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EPR SPECTRUM FOR $NiSiF_6 \cdot 6H_2O$ AT LOW TEMPERATURES

BY J. CZAKON

Institute of Physics, Silesian University, Katowice*

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The Tanaka and Kondo method of calculating the absorptive part of the magnetic susceptibility has been applied for $NiSiF_6 \cdot 6H_20$. It was found that the above mentioned method is very sensitive even to small changes in the parameter $D^{-1}J$. The position of the two main maxima of $\chi''(h)$ remains in agreement with the experimental data of Svare and Seidel for $D^{-1}J = 0.078$. If the molecular field method is used for the calculation of mean values then the EPR line becomes narrower.

The EPR spectrum for $NiSiF_6 \cdot 6H_2O$ has been investigated both theoretically [1, 2] and experimentally [3]. For this compound the exchange interaction between Ni ions is much smaller than the crystalline field anisotropy parameter D. In such a case one can make use of Kubo's linear response theory [4] to investigate the reaction of the system to the time dependent external magnetic field. The shape of the EPR line [1] is just the result of the existence of exchange interaction which is weaker than the crystalline field. The calculations in [1] have been performed under the assumption that the correlations between nearest neighbour spins are negligibly small above the temperature of phase transition and this transition does not effect the values of the moment of the third spin component considerably. On the basis of [1] it has been found by the present author, after laborious numerical calculations, that the position of the main maximum of $\chi''(h)$ is very sensitive even to small changes in the parameter $p = JD^{-1}$ where J stands for the exchange integral and D denotes the crystalline field parameter. The EPR line becomes narrower if the existence of the molecular field [5] in the calculation of spin correlation functions is taken into account. This is shown in Fig. 1*b*.

The measurements for the case of $NiSiF_6 \cdot 6H_2O$ of the absorptive part of magnetic susceptibility $\chi''(h)$ have been performed in a rotating field of frequency $\omega = 30$ GHz [3]. From the measurements of interactions parameters the values $D = 2.24\ 10^{-17}$ erg and $J = 1.75\ 10^{-18}$ erg have been derived. The measurements have been performed in the temperature range 0.4—4.2 K, so in the numerical calculations the values $p = 0.078$,

* Address: Instytut Fizyki, Uniwersytet Śląski, Uniwersytecka 4, 40-007 Katowice, Poland.

$\omega_0 = \frac{\hbar\omega}{D} = 8.88$ should be used and the parameter $t = \frac{kT}{D}$ is contained in the interval 2.56—25.8.

If one assumes $JD^{-1} = 0.1$, $\omega = 10.0$, $t = 2.56$ [1] then it can be noted that the theoretical EPR line (curve *a* in Fig. 1) is considerably shifted towards the right with respect to that derived experimentally by Svare and Seidel [3] (curve *c* in Fig. 1).

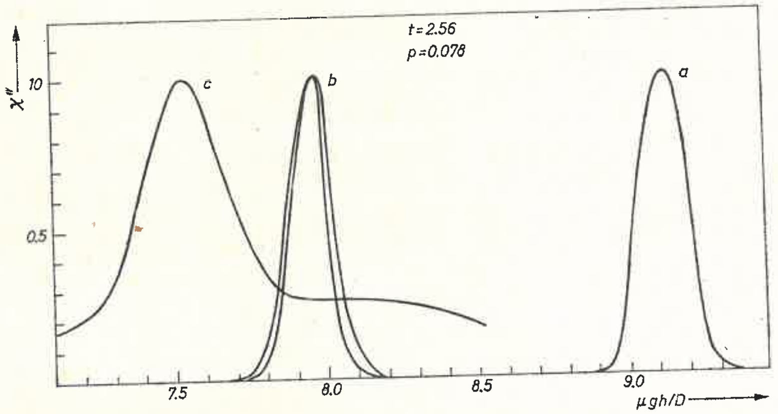

Fig. 1. χ'' versus external magnetic field. The curve *a* represents the result of Tanaka and Kondo for $JD^{-1} = 0.1$, $\omega_0 = 10.0$ and $t = 2.56$. The curve *b* corresponds to the results obtained in the present work for the values $JD^{-1} = 0.078$, $\omega_0 = 8.88$ and $t = 2.56$ and the curve *c* represents the experimental data of Svare and Seidel for the same values of the parameters as in *b*

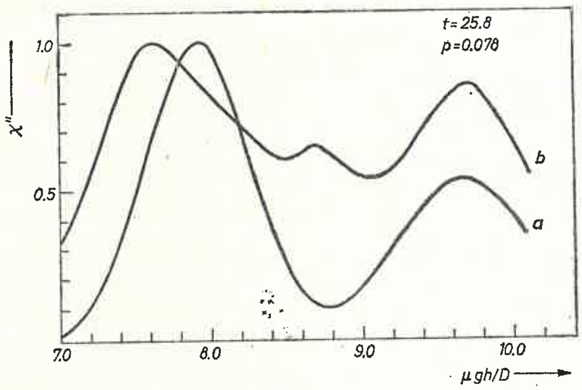

Fig. 2. χ'' versus external magnetic field. The curve *a* represents our result for $JD^{-1} = 0.078$, $\omega_0 = 8.88$, and $t = 25.8$ and the curve *b* corresponds to the experimental data of Svare and Seidel for the same values of parameters as in *a*

A similar situation is observed for higher temperatures. Satisfactory agreement with experimental data is not obtained and the experimental curves are much wider than the theoretical ones (curve *c* in Fig. 1). This is due to the fact that the dipole interactions are not taken into account in the present theory. For higher temperatures ($t = 25.8$ or

$T = 4.2$ K) the agreement with experimental results becomes still weaker inspite of the fact that the positions of the two main maxima nearly coincide with the experimental ones (Fig. 2). The third maximum which appears for $\frac{\mu g h}{D} = 8.7$ (curve b in Fig. 2) cannot be explained within the framework of the present theory. One may suppose that this is due to the presence of such regions in the magnet (e.g. interdomain regions) in which the crystalline field parameter takes on a value different than in the rest of the material and the number of particles taking part in EPR is small in them.

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