Experimental Report

21/02/2014

Proposal:	**4-01-1298**	**Council:**	10/2012	
Title:	Evolution of the zone boundary anomalies in lightly doped La2-xSrxCuO4			
This proposal is continuation of: 4-01-1166				
Research Area:	Physics			
Main proposer:	**RONNOW Henrik**			
Experimental Team:	CHRISTENSEN Niels Bech LANCON Diane PRSA Krunoslav			
Local Contact:	JIMENEZ-RUIZ Monica			
Samples:	La2CuO4 La2-xSrxCuO4, x=0.09			
Instrument	**Req. Days**	**All. Days**	**From**	**To**
IN1	8	7	15/03/2013	22/03/2013

Abstract:

We have discovered anomalies in the spin wave energy and intensity at the (ð,0) point along the zone boundary in the 2D Heisenberg antiferromagnet Cu(DCOO)2•4D2O and in the undoped parent compounds of the high-temperature cuprate superconductors La2-xSrxCuO4 and YBa2Cu3O6+y. This anomaly may be related to RVB-type correlations, and hence the clue to how upon doping the cuprates turn from antiferromagnets to superconductors. A first experiment was performed on IN1 to test this hypothesis, however due to instrumental difficulties only half of the given beamtime could be used. For La2CuO4, the spin wave peaks at very high energy transfer were detected on the IN1 spectrometer with sufficient intensity, which shows the feasibility of the experiment. We therefore propose a continuation of the investigation on the evolution of the zone boundary anomalies upon weak (0-9%) doping and thus ask for 8 days of beamtime.

Experimental report for proposal 4-01-1298

Background

La_2CuO_4 is the parent compound of a high temperature superconductors. It shows antiferromagnetic Heisenberg coupling of spin 1/2 in a 2D square lattice geometry with very weak interplane coupling. Through studies of an insulating physical realisation of the 2D square lattice antiferromagnet Cu(DCOO)24D2O, we have discovered a profound deviation from this renormalized classical behaviour. According to linear spin-wave theory, there should be no dispersion along the zone boundary from $Q = (\pi/2, \pi/2)$ to $(\pi, 0)$, and also no change in the spin-wave amplitude. Yet, There is a 6% decrease the in zone boundary energy at the $(\pi, 0)$ point. Furthermore, the surprising result was that the relatively small 6% zone boundary dispersion is accompanied by an enormous 50% reduction in spin wave amplitude at the $(\pi, 0)$ point.
This discovery has been verified by numerical expansion and quantum Monte Carlo calculations, which however do not shed any light on its origin. The zone boundary anomaly occurs at $(\pi, 0)$, which for antiferromagnetic coupling corresponds to the nearest neighbour distance along the bonds of the lattice. Hence, there must be some sort of correlations between neighbouring spins, not captured by linear spin-wave theory. One type of candidate are RVB correlation. Indeed a variational approach mixing the RVB state and the Neel state to achieve the correct ordered moment the staggered flux phase predicts zone boundary dispersion and intensity variation in the right direction, albeit not quantitatively correct.
If this is the fingerprint of RVB-type correlations, it is of interest to investigate how these correlations evolve as antiferromagnetic order is suppressed by small amounts of doping in the cuprates. Measurements on La_2CuO_4 revealed a zone boundary dispersion opposite to that of the 2DQHAFSL , which can be explained by a four-spin ring-exchange interaction appearing due to the finite hopping matrix element in the cuprates [8]. Yet, both La_2CuO_4 and undoped YBa2Cu3O6+x display the same intensity and line-shape effect as CFTD, which lead to the question how this effect evolve upon doping.

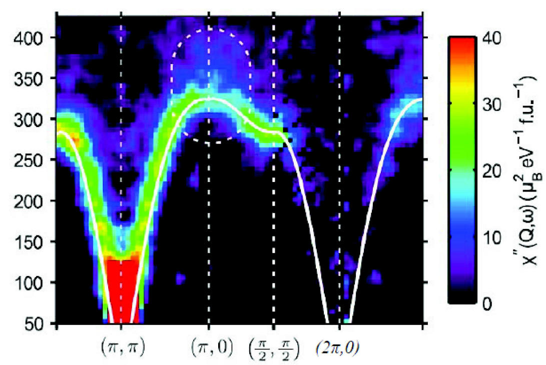


Figure 1: Spin wave dispersion in undoped La_2CuO_4 showing a 13% ZB maximum at $(\pi, 0)$. [2]

This experiment was an attempt to use the specificity of hot neutron triple axis spectrometry to obtain high quality energy scans at the $(\pi, 0)$ and $(\pi/2, \pi/2)$ positions for the case of the undoped La_2CuO_4 compound and the moderately underdoped (x=0.09)$La_{2-x}Sr_xCuO_4$ at energies transfers up to 360 meV.

Experimental set-up

The IN1 spectrometer was in the W configuration with a Cu331 monochromator to maximize the flux at high incident energy, and a Cu200 analyser. Two choices of fixed k_f were tried : $k_f = 7.5$ Å^{-1} and $k_f = 8.5$ Å^{-1}. Each choice of k_f was accompanied by the according choice of filters to remove strong spurious signal such as the second harmonics and higher contamination. Erbium, samarium, indium and hafnium were tried, in front or after the sample. Two difference choices of collimations were also tried : open configuration and 40' collimation before monochromator and analyser.
The La_2CuO_4 sample was aligned with the reciprocal axis a* and b* in the scattering plane. The sample was placed in a cryostat with a large diameter vacuum box (110 cm) and cooled to 2.5 K.

Measurements

Part 1 We attempted to detect the spin wave at both $(\pi, 0)$ and $(\pi/2, \pi/2)$ Q equivalent points with energy scans from 200 to 360 meV. $(\pi, 0)$ and $(\pi/2, \pi/2)$ equivalents were at large Q values, which was necessary to close the scattering triangle at such high energy transfers. The figure shows the results for a number of Q points with the following set-up: $k_f = 8.5$ Å^{-1}, an erbium filter, 17 mn per points, no collimation.

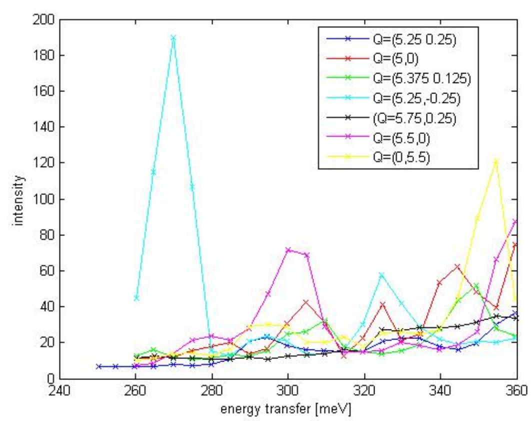
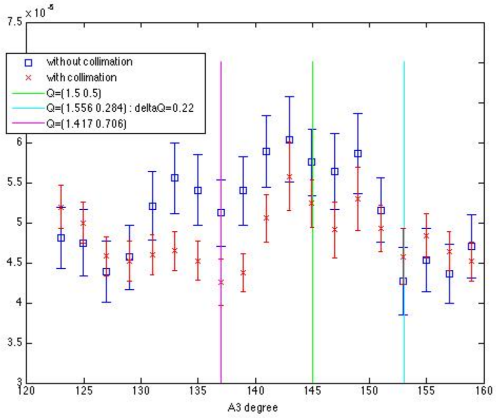


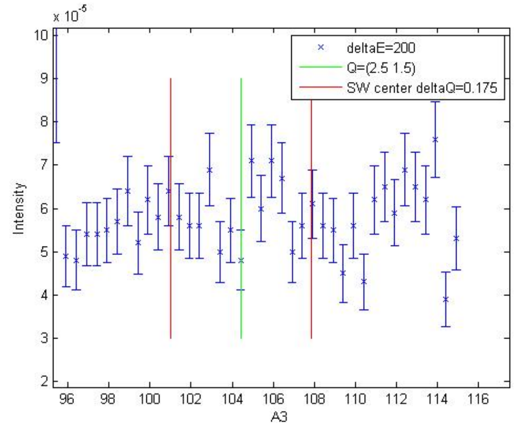
Figure 2: Energy scans at Q equivalents of $(\pi, 0)$ and $(\pi/2, \pi/2)$, with $k_f = 8.5$ Å^{-1}

The scans show a lot of spurious signals with a lot of variation depending on the Q position in the brillouin zone, some of which easily identified as higher harmonics. The spin wave signal (expected depending on the Q point between 280 and 320 meV) could not be extracted from this data.

Part 2 In order to identify the energy upperbound at which we are able to detect the spin wave, we did a series of scans at lower energy transfers at the $(\pi/2, \pi/2)$ position. With a fixed set-up of $k_f = 7.5$ Å^{-1}, we tried the two collimation possibilities and used indium and hafnium filters. The result of this study consists of A3 scans around $(\pi/2, \pi/2)$ position performed at energy transfers ΔE =50,75,100 and 200 meV. Shown here are the scans at ΔE =100 and 200 meV where the spin wave and its double peak feature is shown at 100 meV but is not clearly visible at 175 meV.



(a) A3 scan around Q=($\pi/2, \pi/2$) at fixed energy transfer ΔE =100 meV, both with and without collimation. Lines indicate corresponding points in Q spaces



(b) A3 scan around Q=($\pi/2, \pi/2$) at fixed energy transfer ΔE =200 meV, without collimation

Figure 3: A3 scans at fixed energy transfers around Q=($\pi/2, \pi/2$)

References

[1] P. W. Anderson, P. A. Lee, M. Randeria et al., *J Phys. Condens. Matter 16* **R755** 2004

[2] N. Headings, SM Hayden et al. *Phys. Rev. Lett.* **105** 2010

[3] R. Coldea et al. *Phys. Rev. Lett.* **86** 2001

[4] H. M. Ronnow et al. *Phys. Rev. Lett.* **87** 2001