Experimental report

10/09/2018

Proposal: 5-42-379 **Council:** 4/2014

Title: 24-spin clusters in the mineral boleite: correlations in spin-liquid droplets?

Research area: Physics

This proposal is a new proposal

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Samples: boleite/KPb26Ag9Cu24Cl62(OH)48

Instrument	Requested days	Allocated days	From	To
IN3	0	5		
IN12	3	0		
D7	7	7	01/10/2014	08/10/2014

Abstract:

The crystal structure of the mineral boleite contains Cu2+ ions (each with S=1/2) forming truncated cube clusters of linked triangles. Susceptibility, neutron scattering and exact diagonalization calculations suggest that effective S=1/2 degrees of freedom emerge on the triangles, followed by condensation of these into a singlet state at lower temperature. We hypothesize that the resulting cube of effective S=1/2 degrees of freedom is a fragment of the full S=1/2 dimer problem on the cubic lattice, where a spin liquid groundstate exists. The clusters in boleite afford an intermediate situation, accessible to both experiment and exact diagonalization, in which a spin liquid "droplet" can be studied. Here we propose to characterize the wavevector and temperature dependence of the spin correlations.

24-spin clusters in the mineral Boleite: correlations in spin-liquid droplets? D7, September 2014

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Unconventional ground states and excitations, combined with the possibility of direct connection with quantum many body theories, drive the study of low dimensional, frustrated, magnetic materials with $S = 1/2$ magnetic moments [1]. Boleite ($KPb_{26}Ag_9Cu_{24}Cl_{62}(OH)_{48}$) has so far only been studied crystallographically at room temperature [2, 3]. We here report the preliminary findings of the elastic neutron studies performed at D7, ILL on 2.2 g of the mineral Boleite.

An interesting possibility in frustrated magnets is the formation of composite degrees of freedom from small clusters of spins. For example, in $La_3Cu_2VO_9$ [4], strongly coupled clusters of four triangles of $S = 1/2$ are thought to form effective $S = 1/2$ degrees of freedom, which in turn begin to interact, and may then form a spin liquid at low temperature. The mineral Boleite ($KPb_{26}Ag_9Cu_{24}Cl_{62}(OH)_{48}$) contains highly frustrated 24-atom clusters of Cu^{2+} ions as shown in figure 1. The triangles are formed by oxygen mediated bond with an angle of 125.15°. Between the triangles are side bond also formed by oxygen bridges with an angle of 94.65°. This is shown in figure 1.

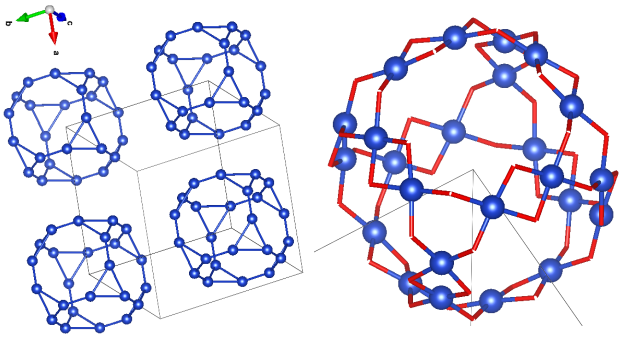

Figure 1: **Left:** A simple illustration of four Copper clusters leaving out all other atoms in the unit cell. **Right:** One Copper cluster with 24 atoms drawn with the mediating oxygen bonds.

We performed two elastic experiments at D7 on the same sample of Boleite. The 7 crystals were co-aligned and mounted on an Al holder without use of glue in the (h h k) plane, as shown in figure 2. The system is cubic with a lattice parameter of a=15.128 Å at 2 K.

Figure 2: Photo of the co-aligned samples on the aluminum holder with a total mass of 2182 mg.

Results

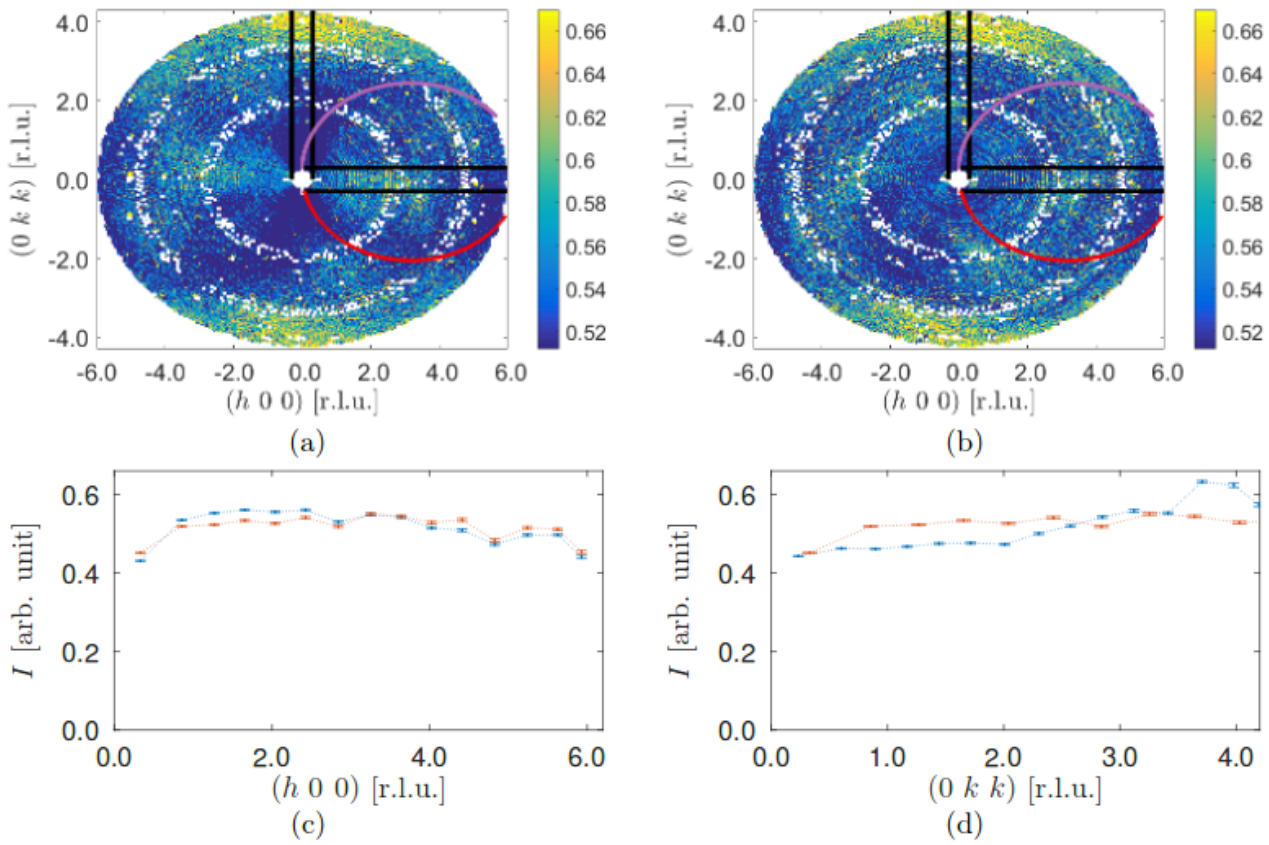

Figure 3: The NSI neutron scattering component separated from the total scattering from boleite by polarization analysis on D7. Color plot of energy integrated NSI neutron scattering intensity at T= 1.5 K (a) and T= 300 K (b). The colorscale, shown to the right of the plots, are given in arbitrary units. The overlayed colored and curved lines represent the position in (h k k) of a single sample holder pillarâs absorption of incoming (red) and outgoing (purple) neutrons from the center of the sample holder. The overlayed straight black lines show the area in q-space of the 1D plot of the NSI scattering intensity along (h 0 0), shown in (c), and (0 k k), shown in (d). The NSI scattering intensity in (c-d) is binned and shown for both T= 1.5 K (blue) and T= 300 K (red).

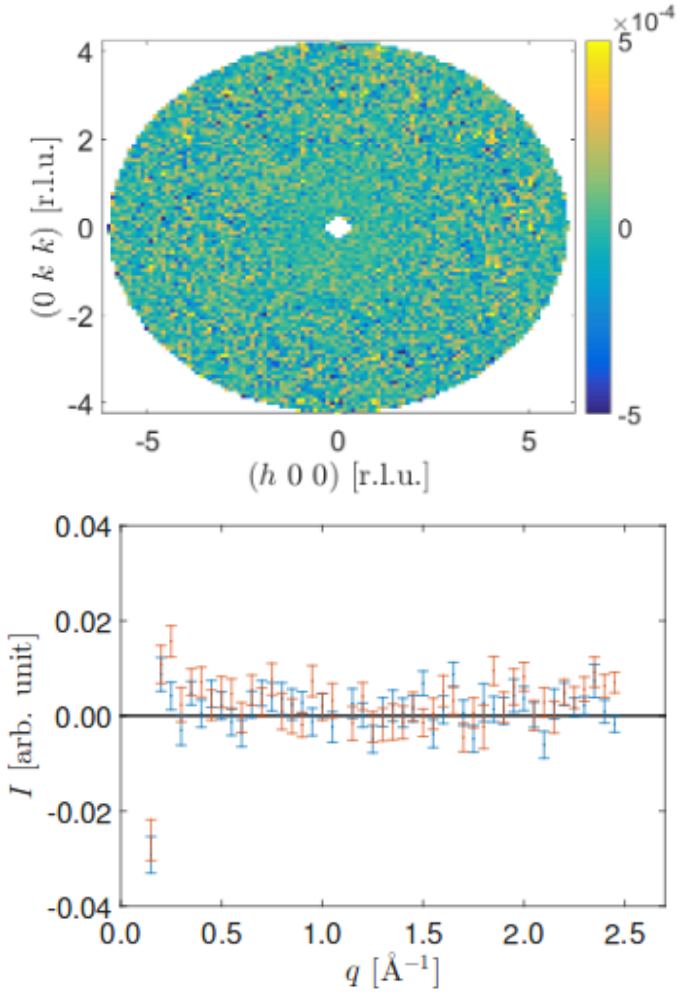

Figure 4: The magnetic scattering component from boleite. The intensity is normalized to peak intensity of the NSI scattering component, for T = 1.5 K. The magnetic and NSI scattering components are separated with polarized neutron analysis on D7. (Top) Magnetic scattering component as function og (h k k), at T= 1.5K. (Bottom) Powder average of magnetic scattering component of the total scattering from boleite, at T= 1.5 K (blue) and T= 300 K (red)

[1] B. Normand et al., Cont. Phys. **50**, 533 (2009)

[2] R. C. Rouse, Journ. of Solid State Chem. **6**, 86-92 (1973)

[3] M. Cooper et al., CA Mineralogist **38**, 801 (2000)

[4] J. Robert, *et. al*, Phys. Rev. B **77**, 054421 (2008)

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