Experimental report

08/02/2024

Proposal:	**5-41-1211**	**Council:**	4/2023

Title: Magnetic Structure of the spin-1/2antiferromagnetic XXZ chain PbCo2V2O8 in a transverse (1,1,0) magnetic field

Research area: Physics

This proposal is a new proposal

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Samples: PbCo2V2O8

Instrument	Requested days	Allocated days	From	To
D23	6	4	29/10/2023	02/11/2023
ORIENTEXPRESS	1	1	06/11/2023	07/11/2023

Abstract:

The one-dimensional (1D) spin-1/2 antiferromagnetic with Heisenberg-Ising (XXZ) anisotropy, is a fascinating model system to explore fundamental physics such as quantum phase transitions and exotic ground states and excitations. Although no long-range magnetic order is expected in the pure 1D case, real materials which have interchain coupling develop long-range magnetic orders that reflect the nature of these ground states. The ACo2V2O8 compounds (A=Sr, Ba) are great physical realizations of the Heisenberg-Ising spin-1/2 chains. They show exotic physics in zero field as well as [1,0,0] and [0,0,1] applied fields with complex magnetic phases and excitations that can be used to test physics concepts. We have discovered a previously unreported phase for the [1,1,0] transverse field direction that is accessible in only the newly synthesized PbCo2V2O8 member of this family due to its lower energy scale. The aim of this experiment is to determine the magnetic structure of this field-induced phase using single crystal neutron diffraction.

EXPERIMENTAL REPORT

ON EXPERIMENT PERFORMED AT JCNS INSTRUMENT AT ILL OR SNS

Proposal number:	5-41-1211		
Experiment title:	**Magnetic Structure of the spin-1/2 antiferromagnetic XXZ chain $PbCo_2V_2O_8$ in a longitudinal (0,0,1) magnetic field**		
Instrument	D23		
Dates of experiment:	29/10/23 – 02/11/23	**Date of report:**	08/02/24
Experimental team: **Names**	**Addresses**		
	Cintli Aguilar Maldonado, Konrad Puzniak, Ralf Feyerherm, Nazmul Islam, Bella Lake		
Local Contact:	Eric Ressouche, Karin Schmalzl		

Abstract

The one-dimensional (1D) spin-1/2 antiferromagnetic with Heisenberg-Ising (XXZ) anisotropy, is a fascinating model system to explore fundamental physics such as quantum phase transitions and exotic ground states and excitations. Although no long-range magnetic order is expected in the pure 1D case, real materials which have interchain coupling develop long-range magnetic orders that reflect the nature of these ground states. The $ACo_2V_2O_8$ compounds (A=Sr, Ba) are great physical realizations of the Heisenberg-Ising spin-1/2 chains. They show exotic physics in zero field as well as [1,0,0] and [0,0,1] applied fields with complex magnetic phases and excitations that can be used to test physics concepts.

Introduction

One dimensional (1D) spin-1/2 antiferromagnets with Heisenberg-Ising (XXZ) anisotropy have been a topic of recent study, in particular using the $ACo_2V_2O_8$ family (A=Sr, Ba) which represent model materials to explore fundamental physics. The characteristic 4-fold screw chains of magnetic ions (Co^{2+}) along its tetragonal c-axis with effective spin-½ exhibit a strong antiferromagnetic intrachain coupling, while the weak interchain coupling gives rise to long-range, antiferromagnetic Neel order at low temperatures. In zero magnetic field these compounds have a spinon continuum above the Neel temperature $T_N \sim 5$ K which is used to demonstrate spinon confinement on cooling below T_N where the continuum is replaced by sharp bound-spinon modes [1,2].

Exotic physics arises as a magnetic field is applied parallel to the easy axis (c-axis) namely a longitudinal field. The Neel antiferromagnetic order (NAF) is suppressed to much lower values ($T_N < 1$ K) and above a critical field $\mu_0 H_{c1}$ the system undergoes a transition to a longitudinal spin density (LSDW) and then another transition at $\mu_0 H_{c2}$ to a transverse canted antiferromagnet (TAF) [3,4]. The phase diagram for the longitudinal magnetic field versus temperature was found by several techniques including neutron diffraction, NMR and specific heat for $BaCo_2V_2O_8$, and $SrCo_2V_2O_8$ [5,6]. Neutron diffraction revealed a commensurate to incommensurate transition at $\mu_0 H_{c1}$ above which the magnetic reflections can be indexed by propagation vector $k_{IC} = (0, 0, 1\pm\delta l)$, while the magnetic order above $\mu_0 H_{c2}$ is also incommensurate along the c-axis. Within these field-induced phases spinon pair excitations (psinons) and bound states of magnons (Bethe Strings) have been discovered and explored using inelastic neutron scattering and terahertz spectroscopy [6,7].

We have synthesized a new family member namely $PbCo_2V_2O_8$, and powder measurements showed it to have very similar magnetic properties to $SrCo_2V_2O_8$ and $BaCo_2V_2O_8$. The magnetic structure in zero field is the same for all three family members [8] and the *H-T* phase diagram for longitudinal and transverse field parallel to [1,0,0] are similar except that $PbCo_2V_2O_8$ has a lower energy scale. The *H-T* phase diagram of $PbCo_2V_2O_8$ as a function of temperature and longitudinal magnetic field (the phases have to be confirmed) is presented in fig. 1 below.

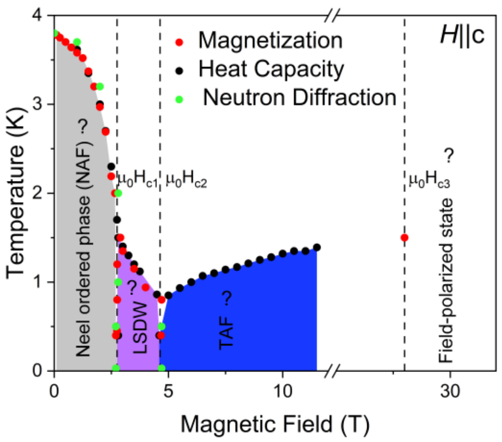

Figure 1. Phase diagram of $PbCo_2V_2O8$ as a function of longitudinal magnetic field H∥c and temperature. The different colored regions indicate the different magnetic phases. The gray phase is identified as a Néel antiferromagnetic phase. The purple phase might have longitudinal spin density wave order, whereas the blue phase might be a transverse antiferromagnetic phase, although these field-induces phases have yet to be confirmed [8].

The phase diagram reveals a suppression of the Neel ordering temperature and transitions to two field-induced phase at $\mu_0 H_{c1} = 2.7$ T *and* $\mu_0 H_{c2} = 4.6$ T with increasing field. Although the nature of these phases is as yet unknown we anticipate that they are similar to those of $SrCo_2V_2O_8$ and $BaCo_2V_2O_8$.

Sample Details and Instrumental Configurations

The neutron diffraction measurements were collected, below T_N at 30 mK and the single crystal neutron diffraction was performed on a small cylindrical-shaped crystal (weight 1 g, diameter 5 mm, and length 6 mm) at the D23 neutron diffractometer. The single crystal was previously aligned on the Orient Express neutron Laue diffractometer. The sample was then installed on D23 in a vertical field orange cryomagnet (equipped with a dilution insert) with the c-axis aligned along the magnetic field. A maximum longitudinal magnetic field of 13 T (H∥c) could be reached and the incident wavelength of the neutron beam is $\lambda = 1.28$ Å.

Objectives

The main goal of this experiment was to determine the magnetic structure of $PbCo_2V_2O_8$ in a longitudinal [0,0,1] magnetic field.

Experimental Results

Powder and single crystalline samples of $PbCo_2V_2O_8$ have been studied in our research group where it has been proved to be isostructural to $SrCo_2V_2O_8$ with space group I41cd (No. 110). $PbCo_2V_2O_8$ develops long-range Neel antiferromagnetic order below $T_N = 3.8$ K, its magnetic structure at 0 T is the same as the other members of the $ACo_2V_2O_8$ family with a propagation vector $q = (0, 0, 1)$. The spins point mostly parallel to the tetragonal c-axis and align antiferromagnetically along the screw chains following the Γ5 irreducible representation [8]. The aim of this experiment was to determine the magnetic structure of field-induced phases using single crystal neutron diffraction. For this purpose, a single crystal of $PbCo_2V_2O_8$ was prepared and cut to appropriate dimensions for the experiment. The sample was aligned with the [0,0,1] direction vertical and parallel to the magnetic field direction and glued with X60 glue into a copper sample holder with the pertinent size for the 15 T vertical magnet with ^{3}He insert experimental setup. A copper monochromator was required to provide a neutron wavelength of 1.28 Å and the ^{3}He insert was also required to achieve temperatures down to 30 mK.

As reported for $SrCo_2V_2O_8$ a commensurate to incommensurate transition occurs at $\mu_0 H_{c1}$ = 3.9 T where the LSDW phase begins and given the similar behavior in all members of the family, $PbCo_2V_2O_8$ is expected to have the same behavior at $\mu_0 H_{c1}$ = 2.7 T. A field dependence of the magnetic reflection (2, 3, 0), up to 6 T, is shown in fig 2 [9]. The peak broadens, however at higher fields, above 2.7 T, we could not observe the two satellite reflections: (2, 3, δl) and (2, 3, -δl) expected if there is incommensurate order [4,10]. One of the possible explanations for this is due to the experimental setup, which did not allow us to have the best resolution along c direction (since the 15 T vertical magnet has a very limited vertical access of -2 to 2 degrees and no collimator was used) to resolve the splitting. It should be emphasized that the focus of the previous experiment was to measure the [1,1,0] field direction [11], thus the setup was not optimized for a measurement along [0,0,1] field direction. A followup experiment using a vertical collimator along with avertical magnetic that has wide vertical angular access, or alternatively a horizontal magnet would clarify the situation.

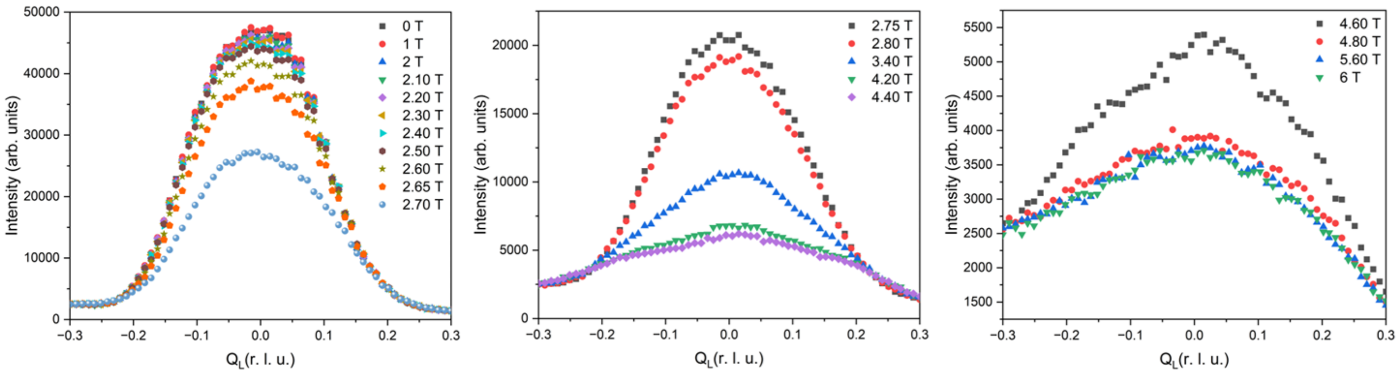

Figure 2. Field dependence of magnetic reflection (2,3,0) up to 6 T [9].

References

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