron into its separate degrees of freedom[2]. The separation of the electron into independent quasi-

separate itself completely from the holon. When instead of creating a hole, as typically is done in a photoemission experiment, an electron is excited from one copper 3*d* orbital to another, the phenomenon of spin–orbital separation can in principle occur (Fig. 1a). The orbiton created in this manner may also deconfine after exciting a spinon, thus splitting the electron into its orbital and spin degrees of freedom[8].

Here we use high-resolution resonant inelastic X-ray scattering (RIXS) to search experimentally for spin–orbital separation in the quasi-1D copper oxide Sr_2CuO_3 (for material details, see Supplemen-

Outline

- Spin-orbital separation
- Orbitons and spinons as an example of fractionalized quasiparticles
- What are quasiparticles and fractionalization and why are they important?
- Observing orbitons in a condensed matter setting using resonant inelastic X-ray scattering
- Analysis of the paper
  - Criticism
  - Citation analysis

Spin-charge separation

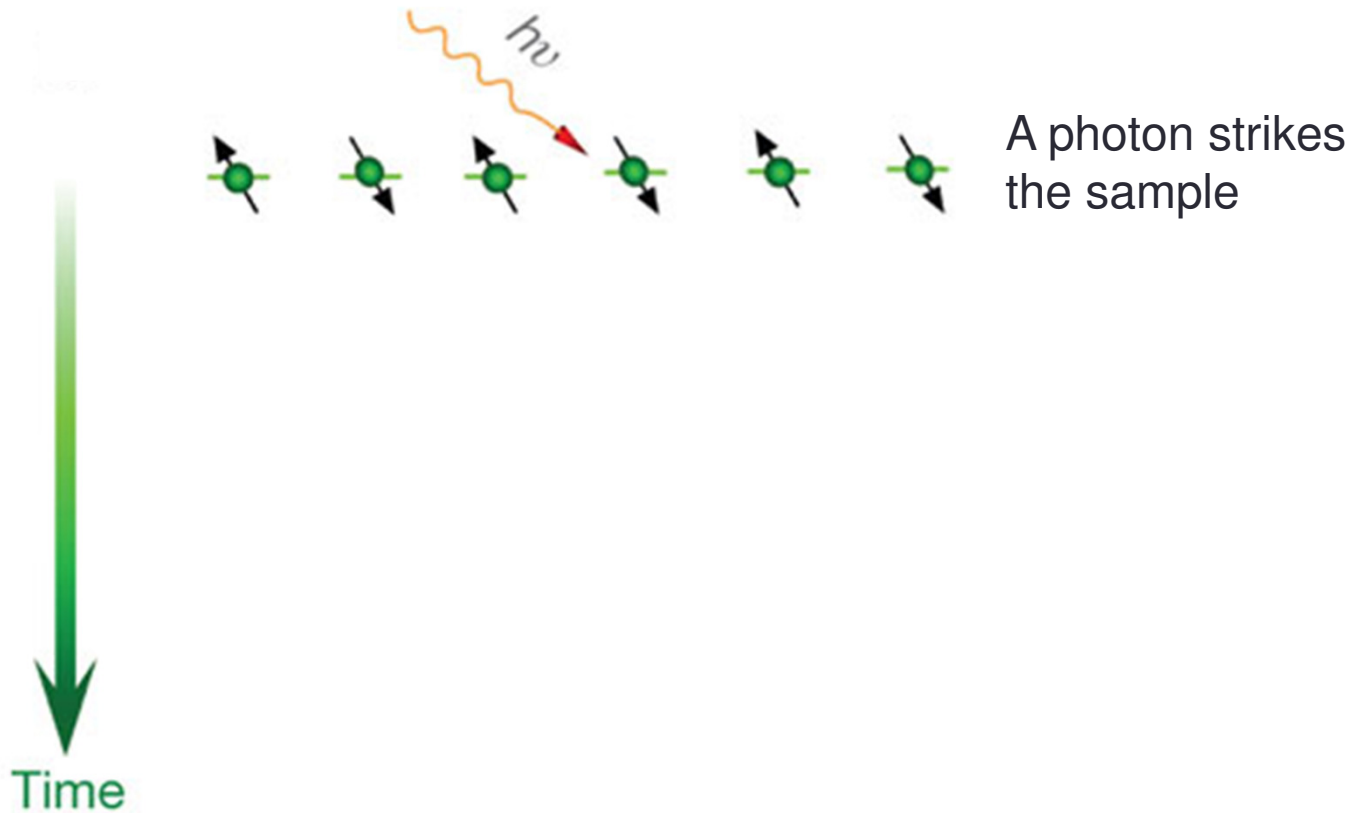
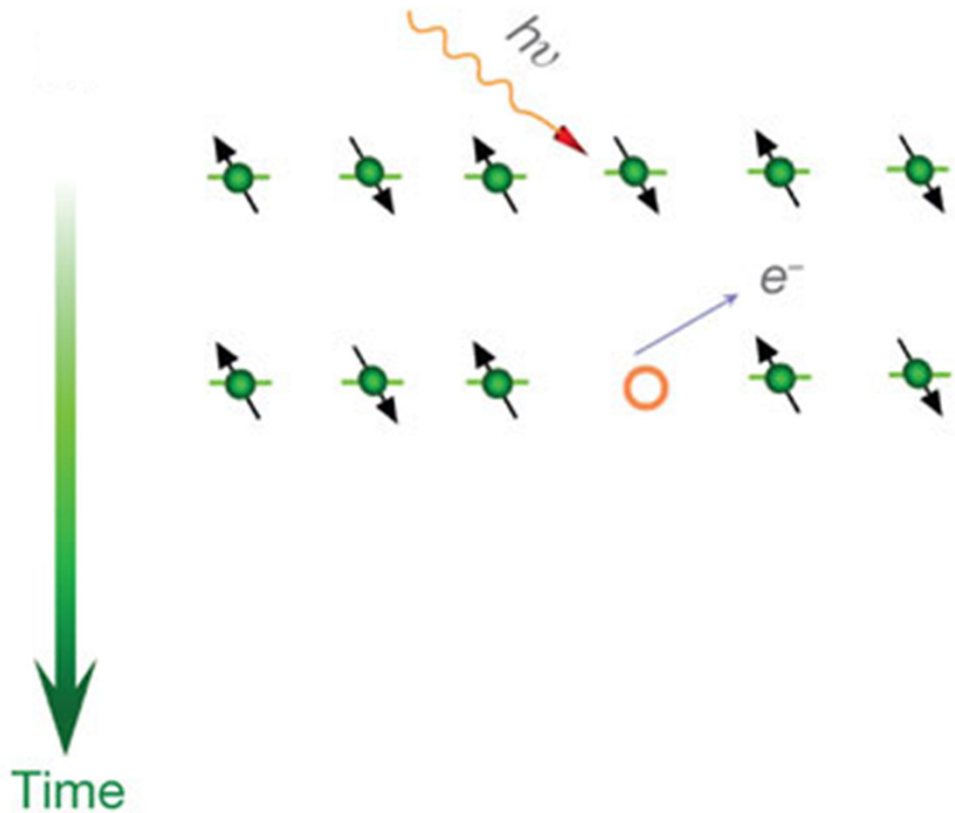


Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

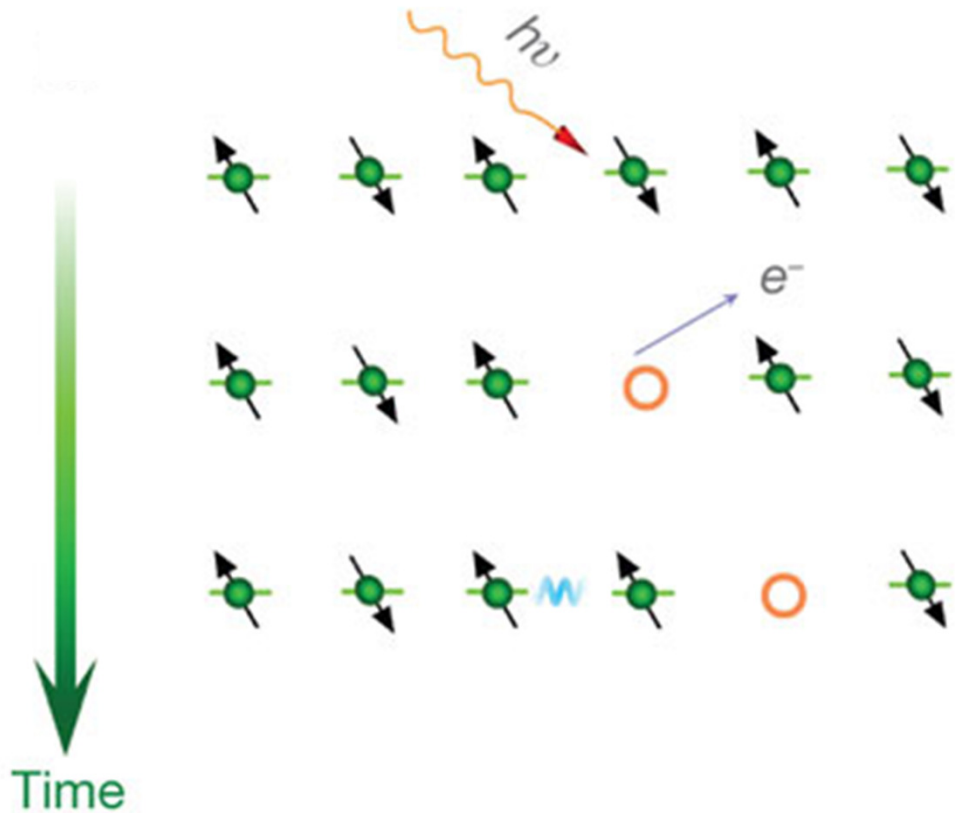
Spin-charge separation



An electron is ejected

Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

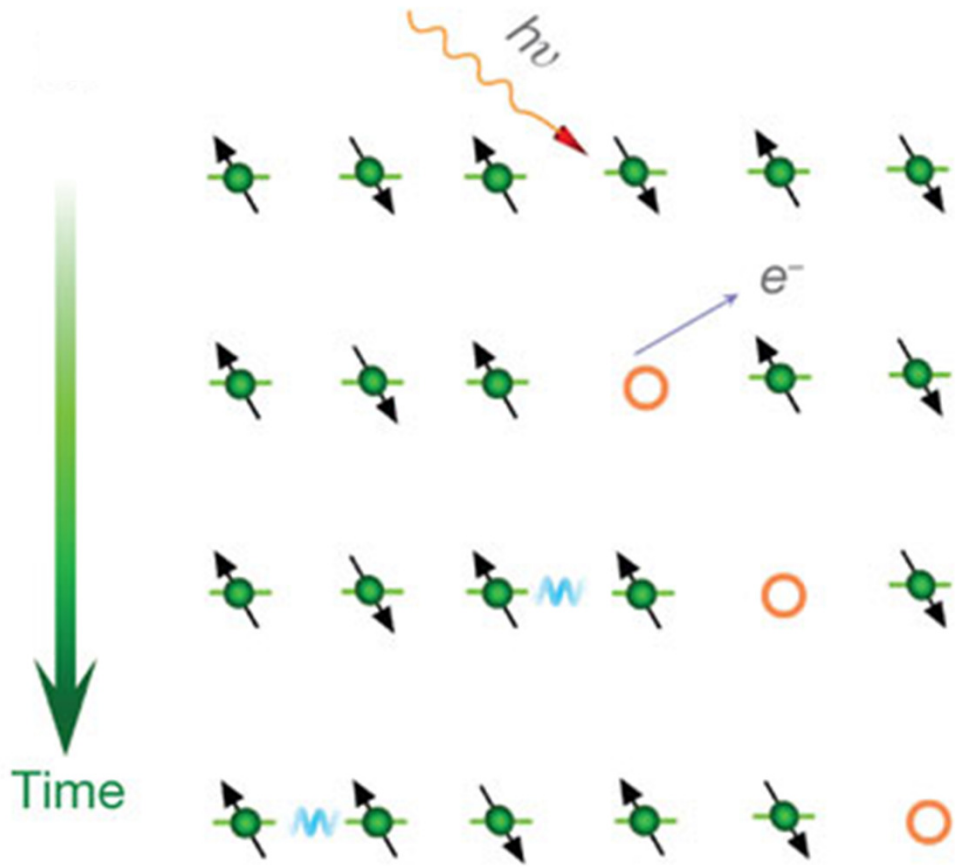
Spin-charge separation



The vacancy is filled, bringing two “up” spins together

Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

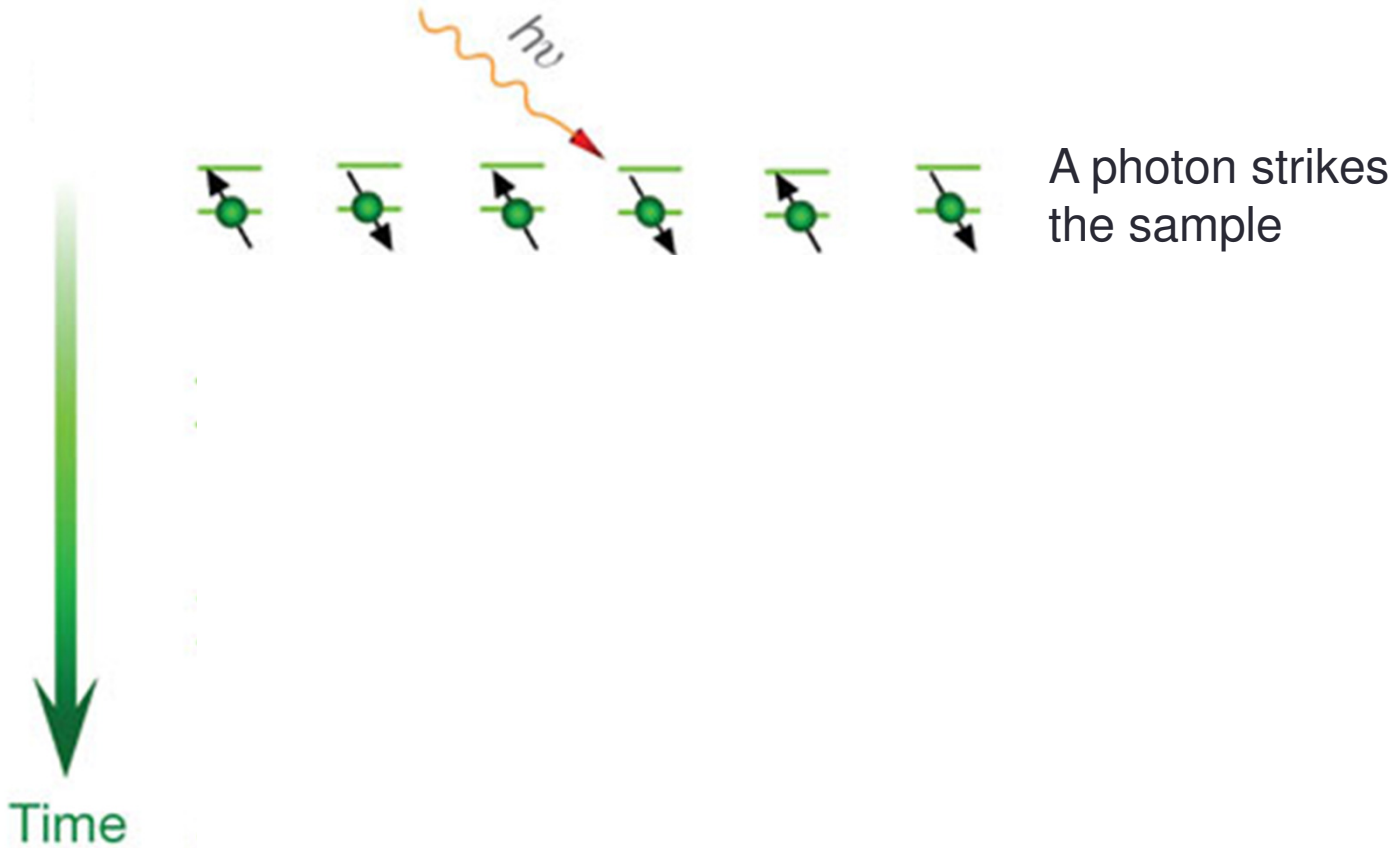
Spin-charge separation



The spin and hole
Travel away in opposite
directions

Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

Spin-orbital separation



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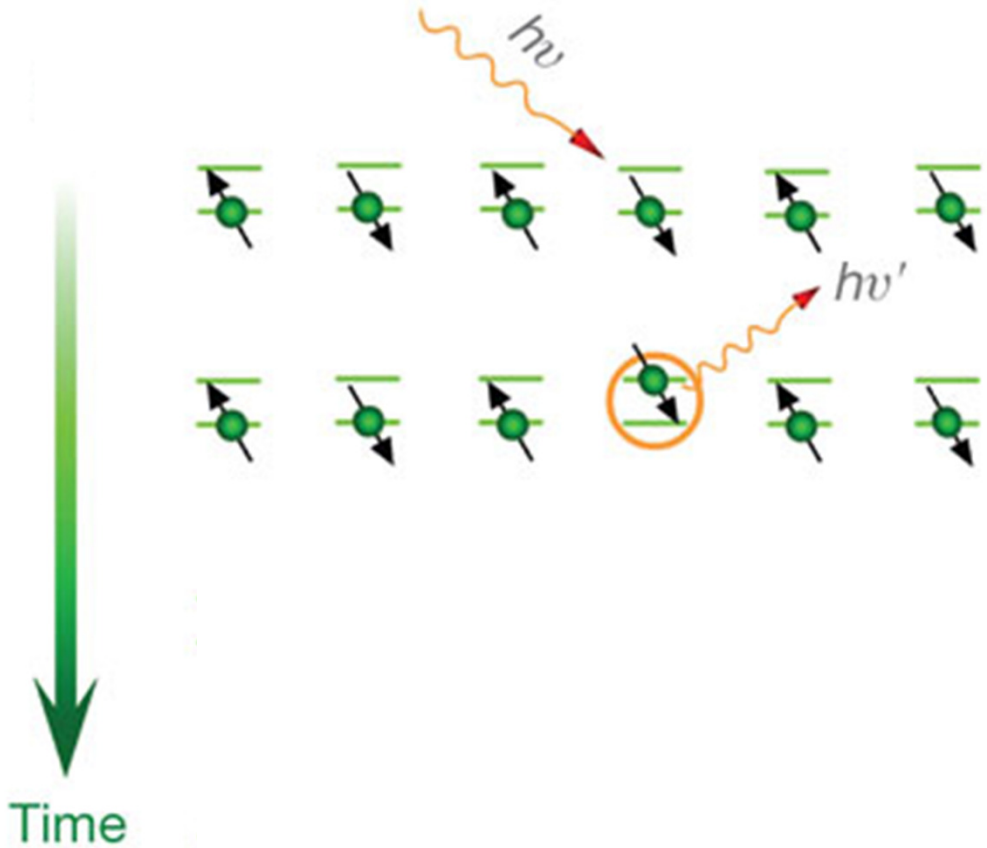
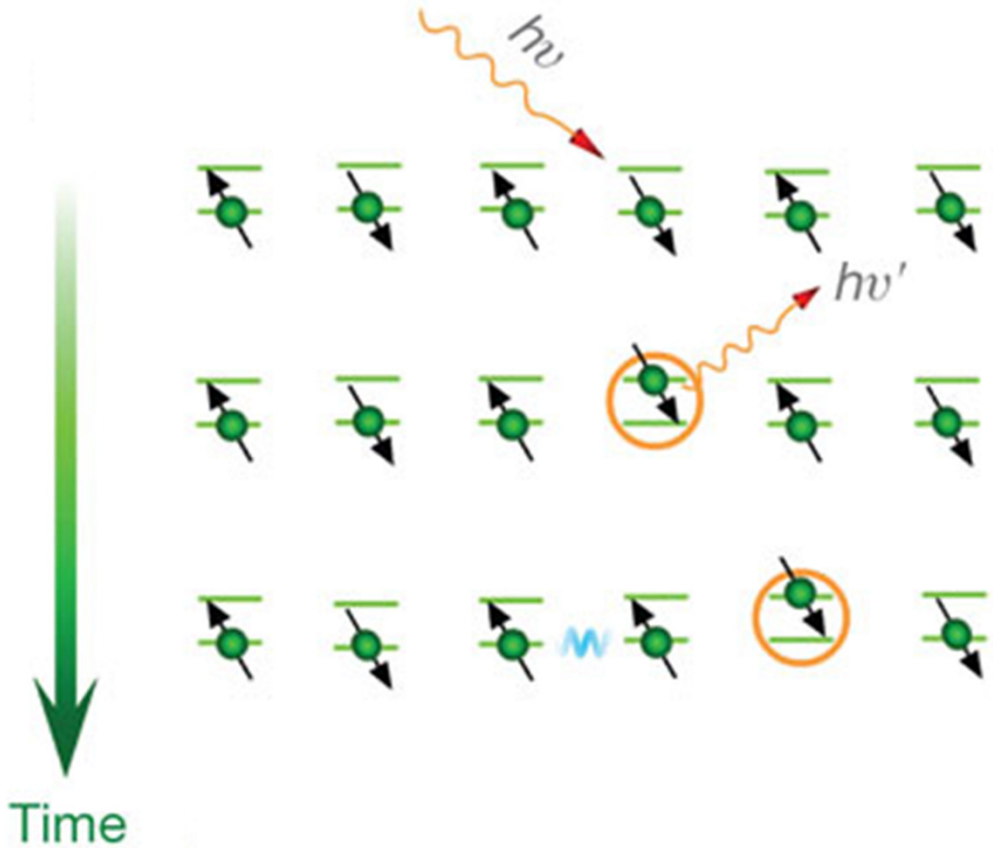
Spin-orbital separation



An electron is excited to a higher orbital

Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

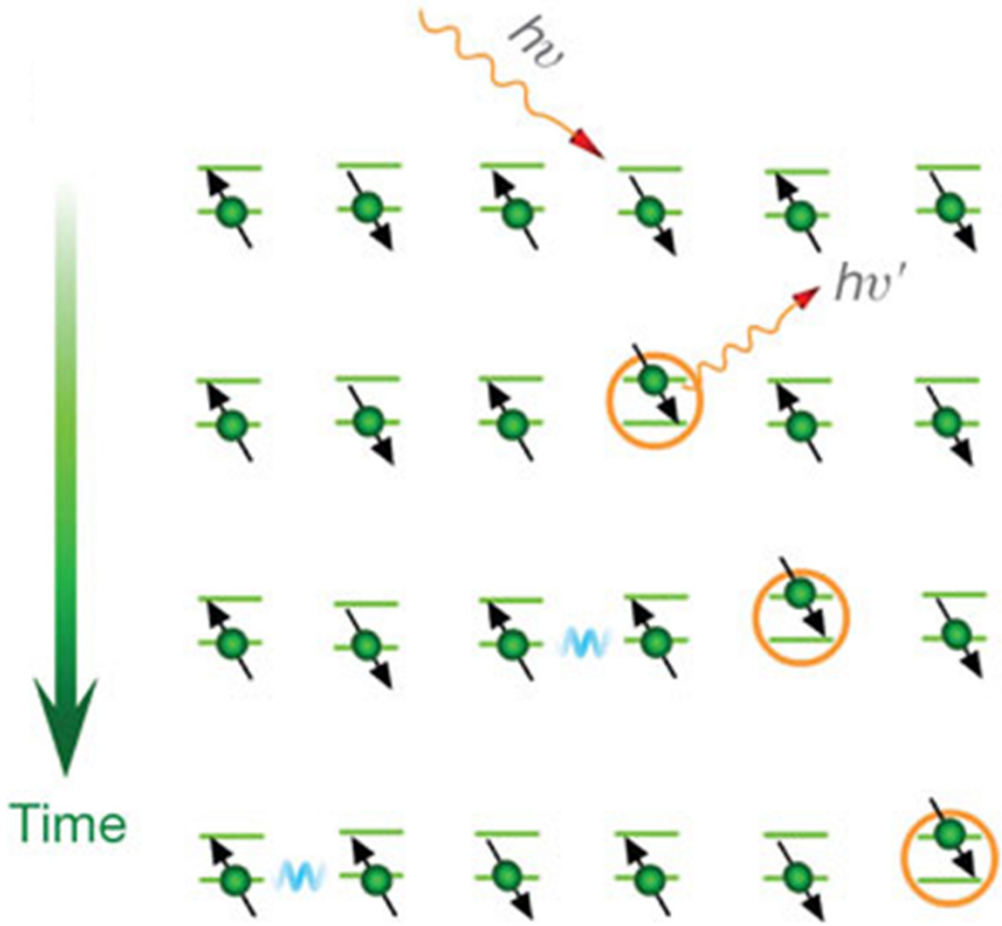
Spin-orbital separation



The excited electron swaps with its neighbor

Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

Spin-orbital separation



An orbiton and a spinon are carried away

Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

Why spin-orbital separation is important

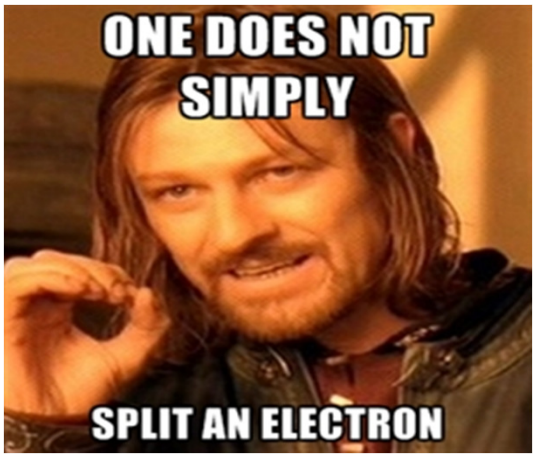
- One example of particle fractionalization
- Key characteristic of 1D physics
- Predicted in the 70s, but only spin-charge separation had been observed
- Related to one explanation of high T_C superconductors

Quasiparticles, fractionalization, and deconfinement

"High energy" physics at low energy

Quasiparticles

- Spin-orbit separation can be viewed as "splitting" the electron into a spinon and orbiton.
- Does that mean spinon and orbiton are fundamental particles?
- First of all, What is a 'fundamental particle'?



"Fundamental Particles" are excitations of the underlying Quantum fields of fundamental interactions

But are they relevant for the description for any phenomena?

Not necessarily. We need to ask about energy scales, number of particles involved etc

Quasiparticles 2

- Most of condensed matter phenomena can be described by quasiparticles. - Introduced by Lev Landau

- They are excitations of macroscopic many particle fields.

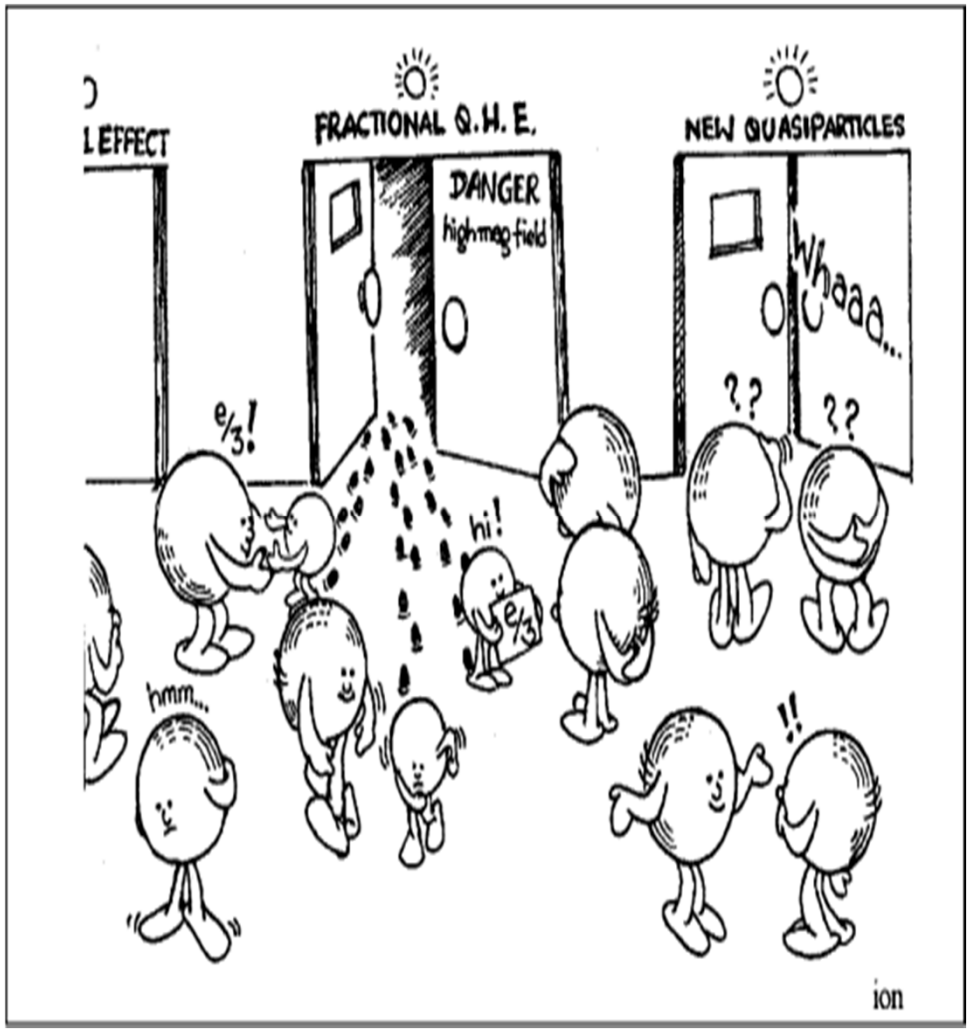
- Quantum numbers ≠ Multiples of elementary particles (‘More is Different’)

- Fractional charge, spin

- Different kind of statistics in low dimensions.

P.W. Anderson, More is different—Broken symmetry and nature of hierarchical structure of science. *Science* **177**, 393 (1972).

Quasiparticle factory



Ingredients:

- Many body physics
- Strong interaction
- Low Dimensions

- Example: Composite Fermions
- High magnetic field
- Strong Interaction
- 2 dimensions
- CF=electron+quantized flux
- But Fractional Charge!!

Our current ingredients

- 1-Dimension + Strong correlation = Fractionalization + Spin-Charge-Orbital deconfinement.

- Are these just ‘theoretical concepts’ or experimentally observable?

- What experimentally-observable phenomena do these ideas predict?
  - Search for particle like patterns in the spectral functions of scattering experiments like ARPES, RIXS.

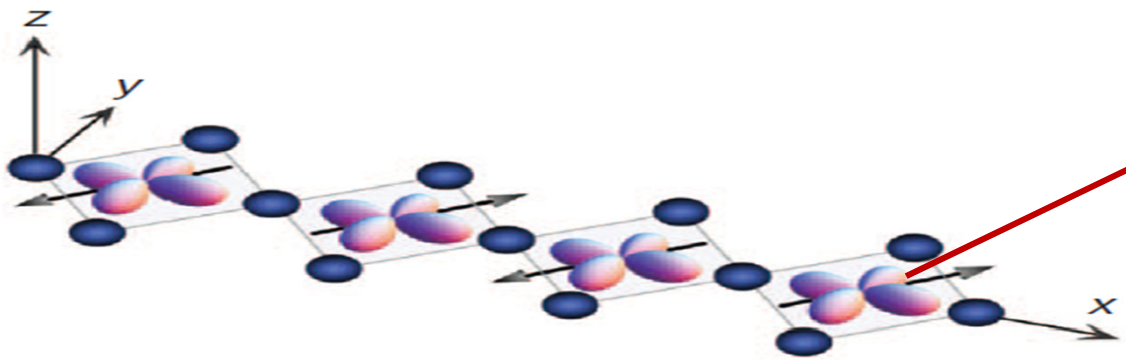
Strong interactions make strong impact

- For interactions in dimensions d>1, Landau Fermi Liquid theory works.

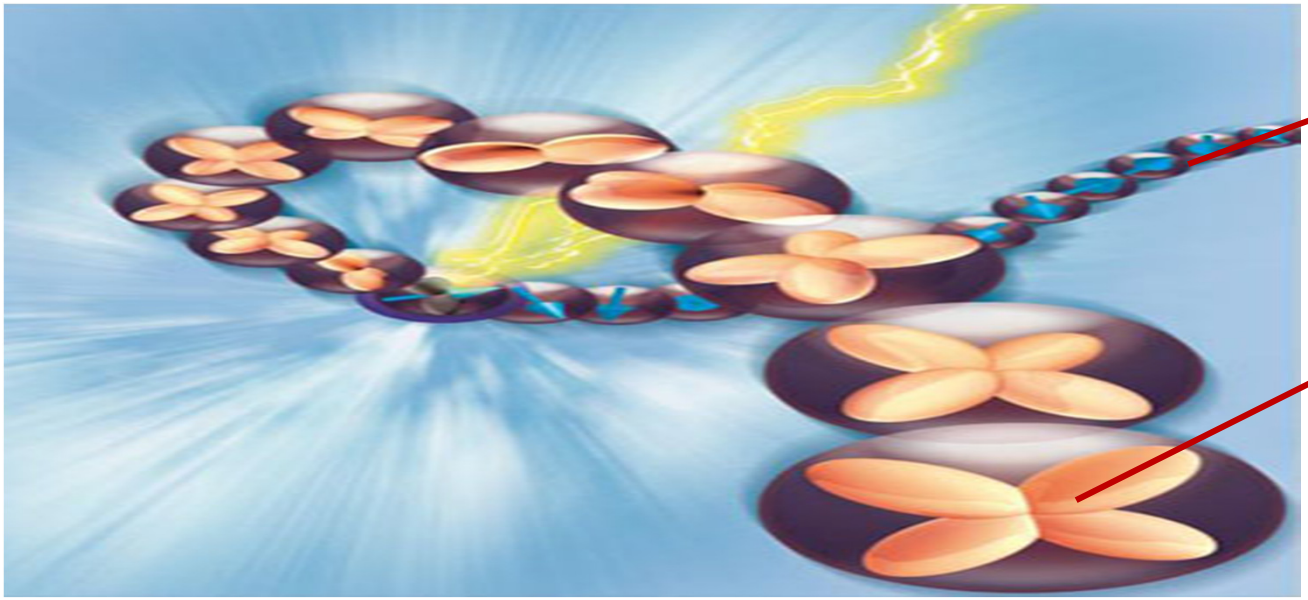
  LFL theory: Quasiparticles are electrons“dressed” by the interactions and have renormalized mass, charge, etc.
- Interactions in one dimension :
  - **Tomonaga-Luttinger liquid theory**: predicts spin-charge separation into excitations called spinons and holons, respectively
  - Spin-orbital separation also recently predicted.
- Experiment: Not a peak in spectral function but a power law decay.

T. Giamarchi, *Quantum Physics in One dimension*, Oxford Science Publications (2004).
K. Wohlfeld, M. Daghofer, S. Nishimoto, G. Khaliullin, & J. van den Brink, *Intrinsic coupling of orbital excitations to spin fluctuations in Mott insulators*. *Phys.Rev. Lett.* **107**, 147201 (2011).

Artists impression of spin-orbit separation



Bound state with spin and orbital angular momentum



Spinons

Orbitons: xz, yz and xy orbitals

Physicist's impression of S-O separation

$$H = -J_O \sum_{j,\sigma} (c_{j\sigma}^{+} c_{j+1,\sigma} + \text{h.c.}) + J \sum_{j} \mathbf{S}_j \bullet \mathbf{S}_{j+1} + E_O \sum_{j} (1 - n_j)$$

A t-J model: Kugel-Khomskii Hamiltonian

J_o - Orbital Exchange constants

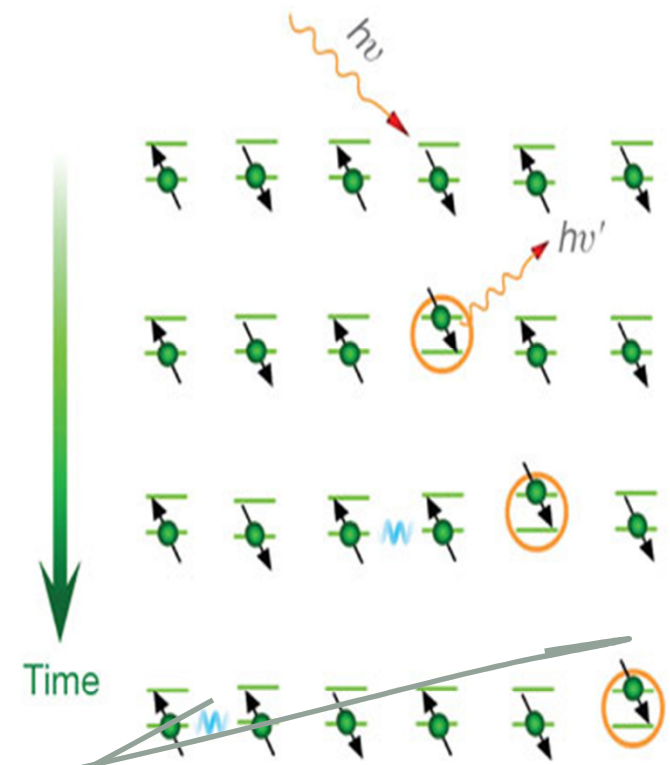
$c_{j,\sigma}$ - Destruction operators of particles in xz orbitals

J - Spin exchange constants

S_j - Spins on the particles in $x^2 - y^2$ orbitals

E_o – xz-orbital exchange energy

$(1 - n_j)$ -counts the particles in xz state.



Spin-orbit separation ansatz

- Deconfinement: Analogous to quark deconfinement of QCD!
- Spinons and orbitons move separately.

$$c_{i\sigma}^{\dagger} = s_{i\sigma}^{\dagger} o_i$$

$\varepsilon_o(k) = E_o - 2J_o \cos(k)$ Orbiton Dispersion

$\varepsilon_s(k) = -2J\cos(k)$ Spinon Dispersion

Spectral function for orbital excitation in RIXS

$$c_{q\sigma}^{\dagger} = \sum_k o_{q-k} s_{\sigma k}^{\dagger}$$

Resulting orbital Excitation spectrum

$$E(q) = E_o \pm 2J_0 |\sin(k)|$$

Observing orbiton quasi-particles experimentally

Why look for orbitons in Sr_2CuO_3?

- Sr_2CuO_3 possesses all the necessary ingredients for fractionalization:
  - One-dimensional
  - Strong antiferromagnetic interactions

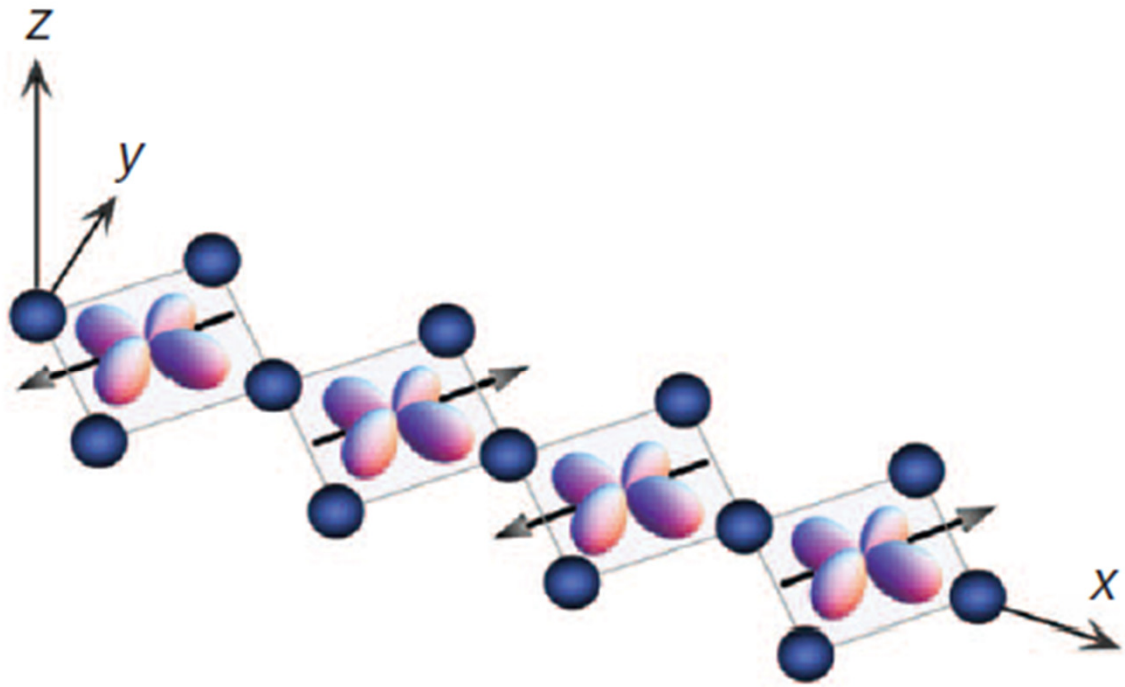
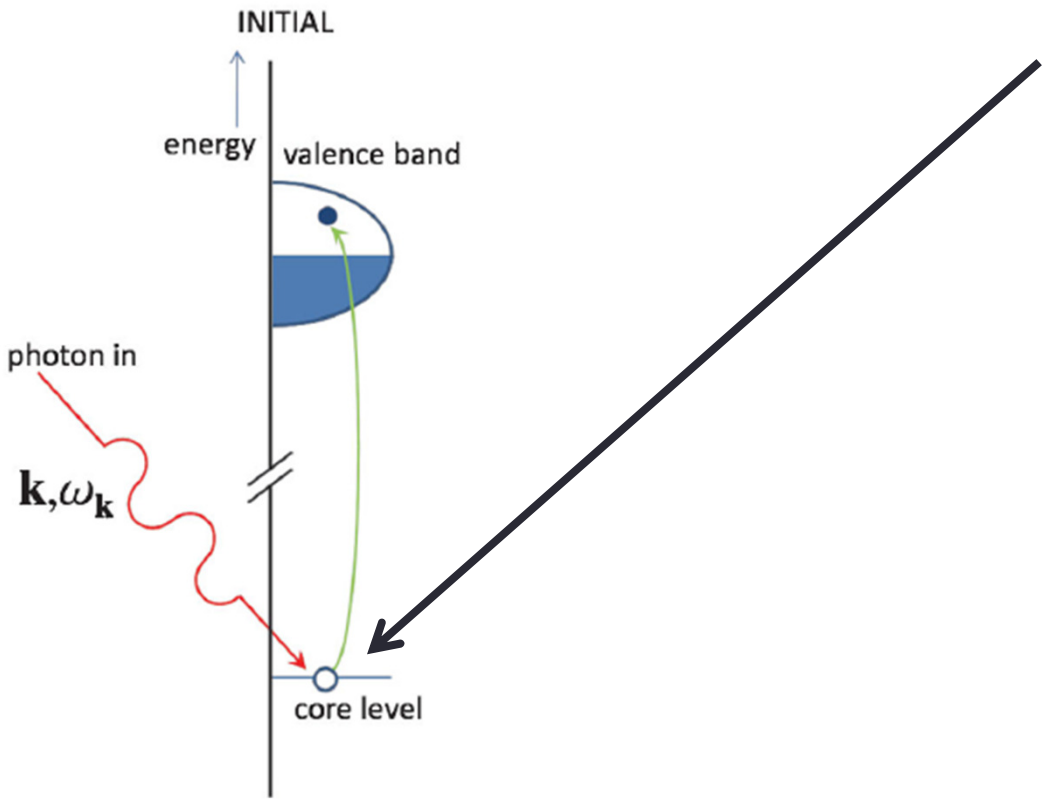


Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

Using RIXS to study quasiparticle excitations

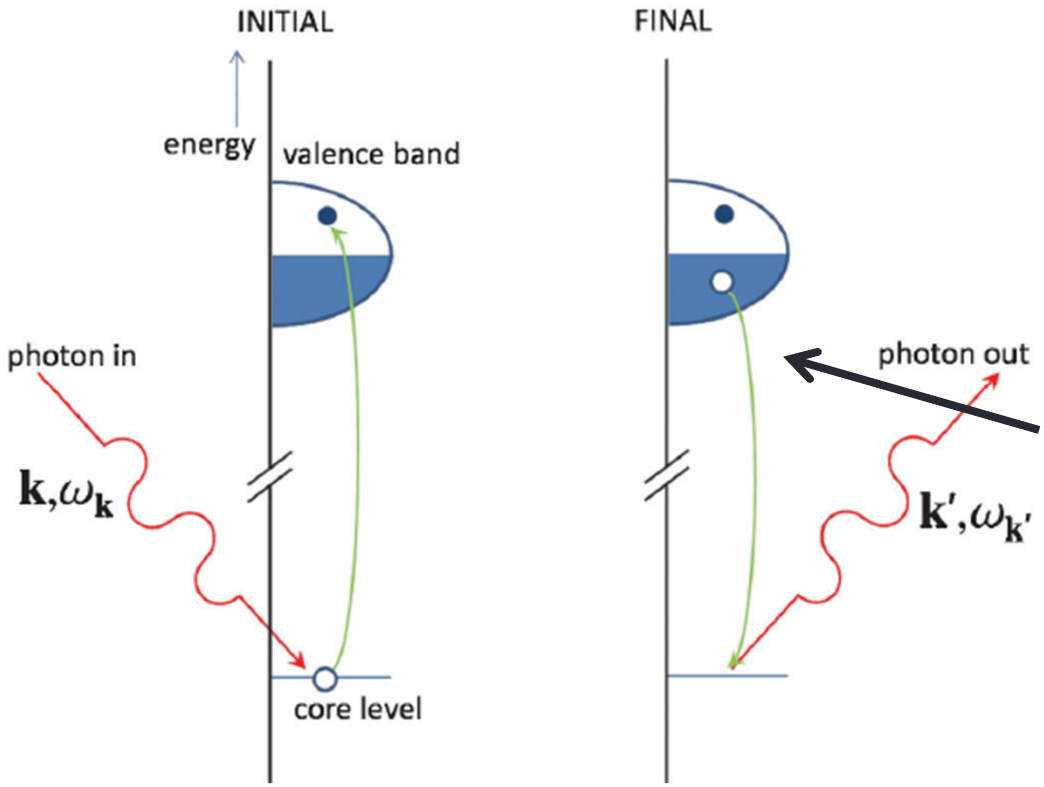


First, an X-ray of known energy, momentum, and polarization is used to move a core-level electron in the solid to an excited state.

- Resonant Inelastic X-ray Scattering (RIXS) is a powerful technique used to measure the dispersion relations of the quasiparticle excitations of solids.

Figure from Luuk J.P. Ament, *et al.*, Resonant inelastic X-ray scattering studies of elementary excitations. *Rev. Mod. Phys.* **83**, 705 (2011).

Using RIXS to study quasiparticle excitations



First, an X-ray of known energy, momentum, and polarization is used to move a core-level electron in the solid to an excited state.

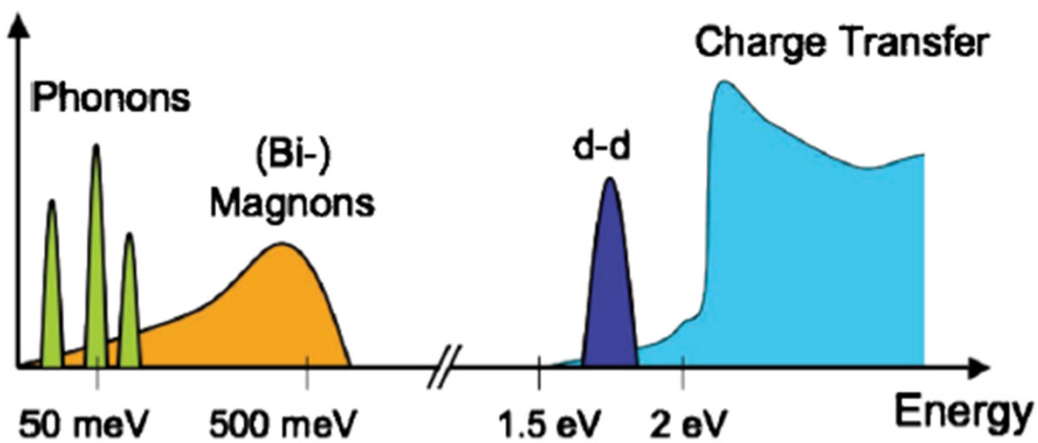
Then a valence electron fills the empty core level, emitting an X-ray. The difference between the two X-rays yields information about the excited state.

- Resonant Inelastic X-ray Scattering (RIXS) is a powerful technique used to measure the dispersion relations of the quasiparticle excitations of solids.

Figure from Luuk J.P. Ament, *et al.*, Resonant inelastic X-ray scattering studies of elementary excitations. *Rev. Mod. Phys.* **83**, 705 (2011).

Advantages of RIXS

- X-rays carry significant momentum (unlike photons in optical spectroscopy), allowing excitation dispersion relations to be measured.
- Energy, momentum, and polarization of X-rays can all be measured.
- Many different types of quasiparticle excitations can be studied with RIXS.



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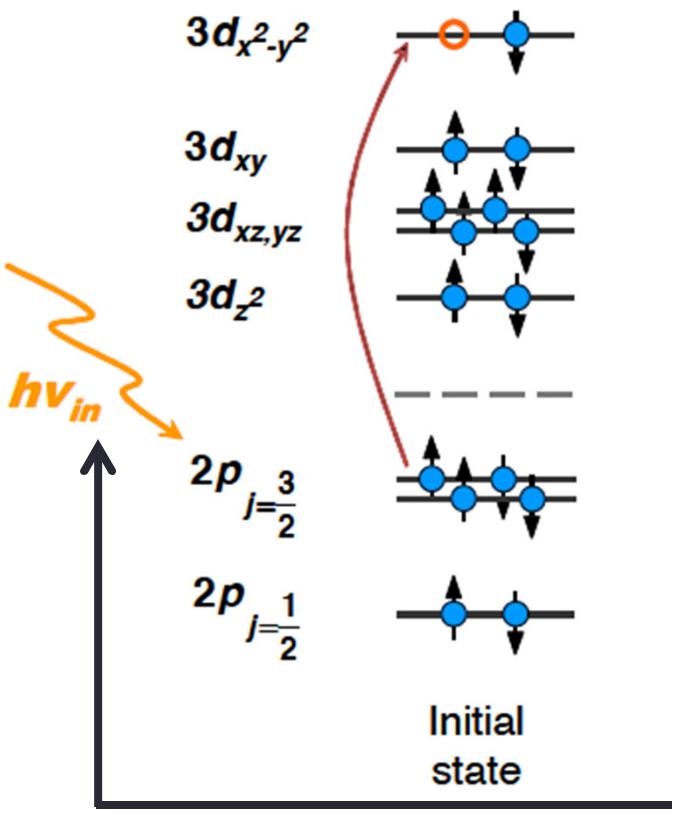
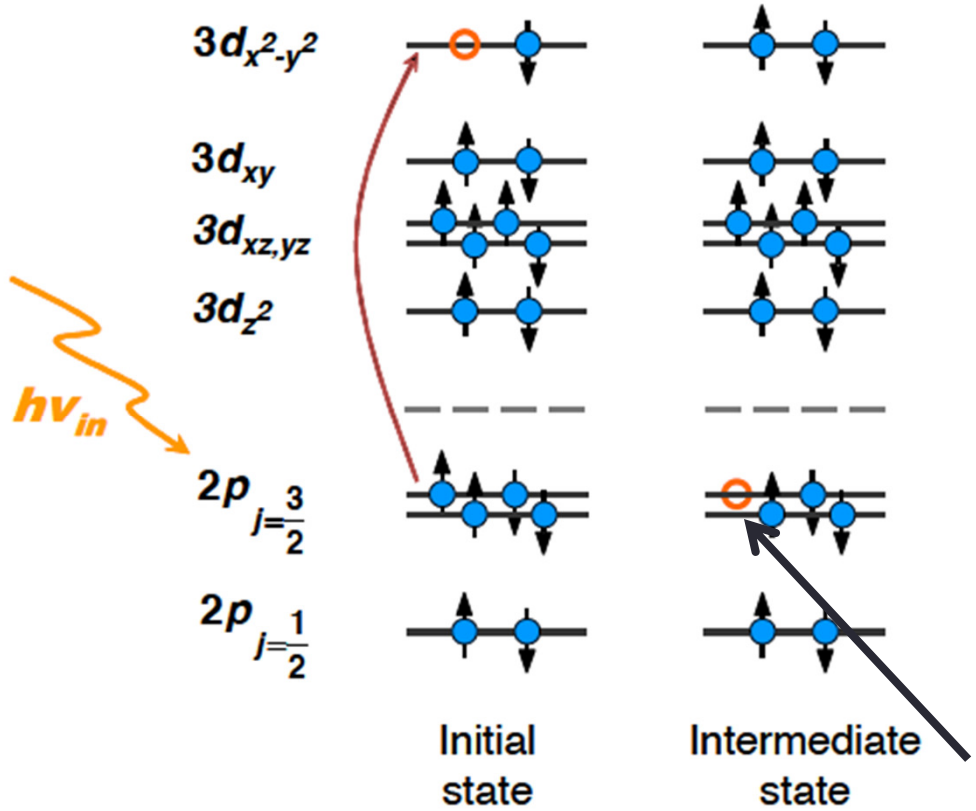
Using RIXS to observe orbitons in Sr_2CuO_3



X-ray excites a core-level Cu electron to an unoccupied *d* orbital

Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

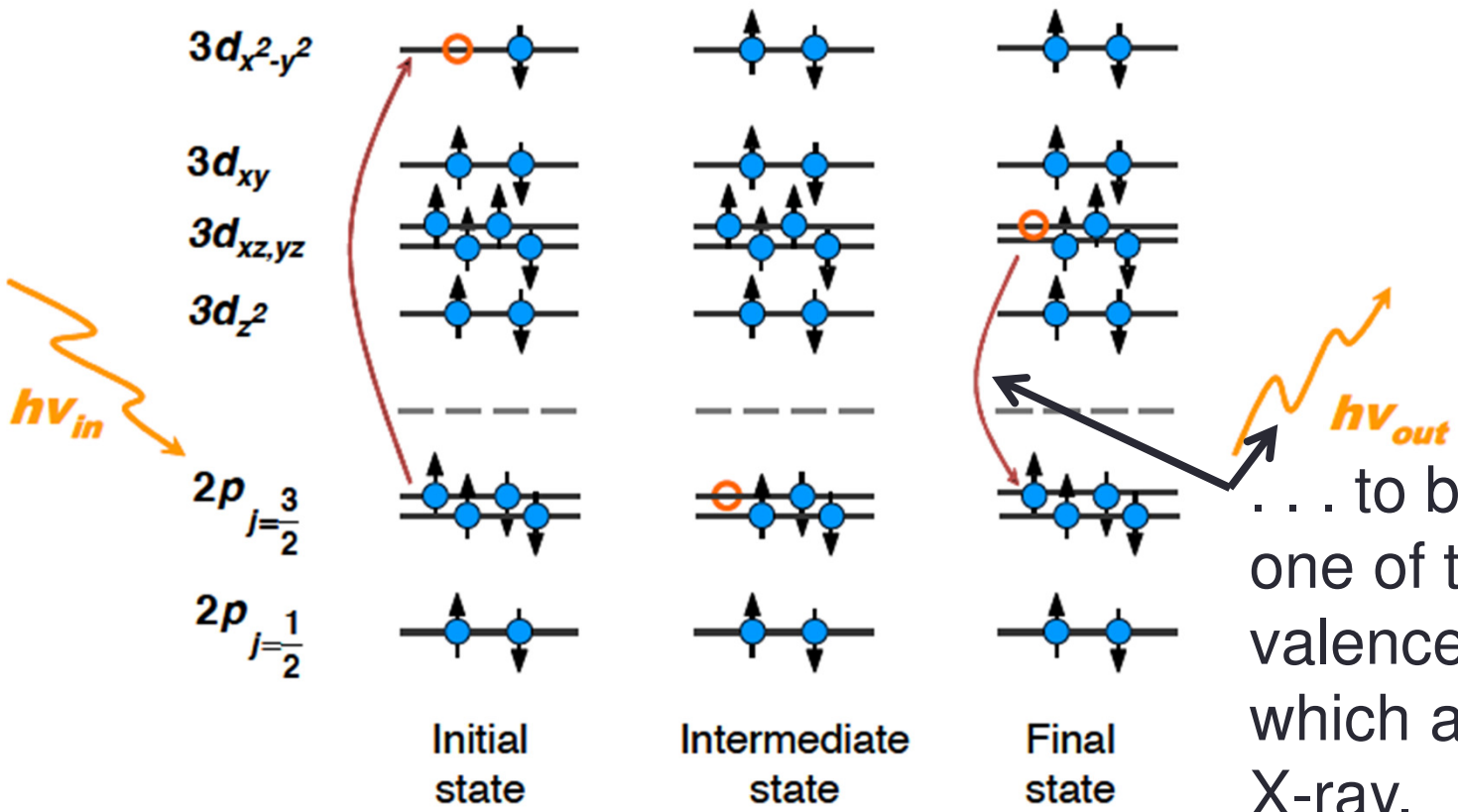
Using RIXS to observe orbitons in Sr_2CuO_3



The excited core electron leaves behind an unoccupied core orbital . . .

Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

Using RIXS to observe orbitons in Sr_2CuO_3



. . . to be filled by one of the other valence electrons, which also emits an X-ray.

The energy and momentum change between the two X-rays give information about the orbiton created.

Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

RIXS spectrum of orbitons

- The dispersion of elementary excitations in Sr_2CuO_3 measured by the authors using RIXS is shown at right (note the holon dispersion is at higher energy and is omitted)

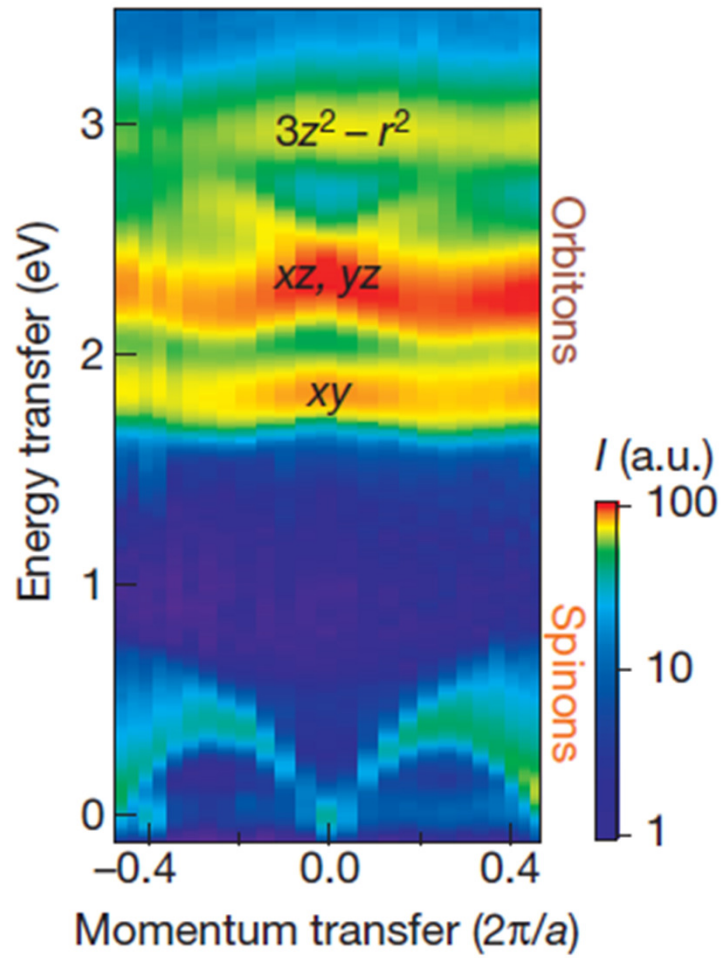


Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

RIXS spectrum of orbitons, continued

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- The lower curve is shown to belong to spinons

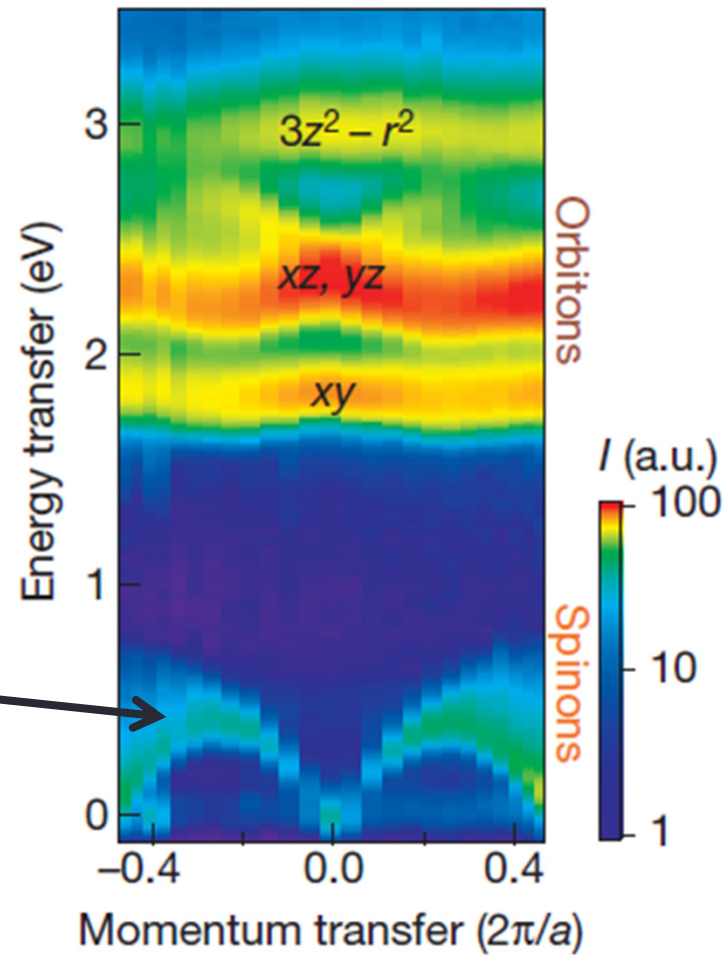


Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

RIXS spectrum of orbitons, continued

- The dispersion of elementary excitations in Sr_2CuO_3 measured by the authors using RIXS is shown at right (note the holon dispersion is at higher energy and is omitted)
- The lower curve is shown to belong to spinons
- The authors argue the upper curves are due to orbitons.

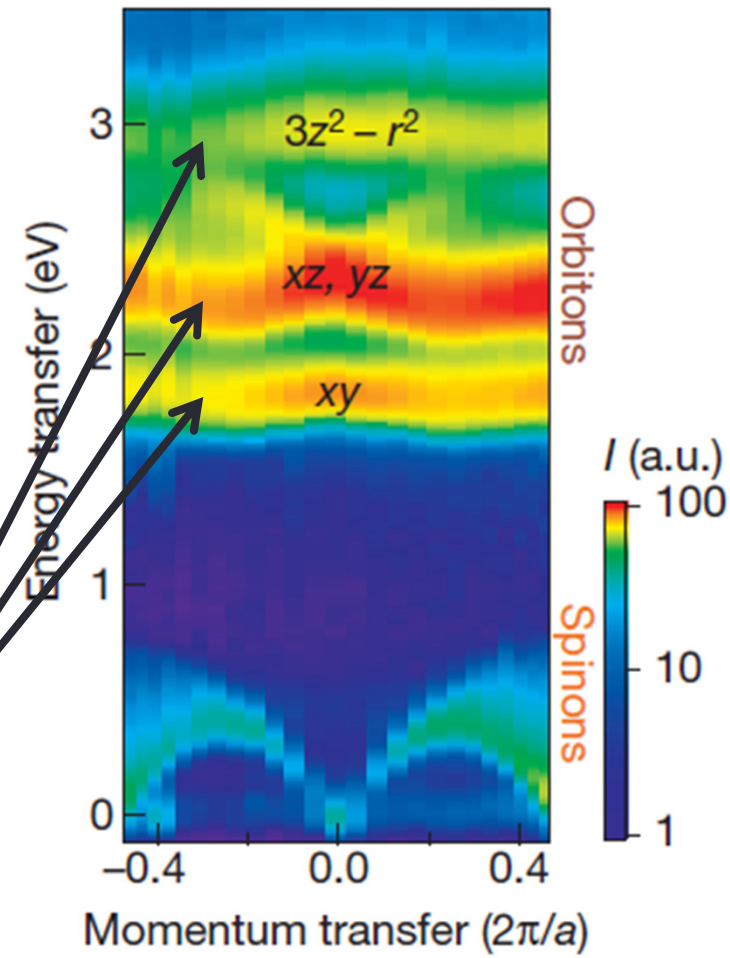
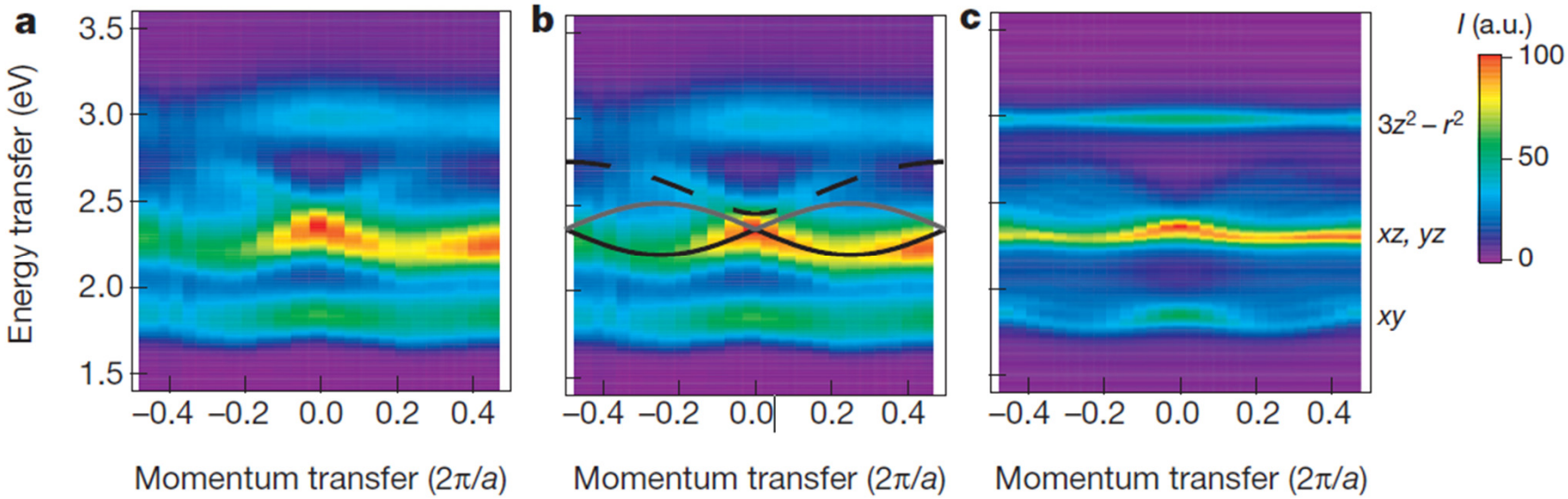


Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

RIXS spectrum of orbitons: comparison with theory



- The experimental orbiton spectrum measured by RIXS (a) compares well with the predictions of the orbital-spin separation ansatz (b) and simulations done on a system of 28 lattice sites (c).

Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

Criticism of J. Schlappa, *et al.*

- While the authors carefully determined which dispersion was due to spinons, they completely ignored holons, which raises questions about their identification of specific dispersions as orbitons

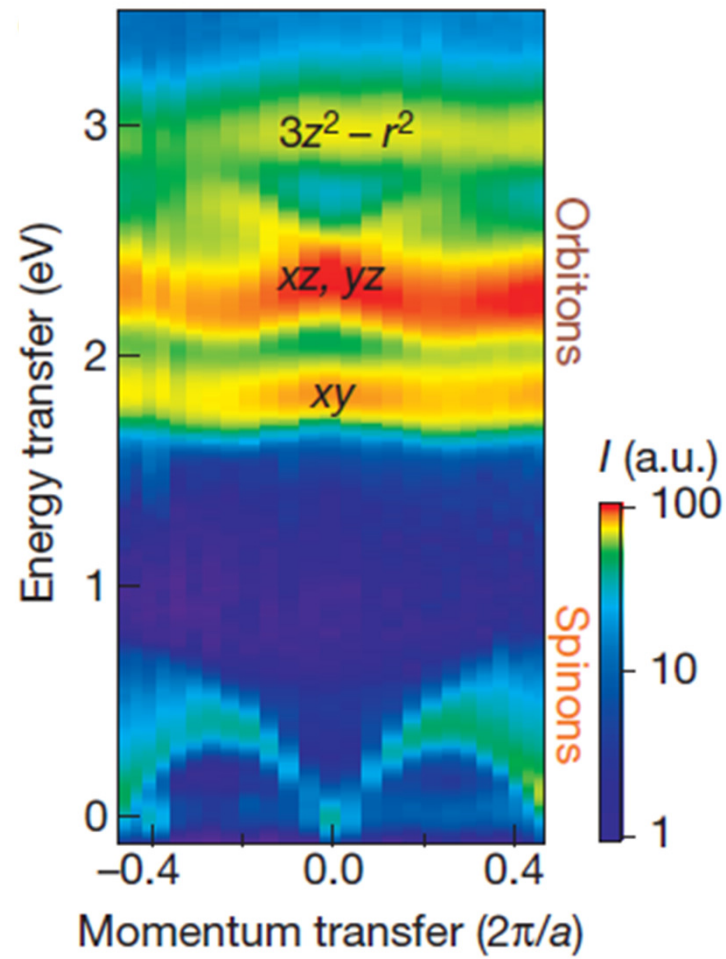
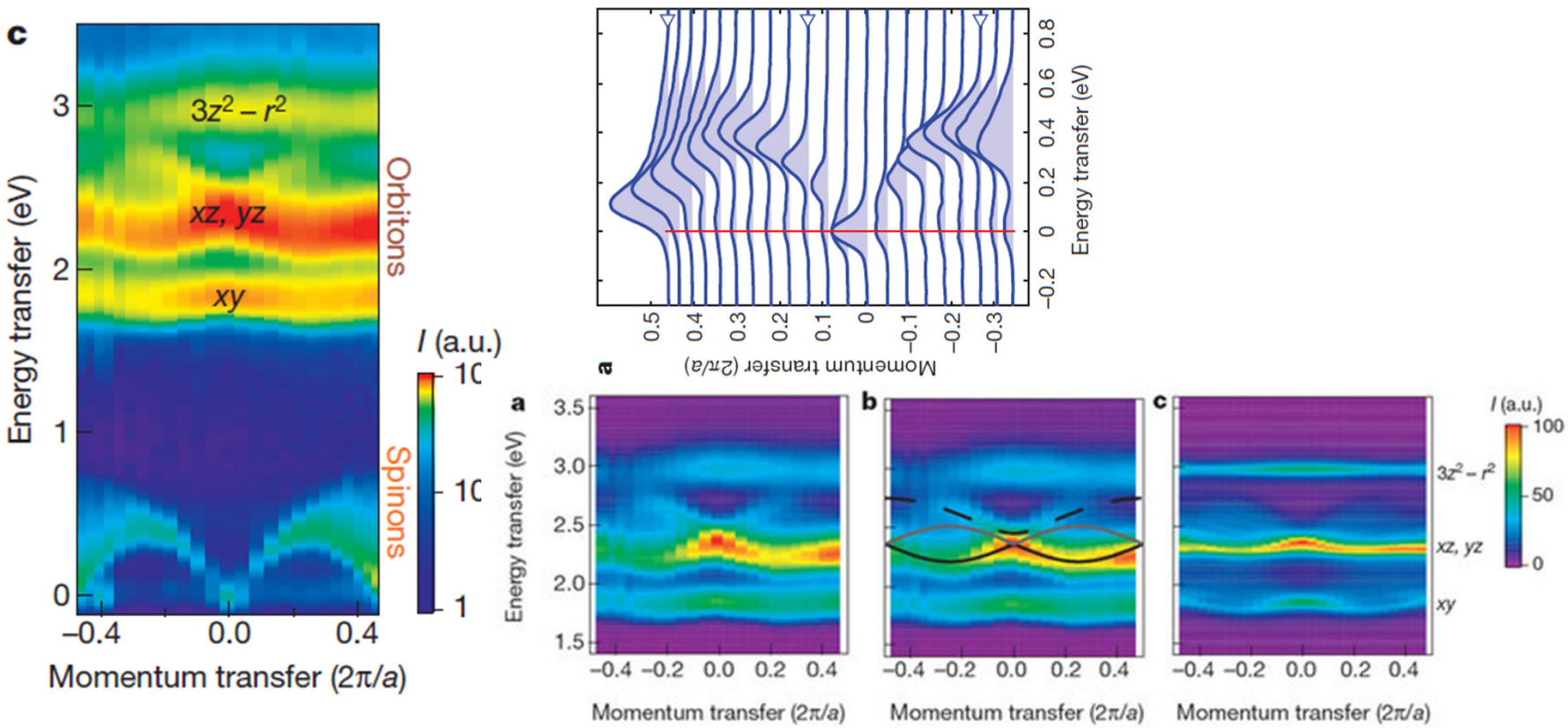


Figure from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

More criticism of Schlappa, *et al.*

- The authors appear to milk their data, recycling the same data in plot after plot (see Figures 1, 3, and 4 below).



Figures from J. Schlappa, *et al.*, Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3 *Nature* **485**, 82 (2012).

Citation analysis

- This article was published on May 3, 2012, and has been cited eight times since then. Citing papers include
  - Another RIXS experiment involving magnetic excitations in the 2D material La_2CuO_4[1]
  - A review article on spin-orbital entanglement in transition metal oxides[2]
  - A computational paper on the one-dimensional antiferromagnet $CaIrO_3$[3]
- No citing publications focus on orbitons, perhaps because the paper is so recent.

1. M.P.M. Dean, *et al.*, Spin excitations in a single La_2CuO_4 layer. *Nat. Mat.* **11**, 850 (2012).
2. Andrzej M. Oleś, Fingerprints of spin-orbital entanglement in transition metal oxides. *J. Phys.: Condens. Matter* **24** 313201 (2012).
3. Post-perovskite $CaIrO_3$: A j = 1/2 quasi-one-dimensional antiferromagnet. *Phys. Rev. B* **85**, 235147 (2012).

Acknowledgements

This presentation was based on the paper “Spin-orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3” by J. Schlappa, *et al.*

We gratefully acknowledge useful suggestions and criticism from Dr. Cooper.