Contribution ID : **66** Type : **Oral**

Comparing inelastic neutron scattering with theory to understand the complex magnetic interactions in a low-dimensional frustrated magnet

Friday, 13 November 2020 11:50 (12)

Frustrated magnetic systems have gained a lot of recent interest as they can exhibit exotic magnetic quantum states such as spin-liquid and spin-nematic states [1,2]. The natural mineral atacamite, $Cu_2Cl(OH)_3$, is one such material which has been reported to exhibit magnetic behaviour characteristic of a frustrated quantum magnet [3]. It also shares structural similarity with another cuprate, herbertsmithite, whose kagomé lattice is predicted to host a spin liquid ground state [4].

Little is understood about the magnetic properties of the natural orthorhombic structure of atacamite in contrast to its other structural polymorphs. This work studies this lesser understood orthorhombic atacamite, where Cu^{2+} ions form a pyrochlore lattice. The novel magnetic interactions and quantum states in materials like atacamite lends itself to spintronic applications where understanding spin interactions can unveil opportunities for intentionally manipulating these spins.

Time-of-flight inelastic neutron scattering measurements on single crystalline atacamite have been performed at Pelican with an incident wavelength of 4.69Å. Excitations were observed at 1.5K, and weakened as temperature was increased beyond the antiferromagnetic transition temperature of T_N = 9.0K [5] to 20K. The strongest dispersion was found along the H00 direction with two nested modes observed up to an energy transfer of 3meV. Relatively weak dispersion was seen along 00L, and a flat mode was observed in out-of-plane scattering covering a narrow section in 0K0.

Ab initio band structure calculations have indicated a 1D sawtooth chain model for the dominant magnetic exchange paths in atacamite [6]. This chain model can be consolidated with our neutron scattering measurements and SpinW calculations. However, the relative magnitudes and directions of the predicted exchange couplings indicate the strongest interactions to be along 0K0, and this does not agree with the strongest dispersion measured experimentally in the H00 direction at zero field.

To better understand the interactions in atacamite, in-field time-of-flight measurements have also been conducted in magnetic fields up to 6.5T, applied along the crystallographic *b*-axis. Data were collected using Pelican and the new open geometry, fully compensated, 7T vertical magnet.

We will present the results of these inelastic neutron scattering measurements along with corresponding SpinW calculations to address the inconsistencies between theory and data when considering the exchange interactions in atacamite.

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Session Classification : Magnetism & Condensed Matter

Track Classification : Magnetism & Condensed Matter