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Investigation of NMR in a quasi-one-dimensional antiferromagnet CsMnBr_3

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Abstract

The NMR spectrum of CsMnBr_3 has been studied. It splits into 3 branches in agreement with the theory of an triangular antiferromagnet. All branches are affected by a dynamic interaction with the electronic AFMR mode.

Keywords: Hyperfine interaction, NMR, One-dimensional systems, Triangular lattice

CsMnBr_3 is a hexagonal crystal, which becomes antiferromagnetic at $T_N = 8.3$ K. Neutron scattering data [1] have shown that CsMnBr_3 is an easy plane antiferromagnet with a quasi-one-dimensional triangular spin structure. Two features established in [2,3,4] are important for understanding our NMR results: 1. The magnetic field \mathbf{H} applied in the easy plane adjusts one pair of the 6 sublattices perpendicular to \mathbf{H} and rotates the other two pairs towards one another until the triangular structure is transformed into a quasi-collinear structure above $H_c = 64$ kOe. 2. The AFMR spectrum contains one low frequency mode at $\nu_{e1} = \gamma_e D(H^3/H_c^2)$.

We have studied the NMR spectrum of CsMnBr_3 in a wide range of frequencies (200 - 500 MHz) and in magnetic fields up to 80 kOe. The static and the RF fields were applied in the basal plane. The measurements were performed in the temperature range between 1.3 K and 3.0 K. Preliminary results of these measurements have been published in [5].

The resonance frequency ν_{n0} of the nuclear spins of Mn^{2+} is mainly defined by the hyperfine field $H_{hf} = -A\langle S \rangle / \gamma_n \hbar$, where A is the hyperfine interaction constant and $\langle S \rangle$ the average spin of the magnetic ion. Using the relations for the magnetic field dependence of the angles θ_i between the sublattice magnetizations and the magnetic field given in [2] we have calculated the field dependence of the NMR frequencies ν'_{n10} for two sublattice magnetizations oriented perpendicular to \mathbf{H} and ν_{n20} and ν_{n30} for two

other pairs of sublattices. They are represented in Fig.1 by dotted lines 1', 2, 3.

The real NMR spectrum of CsMnBr_3 , which we have observed is indicated in Fig.1 and 2 by dots. It was found to split into 3 branches which agrees well with a theoretical prediction for triangular antiferromagnets. It also clearly demonstrates

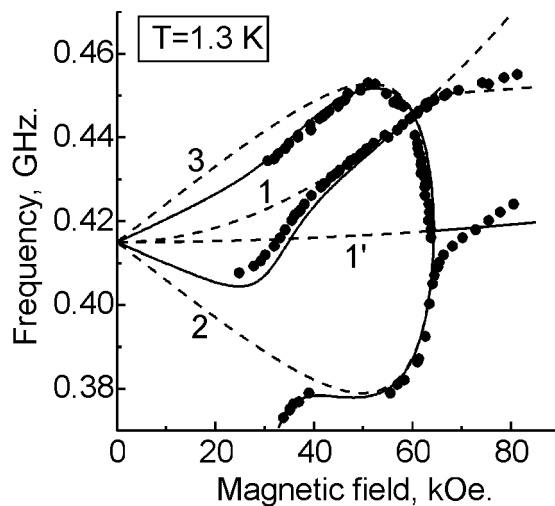


Fig. 1. NMR spectrum of CsMnBr_3 (high frequencies).

the deformation of the spin triangles at the transition to the collinear structure. All three NMR branches are affected by a strong dynamic interaction with the low frequency electronic (AFMR) mode. This interaction gives rise to a frequency shift ("pulling").

Above 45 kOe the effect of pulling becomes very small. In Fig.1 the experimental points for the upper - 3 and the lowest - 2 branches are in satisfactory agreement with the corresponding calculated curves. But for the middle branch - 1' we have observed an unexpected behavior. We can not give an explanation for it but propose the following empiric relationship for the field dependence of the frequency ν_{n10} in the absence of a dynamic interaction: $\nu_{n10} = \nu'_{n10}(1 + cH^2)$, where $c = 1.92 \times 10^{-5} \text{ kOe}^{-2}$. In Fig.1 this relation is represented by the dotted line 1.

In previous publications [6,7,8] the pulling of the NMR and AFMR spectrums was calculated only for 2- or 4- sublattices collinear antiferromagnets. Recently Zaliznyak and co-authors [9] have calculated the frequencies of

coupled oscillations in CsMnBr₃ for the lowest AFMR mode and for all three NMR branches. But his relations can be used only below $\approx 30 \text{ kOe}$ when the magnetic structure is practically not distorted by the applied field. Here we are presenting the result of more complicated calculations.

The equation derived for the frequencies of all 4 modes (three quasi-nuclear and one quasi-electron) is the following:

$$\nu_{el}^2 - \nu^2 = \frac{1}{3} \frac{\nu_{T0}^2}{\nu_{n0}^2} \sum_{i=1}^3 \frac{(\nu^2 + \nu_{ni}^2 - \nu_{ni0}^2) \nu_{ni}^2}{(\nu_{ni0}^2 - \nu^2)}, \quad (1)$$

where ν_{n10} is given by (1) (curve 1) and ν_{ni0} for $i = 2, 3$ are represented by curves 2,3 calculated using the relations from [2]. The equations for ν_{ni} follow:

$$\nu_{ni}^2 = \nu_{n0}^2 \left(1 - \frac{\gamma_n H}{\nu_{n0}} \cos(\theta_i) \right); \quad (2)$$

θ_i are the angles between the sublattice magnetizations and the applied field. In the equations for the coupled oscillations (1) there are two parameters: ν_{T0} and ν_{n0} . The value of the first corresponds to the gap in the AFMR mode; we used for it the value obtained in the experiments of Zaliznyak et al. [9]. The second parameter - ν_{n0} is equal to the NMR frequency at $H = 0$. Its value was derived from the best fit of the calculated NMR spectrum to our experimental data. This best fit is represented by solid lines in Fig.1 and 2. All the experimental data below $H_c = 64 \text{ kOe}$ agree well with the calculated curves. From the obtained value $\nu_{n0} = 415 \text{ MHz}$ (using $A = -1.53 \cdot 10^{-18} \text{ erg}$ [10]) we have calculated the average spin of Mn²⁺ in CsMnBr₃ to be $\langle S \rangle = 1.8$.

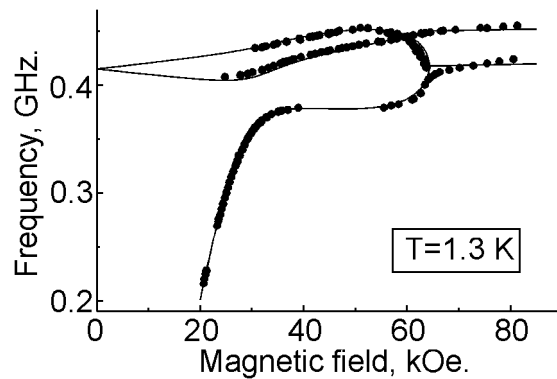


Fig. 2. NMR spectrum of CsMnBr₃.

This corresponds to the following reduction of the spin momentum due to magnetic quantum fluctuations: $\delta S/S = (S - \langle S \rangle)/S = 28\%$. This value is in a good agreement with the data received by other methods [1,4].

It is surprising that above H_c , where to a first approximation CsMnBr₃ should behave like a quasi-two-sublattice antiferromagnet with one NMR frequency, we have observed two branches of NMR.

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