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# Influence of quantum fluctuations on the ground state of quasi-one-dimensional triangular antiferromagnet $CsMnI_3$

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**Abstract**

$^{55}$Mn NMR in the quasi-1D triangular antiferromagnet $CsMnI_3$ was investigated. Six NMR modes corresponding to six spin orientations of Mn ions in elementary magnetic cell were observed. The difference between average values of the Mn spins $\langle S \rangle$ in magnetically nonequivalent antiferromagnetic chains was found. We have determined a new magnetic phase of $CsMnI_3$ in a magnetic field parallel to the hexagonal axis in the range 39–52 kOe. Calculations indicate that the new phase is a result of the difference between the $\langle S \rangle$ values in neighbouring antiferromagnetic chains. 

*Keywords:* $CsMnI_3$; Ground state; NMR; Quantum fluctuation; Quasi-1D; Spin reduction; Triangular antiferromagnet

We have investigated the $^{55}$Mn NMR in quasi-1D triangular antiferromagnet (AF) $CsMnI_3$. The low-field magnetic structure of this substance consists of AF chains along the hexagonal axis $C_6$. One-third of the chains have spins directed along $C_6$, while the other spins are at angle $\Theta \approx \pi/3$ to it (Fig. 1). $^{55}$Mn NMR was observed in single crystal samples at the magnetic fields 5–80 kOe, at frequencies 250–450 MHz and temperatures 1.3–4.2 K with $\alpha$ continuous-mode spectrometer. The $^{55}$Mn NMR spectrum for $H \| C_6$ at $T = 1.3$ K is presented in Fig. 2. It consists of five modes corresponding to six magnetic sublattices. The frequency of the sixth NMR mode is equal to zero for this field orientation. The nuclear frequency pulling due to interaction with ESR [1] is clearly seen in this spectrum. The calculation of NMR spectrum for AF with six sublattices is given in Ref. [2]. It was used to determine the unpulled NMR frequencies $\omega_{ni} = \gamma_n |A \langle \boldsymbol{S} \rangle_i + \boldsymbol{H}|$ as well as $\langle \boldsymbol{S} \rangle_i$ and the angles between sublattices and magnetic field ($\gamma_n$ is the gyromagnetic ratio, $A$ is the hyperfine constant, $\langle \boldsymbol{S} \rangle_i$ is the averaged spin of the $i$th magnetic sublattice).

The $^{55}$Mn NMR spectrum is quite complicated, but it is easy to determine the main features of $CsMnI_3$ magnetic structure. Thus, at $H \to 0$ two strongly field dependent NMR modes converge to $\omega_{n1} = 417$ MHz while the other modes converge to $\omega_{n2} = 388$ MHz. This proves that nonequivalent AF chains have small and different mean spins $\langle S \rangle_1 = 1.86$, $\langle S \rangle_2 = 1.74$, in comparison with $S = \frac{5}{2}$ for $Mn^{2+}$ ion. This phenomenon is caused by quantum fluctuations and was predicted in Ref. [3]. At fields $H > 52.5$ kOe only one NMR mode is observed. Therefore, all $Mn^{2+}$ spins are equal and have equivalent orientation in the external field, i.e. the well-known spin-flop phase is realised. At $H = 39$ kOe, the strong transformation of all NMR modes occurs because of transition to the new magnetic phase 3. It differs from the low-field phase by turning all spins at angle $\approx \pi/6$. The calculated NMR spectrum based on magnetic structures of phases 1 and 3 is presented in Fig. 2 by solid lines. Phase 3 takes place also at small angles between the magnetic field and the $C_6$ axis. This phase was observed for the first time.

We have calculated the energy difference between phases 1 and 3 taking into account the difference of mean spin values in nonequivalent AF chains [4]. Phase 3 exists only if $\langle S \rangle_1 \neq \langle S \rangle_2$. The calculated transition field in this phase is 37.8 kOe (measured values of $\langle S \rangle_1$

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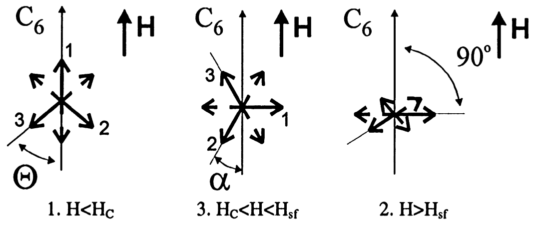


Fig. 1. Magnetic phases of $CsMnI_3$ for $H||C_6$.

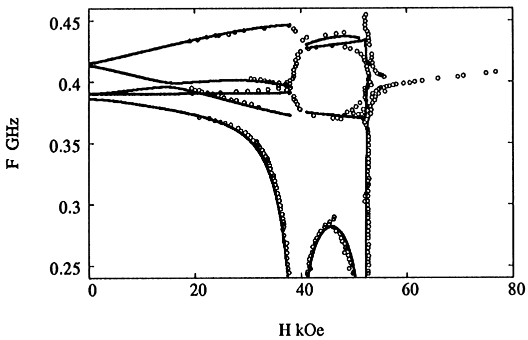


Fig. 2. $^{55}$Mn NMR spectrum for $H||C_6$ at $T = 1.3$ K.

and $\langle S \rangle_2$ in $CsMnI_3$ were taken). We have determined also other magnetic parameters for this substance. Fig. 3 shows the field dependence of spin triangle deformation obtained from NMR spectrum at $\varphi = 20°$ between the magnetic field and the $C_6$ axis. The solid line is our calculation [4]. The field dependencies of $\langle S \rangle$ at different $\varphi$ for $Mn^{2+}$ ions are shown in Fig. 4 [2,5]. At $\varphi = 20°$ and 90° only $\langle S \rangle_2$ is presented. Microscopic calculations are needed for the quantitative analysis of these data, although qualitatively they are in good agreement with the theory of suppression of quantum fluctuations.

Thus, the new phase 3 in $CsMnI_3$ at fields directed close to the $C_6$ axis exists because of the anisotropy of mean spins in nonequivalent AF chains. This anisotropy is a consequence of anisotropy of the quantum fluctuations in quasi-1D six-sublattice AF. Up to now, all

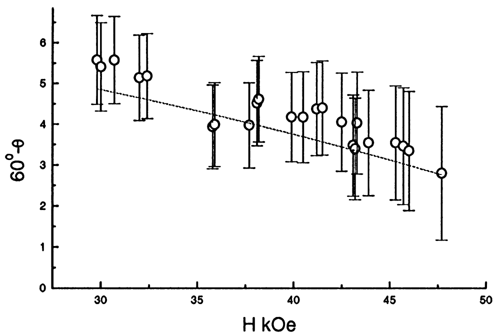


Fig. 3. Field dependence of angle $\Theta$ between spins 2 and the $C_6$ axis.

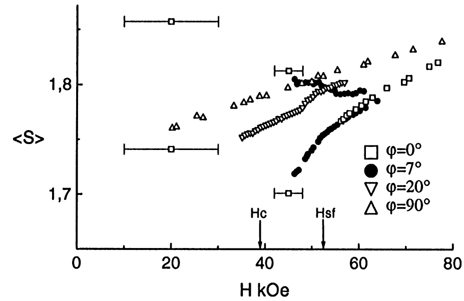


Fig. 4. Field dependence of mean $Mn^{2+}$ spins for different angles $\varphi$ between H and the $C_6$ axis.

known effects of quantum fluctuations in magnetic systems were either the decreasing of mean spin magnitude (reduction), or the total destruction of magnetic order (as in pure 1D substances). Existence of a magnetic phase caused by quantum fluctuations was discovered for the first time.

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