Experimental report

19/12/2016

Proposal:	**4-04-457**	**Council:**	4/2012
Title:	Spin dynamics in dimers of entangled Cr7Ni rings		
Research area:	Physics		

This proposal is a new proposal

Main proposer:	**Paolo SANTINI**
Experimental team:	Michael BAKER Simon ANSBRO Robert WOOLFSON George WHITEHEAD Tatiana GUIDI Alessandro CHIESA Giuseppe AMORETTI Paolo SANTINI Stefano CARRETTA
Local contacts:	Hannu MUTKA

Samples: {Cr7NiF3(C8H14NO5)(O2CC(CH3)3)15}2(N2C10H8)

Instrument	Requested days	Allocated days	From	To
IN5	10	7	27/05/2013 08/12/2014	29/05/2013 15/12/2014

Abstract:

Supramolecular complexes containing linked molecular nanomagnets (antiferromagnetic rings) have been demonstrated to display entanglement and to be excellent candidates for quantum infgormation processing. So far coupling and entanglement have only been demonstrated indirectly by macroscopic techniques like susceptibility or by fitting model hamiltonians to Electron Paramagnetic Resonance data. Inelastic neutron scattering can provide a much more direct characterization of the form of the coupling and of the associated ring-ring entanglement. In particular, the full pattern of real-space dynamical correlation functions between pairs of individual atomic spins can be extracted from INS data by exploiting the position-sensitive detectors of IN5.

we propose to study a supramolecular complex of two Cr7Ni rings linked through pyrazine. By applying an exernal field it will be possible to switch the ground-state structure from entangled to factorized, an to extract the resulting modification of the spin dynamics.

Spin dynamics in a dimer of entangled Cr_7Ni rings

Proposal number 4-04-457

Main proposer - Paolo Santini
Local contacts - Hannu Mutka, Jacques Ollivier

Participants
E. Garlatti , T. Guidi , S. Ansbro, P. Santini , G. Amoretti, J. Ollivier, H. Mutka,
G. Timco, I.J. Vitorica-Yrezabal, G.F.S. Whitehead, R.E.P. Winpenny, S. Carretta

Molecular nanomagnets (MNM) are molecules with a magnetic core surrounded by an organic ligand sheath, which acts to limit the number of possible exchange pathways. One of the most exciting applications for these compounds is in quantum information processing. A crucial resource for this application is entanglement and supramolecular systems of weakly coupled MNMs are an ideal playground to investigate it. So far entanglement between molecular subunits has only been experimentally demonstrated in a $(Cr_7Ni)_2$ dimer by exploiting susceptibility as an entanglement witness or by fitting a trial model Hamiltonian to EPR data. This system is a supramolecular cluster consisting of two antiferromagnetic Cr_7Ni-purple rings, linked through a pyrazine unit, directly connecting the two Ni ions (see Fig.1). This link leads to a weak exchange interaction between the two ions and thus to entangled eigenstates for the dimer.

By exploiting the $(Cr_7Ni)_2$ dimer as a benchmark, we want to demonstrate that through 4D-INS we can obtain a quantification of the entanglement by measuring $S(\mathbf{Q},\omega)$ in large portions of the reciprocal space. Indeed, the INS cross-section yields direct information on the dynamical inter-ring spin-spin correlations, which are a signature of entanglement between the qubits.

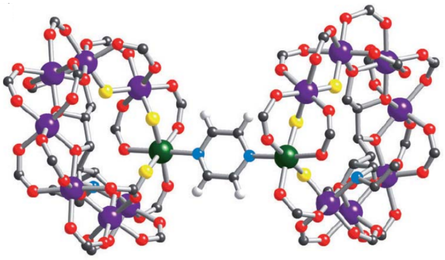

Figure 1: Molecular structure of the supramolecular dimer of formula $[Cr_7NiF_3(C_7H_{12}NO_5)(O_2CC(CH_3)_{15})]_2(N_2C_4H_4)$ (magenta, Cr; green, Ni; yellow, F; red, O; light blue, N; grey, C; $C(CH_3)_3$ groups and all H atoms omitted for clarity).

We have mapped out a large volume of $S(\mathbf{Q},\omega)$ for the $(Cr_7Ni)_2$ dimer using the time-of-flight spectrometer IN5. 6 single crystals were mounted in a specifically designed Al sample holder and covered in fomblin oil to protect the crystals.

Spectra were collected at wavelengths of 5 and 7.5 Å at a temperature of 1.2 K and a magnetic field of 2.5 T. The magnetic field was used to select a factorised ferromagnetic ground state for the dimer, so that we were able to investigate the entanglement between the rings in the entangled excited states. In addition, from an experimental point of view, in presence of a sizeable magnetic field we have been able to better resolve the small splitting between the two transitions from the factorised ground state towards the two entangled excited states (see Fig. 2).

The **Q**-dependence of the two low-energy excitations were explored by rotating the sample throughout the full 360 degrees for the 5 Å and throughout 180 degrees for the 7.5 Å data in 1 degree steps and then stitching together the data in Horace.

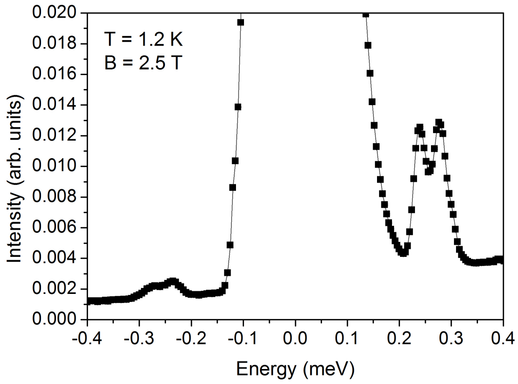

Figure 2: Measured INS spectrum of Cr_7Ni dimer as a function of energy, measured at 7.5 Å with a temperature of 1.2 K and magnetic field of 2.5 T. The two transitions from the factorised ground state towards the two entangled excited states clearly visible in both the energy-loss and energy-gain sides.

In general, the measurement proceeded well and we were able to obtain a good statistics in the 8 days allocated for the measurement. The **Q**-dependence has been extracted for each of the two transitions shown in Fig.3.

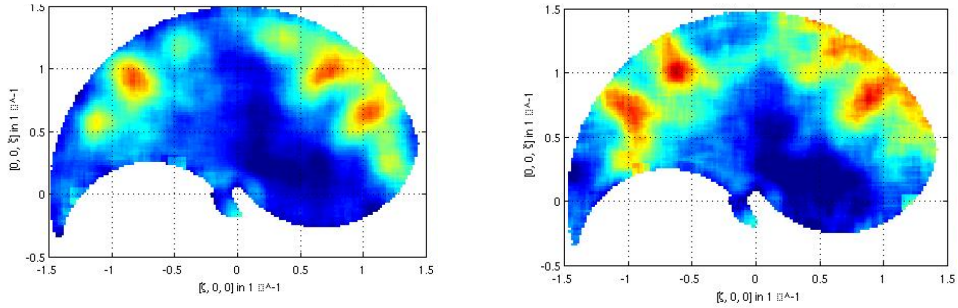

Figure 3: Constant energy maps for the low energy transition (left) and high energy (right) in the dimer of the horizontal component Qx-Qz and fully integrated over the full Qy data range

We have been able to obtain high quality data on IN5 and thus with suitable data treatment accounting for the self-attenuation of the crystals as well as separating the magnetic signal from the non-magnetic, we are confident that it will be possible not only to demonstrate the presence of entanglement in the eigenstate of the dimer but also to quantify it through the concurrence. Indeed the preliminary results show directly the presence of entanglement from the short-Q modulation in the constant energy plots (see Fig.3), reflecting inter-ring (long-distance) spin-spin correlations.