Experimental report

08/02/2022

Proposal: **4-03-1750** **Council:** 10/2020

Title: Quantum Critical point of a Spin-1/2 antiferromagnetic XXZ chain in alongitudinal magnetic field

Research area: Physics

This proposal is a new proposal

Main proposer: **Bella LAKE**

Experimental team: Martin BOEHM
Jie MA

Local contacts: Martin BOEHM

Samples: $BaCo_2V_2O_8$

Instrument	Requested days	Allocated days	From	To
THALES	6	5	02/06/2021	08/06/2021

Abstract:

A spin-1/2 anisotropic XXZ spin chain in a longitudinal field applied parallel to the easy axis shows exotic physics. Above a critical field, the long-range antiferromagnetic order is destroyed and the system enters a gapless critical regime known as a Tomonaga Luttinger Liquid. In this phase as well as spinon-pair excitations (known as psinons), bound states of magnons can also be excited, these are known as Bethe strings which we have verified experimentally. In this proposal we wish to study the quantum critical phase transition between the Neel ordered and the quantum critical regime. Our measurements will focus on the search for Energy/Temperature critical scaling which is a signature of such a quantum critical point.

EXPERIMENTAL REPORT

ON EXPERIMENT PERFORMED AT JCNS INSTRUMENT AT ILL OR SNS

Proposal number:	4-03-1750		
Experiment title:	Excitations in the spin-1/2 antiferromagnetic XXZ chain in a longitudinal magnetic field		
Instrument	ThALES		
Dates of experiment:	02/06/2021 – 08/06/2021	**Date of report:**	02/02/2022
Experimental team: Names	Bella Lake, Konrad Puzniak, Jie Ma		
Local Contact:	Martin Boehm, Paul Steffens		

Introduction:

The one-dimensional (1D) spin-1/2 antiferromagnet (AFM) with Heisenberg-Ising (XXZ) anisotropy is an ideal model system to explore fundamental physics concepts. In zero applied magnetic field, this system hosts spinon excitations - quite different from the magnons of conventional three-dimensional (3D) magnets which have integer spin. A very interesting spin-1/2 quasi-1D antiferromagnetic XXZ material is $BaCo_2V_2O_8$ [1]. This compound crystallizes in the tetragonal space group I 41/a cd. The Co2+ions have effective S=1/2 moments that are arranged in screw chains along the c-axis. The Co2+ions are coupled by strong antiferromagnetic interactions within the screw chains which have partial Ising (XXZ) anisotropy where the interaction strength is J= 5.6 meV and the anisotropy parameter is ε= 0.46 with the c-axis being the easy-axis. Weak interchain coupling gives rise to long-range magnetic order below T_N= 5.5 K. The spins are aligned antiferromagnetically along the screw chains. Detailed single crystal neutron diffraction measurements of the magnetic structure were performed on D23 [2]. They revealed that this staggered field competes with the Ising anisotropy causing the quantum phase transition at 10 T 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 [1]. 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.

The behavior of $BaCo_2V_2O_8$ in a transverse magnetic field applied perpendicular to the easy-axis is very interesting. The transverse field suppresses long-range magnetic order and results in a 1D Quantum Critical Point (QCP) at B_{1Dc}= 4.7 T and a 3D QCP at B_{3Dc}= 10.3 T. The 1D QCP has a class of universality described in terms of the E_8 Lie algebra which is characterized by 8 gapped excitations whose gaps are theoretically predicted to have precise values and have been observed by inelastic neutron scattering and terahertz spectroscopy.

A longitudinal magnetic field applied parallel to the easy axis also shows exotic physics. Above a critical field, the long-range antiferromagnetic order is destroyed and the system enters into 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 H. Bethe in 1931 [3].

Sample Details and Instrumental Configurations:

During the measurements a longitudinal magnetic field was applied along the (0,0,1) direction, which is longitudinal (or parallel) to the spin direction in zero magnetic field. Measurements took place at T = 1.50 K within the horizontal (H, K, 0) scattering plane. The triple axis spectrometer measurements were performed over the energy range from E= 0 to E= 15.30 meV in the steps of 0.10 meV. All the data were measured at a fixed final wavevector: k_f = 1.50 $A^{\circ-1}$. The resolution was ΔE= 0.17 meV at k_f =1.50 $A^{\circ-1}$.

Results:

We recorded the experimental scans between B= 0.0 T and B= 15.0 T. In figure 1. The color maps of the inelastic neutron scattering intensity measured on ThALES spectrometer at T=1.5 K, showing the field dependence of the excitation spectrum of $BaCo_2V_2O_8$ in longitudinal magnetic fields up to B=14.9 T for the wavevector Q= (3.25,0,0) are presented (left plot) and Q = (2.3,2.3,0) (right plot). As we look closely to the part of the **left map** which starts at magnetic field higher than B= 5 T and for energies higher than E=10 meV, we can see a weak line corresponding to the 3-string excitation (marked by a black line in figure 1.), that was observed in a case of $SrCo_2V_2O_8$ [4]. Also, we may observe a strong line (below the 3-string excitation) corresponding to the 2-string excitation (marked by a green line in figure 1.) and another line corresponding to the psinon-psinon excitation (marked by a pink line in figure 1.), that was found in the case of $SrCo_2V_2O_8$ [4]. As we look closely to the part of the **right map** which starts at magnetic field higher than B= 5 T and for energies lower than E= 5 meV, we can see a strong line corresponding to the psinon-antipsinon excitation (marked by the lower pink line in figure 1.). This is consistent with an observation of the psinon-antipsinon excitation that was found in the case of $SrCo_2V_2O_8$ [4]. Additionally, another line has been added to figure 1. corresponding to the 2-string excitation, also found in a case of $SrCo_2V_2O_8$ (upper green line in figure 1.) [4].

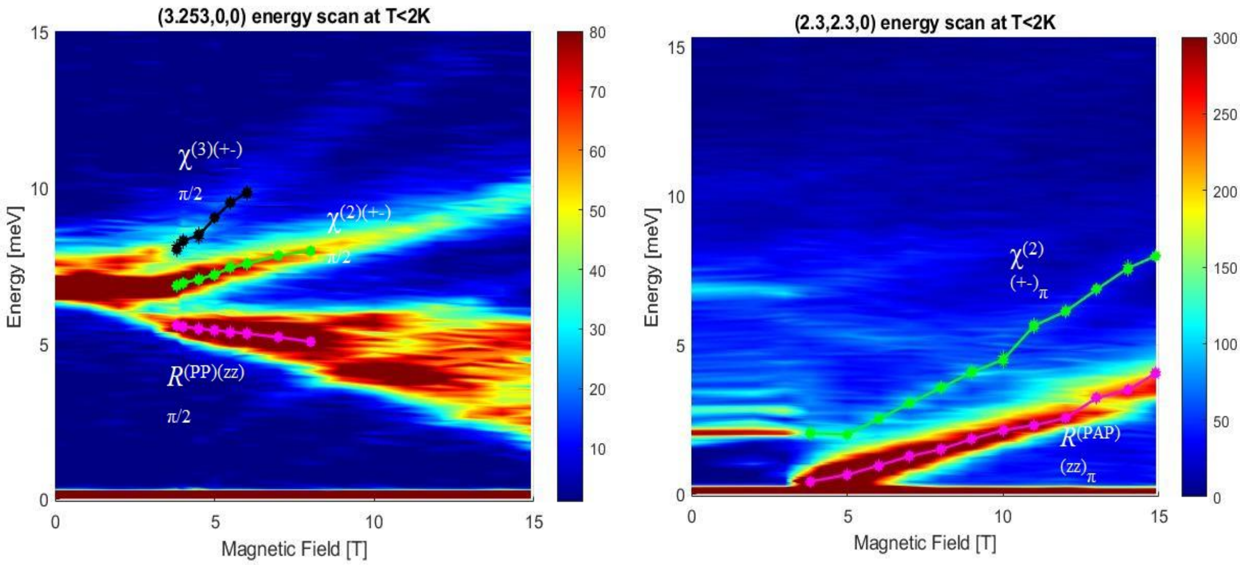

Figure 1: Energy vs. magnetic field wavevector maps measured at T= 1.50 K and k_f = 1.50 $A^{\circ-1}$ for: Q = (3.253,0,0) (left plot) and Q = (2.3,2.3,0) (right plot).

Conclusions:

We have accomplished the goals set in our experiment. Especially, we could confirm the existence of: 3-string excitation, 2-string excitation, psinon-psinon excitation and psinon-antipsinon excitation in $BaCo_2V_2O_8$ in a longitudinal magnetic field by means of inelastic neutron scattering measurements.

Bibliography:

[1] S. Kimura *et al.*, J. Phys. Soc. of Japan **82**, 033706 (2013).
[2] Q. Faure *et al.*, Nat. Phys. **14**, 716 (2018).
[3] H. Bethe, Zeitschrift für Physik **71**, 3-4 (1931).
[4] A. K. Bera, B. Lake *et al.*, Phys. Rev. B **96**, 054423 (2017).