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QUASICRITICAL BEHAVIOUR OF THE NMR AND μSR RELAXATION IN YMn_2D_x

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The magnetic and structural properties of YMn_2 are strongly influenced by introduction of hydrogen (deuterium) in the structure, however, it only slightly modifies the noncollinear antiferromagnetic structure of the compound. The temperature dependences of the NMR relaxation times T_1 and T_2 of deuterium and the zero-field relaxation of muons in YMn_2D_x were measured at temperatures above the magnetic ordering temperature T_N. The corresponding relaxation rates are described by the empirical expression $(T/T_N - 1)^{-\eta}$, where the exponent η increases linearly with deuterium concentration x. To explain this behaviour, the Moriya theory of spin fluctuations was used. The expressions for NMR and μSR relaxation rates have been calculated. The resultant formulae agree well with the experiment, giving reasonable values of fitting parameters. The results obtained are discussed in terms of spin fluctuation excitation spectrum.

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The C15 Laves phase compound YMn_2 and its hydrides (deuterides) have very intriguing properties above their magnetic ordering temperature T_N. The NMR relaxation times T_1 and T_2 of deuterium and the muon depolarisation rate λ of these materials exhibit a critical divergence as T_N is approached from above [1–3]. It is interesting that their temperature dependence above T_N can be described by nearly the same function of temperature T

$$F(\delta) = \text{const}\ \delta^{-\eta}, \tag{1}$$

where $\delta = (T - T_N)/T_N$ is the reduced temperature, the exponent η depends linearly on the deuterium concentration x and the constant prefactor of course depends on the quantity under consideration. The dependence of η on x is shown in Fig. 1.

We call the behaviour described by Eq. (1) "quasicritical", because the function $F(\delta)$ has a singularity when T approaches the critical temperature T_N but on the other hand the true critical exponent should not depend on the chemical composition of the material but only on the model Hamiltonian [4]. Thus we have to look for another formula which would explain this behaviour. It is clear that spin fluctuations play an important role in the vicinity of the temperature where the

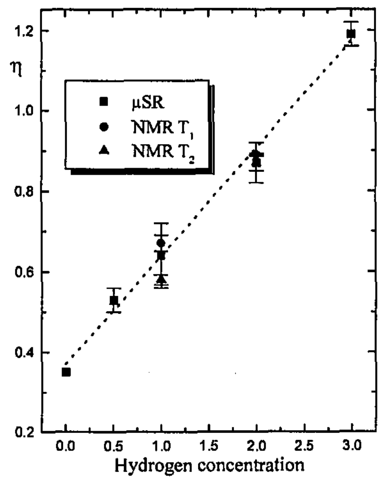

Fig. 1. Dependence of the exponent η on the deuterium concentration x.

phase transition takes place. Therefore, we refer to Moriya's theory of spin fluctuations [5]. This theory was originally formulated to describe the NMR relaxation rates near the transition temperature and we think that it can also be used to describe the muon depolarisation as it is caused by the same physical interaction. According to Moriya's theory [5] the spin-lattice relaxation time T_1 for a cubic crystal can be written as follows:

$$\frac{1}{T_1} = \frac{2A^2 k_B T}{\hbar^2 g^2 \mu_B^2} \frac{1}{N} \sum_k \frac{\chi(k)}{\Gamma_k}, \tag{2}$$

where A is a hyperfine constant, N is the number of magnetic atoms in the sample, $\chi(k)$ is a staggered susceptibility, Γ_k determines the decay of the time correlation function

$$f_k(t) = \exp(-\Gamma_k t) \tag{3}$$

and other symbols have their usual meanings. For an antiferromagnet the susceptibility can be written as

$$\chi(\boldsymbol{k}) = \frac{g^2 \mu_B^2 S(S+1)/3k_B T_N}{\delta + [1 - J(\boldsymbol{k})/J(\boldsymbol{K}_0)]}, \tag{4}$$

where S is the spin of magnetic ion, $J(\boldsymbol{k})$ is the Fourier transform

$$J(\boldsymbol{k}) = \sum_j \exp\left[i\boldsymbol{k} \cdot (\boldsymbol{R}_j - \boldsymbol{R}_{j'})\right] J_{jj'} \tag{5}$$

of the exchange coupling constant $J_{jj'}$ and $\boldsymbol{K}_0$ is the antiferromagnetic wave vector. The second term in the denominator in Eq. (4) can be approximated as

$$1 - J(\boldsymbol{k})/J(\boldsymbol{K}_0) = \gamma \kappa^2, \tag{6}$$

where $\boldsymbol{\kappa} = \boldsymbol{k} - \boldsymbol{K}_0$. Then we can write

$$\chi(\boldsymbol{k}) = \frac{C_1}{\delta + \gamma \kappa^2} \tag{7}$$

or

$$\chi(\boldsymbol{k}+\boldsymbol{K}_0)=\frac{C_1}{\delta+\gamma\kappa^2}. \tag{8}$$

The decay rate Γ_k for an antiferromagnet we can approximate after [5] as

$$\Gamma_{\boldsymbol{k}+\boldsymbol{K}_0}=\Lambda'+\Theta' k^2, \tag{9}$$

where $\Lambda'\propto T-T_{\mathrm{N}}$ above T_{N} and Θ' remains finite as the transition temperature is approached. Thus we can write

$$\Gamma_{\boldsymbol{k}+\boldsymbol{K}_0}\cong C_2\delta+\Theta' k^2. \tag{10}$$

Now we can do the summation in Eq. (2)

$$\frac{1}{N}\sum_k\frac{\chi(\boldsymbol{k})}{\Gamma_k}=\frac{1}{N}\sum_k\frac{\chi(\boldsymbol{k}+\boldsymbol{K}_0)}{\Gamma_{k+K_0}}=\frac{1}{N}\sum_k\frac{C_1/C_2}{(\delta+\gamma k^2)[\delta+(\Theta'/C_2)k^2]}. \tag{11}$$

Moriya arbitrarily assumed $\Theta'/C_2=\gamma$ (Ref. [5], p. 384) and obtained the asymptotic form

$$\frac{1}{T_1}=\text{const } \delta^{-1/2} \tag{12}$$

for an antiferromagnet when $T\to T_{\mathrm{N}}$. He also stressed that the anomalous increase in the relaxation rate should be observed in a very narrow temperature range. We however observe such quasicritical behaviour of the relaxation rates T_1, T_2 and the muon depolarisation rate λ in a rather wide temperature range which cannot be described by means of the universal exponent 1/2. Thus we abandon Moriya's assumption and define a parameter α

$$\alpha=\frac{\gamma C_2}{\Theta'}. \tag{13}$$

Then we can write

$$\frac{1}{T_1}=\text{const } T\frac{1}{N}\sum_k\frac{1}{(\delta/\gamma+k^2)(\alpha\delta/\gamma+k^2)} \tag{14}$$

and if we approximate the summation by integration we obtain for $\alpha\neq 1$

$$\frac{1}{T_1}=\text{const } T\left(\frac{\delta}{\gamma}\right)^{-1/2}\left\{\frac{1}{1-\alpha}\arctan\left[k_{\max}\left(\frac{\delta}{\gamma}\right)^{-1/2}\right]\right.$$
$$\left.+\frac{\alpha^{1/2}}{\alpha-1}\arctan\left[k_{\max}\left(\frac{\alpha\delta}{\gamma}\right)^{-1/2}\right]\right\}, \tag{15}$$

where $k_{\max}$ is a cut-off parameter. It is easily seen that in the vicinity of the transition point, i.e. $\delta\to 0$, we recover Moriya's result because the function arctangent then goes to a finite value. The same form should describe the behaviour of $1/T_1$ and λ. We fitted our function to our experimental data for different deuterium concentrations x using $k_{\max}$, γ, α as the fitting parameters but keeping the transition temperature T_{N} fixed. The results are shown in Fig. 2.

The best values of the fitting parameters are given in Table.

In conclusion we can say that the behaviour of the NMR relaxation rates $1/T_1$, $1/T_2$ and the muon depolarisation rate λ in YMn_2D_x, which are well repro-

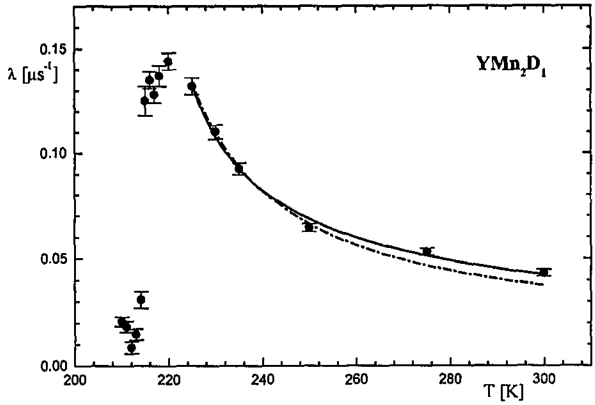

Fig. 2. The dependence of the muon relaxation rate λ on temperature T (broken line — theory, solid line — fitting to the experiment).

TABLE

The best values of the fitting parameters: γ, $k_{\max}$, and λ_0 for some deuterium concentrations and respective temperature T_N.

x	0.5	1.0	2.0	3.0
γ	0.0754	0.0512	0.0224	0.0045
$k_{\max}$	0.0260	0.0467	0.0485	0.0757
α	9.64×10^{-8}	1.087×10^{-12}	9.42×10^{-6}	2.915×10^{-10}
λ_0 [s^{-1}]	2.55×10^{-4}	4.27×10^{-4}	8.21×10^{-3}	0.0406
T_N [K]	245	205	243	325

duced by the empirical formula given by Eq. (1), can be explained within the spin fluctuations theory in a wide range of temperatures above the transition point.

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