Experimental report

31/01/2022

Proposal: **4-05-787** **Council:** 10/2019

Title: Bethe string excitations at low magnetic fields in the Spin-1/2 antiferromagnetic XXZ chain SrCo2V2O8

Research area: Physics

This proposal is a continuation of 4-05-700

Main proposer: **Bella LAKE**

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Local contacts: Martin BOEHM

Samples: SrCo2V2O8

Instrument	Requested days	Allocated days	From	To
THALES	7	7	02/03/2021	09/03/2021

Abstract:

A spin-1/2 anisotropic XXZ spin chain in a longitudinal field applied parallel to the easy access shows exotic physics. Above a critical field, the long-range antiferromagnetic order is destroyed and the system enters a gapless critical regime. As well as spinon-pair excitations (known as psinons), bound states of magnons can also be excited, these are known as Bethe strings and were first predicted by Hans Bethe in 1931 but have only been verified very recently by our terahertz and inelastic neutron scattering measurements on the model magnet SrCo2V2O8. Detailed comparison of our data to a newly developed Bethe Ansatz theory was able to provide quantitative proof of these excitations. The goal of this proposal is to perform a thorough investigation of the excitations using the Thales spectrometer in the low field critical region of SrCo2V2O8 where deviations from linear field dependence are anticipated and the theory breaks down. Therefore our experimental insights will provide important inputs for the theoretical understanding.

EXPERIMENTAL REPORT

ON EXPERIMENT PERFORMED AT JCNS INSTRUMENT AT ILL OR SNS

Proposal number:	4-05-787		
Experiment title:	Quantum Critical point of a Spin-1/2 antiferromagnetic XXZ chain in a transverse magnetic field		
Instrument	ThALES		
Dates of experiment:	03/03/2021 – 10/03/2021	**Date of report:**	27/01/2022
Experimental team: Names	Bella Lake, Konrad Puzniak, Anup Bera		
Local Contact:	Martin Boehm, Paul Steffens		

Introduction:

$SrCo_2V_2O_8$ has a tetragonal crystal structure (I41cd a=b=12.27 Å, c=8.42 Å). The Co^{2+} ions have effective S=1/2 moments that are arranged in screw chains along the c-axis. There are 4 screw chains per unit cell, 2 rotate clockwise and 2 anticlockwise. The Co^{2+} ions are coupled by strong antiferromagnetic interactions within the screw chains which have partial Ising (XXZ) anisotropy where the interaction strength is J= 7.0 meV and the anisotropy parameter is ε= 0.56 forcing the spins to point along the c-axis.

Weak interchain coupling gives rise to long-range magnetic order below T_N = 5.2 K [1]. The spins are aligned antiferromagnetically along the screw chains and ferromagnetically (antiferromagnetically) along the **a** (**b**) direction respectively resulting in twinning. The ordering wavevector is k_1= (1,0,0).

In a transverse magnetic field applied along the [1,0,0] direction, $SrCo_2V_2O_8$ undergoes a transition at the field of H_C [100] ~7 T (fig. 1). The effects of a [1,0,0] transverse magnetic field have been also explored in the related compound $BaCo_2V_2O_8$ which has a very similar structure to $SrCo_2V_2O_8$.

$BaCo_2V_2O_8$ also shows suppression of long-range antiferromagnetic order at the surprisingly low field of 10T. This was attributed to the anisotropic g-tensor with off-diagonal terms which arises from the 4-fold screw chain structure of the Co^{2+} ions. Consequently, a uniform field applied along [1,0,0] produces an effective staggered field along the [0,1,0] direction [2].

Detailed single crystal neutron diffraction measurements of the magnetic structure were performed on D23 [3]. They revealed that this staggered field competes with the Ising anisotropy causing the quantum phase transition at 10T where the spins rotate from antiferromagnetic order along the c direction to point antiferromagnetically along the b direction, perpendicular to both the Ising anisotropy and the field [3]. The zero-field ordering vector k_1= (1,0,0) is replaced by k_2= (0,0,0) above the critical field, while at intermediate fields both wavevectors are present giving a non-collinear structure.

Sample Details and Instrumental Configurations:

This experiment was performed to explore the magnetic excitations in the vicinity of 3D Quantum Critical Point (QCP) at B_C= 6.90 T. The $SrCo_2V_2O_8$ cylindrical single crystal sample (*m*= 2.38 g) was used during the ThALES experiment. All of the data were measured at *T*= 60 mK with the **b** axis aligned along the magnetic field (for this reason, the sample was pre-oriented using the Laue method before the experiment) and at a fixed final wavevector of k_f = 1.35 Å^{-1} and k_f = 1.15 Å^{-1}.

Results:

The experimental schedule allowed us to measure the magnetic excitations at three wave vectors namely:
Q = (2,0,1); *Q* = (0,0,2) and *Q* = (3,0,1). We recorded the experimental scans between *B*= 6.0 T and *B*= 9.0 T. In figure 1. the experimental results are presented. In case result for *Q* = (2,0,1), the low energy mode reaches a minimum energy at the magnetic field of *B* = 6.9 T. This is consistent with the results shown by X. Zhang [4].

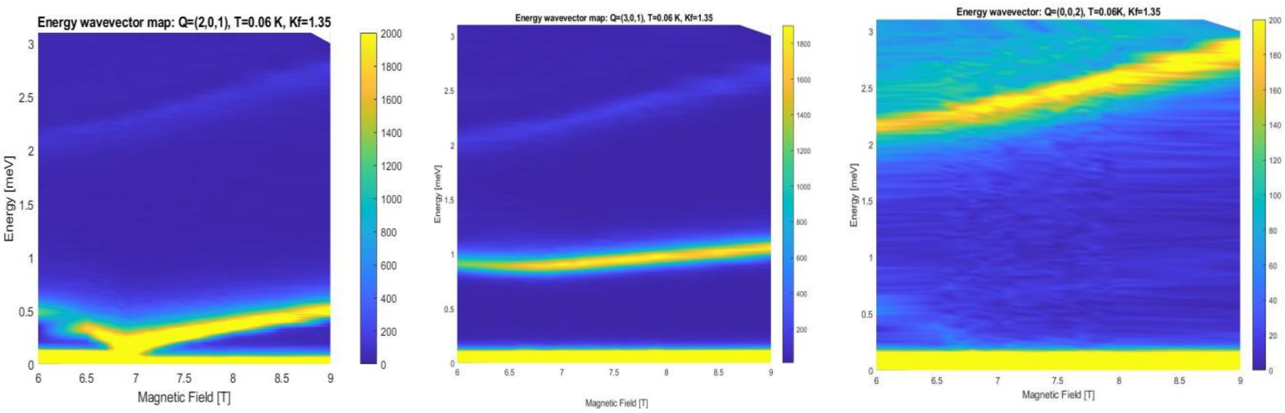

Figure 1: Energy vs. magnetic field wavevector maps measured at T= 0.06 K and k_f = 1.35 $A^{\circ -1}$ for: Q = (2,0,1) (left plot), Q = (3,0,1) (middle plot) and Q = (0,0,2) (right plot).

Conclusions:

We have accomplished the goals set in our ThALES experiment. Especially, we could confirm the existence of 3D QCP in $SrCo_2V_2O_8$ at *B* = 6.9 T in a transverse magnetic field by means of inelastic neutron scattering measurements.

Bibliography:

[1] A. K. Bera, B. Lake *et al.*, Phys. Rev. B **96**, 054423 (2017).
[2] S. Kimura *et al.*, J. Phys. Soc. of Japan **82**, 033706 (2013).
[3] Q. Faure *et al.*, Nat. Phys. **14**, 716 (2018).
[4] X. Zhang *et al.*, Phys. Rev. B **103**, 144405 (2021).