

<b>Proposal:</b>	<b>4-01-1295</b>	<b>Council:</b>	10/2012	
<b>Title:</b>	SeCuO3 – coupled cluster system close to criticality			
<b>This proposal is a new proposal</b>				
<b>Research Area:</b>	Physics			
<b>Main proposer:</b>	<b>ZIVKOVIC Ivica</b>			
<b>Experimental Team:</b>	PRSA Krunoslav SURIJA Vinko			
<b>Local Contact:</b>	BOEHM Martin			
<b>Samples:</b>	SeCuO3			
<b>Instrument</b>	<b>Req. Days</b>	<b>All. Days</b>	<b>From</b>	<b>To</b>
IN8	7	7	07/05/2013	14/05/2013
<b>Abstract:</b> A monoclinic system SeCuO3 has been proposed to consist of linear segments of 4 copper ions, tetramers, with a strong intra-tetramer interactions (~200 K) and with a 3D magnetic order occurring at only 8 K. It represents a rare example of a system where the transition from long-ranged, collective states into local quantum states can be investigated. We plan to perform the initial investigation of magnetic excitations below and above the ordering temperature.				

## Experimental report of the inelastic neutron scattering on $\text{SeCuO}_3$

$\text{SeCuO}_3$  crystallizes in a monoclinic space group  $P2_1/n$  with two distinctive copper sites Cu1 and Cu2 in the unit cell. In our recent publication [1] we have shown that the magnetism of this compound can be modeled as consisting of weakly coupled, localized, magnetic tetramers ( $\text{Cu2} - \text{Cu1} - \text{Cu1} - \text{Cu2}$ ), with intra-tetramer couplings  $J_{11} \sim 220$  K and  $J_{12} \sim 160$  K. The weak inter-tetramer coupling leads to the commensurate 3D antiferromagnetic ordering at  $T_N = 8$  K.

Since isolated tetramers exhibit a singlet ground state, it is especially interesting to observe how this localized picture evolves into 3D spin waves. To this end we have performed an inelastic neutron scattering experiment with thermal neutrons at the IN8 instrument. The sample was  $15 \times 5 \times 5 \text{ mm}^3$  in size, with a mass of around 0.5 g and it has been placed so that the scattering plane has contained vectors  $[101]$  and  $[010]$ . The monochromator used was PG002 and the neutron's final momentum was fixed at  $k_F = 2.662 \text{ \AA}^{-1}$ . We have focused our investigation around (030) Bragg point because of the largest difference in intensities above and below  $T_N$ .

With thermal neutrons we were able to spot two modes: a high energy flat mode around 27 meV and a low energy, possibly acoustic, mode around 2 meV. During the experiment we have also detected a spurion around 17 meV which has been removed from the analysis (the confirmation that it is a spurion has been later attained through the measurements on EIGER instrument at PSI).

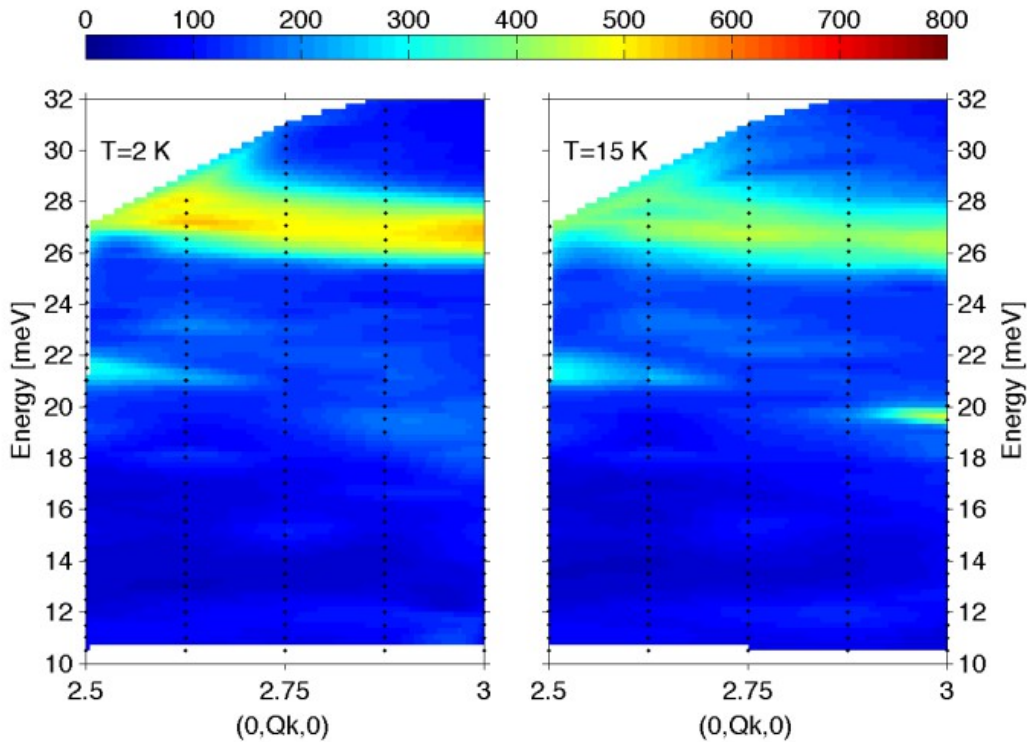


FIG. 1: Longitudinal high energy excitations. Units are counts per minute.

Longitudinal scans  $(0, Qk, 0)$  reveal a weak intensity dependence on the wave vector which might be related to the expected singlet-triplet oscillations.

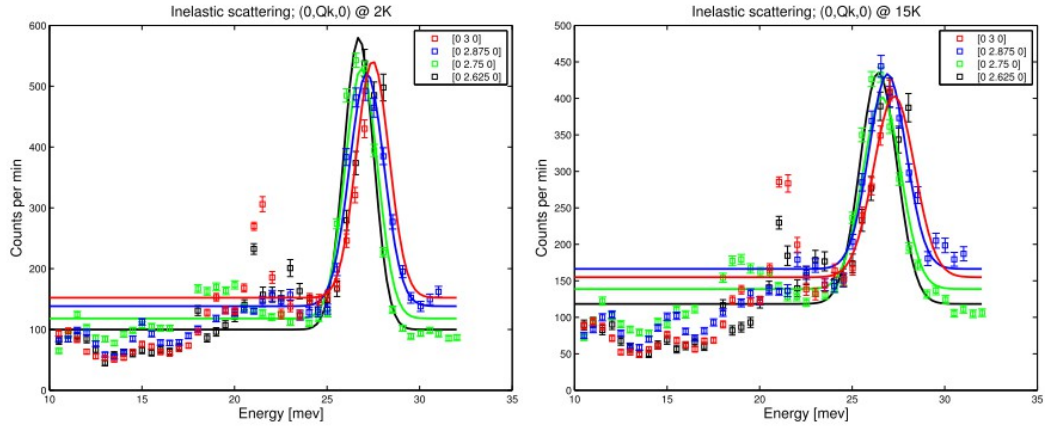


FIG. 2: Longitudinal high energy excitations below (left) and above (right) the transition temperature. Solid lines are Gaussian fits.

On the other hand, the scans along  $(Qk,0,Qk)$  show practically negligible intensity dependence.

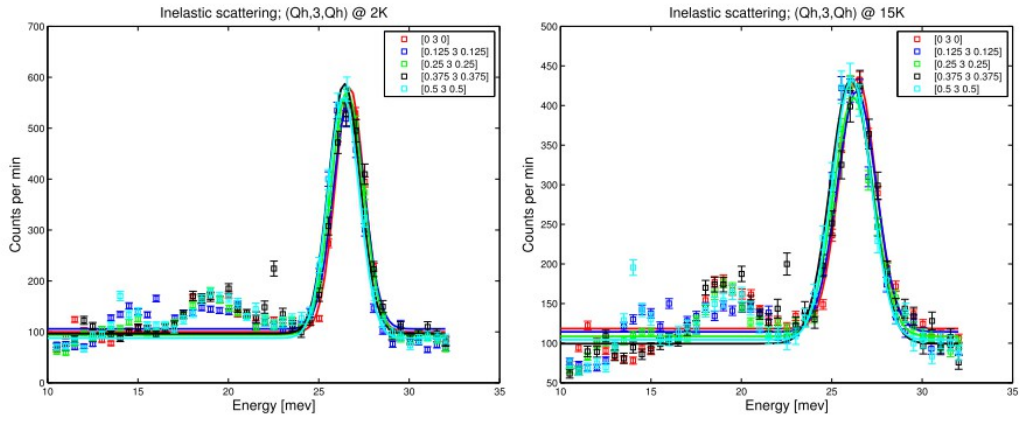


FIG. 3: Transversal high energy excitations below (left) and above (right) the transition temperature. Solid lines are Gaussian fits.

The temperature dependence of the  $(030)$  excitation reveals a gradual decrease in intensity, indicating the magnetic origin.

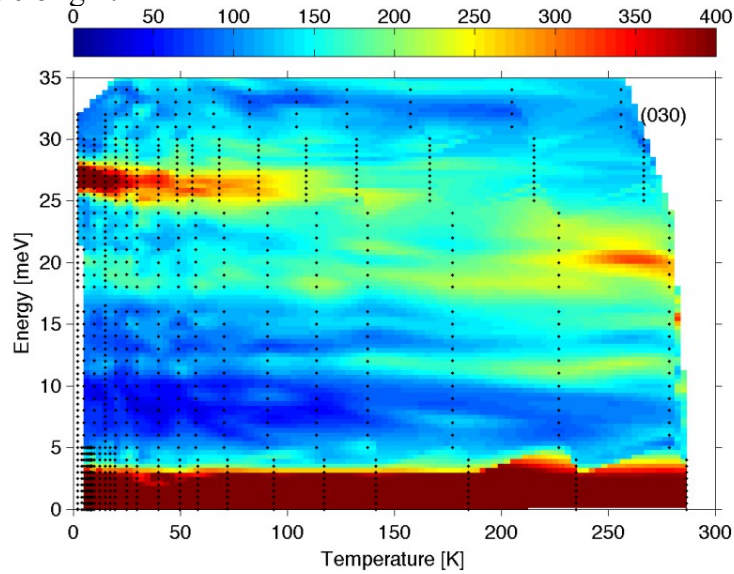


FIG. 4: Temperature scan of the  $(030)$  excitation around 27 meV.

We have also investigated the temperature dependence of the low-energy excitation around 2 meV. Its disappearance above  $T_N$  indicates that it is an acoustic mode related to the long range antiferromagnetic order.

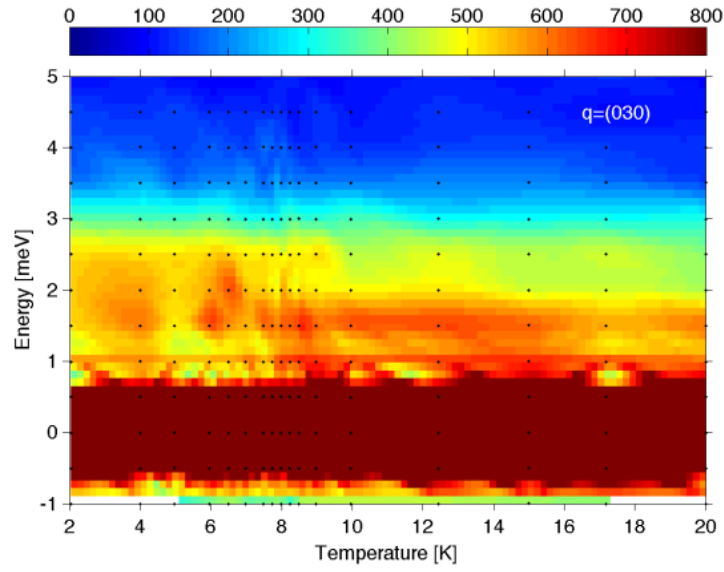


FIG. 5: Temperature scan of the (030) excitation around 2 meV.

[1] I. Živković *et. al.*, Phys. Rev. B, **86**, 054405 (2012).