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

<table>
<thead>
<tr>
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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 \cite{1}. Boleite (KPb\textsubscript{26}Ag\textsubscript{9}Cu\textsubscript{24}Cl\textsubscript{62}(OH)\textsubscript{48}) has so far only been studied crystallographically at room temperature \cite{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\textsubscript{3}Cu\textsubscript{2}VO\textsubscript{9} \cite{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\textsubscript{26}Ag\textsubscript{9}Cu\textsubscript{24}Cl\textsubscript{62}(OH)\textsubscript{48}) contains highly frustrated 24-atom clusters of Cu\textsuperscript{2+} ions as shown in figure 1. The triangles are formed by oxygen mediated bond with an angle of 125.15\degree. Between the triangles are side bond also formed by oxygen bridges with an angle of 94.65\degree. This is shown in figure 1.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{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.}
\end{figure}

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 \AA at 2 K.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure2.png}
\caption{Photo of the co-aligned samples on the aluminum holder with a total mass of 2182 mg.}
\end{figure}
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 pillar’s 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 of $(h k l)$, at $T= 1.5$K. (Bottom) Powder average of magnetic scattering component of the total scattering from boleite, at $T= 1.5$ K (blue) and $T= 300$ K (red)


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Instrument: D7