ESRF	**Experiment title:** Magnetic signal in the Pseudogap phase of $YBa_2Cu_3O_{7-\delta}$	**Experiment number**: HC-5304
Beamline: BM28	**Date of experiment**: from: 26/04/2023 to: 02/05/2023	**Date of report**: 13/09/2023
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Report: Experiment HC-5304 was performed on an untwinned $YBa_2Cu_3O_{6.6}$ sample with a Tc of 63K and a T* around 230K. Measurements were performed with the following configuration : horizontal geometry, π –incident polarisation, a Pt 400 analyser selected the diffracted beam polarisation ($\pi'/\boldsymbol{\sigma}'$) and a point like detector. The sample was placed under a Be dome allowing a cooling from room temperature to 5K using a cold finger. Energy was tuned around copper K-edge (8.997keV) with a Si 111 monochromator. Three main potential signals were investigated during the experiment :

- First, [0 K 0] and [0 K -0.5] reciprocal space positionsd with K=1.5, 2.5, 3.5 was searched by performing H, K and L scans to find the q=1/2 magnetic signal shown to exist in Polarised Neutron diffraction Experiments [1].
- Then, we investigated the [0 K 0] reciprocal space postions were a q=0 Magnetic signal has been observed in both YBCO [2] and $HgBa_2CuO_{4-\delta}$ [3] cuprates by Polarised Neutron Diffraction by doing H and K scans for different temperature and azimutal angle.
- Eventually, the structure of the K-egde of Cu, on the 010 Bragg peak and slighlty off in K, was studied by performing a serie of energy scans at 100K in both polarisation channels.

We will therefore divide this report in three parts corresponding to three main signals investigated.

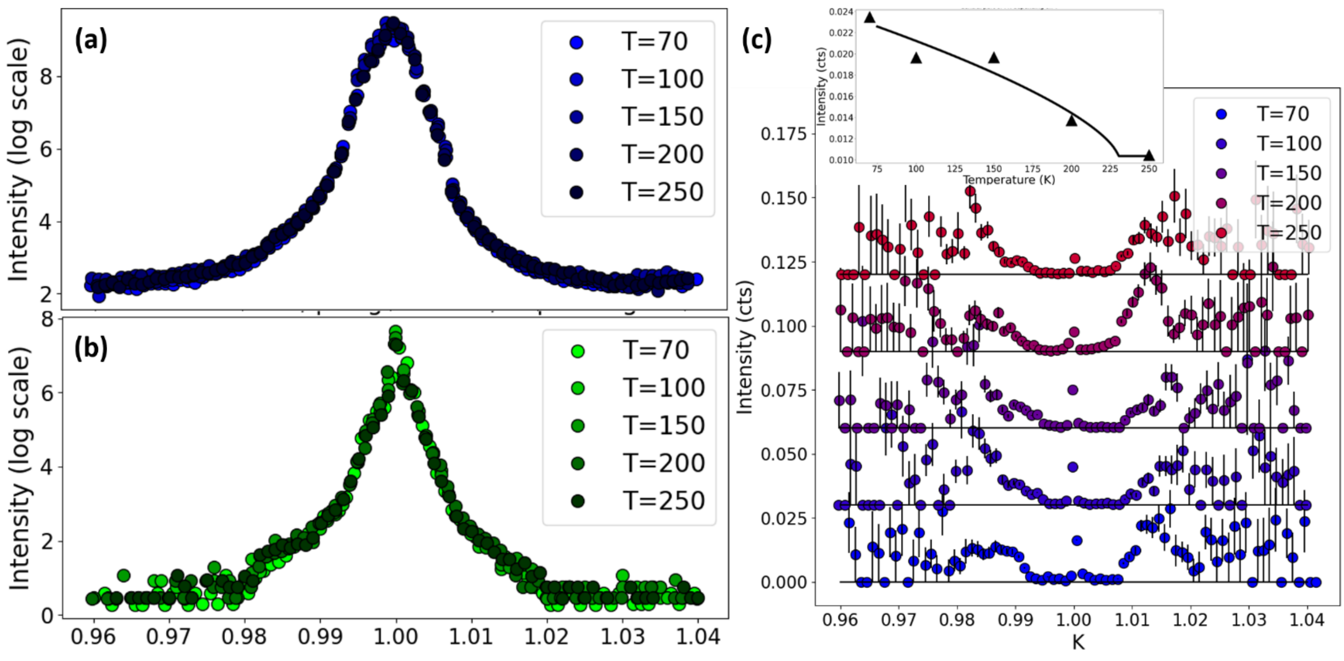

Fig 1. (a) π-π' channel intensity around 010 depending on K at various Temperatures. (b) π–$\boldsymbol{\sigma}$' channel intensity around 010 depending on K at various Temperatures. Data have been fitted by a Pseudo-Voight function then centered on 010 by shifting the fit maximum to K=1 to account for misalignement at each temperature. (c) Flipping ratio around 010 depending on K at various T. The Inset shows the Flipping ratio central intensity summed over 5 points. Error bars caused by statistical uncertainty are smaller than a point. However, other sources of uncertainty caused by data treatement might occur. The black line is an order parameter fit of the data with fixed T* = 230K which gives the function 0.016*(T/230 - 1)^0.67 as a result.

I. CDW and q=1/2 Magnetism

Before searching for the q=1/2 magnetism we looked for the CDW signature in cuprates that should exist at both [0 1.695 0] and [0 1.305 0] [4]. This signal is very weak and is so of the order of magnetude of the one expected from the q=1/2 magnetism, also weak in PND experiments. However, despite an important counting time of up to 20mn by points at some positions we were unable to observed the CDW peaks. Then, we moved on to the [0 K 0] (K=1.5,2.5,3.5) positions but scans there also show no peak above background for the same counting time.

II. q=0 Magnetism teemperature dependence

K scans have been performed on the 010 Bragg at various temperaturs in both π-π' and π-$\boldsymbol{\sigma}$' polarisation channels. The goal of the measurement was to look for differences in shape of the Bragg peak between π-π' and π-$\boldsymbol{\sigma}$' which could be related to a magnetic contribution in the π-$\boldsymbol{\sigma}$' channel. For theoretical reasons we expect the q=0 magnetic contribution found in cuprates to generate a contribution in the π-$\boldsymbol{\sigma}$' to the 010 Bragg peak. Data shows that the Bragg peak in the π-π' channel have a pretty "round" top wheras the π-$\boldsymbol{\sigma}$' ones are more "sharp" **(Fig 1-a,b)**. The general shape and intensity of the peak does not change when increasing temperature up to 250K above the T* of the Pseudogap. By plotting the flipping ratio of the tow channels **(Fig 1-c)** defined as :

$$FR = \frac{I_{\pi-\sigma\prime}}{I_{\pi-\pi\prime}}$$

we observed two effects. First the flipping ratio shows for each temperature an increase in the tail of the peaks caused by the π-$\boldsymbol{\sigma}$' peak being wider than the π-π' one. This enlargement would be the kind of effect expected from a magnetic contribution but this effect does not disappear nor decrease significatively in temperature with suggests it is not caused by the magnetic q=0 signal observed in the Pseudogap by PND. The origin of the enlargement is thus unclear and may lie in a difference of resonnant contribution to the peak between π-π' and π-$\boldsymbol{\sigma}$' channels near the K-edge. Nevertheless, a small peak also appear at the center of the Flipping ratio scan caused by the variation of shape between both polarisations with the π-$\boldsymbol{\sigma}$' one being sharper. Interestingly this sharp Flipping ratio central peak decreases in temperature and is reduced at 250K **(Fig 2,c Inset)**. It thus seems to follow the pseudogap Phase in temperature which indicate it could be the resonnant diffraction equivalaent of the q=0 magnetic signal found by PND.

III. K-edge structure on and slightly off 010

Eventually, energy scans have also been performed on the 010 Bragg peak and at slighlty off K position relative to the peak at 100 K in both polarisation channels. In the π-$\boldsymbol{\sigma}$' at the 010 position we see a sharp peak at 8.9825eV, copper pre-edge energy where Cu 3d orbitals have the most contribution to resonnance **(Fig-2,a)**. By going slightly off the 010 position we see that this structure endures and widens in shape up to spread on the total range of the K-edge from 8.975 to 8.995eV. Such a structure could be related to a resonnant process involving Cu 3d orbital. However its maximum energy increases as we go slighlty off the Bragg peak going up to 8.988 in **Fig 2,d**. It goes against the idea of a resonnant process and tend to point more toward a multiple scattering origin. An azimutal angle (ψ) dependence of the structure could settle the question as multiple scattering peaks quickly disappear in ψ but this have not been performed during this experiment due to lack of time. FDMNES caculations are also in progress to see if we can simulate the structure and confirm a resonnant scattering origin.

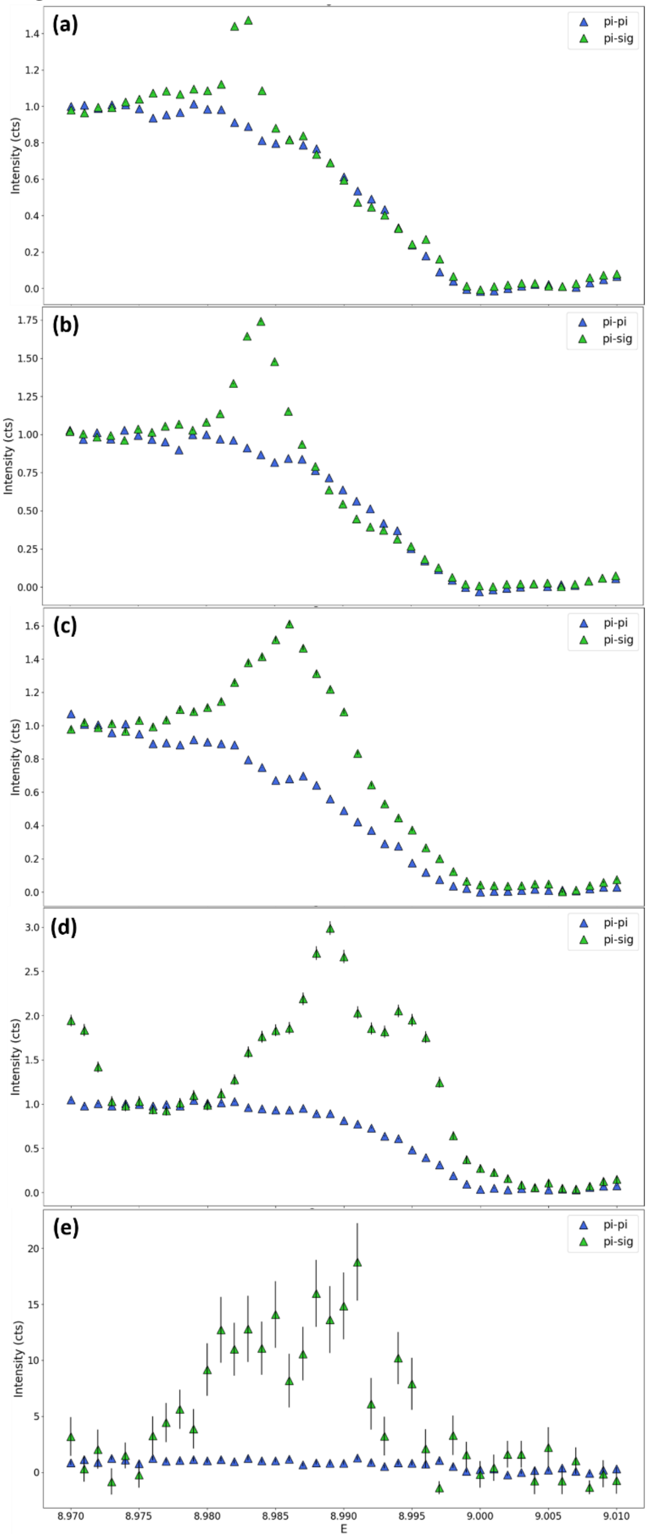

Fig 2. Energy scans around K-edge on respectively : the 010 Bragg peak, slighly of the peak at [0 1-δ 0] (a), [0 1-2δ 0] (b), [0 1-3δ 0] (c) and [0 1-12δ 0] (d) where δ=0.00139 in both polarisation channels. The average of the 10 last point of the scan have been substracted as a background and the average of the first 6 points of the scan have been normlised to unity except for (d) where the normalisation have been done on the 4 to 9 point.

IV. References

[1] D. Bounoua et al, Com Phys 5, (2022) [2] L. Mangin-Thro et al, Nat Com, (2015) [3] Y. Li et al, Nat Lett, (2008) [4] J. Chang et al, Nat Phys 8, (2012)