

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

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It was suggested decades ago and then experimentally verified in the 90s that the electron's spin and charge degree of freedom can separate provided the electrons strongly interact and their motion is confined to one dimension. Here we discuss the case when also the orbital degree of freedom of an electron in the Mott insulator can separate as recently theoretically investigated and experimentally observed in the resonant inelastic x-ray scattering on Sr_2CuO_3 .

The strong Coulomb repulsion between the $\sim 10^{23}$ electrons in transition metal oxide crystals leads to peculiar collective behaviours of electrons and hence various, at first sight counterintuitive, phenomena. One of them is the apparent separation of the two quantum numbers of an electron - the spin $\hbar/2$ and charge e - which happens when the strongly interacting many body electron system is confined into one dimension (1D) [1].

This spin-charge separation phenomenon, as observed in e.g. quasi-1D spin chain of Sr_2CuO_3 [cf. Fig. 1(d)], can be explained as follows: Firstly, the repulsion between electrons in the last valence orbital of the Cu ion in Sr_2CuO_3 crystal is so strong that the electrons almost 'freeze', i.e. become localized on the Cu ions, and there is only a very 'small shuttle' motion of electrons which lowers the energy of the system but which is allowed when the spins of the neighbouring localized electrons form a particular antiparallel (called antiferromagnetic) alignment, cf. Fig. 1(d). Secondly, an even more interesting situation occurs when one of the electrons is taken out from the chain, as e.g. in the angular resolved photoemission (ARPES) experiment, cf. Fig. 1(b). Then the remaining empty site (called a hole) in such a spin chain is formed and this can become mobile in the chain, since when an electron moves and fills in the empty site, the total interaction energy of the system stays unchanged. Next, however, it occurs that when the hole moves, its two quantum numbers, which describe spin and charge, separate: the spin quantum number moves via the so-called spin flips of the spins of the electrons

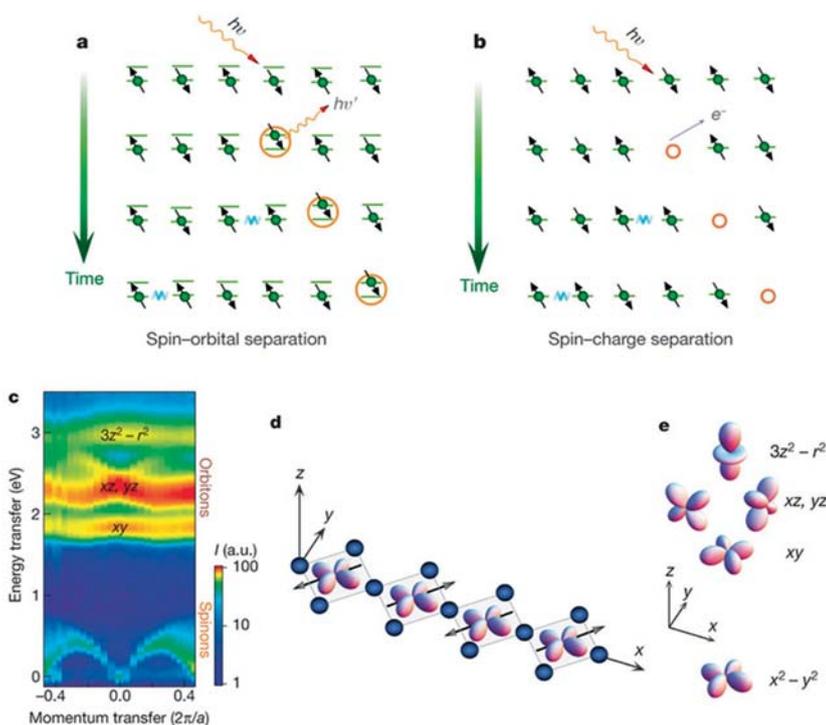


Fig. 1: Spin-orbital separation process in an antiferromagnetic spin chain, emerging after exciting an orbital. **a-b**, Sketch of spin-orbital separation (**a**) and spin-charge separation (**b**), generated in a RIXS and ARPES process, respectively. **c**, RIXS intensity map of the dispersing spin- and orbital excitations in Sr_2CuO_3 vs. photon-momentum transfer along the chains and photon-energy transfer (for details see [3]) - note the large dispersion (~ 0.2 eV) of a π period feature observed between 2.0 and 2.8 eV energy transfer which is the proof of the spin-orbital separation. **d**, Geometry of the CuO_3 chain in Sr_2CuO_3 with the ground state copper $3d x^2-y^2$ orbitals in the middle of each plaquette and oxygen sites at the plaquette corners. **e**, Orbital symmetries of x^2-y^2 and excited $3d$ orbitals. In panels (**c-e**) 'hole' language is used (for details see [3]). Figure adopted from Ref. [3].

while the charge moves via a simple filling of the empty sites by hopping. Although this phenomenon, called spin-charge separation, may sound like a purely theoretical speculation, it indeed was observed in a number of ARPES experiments on various quasi-1D cuprate oxides [2].

The spin-orbital separation phenomenon reported in Ref. [3], in which the IFW team played a leading role in developing the theory, concerns a related yet an entirely novel mechanism. Firstly, it should be noted that due to the binding to the atomic nucleus the electron not only has spin and charge but also an angular momentum quantum number 'corresponding to the quantized atomic orbital it occupies (e.g., *s*, *p* or *d*)' [3]. So, as noted in Ref. [3]: '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' and thus one could indeed talk about separation of spin and orbital quantum numbers. Second, in contrast to the above mentioned ARPES experiment, the electron is now not 'entirely' taken out from the spin chain. Instead in the here discussed resonant inelastic x-ray scattering (RIXS) experiment, the electron is merely moved to another orbital, cf. Fig. 1(a), and forms a so-called orbital excitation.

Nevertheless, the main result of Ref. [3] suggests that, similarly to the above spin-charge separation case, such orbital excitation in the spin chain can move and, moreover, when it moves, again the electron quantum numbers separate - this time, these are the spin and orbital quantum numbers, cf. Fig 1(a). Although the detailed theoretical description of the spin-orbital separation is significantly more involved than of the spin-charge separation [3, 4], its experimental verification in RIXS has turned out to be equally undoubtful: the very well-resolved spectrum shown in Fig. 1(c) clearly shows separate spinon and orbiton branches (for details see caption of Fig. 1) which proves that the spin and orbital quantum numbers indeed separate.

[1] T. Giamarchi „Quantum Physics in One Dimension“ (Clarendon Press, Oxford, 2004) and references therein.

[2] C. Kim et al. Phys. Rev. Lett. 77 (1996) 4054.

[3] J. Schlappa et al. Nature 485 (2012) 82.

[4] K. Wohlfeld et al. Phys. Rev. Lett. 107 (2012) 147201.

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