Experimental report

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Proposal:	**4-01-1512**	**Council:**	4/2016

Title: Investigation of a frustrated quantum magnet with novel interaction scheme

Research area: Physics

This proposal is a new proposal

Main proposer: **Shravani CHILLAL**

Experimental team: Shravani CHILLAL
Bella LAKE

Local contacts: Paul STEFFENS

Samples: SrCuTe2O6

Instrument	Requested days	Allocated days	From	To
THALES	7	6	24/06/2016	30/06/2016

Abstract:

SrCuTe2O6 consists of a 3-dimensional arrangement of spin-1/2 Cu ions. The 1st, 2nd and 3rd neighbor interactions respectively couple Cu2+ into a network of isolated triangles,a highly frustrated hyperkagome lattice consisting of corner sharing triangles and antiferromagnetic chains. Of these, the chain interaction dominates in SrCuTe2O6 while the other two interactions lead to frustrated interchain coupling giving rise to long range magnetic order, however, at suppressed temperatures. This is in contrast to ideal spin-1/2 antiferromagnetic chain which is expected to have a spin liquid ground state with no long-range magnetic order and spinon excitations. Frustrated interchain coupling leads to weak long-range order and modifies the low energy excitation spectrum in a way that reflects the underlying physics arising from the frustration. Therefore, we wish to explore the magnetic excitations of this quantum magnet using inelastic neutron scattering on the THALES spectrometer together with the multiplexed analyzer/detector and the single detector systems. Hence, we request a beamtime of 7 days.

Investigation of a frustrated quantum magnet with novel interaction scheme

$SrCuTe_2O_6$ is a new quantum magnet crystallizing in cubic symmetry (space group $P4_132$ [1]) with the magnetic spin-1/2 Cu^{2+} ions occupying a single Wyckoff site. The Cu^{2+} ions are coupled together by exchange interactions J_1, J_2 and J_3 which in turn, couple them into isolated equilateral triangles, a highly frustrated hyperkagome lattice (network or corner sharing triangles) and uniform chains (running parallel to the **a**, **b**, and **c** axes) respectively. Together, these interactions can give rise to a frustrated network of chains. The DC susceptibility measurements of $SrCuTe_2O_6$ reveal a broad maximum at 32K, which is reminiscent of a one-dimensional spin-1/2 Heisenberg antiferromagnet. The susceptibility can be fitted to a 1D chain model for chain interaction J_3= 49K (4.22meV) [2]. Further, the First principles electronic structure calculations also confirm the 1D nature of the magnetism in the system and find that J_3 is 45K. These calculations also suggest that J_1, J_2 are also significant enough leading to frustrated interchain coupling. This is further confirmed experimentally by the appearance of two successive magnetic transitions at T_{N1}=5.5K and T_{N2}=4.5K in DC susceptibility and heat capacity data [2,3,4].

Ideally, a spin-1/2 AF chain is expected to have a spin liquid ground state with no long range order (LRO) and only spinon continuum instead of the sharp magnon modes. The spinon continuum forms a sinusoidal modulation of the excitation spectra originating at the 1D zone centre with an upper bound of $\pi*J_{chain}$ and a lower bound of $\pi/2*J_{chain}$. The addition of a frustrated interchain coupling chains could give rise to LRO and modify the excitation spectra such that ordered spins affect the low energies while 1D chains still dominate the higher energies. In case of $SrCuTe_2O_6$, we expect the upper and lower bounds of the spinon continuum to be at approximately 14mev and 7mev respectively originating at (1,0,0). A sharp spin wave dispersion is expected at lower energies due to the small frustrated interchain coupling at the 3D AF zone centre. In this experiment we explore both parts of the magnetic excitations in $SrCuTe_2O_6$ using inelastic neutron scattering. For this purpose we make use of two co-aligned single crystals of $SrCuTe_2O_6$ (see Figure 1) oriented in the <hh0>/<00l> scattering plane so that the high symmetric cubic directions <001>, <110> and <111> are accessible for the measurement. To obtain an overview of the magnetic excitation spectra at various energy transfers ranging from 0.5meV – 8meV at 2K and 8K (which correspond to the temperatures above and below the magnetic transitions), we make use of the multi analyser/detector system.

Figure 1 Picture of the single crystal alignment used for the THALES

In first part of the experiment, the excitation spectra is obtained at higher energy which reveal the one dimensional nature of the interactions in the system, in the form of streaks perpendicular (along <hh0>) to the chain direction *c* (<00l>). This feature is visible both above (8K) and below (2K) the magnetic transition temperature as can be seen in Figures 2a-b for energy transfer of 6meV. The excitations above T_N are broader compared to the 2K because of the thermal broadening. As the system has three mutually perpendicular chains running parallel to crystalline *a, b* and *c* directions, we also observe streaks parallel to <001> direction. These streaks are stronger in intensity than the other direction because it is a superposition of two other chains running along *a* and *b* directions.

The effect of magnetic ordering is visible at lower energies. This is clearly evident in Figure 2c-d. At high temperatures, the plot still shows the signatures of the 1D behaviour, i.e., streaks running along <00l> and <hh0> directions, as expected. However, at 2K, the streaks are replaced by sharp blobs of intensity that come as a result of a steep spinwave dispersion of the long range ordered state. This behaviour is very similar to the prototypical 1D chain compound $KCuF_3$, where the antiferromagnetically coupled 1D chains are interacting by a weak ferromagnetic coupling [5]. Therefore, we can conclude that the frustrated J1 and J2 couplings in $SrCuTe_2O_6$ provide the necessary interchain interactions that consequently force the one dimensional system into a three dimensional magnetic order at lower temperatures.

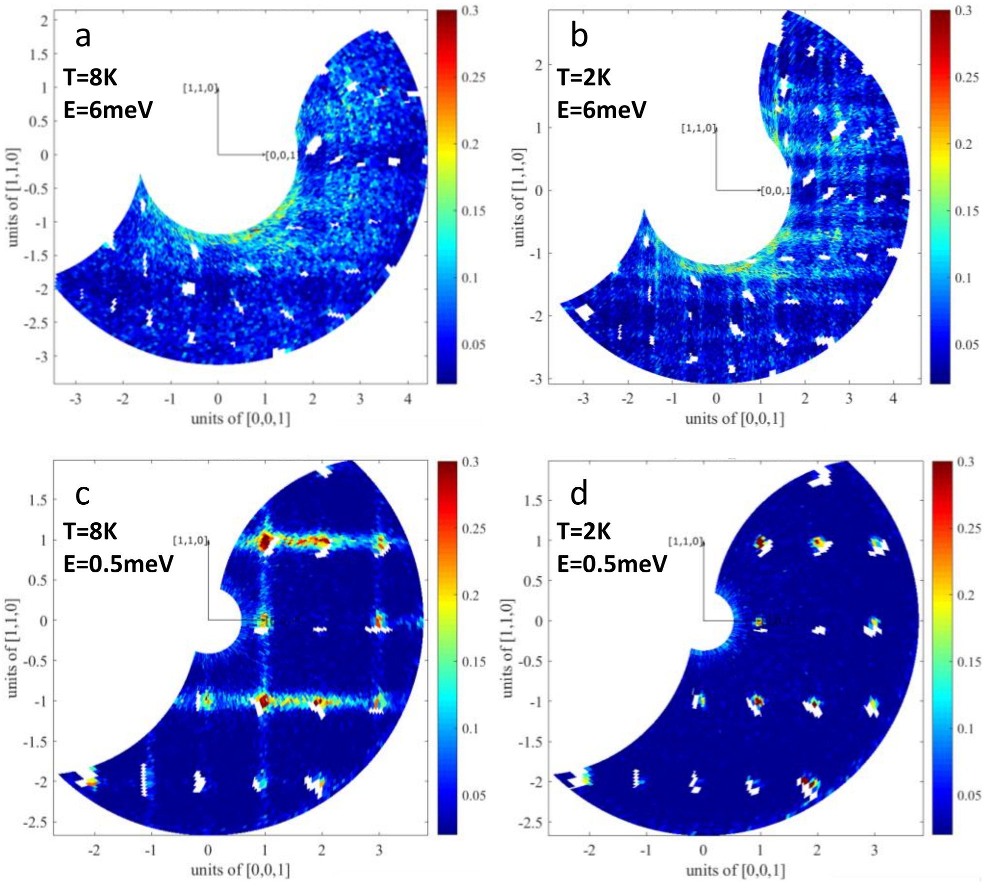

Figure 2: The constant ebergy maps of $SrCuTe_2O_6$ at energy transfers of 6 meV and 0.5 mev at 2K (below T_N) and 8K (above T_N).

References:

[1] L. Wulff, and H. Muller-Buschbaum, Zeitschrift fur Naturforschung **52** 1341 (1997)
[2] N. Ahmed et.al., Phys. Rev B **91** 214413 (2015)
[3] B. Koteswararao et.al., J.Phys.:Condens. Matter **27** 426001 (2015)
[4] B. Koteswararao et.al., APL Mater. **4**, 036101 (2016)
[5] B. Lake et.al., Nature materials **4**, 329 (2005)