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Spin excitations of the one-dimensional $S=\frac{1}{2}$ Heisenberg antiferromagnet Yb_4As_3 under magnetic field

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Abstract

Inelastic neutron scattering experiments on the charge ordered state of Yb_4As_3 have been performed under magnetic field up to about 6 T. The observed dependence of the magnetic response from the one-dimensional Yb^{3+} chains on the applied magnetic field is well understood by the quantum sine-Gordon theory for the staggered field effect due to the existence of the Dzyalosinsky–Moriya interaction.

Keywords: 1D system; Yb_4As_3; Neutron scattering

Yb_4As_3 has an anti-Th_3P_4 type cubic crystal structure at temperatures above about 290 K. Below this temperature, it shrinks slightly along a [1 1 1] direction giving a trigonal structure. It does not undergo any magnetic long range ordering at least down to 45 mK, and shows typical heavy-fermion-like anomalies though its carrier density is very low ($\sim 10^{-3}$ per formula) at low temperatures [1]. The polarized neutron diffraction experiments [2] proved the existence of the charge ordering in the low temperature phase of Yb_4As_3 where four Yb ions aligned along the [1 1 1] direction become mainly tri-valent whereas the rest of 12 Yb ions in a unit cell are almost di-valent. The inelastic neutron scattering experiments [3] revealed that the Yb^{3+} chains caused by the charge ordering exhibit low energy magnetic excitations which are well characterized as those of a one-dimensional (1D) spin $\frac{1}{2}$ Heisenberg system with a nearest neighbor antiferromagnetic coupling (1D-HAF) [4]. The observed C/T value at the low temperature limit (205 mJ/K^2/mol) as well as the broad peak of susceptibility around 20 K are explained well by the 1D-HAF model with the exchange interaction value determined by the neutron scattering experiment ($J = 2.2$ meV). These facts clearly indicate that the "heavy-fermion" behavior in Yb_4As_3, except for the resistivity anomaly, originates from the quantum spin excitations.

On the other hand, experimental results of specific heat under magnetic field exhibit unusual properties, which indicate opening of a gap in the low energy excitations of Yb_4As_3 by applying a magnetic field [5]. This is not consistent with the simple 1D-HAF model, which explains well the properties of the spin degree of freedom of the system at zero magnetic field. In order to shed light on this phenomenon, we performed measurements of spin excitations of Yb_4As_3 under magnetic field. A part of the experimental results has been published elsewhere [6].

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The inelastic neutron scattering experiments were performed on the cold neutron triple axis spectrometers 4F2 at LLB and IN12 at ILL. A single crystal sample ($\sim 8 \times 8 \times 4\,\mathrm{mm}^3$) was set inside a Helmholtz-type superconducting magnet with the [1 −1 0] axis vertical in each experiment. The [1 1 1] direction in the horizontal scattering plane was selected as the unique axis, along which the chains of Yb^{3+} ions are formed in the trigonal phase, by utilizing the strain-cool technique to make a single domain sample [2,3].

We found that, by applying a magnetic field, the spectrum at the 1D wave vector around $q = 1$ $[\pi/d]$ (d: atomic distance in the 1D chain) changes drastically from the gap-less one corresponding to the spinon pair excitation continuum of the 1D-HAF system to a sharp one at a finite excitation energy. The magnetic field dependence of the gap is fitted well by the power law with the exponent $\frac{2}{3}$ as shown in Fig. 1. These results are in good agreement with the theory presented by Oshikawa et al. [7], which argues that the gap is opened by the staggered field alternating along Yb^{3+} chains induced by the uniform magnetic field applied perpendicular to the chains due to existence of the Dzyaloshinsky–Moriya interaction between Yb^{3+} ion pairs in the chains. The observed sharp peak around $q = 1$ under magnetic field can be attributed to the superposition of the scattering from the "soliton mode" and "breather mode" which are predicted by the quantum sine-Gordon theory applied to the present system [7,8]. In order to get more detailed information on the nature of the excitations, we have performed a high-resolution inelastic neutron scattering experiment at the cold neutron triple axis spectrometer IN14 at ILL (incident neutron energies of 3–5 meV). Fig. 2 depicts the spectra at the same 1D wavevector of $q = 1$ but with different

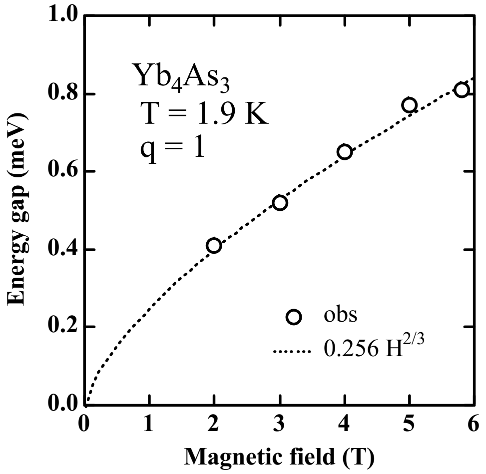

Fig. 1. Magnetic field dependence of the energy gap at $q = 1$.

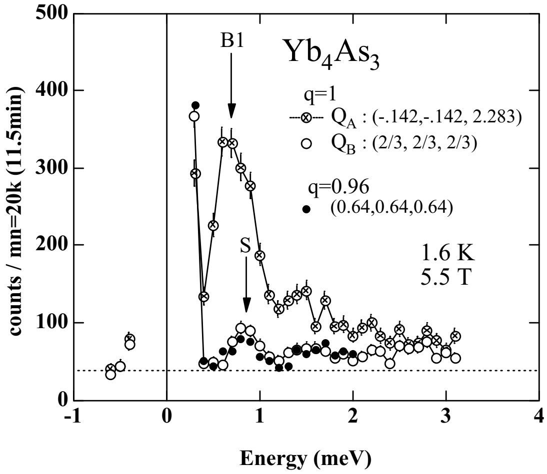

Fig. 2. Spectra under magnetic field of $H = 5.5\,\mathrm{T}$ for the one-dimensional wave vector of $q = 1$ $[\pi/d]$ with two different scattering vectors and for $q = 0.96$.

scattering vectors $Q_A = (-0.142, -0.142, 2.283)$ and $Q_B = \left(\frac{2}{3}, \frac{2}{2}, \frac{2}{3}\right)$ at 1.6 K under $H = 5.5\,\mathrm{T}$. Clear peaks are observed at about 0.8 meV in both cases although the peak positions of the spectra are slightly different. Since the lightest breather (B1) and soliton (S) modes are associated with the spin fluctuations parallel ($\|$) and perpendicular ($\perp$) to the chain direction ([1 1 1]), respectively [8], the peaks can be attributed to the superposition of the two modes at Q_A and pure soliton mode at Q_B because neutron magnetic scattering cross section is proportional to the component of spin fluctuation perpendicular to the scattering vector. Actually, the peak at Q_A is mainly due to the lightest breather mode because the intensity of the soliton mode is expected to be smaller than that of the breather mode by about a factor 4 due to the anisotropy of the g-factor ($g_{\|}/g_{\perp} = 2.3$) [9] and also to the scattering angle dependence of the cross section of each spin fluctuation. This is consistent with the fact that the intensity of the spectrum at Q_B (pure soliton mode), which is proportional to $g_{\perp}^2$ is very small compared to that at Q_A. In Fig. 2, the spectrum of the soliton mode at $q = 0.96$ [$Q = (0.64, 0.64, 0.64)$], where spin excitation is expected to be gap-less if there is no staggered field effect [4], is also shown. The spectrum is almost same as that at Q_B, indicating that the soliton mode shows little dispersion around these points.

Thus, we could identify both breather and soliton modes which are predicted by the quantum sine-Gordon theory [8], in which the similar gap-opening phenomenon in Cu benzoate [10] is discussed. We measured also the magnetic field dependence of spectra at several medium q values ($0.3 \leqslant q \leqslant 0.7$), where spin excitation energy becomes higher than about 2 meV [3], using a high-resolution configuration. However, they show little change under magnetic field. This fact indicates that the staggered field influences the whole excitation spectrum and its effect cannot be regarded as a simple perturbation to the 1D-HAF model in the present case.

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