FIELD DEPENDENCE OF SPIN WAVES IN THE KONDO LATTICE $CeCu_2$*

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The Kondo lattice compound $CeCu_2$ shows an antiferromagnetic ordering below $T_N = 3.5$ K. The two moments in the primitive crystallographic unit cell are aligned antiparallel to each other and oriented along the orthorhombic $c-$axis even though the a-axis is the easy axis of magnetization. This can be explained by a strongly anisotropic antiferromagnetic exchange in the ac-plane which cancels out the crystal field anisotropy. The measurements of the spin wave dispersion at 1.5 K that we present in this paper for zero field and for 5 T in a-direction verify this assumption. Preliminary model calculations using the program package *McPhase* reproduce qualitatively the measured dispersion curves.

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1. Introduction

$CeCu_2$ is a Kondo lattice compound which shows antiferromagnetic ordering at $T_N = 3.5$ K [1] with the propagation vector (000) and a Kondo temperature of $T_K = 4$ K as derived from an extrapolation of the neutron quasi-elastic line width [2]. The two magnetic moments in the primitive crystallographic unit cell ($CeCu_2$-structure, space group Imma; magnetic = chemical unit cell) are aligned antiparallel to each other and oriented along the orthorhombic c-axis. The magnetic structure is shown in Fig. 1. It is surprising that the easy axis of magnetization is the a-axis while the moments are oriented along the c-direction. A possible scenario for such a situation is that the antiferromagnetic exchange is strongly anisotropic in

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the nearly hexagonal ac-plane and competes with the crystal field anisotropy. The low-field susceptibility is different for all three crystallographic directions ($\chi_a > \chi_c > \chi_b$). It shows a peak at T_N only for χ_c [1, 3]. The magnetization curves at $T = 2\,K$ in the ordered state as shown in Fig. 2 are also strongly anisotropic. The field induced ferromagnetic state seems to be reached already for fields in a-direction of the order of 2 T. Saturation in the other directions is reached only at considerably higher fields and with lower saturation moments: 15 T ($1\mu_B$) for the c-direction, 30 T ($0.5\mu_B$) for the b-direction [4].

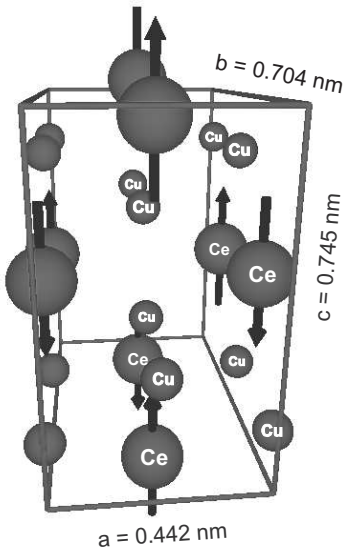

Fig. 1. Magnetic structure of $CeCu_2$ (after [1]).

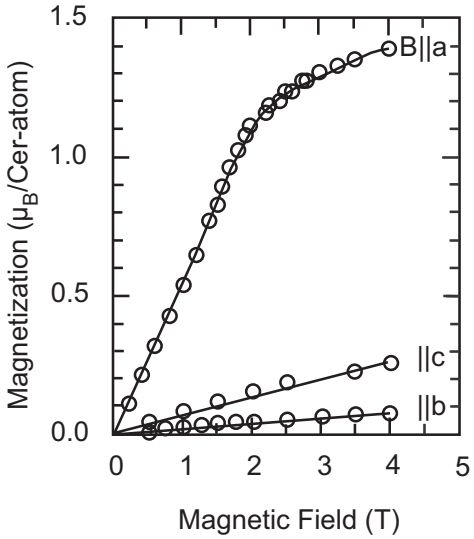

Fig. 2. Magnetization measurement of $CeCu_2$ at 2 K along the main crystallographic directions (from [1]). Lines are guide to the eyes.

2. Experimental details and results

The measurements of the spin wave dispersion at $T = 1.5\,K$ and as function of the magnetic field along the a-direction were performed on the cold triple-axis spectrometer IN12 at ILL Grenoble. The $CeCu_2$ single crystal was the same as that used for the measurements of the crystal field (CF)–phonon interaction [5]. In this paper we present the results for the dispersion along (0k0) in zero field and at 5 T ($H \parallel a$). Due to the symmetry of the magnetic lattice there are two spin wave modes, but only one spin wave mode is visible for scans along (0k0). The experimental results are displayed in Fig. 3. The measured dispersion curve in zero field differs drastically from that at 5 T.

The error bars indicate the measured full width at half maximum of the peaks. The widths are only slightly larger than the instrumental resolution indicating that the collective excitations in the magnetically ordered state of the Kondo compound are nearly unaffected by the Kondo effect. The full lines in the figure indicate results of a preliminary fit using the *McPhase* [7] program which will be discussed in detail in the next section.

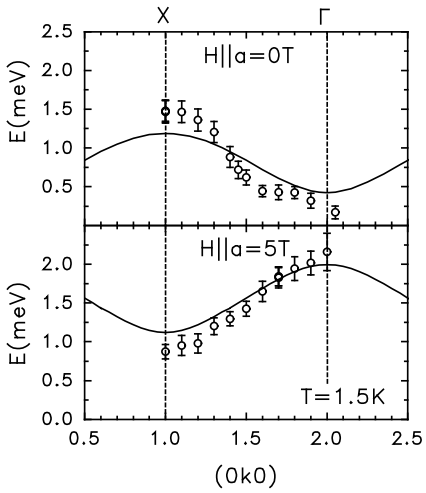

Fig. 3. Dispersion of magnetic excitations at different fields in a-direction. The data points are experimental results and the error bars indicate the measured full width at half maximum of the peaks. The lines are results of a calculation assuming an **anisotropic** exchange interaction (see text).

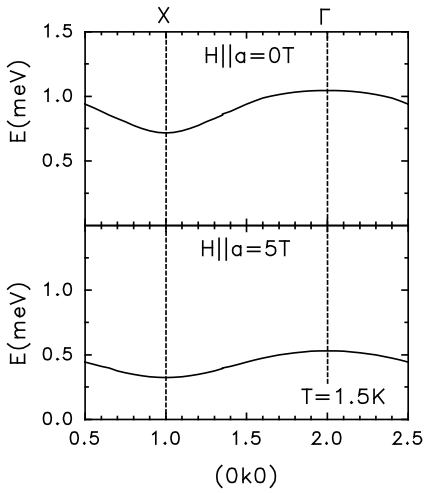

Fig. 4. Calculated dispersion curves with an **isotropic** exchange interaction in $CeCu_2$ in zero field and for a field of 5 T in a-direction. The lines are results of a calculation using the *McPhase* [7] program.

3. McPhase calculations

For the preliminary calculations only nearest neighbor exchange interactions up to a maximum distance of 0.876 nm have been applied (the present aim was only to show the qualitative difference between isotropic and anisotropic exchange). The following parameters were used for the calculations: in both cases the single ion anisotropy due to the crystal field was modeled by an anisotropic Kramers doublet groundstate with saturation moments 1.37, 0.5 and $0.94\mu_B$/Ce-atom for the a-, b- and c-direction, respectively. The exchange interaction $\boldsymbol{H}_{ex}$ was treated in mean-field approximation

$$\boldsymbol{H}_{\rm ex} = -\frac{1}{2}\sum_{ij,\alpha\beta} \boldsymbol{J}_i^{\alpha}\mathcal{J}_{\alpha\beta}(ij)\boldsymbol{J}_j^{\beta}\,, \tag{1}$$

where $\boldsymbol{J}_i^{\alpha}$ denotes the Cartesian coordinates of the angular momentum of the Ce atom at the lattice position i. Using the (diagonal) exchange tensor given in column 4–6 of Table I the observed magnetic structure (Fig. 1) can be reproduced. The excitation spectrum was calculated in the random phase approximation [6, 7] for zero field and is shown in Fig. 3. According to the calculation in a field of 5 T parallel to the a-direction the ferromagnetically aligned spin configuration is stable and the form of the dispersion changes because of the anisotropy of the exchange interaction.

TABLE I

Exchange interaction constants used in the *McPhase* calculation for $CeCu_2$. Column 1–3 denote the relative position of the Cerium neighbor in units of the lattice constants. The anisotropic exchange constants are shown in column 4–6 and the last column contains the isotropic exchange constants (see text).

$x_i - x_j$ [a]	$y_i - y_j$ [b]	$z_i - z_j$ [$c4$]	$\mathcal{J}_{aa}(ij)$ [μ eV]	$\mathcal{J}_{bb}(ij)$ [μ eV]	$\mathcal{J}_{cc}(ij)$ [μ eV]	$\mathcal{J}_{\rm iso}(ij)$ [μ eV]
+0.0	+0.5	+0.0766	+29.9	−86.5	−72.0	−18.0
+0.5	+0.0	−0.4234	−13.9	+13.2	−10.6	−2.65
+1.0	+0.0	+0.0	+18.3	−88.0	+7.10	+1.78
+0.5	+0.0	+0.5766	+11.0	−48.7	−35.7	−8.93
+0.5	+0.5	+0.5	−5.27	+21.8	−6.08	−1.52
+1.0	+0.5	+0.0766	+10.6	−44.7	−20.9	−5.23
+0.0	+1.0	+0.0	+3.86	−37.5	+14.7	+3.68
+1.5	+0.0	−0.4234	+4.96	+14.3	−4.60	−1.15
+0.0	+0.0	+1.0	+1.00	−6.46	+23.9	+5.98
+0.0	+0.5	−0.9234	+1.48	−7.26	−3.66	−0.92
+1.5	+0.0	+0.5766	+1.36	−8.30	−0.76	−0.19
+0.5	+1.0	−0.4234	+0.85	−2.88	−2.59	−0.65
+1.0	+1.0	+0.0	−0.28	−5.00	+0.57	+0.14
+1.5	+0.5	+0.5	+0.81	+0.63	−0.65	−0.16
+0.5	+1.0	+0.5766	+0.09	−5.00	+0.58	+0.15
+1.0	+0.0	+1.0	−0.83	−2.61	−2.67	−0.67
+0.0	+0.5	+1.0766	+0.99	−2.92	+1.56	+0.39

In order to underline the conclusion, that the exchange interaction has to be anisotropic in $CeCu_2$ the dispersion of the excitations was also calculated assuming an isotropic exchange (*i.e.* $\mathcal{J}_{aa} = \mathcal{J}_{bb} = \mathcal{J}_{cc} = \mathcal{J}_{\rm iso}$). The result of this calculation is shown in Fig. 4 and has been obtained using the exchange constants given in the last column of Table I. In this model the dispersion has a global minimum at the Γ-point corresponding to the acoustic mode and the form does not change by applying a field of 5 T which induces a ferromagnetic structure. Note that due to the isotropy of the exchange in this calculation the moments are aligned by the crystal field parallel to the a-direction in zero field (this is also in contrast to the experimental observation).

Finally we want to remark that the present case is different from the situation of the anisotropic exchange in $NdCu_2$ that has been described in detail in Ref. [6]. While we have to invoke an anisotropic exchange in $CeCu_2$ within the ac-plane ($\mathcal{J}_{aa} \neq \mathcal{J}_{bb} \neq \mathcal{J}_{\rm cc}$), we could explain the spin waves in $NdCu_2$ by an isotropic exchange within the ac-plane ($\mathcal{J}_{aa} = \mathcal{J}_{cc} \neq \mathcal{J}_{bb}$).

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