Experimental report

14/05/2025

Proposal: 4-05-879 **Council:** 4/2023

Title: Unravelling the nature of the magnetic exchange in a model spin dimersystem

Research area: Physics

This proposal is a new proposal

Main proposer: Leonie Christine SPITZ

Experimental team: Leonie Christine SPITZ
Federico PISANI

Local contacts: Bjorn FAK

Samples: Cu(DCOO)2 4D2O

Instrument	Requested days	Allocated days	From	To
PANTHER	2	1	05/06/2024	07/06/2024

Abstract:

The magnetic exchange interactions in low-dimensional quantum spin systems are a central focus in the search for the origin of the electron pairing mechanism giving rise to high temperature superconductivity. This lead to a surge in interest in simple model systems in which to study the nature of magnetic exchange. Cu(II) acetate, which hosts strongly coupled Cu2+ spin pairs which are almost isolated from other pairs, has attracted interest as a simple model system due to its many favorable characteristics and suitability for a range of different experimental techniques. However, the nature of the magnetic exchange between neighboring Cu2+ spins has never been experimentally verified. We propose to fill this gap by studying the magnetic form factor of the singlet-triplet transition in Cu(II) acetate using inelastic neutron scattering. Its momentum dependence will give us the necessary information to distinguish between direct exchange and a superexchange mechanism. The knowledge of the nature of the magnetic exchange in Cu(II) acetate will pave the way to pioneering time-resolved out-of-equilibrium studies on this low-dimensional quantum magnet.

Description of the experiment

In this experiment, we measured the momentum dependent neutron magnetic form factor of the singlet to triplet transition of the isolated antiferromagnetic Heisenberg dimers in Cu(II) acetate monodeuterate at the thermal TOF neutron spectrometer PANTHER. A single crystal weighing 3.25 g was mounted on an aluminum sample holder and oriented with its b-axis vertical in order to have the (*H0L*) plane in the equatorial plane of the instrument. Spectra were collected at a base temperature of *1.5K* at an incident energy of E_i *= 76 meV* in rotation steps of 1°.

Results

The singlet to triplet transition was found at *ΔE = 36.5 meV* as shown in figure 1a. Figure 1b shows its momentum dependence in the *(H0L)* plane. The dimers are oriented along *(1 0 -1),* and exist in two opposite orientations along the *b*-axis. Hence, we measure a projection of the dimer in the *(H0L)* plane.

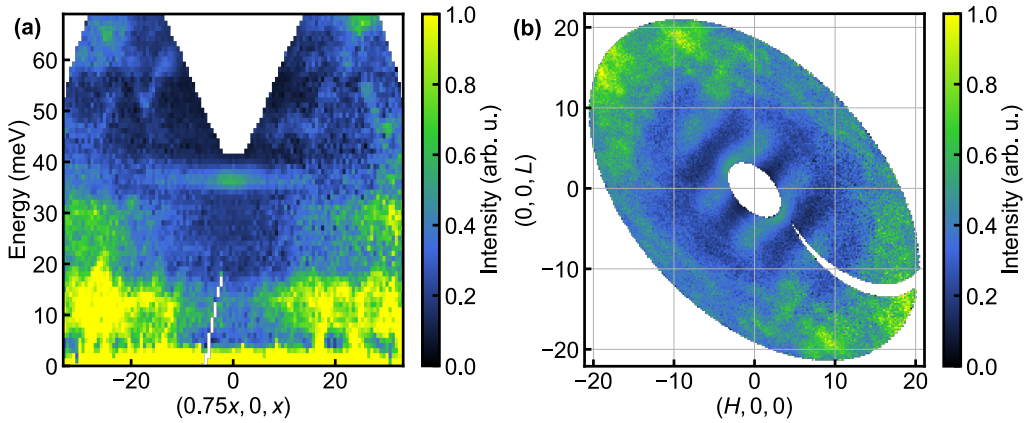


Figure 1: Neutron differential cross section of the singlet to triplet excitation at *ΔE = 36.5* meV. (a) Energy versus reciprocal space cut centred at (3.45 0 -3.28) with integration range *-0.3 ≤ K ≤ 0.3* showing the singlet-to-triplet excitation. (b) Constant energy cut with integration range *35 ≤ E ≤ 38* meV.

The component of the spectral function $S_{zz}(k,\omega)$ forms parallel rods perpendicular to the dimer axis. Figure 2a shows the measured neutron magnetic form factor along such a rod, while 2b shows the oscillating intensity along the dimer axis which follows

$$S_{zz}(k,\omega) \propto (1-\cos(k\cdot R))\delta(\hbar\omega + \Delta E)$$

where *R* is the distance between the Cu atoms in a dimer projected on the *(H0L)* plane. This simple model was used to fit the oscillations in Figure 2b.

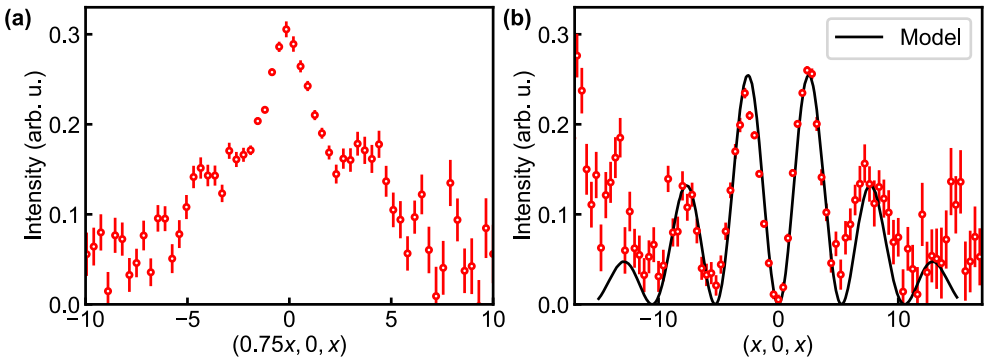


Figure 2: Cuts of the neutron magnetic form factor perpendicular (a) and parallel (b) to the dimer axis with integration ranges $0.3 \leq K \leq 0.3$ and $33 \leq E \leq 39$ meV.

Outlook

We are in the midst of performing calculations of the neutron magnetic form factor that will allow us to retrieve information on the symmetry of the electronic wave functions and with it the nature of the magnetic exchange interactions between the Cu^{2+} ions.