Summary on "Observing spinons and holons in 1D antiferromagnets using resonant inelastic x-ray scattering."

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We propose a method to observe spinon and anti-holon excitations at the oxygen K-edge of Sr_2CuO_3 using resonant inelastic x-ray scattering (RIXS). The evaluated RIXS spectra are rich, containing distinct two- and four-spinon excitations, dispersive antiholon excitations, and combinations thereof. Our results further highlight how RIXS complements inelastic neutron scattering experiments by accessing charge and spin components of fractionalized quasiparticles

Introduction:- One-dimensional (1D) magnetic systems are an important playground to study the effects of quasiparticle fractionalization [1], defined below. Hamiltonians of 1D models can be solved with high accuracy using analytical and numerical techniques, which is a good starting point to study strongly correlated systems. The fractionalization in 1D is an exotic phenomenon, in which electronic quasiparticle excitation breaks into charge ("*(anti)holon*"), spin ("*spinon*") and orbit ("*orbiton*") degree of freedom, and are observed at different characteristic energy scales. Spin-charge and spin-orbit separation have been observed using angle-resolved photoemission spectroscopy (ARPES) [2] and resonant inelastic x-ray spectroscopy (RIXS) [1], respectively.

RIXS is a spectroscopy technique that couples to spin, orbit and charge degree of freedom of the materials under study. Unlike spin-orbit, spin-charge separation has not been observed using RIXS to date. In our work, we propose a RIXS experiment that can observe spin-charge separation at the oxygen K-edge of doped Sr_2CuO_3, a prototype 1D material. Spin-orbit separation [1] and recently, four-spinon [3] was observed at Cu L_3-edge and oxygen K-edge, respectively of Sr_2CuO_3. Our proposed experiment requires Sr_2CuO_3 to be doped, which can indeed be doped with Zn, Ni or Co [4], making it an ideal material to test our prediction. We also predict that apart from spinon and holon, one can observe combinations of them. Our electron-doped 1D chain can shed some light on the nature of excitations in doped two-dimensional (2D) cuprates, which are of interest to the scientific community due to their superconducting nature. Recently, a gapped collective mode [5] was observed in electron-doped 2D cuprate using RIXS, but is absent in hole-doped. It was attributed to charge excitations, though the composition of this excitation is still an open question.

Methods: - Sr_2CuO_3 consists of CuO_4-plaquettes, namely a Cu at the center and four Os at the vertices of a square, that run along a chain and the ground state character is predominantly of the form $\alpha\left|d^9\underline{L}^0\right\rangle + \beta\left|d^{10}\underline{L}^1\right\rangle$ (with $\alpha \approx 0.8$), where d refers to Cu and L to O. We integrate out the oxygen in the model and assume a net-spin moment on the Cu-atom that couples *antiferromagnetically* in the chain. The low energy excitations of Sr_2CuO_3 are studied using a t-J model, and the Hamiltonian is given by $H = -t\sum_{i,\sigma} c^{\dagger}_{i,\sigma}\, c_{i,\sigma} + J\sum_i(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \hat{n}_i\, \hat{n}_{i+1})$. Here, $c_{i,\sigma}$ annihilates a hole on site-*i* with spin-σ. $\boldsymbol{S}_i$ and $\hat{n}_i$ are the spin and hole-occupancy at site-*i*. Also, t and J are the hopping and *super-exchange* parameters used in the model.

To capture the RIXS spectra, we use Kramers-Heisenberg formalism [6], which is given by $I_{RIXS} = \sum_f \left|A_{fi}\right|^2 \delta(E_f - E_g + \Omega)$. Here, the RIXS spectral function is given by $A_{fi} =$

$\sum_{i,n} e^{iq\cdot R_i} \frac{\langle f|D^\dagger|n\rangle\langle n|D|i\rangle}{E_g+\omega_{in}-E_n+i\Gamma_n}$. $|i\rangle, |f\rangle, |n\rangle$ are the ground, final and intermediates states with E_g, E_f, and E_n energies, respectively. Γ_n is a lifetime broadening for the intermediate-state. Here, the dipole operator, $D = \sum_{i,\sigma}(d_{i,\sigma} - d_{i+1,\sigma}), s_{i,\sigma}^\dagger$. $s_{i,\sigma}^\dagger$ creates a core hole in the orbital 1s of oxygen, and the relative phase between $d_{i,\sigma}$ and $d_{i+1,\sigma}$ is to account for the phase of hybridizing $2p$-orbital of oxygen in the cuprate. The core-hole on oxygen locally modifies the *super-exchange* between two adjacent copper atoms.

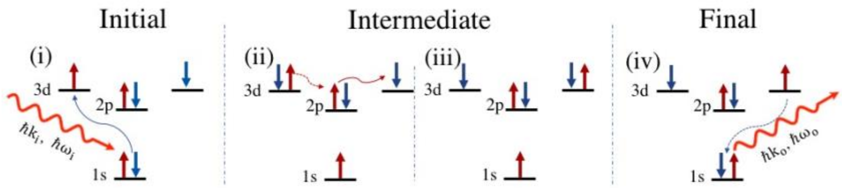

Figure 1: Spin flip mechanism at the oxygen K-edge. Hybridization between the Cu and O orbitals allows an incident photon to excite an O 1s electron into the $3d_{x^2-y^2}$ orbital on one of the two neighboring Cu sites, creating a Cu d^{10} upper Hubbard band excitation in the intermediate state (panel i). The d^{10} excitation can transfer to the other neighboring Cu site via two Cu-O hopping processes [(panel ii) & (panel iii)]. Finally, the extra electron decays back into the O 1s core level, leaving the system in a final state with a net double spin-flip (panel iv).

Direct spin flip is forbidden at this edge and the magnetic excitations occur via a double spin-flip mechanism as shown in **Figure 1**. The RIXS spectra shown in Figure 2 is calculated using the Lanczos method, a numerical method that allows to solve exactly a small cluster, on a 20-site cluster with a fixed number of holes in the system. Dynamical spin $[S(q,\omega)]$ and charge $[N(q,\omega)]$ structure factor were also calculated using an approximate but very accurate technique called density matrix renormalization group (DMRG) on an 80-site lattice to clarify the nature of the evaluated RIXS excitations.

<u>*Results*</u>: - RIXS spectra for the doped 1D AFM chain is shown in Figure 2. Figure 2(a) and Figure 2(b) shows the RIXS spectra for 5% and 10% electron-doping, respectively in the 1D chain. Figure 2(c), Figure 2(d), and Figure 2(e) are the cuts at $q = (\frac{\pi}{a}, \frac{\pi}{2a})$ and 0, respectively for the 1D doped chain compared to an undoped.

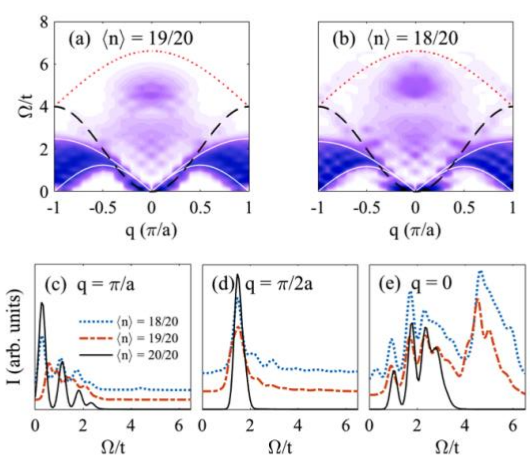

Figure 2. Calculated RIXS spectra at for N = 20 site doped t-J chain with (a) one (b) two electrons-doping. The white, black and red lines overlay shows the boundaries for TS-continuum, antiholonic excitation and upper bound for antiholon-TS excitations, respectively. Panels (c), (d), and (e) compare the doped RIXS spectra with the undoped case for momentum transfers of q = $(\frac{\pi}{a}, \frac{\pi}{2a})$, and 0, respectively.

In the evaluated RIXS spectra, there are four basic features: i) a continuum within the white overlay below 2.5t ($\approx \pi J$), ii) a continuum, predominantly at q = 0 and below 4t in energy but outside white overlay, iii) a cosine-like dispersing peak with bandwidth 4t highlighted by black line, iv) a continuum above 4t at q = 0 with an upper bound highlighted by red overlay.

The RIXS spectra can be explained by making use of the fact that spin-charge separation occurs in 1D; understanding the excited states as a product of non-interacting chargeless spin$-1/2$ "spinons" and spinless charge "anti-holons": $|\psi\rangle = |\psi_s\rangle \otimes |\psi_{\bar{h}}\rangle$ [7]. Spinon is defined by a dispersion relation given by $\omega_s(k) = \frac{\pi J}{2} |\sin(ka)| \; \forall \; k \in [0, \pi)$, and are always created in pairs in RIXS to preserve the total spin of the system. The band of one anti-holon is given approximatively by $\omega_{\bar{h}}(k) = -2t \; cos(ka + \phi) \; \forall \; k \in [0,2\pi)$ [8]. Using the idea of these fractionalized particles, it is concluded that the feature –(i) is due a predominantly two-spinon (TS) continuum, (ii) is four-spinon (FS) continuum, (iii) is an anti-holon excitation, and (iv) is a two-spinon anti-holon (TS-$\bar{h}$) continuum. Feature-(i) and (iii) are independently confirmed to be spinons and antiholons, respectively using DMRG calculations, which resemble $S(q,\omega)$] and $N(q,\omega)$, respectively (details not here).

Conclusion: - We have shown that spinon and anti-holons can be observed at the oxygen K-edge of doped Sr_2CuO_3. The low-energy RIXS spectra should consist of two-spinon (TS), four-spinon (FS), anti-holon and two-spinon anti-holon (TS- $\bar{h}$), which is understood in the picture of fractionalized particles. Expanding our analysis of the antiholonic picture to the 2D cuprate can shed light on the nature of gapped collective mode observed in electron-doped 2D cuprate [5].

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