Resonant Inelastic X-ray Spectroscopy on $LiCu_3O_3$

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Abstract

In this paper we investigate the resonant Soft X-ray spectra of $LiCu_3O_3$ on the copper$L_{2,3}$ edges. Various copper compunds exhibits a strong magnetic responce, whether ferromagnetic or antiferromagnetic, which is also the case in this material. It consists of 4 layers in the unit cell: 2 layers with CuO and 2 layers Cu^{1+}. In the later sections we have a look onto the optical spectra mentioned before and the x-ray absorption spectra. We further analyze the magnetic behaviour in terms of circular and linear magnetic dichroism. The resonant sofr x-ray spectra show a significant feature, namely one can directly extract the whole complex refractive index with no need of using the Kramers-Kronig transformation. Moreover the consistency of this relations (and its extensions for small energy ranges) can be investigated.

I. INTRODUCTION

In the past recent years there is a continuous growth in interest of developing new techniques of probing magnetic properties of transition metal (TM) compundsand rare earths (RE). Usually one would use the standard inelastic neutron scattering (INS) technique, but in the following paper we will introduce you to a developing technique to do so. Moreover the resonant inelastic x-ray scattering (RIXS) spectra provide one with various optical properties of the material. In general one directly obtains the real and imaginary part of the refractive index, which rises the possibility to develop new numerical methods for the Kramers-Kronig (KK) transformation, which are very useful in alayzing various data from optical measurments.

II. THEORETICAL BACKGROUND

The core understanding in x-ray spectroscopies lies in the us of sceond-order perturbation theory with a interaction hamiltonian directly related to the vector potential of the incoming wave. In general neglecting the interactionn bewtween electrons one can show that the vector potential $\vec{A}(\vec{r})$ enters the hamiltonian through the kinematic part of the energy, namely:

$$\hat{H} = \sum_i \frac{(\vec{p}_i - e\vec{A}_i)^2}{2m_i}, \tag{1}$$

where $\vec{p}_i$ and m_i are the momentum and mass of the i-th electron. Considering the interaction of the electrons, the ligand field and making use of Fermi's goldern rule one can obtain the RIXS amplitude as [1]:

$$\sigma(\hbar\omega, \hbar\omega') = \sum_f \left| \sum_n \frac{\langle f|\hat{D}_2|n\rangle\langle n|\hat{D}_1|i\rangle}{E_n - E_g - \hbar\omega - i\Gamma_i} \right|^2 \times \delta(\hbar\omega - \hbar\omega' + E_g - E_f), \tag{2}$$

where $\hat{\vec{D}}_{1,2} = \vec{\epsilon}_{1,2} \cdot \hat{\vec{p}}\ exp(\pm\vec{k}_{1,2} \cdot \vec{r})$ is the dipole transition operator with $\vec{\epsilon}_{1,2}$ and $\vec{k}_{1,2}$ being the polarisation and wave vector of the incoming (1) and outgoing (2) wave. The ground, intermediate and final states are denoted as $|i\rangle$, $|n\rangle$ and $|f\rangle$ respectively, where the sum is taken out over all intermediate and final states. The corresponding energies to these states are: E_i, E_n and E_f. The Fig.1 shows the common RIXS process, which involves core hole-electron coulomb interaction, causeing the creation of a hole in the valence shell.

*A thank you or further information

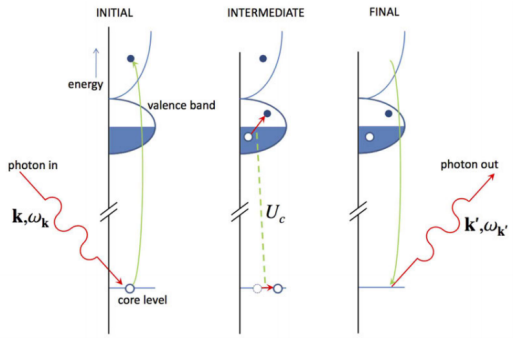

Figure 1: *Typical RIXS process involving creaion of a hole in the valence shell due to core hole-electron coulomb interaction [3] (Pciture taken from [3])*

III. Polarization

IV. RIXS spectra

V. X-ray Absorption Spectroscopy

As mentioned before RISX can be essentially seperated into x-ray absorption (XAS) and x-ray photoemission spectroscopy (XPS) with some intermediate interaction described by the green's function of the Kramers-Heisenberg Hamiltonian. The XAS spectrum is directly proprtional to the absorption of the crystal which gives information on magnetic properties of the material. The difference in the absorption using left- and right-cirular polarized x-rays in claed circular magnetic x-ray dichroism (CMXD) (the similiar differnec in linear polarized light is called LMXD). In order to obtain the CMXD one needs to preserve only the relevant resonances at the copper L_3 and L_2 edges, which means one needs to model and substract the background assossiated with the excitation of the core electrons into the continuum. The way to do so is to use user-defined bakground function (using for example the arcus tangent) or using the shirley algorithm [4, 5], this is shown in the Fig. S2. One directly notice that the Shirley algorithm is fitting the backgound much better. Thus for different polarizations this method was used and the corresponing aborption spectra ar drawn in Fig.S3. Now one can proceed to evaluate the CMXD and

Table 1: *Example table*

Name		
First name	Last Name	Grade
John	Doe	7.5
Richard	Miles	2

LMXD on the copper L edges

As was stated by Haverkort [6] one can use the absorption spectra and their corresponding polarizations to evaluate the conductivity tensor. First of all it is needed to use symmetries to break down the form of the tensor. The relation mentioned in [6] is

VI. Results

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$$e = mc^2 \tag{3}$$

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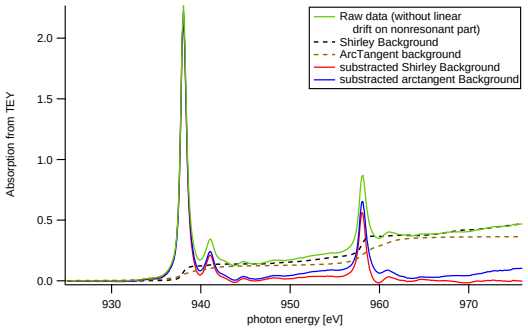

Figure 2: *Absorption spectra and modelled background with two different methods*

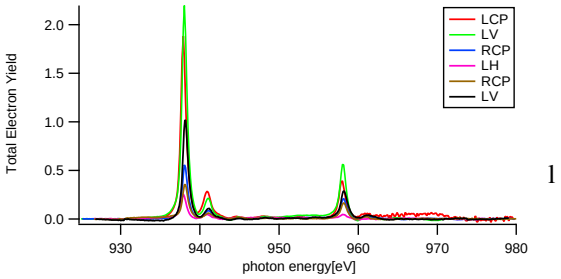

Figure 3: *Absorption spectra and modelled background with two different methods*

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VII. Discussion

i. Subsection One

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ii. Subsection Two

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