Experimental report

17/10/2016

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Title: Spin Hamiltonian of the spin-1/2 chain system beta-TeVO4

Research area: Physics

This proposal is a new proposal

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Samples: TeVO4

Instrument	Requested days	Allocated days	From	To
THALES	3	3	30/10/2015	02/11/2015

Abstract:

Spin-nematic correlations are predicted as a generic feature of the frustrated ferromagnetic zigzag S=1/2 J1-J2 chain model. The ultimate experimental evidences however are rather limited, i.e. for LiCuVO4, so their number should be extended.
The proposed INS experiment aims to measure spin excitations in a new frustrated ferromagnetic zigzag S=1/2 J1-J2 chain compound beta-TeVO4.
The data will be used for determination of the effective spin Hamiltonian.

Spin Hamiltonian of the spin-1/2 chain system β-TeVO$_4$

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We performed inelastic neutron scattering experiments on five co-aligned single crystals ($\sum_i m_i = 0.8\,g$) of β-TeVO$_4$. We have investigated the energy range between 0.25 and 4 meV. Our results show that at 1.5 K ($T < T_{N3} = 2.25$ K) several dispersing magnon modes develop along h (along the a axis), whereas along l (along the chain c direction) only a low-energy part of a very steeply dispersing mode is found. Finally, a magnon gap at **q** *= (0.8 0 0.42) that amounts ~0.6 meV is found to narrow with increasing temperature and close at T_{N3}.*

The β-TeVO$_4$ system has a monoclinic unit cell ($P2_1$/c) with parameters: $a = 4.379(2)$ Å, $b = 13.502(4)$ Å, $c = 5.446(2)$ Å, and $\beta = 91.72(5)^\circ$ [1]. The zigzag chains are formed by corner-sharing VO$_5$ pyramids, making it a candidate for a spin-1/2 chain system with competing nearest- and next-nearest-neighbor interactions. The magnetic susceptibility has a maximum at ~15 K, while at low temperatures three magnetic phase transitions are found at $T_{N1} = 4.65$ K, $T_{N2} = 3.28$, and $T_{N3} = 2.28$ [2]. These were ascribed to the transitions between the paramagnetic and the spin-density-wave (SDW) state, the SDW and the stripe state, and finally between the stripe and the vector-chiral (VC) state [3]. Magnetic excitations in the VC magnetic ground state were investigated by antiferromagnetic resonance measurements on single-crystal sample and inelastic neutron scattering on powder sample. Both experiments indicate pronounced excitation at ~1 meV, while neutron experiment shows additional broad feature at ~2.5 meV. To explore the magnetic excitations better, we now performed inelastic neutron experiment on single crystals on the THALES spectrometer at ILL.

Our experiment employed 5 co-aligned ($\delta\phi < 3$ deg) single crystals having a total mass of ~0.8 g and the a and c axis defining the scattering plane. The THALES instrument is a Three Axis Low Energy Spectrometer and is thus most suited to explore excitations up to 3 meV with energy resolution at the elastic line of ~0.1 meV. Hence, we focused on the excitation spectrum above 0.25 meV and at 1.5 K, i.e., in the VC phase, where long-range magnetic order should yield well-defined sharp magnon features. The majority of the data are the energy scans, which were performed at fixed (h and l) positions across the reciprocal space. These were complemented by several **q**-scans at fixed energy, along the chosen **q**-directions.

The results for the behavior along h are summarized in the map representation in Fig. 1. The excitation spectrum has two dominant types of features. (i) First are the sharp low-energy modes below ~1.2 meV. In particular, one mode seems to be gap-less, coming out of the (0.8 0 0.42) magnetic reflection, whereas the second seems to have a gap of ~0.6 meV. The dispersion of these modes reach a maximum of ~1.2 meV at the edge of the Brillouin zone. (ii) Second are broad features above ~1.3 meV. Compared to sharp modes at lower energies these modes have a more step like shape, which suggests that they might be a lower boundary of the spinon continuum. The observed behavior thus seems to combine signatures of 1D (continuum) and 3D (sharp features) spin correlations, suggesting that β-TeVO$_4$ is indeed a good spin-chain model system.

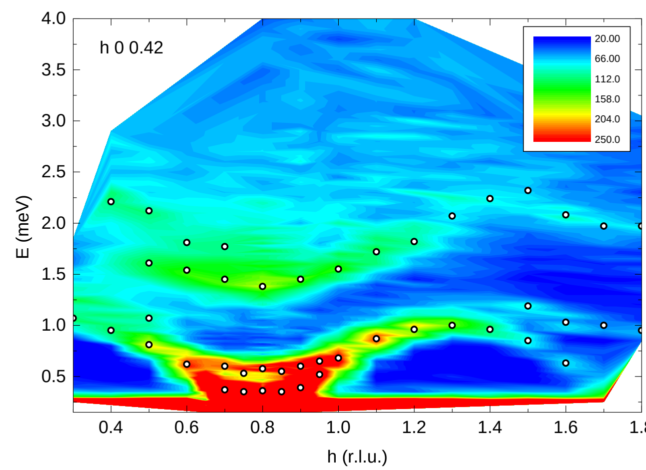

Figure 1: $E(h)$ map along $-h\,0\,-0.42$.

On the other hand, the results along the l direction show a very sharp mode, coming out of the magnetic reflection, which losses intensity above 2.5 meV (Figure 2). The observed response is in line with high-energy inelastic neutron scattering results, suggesting that intrachain exchange interactions are much higher than interchain ones.

Finally, we investigated the temperature dependence of the observed magnon gap. The corresponding energy scans at the magnetic peak position are shown on Figure 3. Clearly, the magnon gap reduces with increasing temperature and seems to completely collapse at $T \sim T_{N3}$. This is in line with the suppression of the VC order, where sharp magnon excitations are expected, whereas in the SDW the magnon features are expected to broaden.

[1] G. Meunier et al., J. Sol. Stat. Chem. **6**, 67 (1973).

[2] Y. Savina et al., Phys. Rev. **B 84**, 104447 (2011).

[3] M. Pregelj et al., Nature Comm. **6**, 7255 (2015).

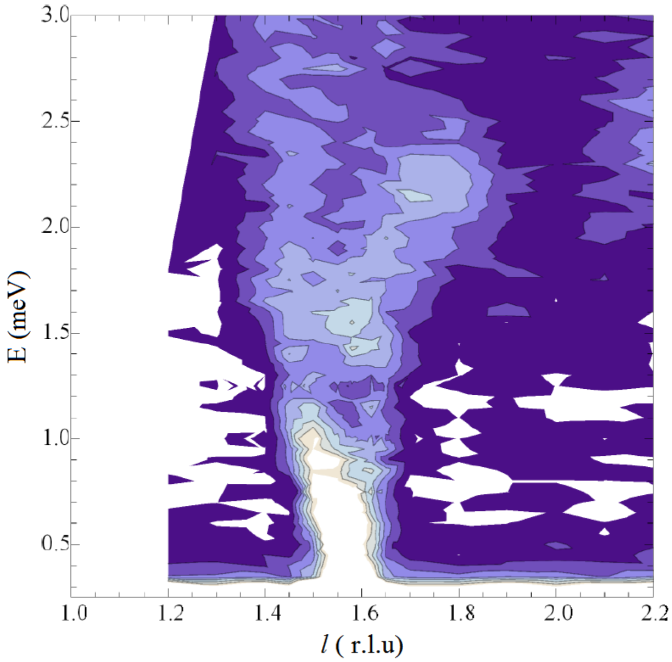

Figure 2: $E(l)$ map along $0.2\ 0\ l$.

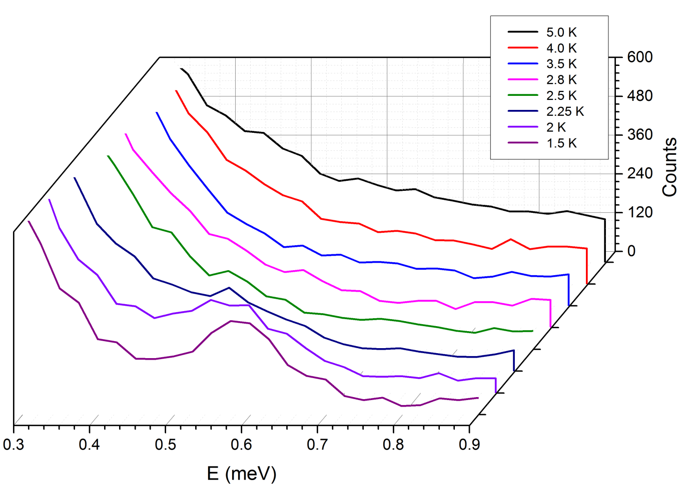

Figure 3: Temperature dependence of the magnong mode at 0.8 0 0.42