Evidence for magnons and solitons in the one-dimensional $S = \frac{1}{2}$ antiferromagnet Yb_4As_3

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Abstract

By means of low-temperature measurements of the specific heat, C, and thermal expansion, $\alpha = l^{-1}\partial l/\partial T$, the magnetic properties of the quasi-one-dimensional (quasi-1D), $S = \frac{1}{2}$ Heisenberg antiferromagnet Yb_4As_3 were investigated. In finite magnetic fields distinct anomalies were found which are pronounced differently strongly in both quantities: (i) the in-T linear contribution dominating the low-T specific heat becomes reduced with field and (ii) a peak is induced at slightly higher temperatures. The latter feature being much more pronounced in $\alpha(T, B)$ is well described by the classical sine-Gordon (SG) soliton solution of a 1D Heisenberg antiferromagnet with a weak easy-plane anisotropy.

Keywords: Yb_4As_3; Spin chains; Specific heat

One of the unique properties of the rare-earth pnictide compound Yb_4As_3 is the charge-ordering transition at $T_{co} = 293$ K [1] which leads to the formation of 1D Yb^{3+} ($S = \frac{1}{2}$) chains. Upon cooling below T_{co} the smaller Yb^{3+} ions order along one of the possible four space diagonals, e.g., parallel to the $\langle 111 \rangle$ axis which usually results in the formation of a multidomain low-T structure. Since the transition at T_{co} is accompanied by a trigonal distortion, i.e. a shortening of the Yb^{3+} chains, a preferential orientation of the domains can be induced by the application of uniaxial stress prior to cooling through T_{co}. The existence of antiferromagnetic (afm) $S = \frac{1}{2}$ Heisenberg chains at low temperatures was clearly confirmed via inelastic neutron-scattering experiments [2].

In this paper we report additional features in the low-energy magnetic excitation spectrum of these $S = \frac{1}{2}$ spin chains that were found in response to a magnetic field.

The experiments were carried out on high-quality single crystals prepared as described in Ref. [1]. For the specific-heat measurements, a microcalorimeter from Oxford Instruments was used. Details concerning the thermal-expansion measurements are given elsewhere [3].

Fig. 1 shows low-temperature specific-heat data taken at varying fields up to 12 T aligned perpendicular to the $\langle 1\ 1\ 1 \rangle$ direction of the majority domain of the crystal. The large in-T linear specific heat, γT, found in zero field is consistent with the low-energy linear dispersion relation of magnons in the 1D $S = \frac{1}{2}$ antiferromagnet (AFM) [4]. As is demonstrated in Fig. 1 the effect of a magnetic field on the low-energy magnetic excitations is twofold: (i) the in-T linear specific heat becomes suppressed below its zero-field value and (ii) a broadened peak develops at slightly higher temperatures which grows in size and shifts to higher temperatures with increasing fields. Fig. 2 shows that the latter feature, depending on the actual domain configuration and field orientation (see below), is much more strongly pronounced in the coefficient of thermal expansion. Since in the $\alpha(T, B)$ experiments small uniaxial pressure could be applied along the measuring direction, we were able to study this contribution for different domain-structure configurations. A detailed quantitative analysis of these studies reveals a clear

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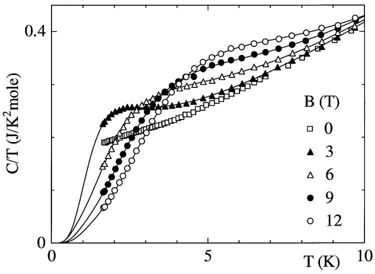

Fig. 1. $C(T, B)$ of Yb_4As_3 at varying magnetic fields. Solid lines are fits described in the text.

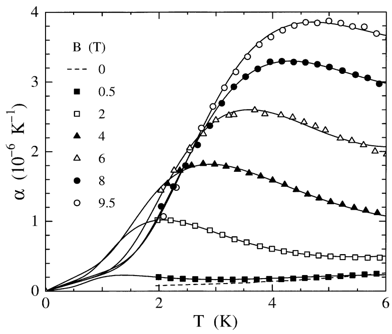

Fig. 2. $\alpha(T, B)$ of Yb_4As_3 with a domain configuration (defined in the text) $x = 0.35$ at varying magnetic fields. Solid lines are fits according to Eq. (4) of [3].

correlation between the magnitude of the anomaly in α, α_{max}, and the domain configuration, i.e. the volume fraction x of the sample in which the spin chains run parallel to the measuring direction [3]: with increasing x, α_{max} reduces monotonically and extrapolates to $\alpha_{max} = 0$ for $x = 1$. Since the latter configuration corresponds to a monodomain structure with B aligned parallel to the spin chains, this correlation implies that a finite field component perpendicular to the chains is required to induce the anomaly.

The suppression of the in-T linear specific heat in finite fields was ascribed in Ref. [5] to the field-induced opening of a gap, δ, in the spin-excitation spectrum due to a weak inter-chain coupling. On the other hand, a quite similar phenomenology in $C(T, B)$, i.e. a reduction of the low-T data and the formation of a peak for the 1D $S = \frac{1}{2}$ Heisenberg AFM Cu benzoate has been attributed to the formation of a field-induced gap, Δ, of unknown origin [6]. As possible causes for the gap exchange anisotropies [6], an alternating g-tensor [6,7] and the Dzyaloshinskii–Moriya interaction [7] have been discussed.

As for the field-induced peak anomaly in Yb_4As_3, in Ref. [3] it was found that it is well described by classical SG solitons in a 1D afm Heisenberg chain employing a weak easy-plane exchange anisotropy. Since solitons exist only for fields perpendicular to the spin chains, this mechanism provides a quite natural explanation for the highly anisotropic field response found in our $\alpha(T, B)$ measurement. The solid lines in Figs. 1 and 2 represent fits according to the soliton model given in Eqs. (3) and (4) of Ref. [3]. For the specific heat, where the magnon contribution is predominant in small fields, a term $C_{magn}/T \propto \exp(-\delta(B)/k_B T)$ was included in the fitting procedure to account for a field-induced gap, $\delta(B)$, in the spin-excitation spectrum. Note that such a separation into a magnon and soliton part is a consequence of our classical approach. The field dependence of the soliton energy E_s derived from these fits is shown in Fig. 3. The figure also includes $E_s(B)$ data taken from fits on various data sets shown in Ref. [3]. For small fields $E_s(B)$ follows a linear field dependence (broken line) in accordance with the classical SG soliton solution [3]. On the other hand, a fit $E_s(B) \propto B^{\varepsilon}$ with $\varepsilon = 0.66$, as suggested in Ref. [8], describes the data much better. A $B^{2/3}$ dependence was observed also for the field-induced gap in Cu benzoate [6] and was explained using a quantum SG model [7]. Thus, our results suggest an alternative description of soliton excitations in the afm $S = \frac{1}{2}$ Heisenberg chain in terms of the quantum SG model.

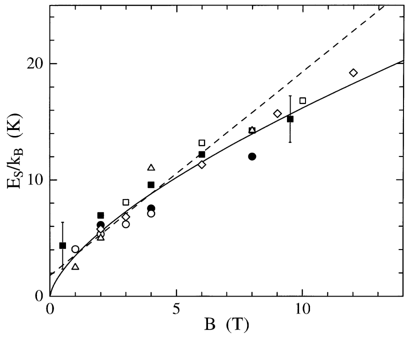

Fig. 3. Field dependence of the soliton energy E_s as derived from the fits in Fig. 1 (◇) and 2 (■) as well as data taken from [3]. Solid line is a fit $E_s(B) \propto B^{0.66}$.

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