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Magnetic excitations in the antiferromagnetic phase of $NdCu_2$

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Abstract. Detailed investigations of the magnetic interactions can be performed by comparing measurements with calculations of dynamical magnetic properties. In this study neutron spectroscopy on single crystals was used to measure the magnetic excitations in the antiferromagnetic phase of $NdCu_2$. This phase is characterized by a stacking of ten ferromagnetically ordered *bc*-planes with a propagation vector of (0.6 0 0).

The magnetic excitations have been calculated in the different magnetic phases, which can be stabilized by a magnetic field along the crystallographic *b* direction (= easy axis). The model is based on a mean field (MF) theory and fluctuations are treated in the random phase approximation (RPA). The dispersion of the magnetic excitations has been calculated using exchange parameters, which have been determined by neutron spectroscopy in the ferromagnetically aligned phase in a magnetic field of 3 T parallel to *b*. For the calculation the program package *McPhase* was used. The results are compared to data of neutron spectroscopy on single crystals.

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The magnetic phase diagram of $NdCu_2$ has been studied for fields aligned parallel to the crystallographic *b* direction, the easy axis of this orthorhombic system [1]. Up to a field of 1 T the zero field antiferromagnetic phase AF1 is stable. Between 1 and 2.5 T a ferrimagnetic phase F1 is found, which is followed by a complicated phase F2 (2.5–2.8 T). For magnetic fields above 2.8 T the moments are aligned ferromagnetically (F3). The phase diagram has been modeled by a numerical MF calculation using the *McPhase* (http://www.mcphase.de) program package.

In order to find out more about the magnetic exchange in this system, the magnetic excitations have been measured and analyzed in the phase F3 of $NdCu_2$. This has lead to a model for the exchange anisotropy in all RCu_2 compounds [2]. In the present paper we report on measurements of the magnetic excitations in the phases AF1 and F1 and compare the data to the predictions of the MF–RPA model.

1 Experimental

The inelastic neutron scattering experiments have been performed on a $NdCu_2$ crystal with dimensions $4 \times 5 \times 7\,mm^3$; the details of the sample are given in [1]. For the measurements in zero magnetic field the 4F2 triple axis spectrometer of the Laboratoire Leon Brillouin (LLB, Saclay) was used. The experiments in magnetic fields parallel to *b* were done on the IN14 and IN12 triple axis spectrometers of the In-

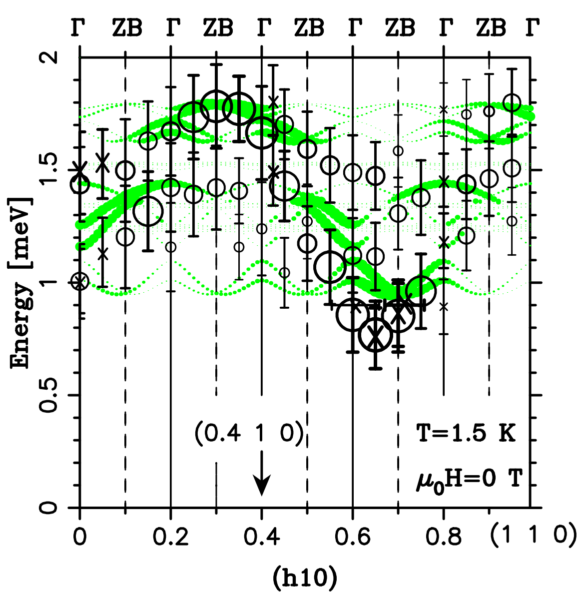

Fig. 1. Dispersion of the magnetic excitations along (h 1 0) in the AF1 phase of $NdCu_2$. The calculation (•) is compared to experimental data measured at 4F2-LLB (○) and IN12-ILL (×). The different sizes of the symbols represent the intensities, *vertical lines* mark the center (Γ) and the zone boundary (ZB) of the magnetic Brillouin zone. The *arrow* indicates the position of the magnetic propagation vector in AF1

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stitute Laue Langevin (ILL, Grenoble) with a 5 T vertical magnet for fields perpendicular to the scattering plane. In addition, the V2 triple axis spectrometer of the Hahn Meitner Institut (HMI, Berlin) was employed together with a 5 T horizontal field magnet to access scattering vectors within the *ab*-plane. At 4F2 and IN14 a graphite filter was used in order to avoid $\lambda/2$ contamination of the primary neutron beam (at $k_f = 1.64\,\text{Å}^{-1}$).

For the measurement of the dispersion of the magnetic excitations a temperature of 1.5 K was stabilized. Energy scans at constant scattering vector $\boldsymbol{Q}$ and scans of $\boldsymbol{Q}$ along the principal crystallographic directions of the Brillouin zone at constant energy have been performed. The data were fitted by a set of Gaussian functions and evaluated by plotting the energy of the excitations versus $\boldsymbol{Q}$ in a plot with different point size corresponding to the intensity maximum of the fitted Gaussian peak. Figure 1 shows such a plot for the dispersion of the excitations in AF1 for $\boldsymbol{q} = (h\,1\,0)$. The calculated magnetic excitations were plotted in the same way and thus can be compared to the measured data.

2 Results and discussion

The calculation is based on the following Hamiltonian:

$$
\begin{aligned}
H &= H_{\text{cf}} + H_{\text{ex}} + H_{\text{Ze}}\,, \\
H_{\text{cf}} &= \sum_{i,lm} B_l^m O_l^m(\boldsymbol{J}_i)\,, \\
H_{\text{ex}} &= -\frac{1}{2}\sum_{ij\alpha\beta} \boldsymbol{J}_i^\alpha \mathcal{J}^{\alpha\beta}(ij)\boldsymbol{J}_j^\beta\,, \\
H_{\text{Ze}} &= -\sum_i g_J \mu_B \boldsymbol{H}\boldsymbol{J}_i\,.
\end{aligned} \tag{1}
$$

Here the first term, H_{cf}, describes the crystal field Hamiltonian of the $4f$ electrons on each Nd^{3+} ion. The second term, which is an order of magnitude smaller, describes the anisotropic bilinear exchange interaction between different Nd ions. The exchange tensor $\mathcal{J}^{\alpha\beta}(ij)$ is assumed to be diagonal and the orthorhombic distortion of the nearly hexagonal crystal is neglected. The third term in (1) is the Zeeman energy due to an applied magnetic field $\boldsymbol{H}$.

Using the Hamiltonian (1) in *McPhase* the magnetic phases have been modeled by a numerical mean field procedure similar to that described in [1], however without considering the effect of inter-doublet mixing. Because the exchange interaction in $NdCu_2$ is long range, the exchange has to be considered up to the 12th nearest neighbor in the *a* direction (corresponding to 26 Å) in order to reproduce the different magnetic structures correctly [3]. A MF–RPA [4, 5] calculation of the magnetic dynamics was based on the results of this simulation of the static properties. Note that this calculation is *not* a fit to the experimental data: the dispersion of the magnetic excitations for the phases AF1, F1 and F2 was calculated using the exchange parameters given in [2].

Figures 1 and 2 show the calculated dispersion in comparison with experimental data in the phases AF1 and F1, respectively. The different sizes of the symbols correspond to the measured or calculated intensities. Part of the data (F1) have already been published [6], however without comparison to this model calculation. The complicated magnetic unit

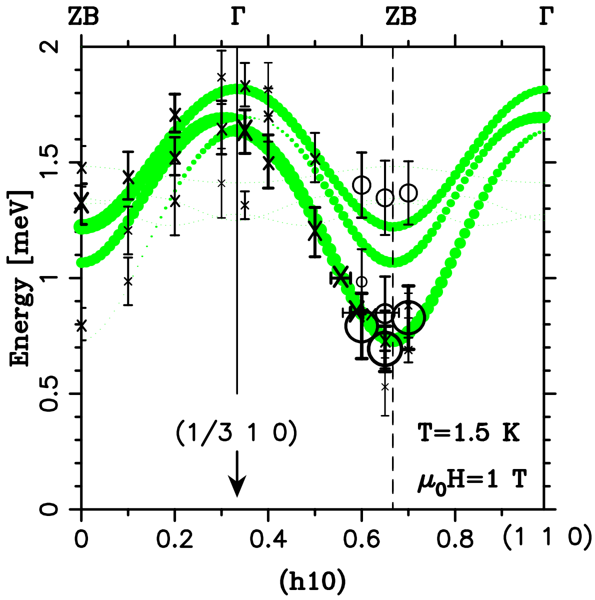

Fig. 2. Dispersion of the magnetic excitations along (h 1 0) in the F1 phase of $NdCu_2$ in a magnetic field of 1 T applied along the b direction. The calculation (•) is compared to experimental data measured at V2-HMI (×), and IN14-ILL (○) [6]. The *different sizes of the symbols* represent the intensities, *vertical lines* mark the center (Γ) and the zone boundary (ZB) of the magnetic Brillouin zone. The *arrow* indicates the position of the magnetic propagation vector in F1

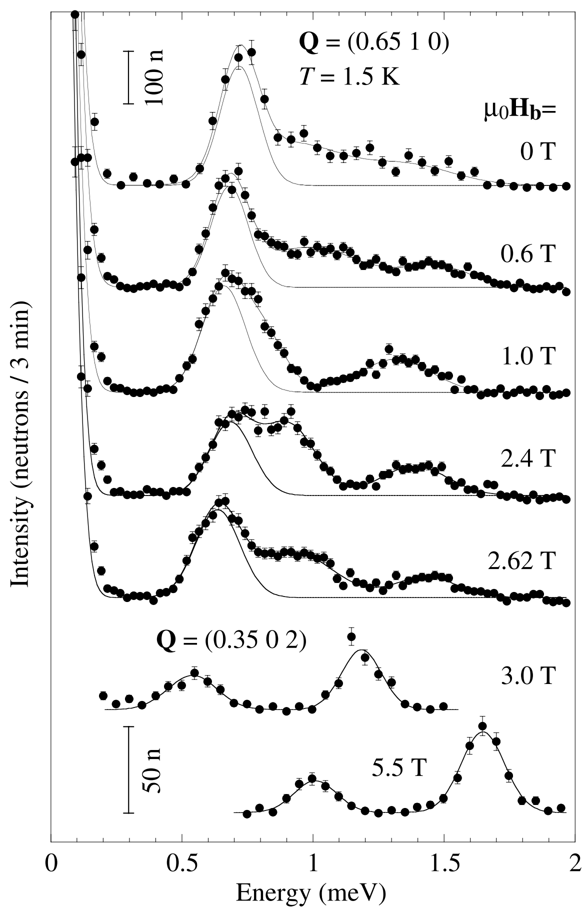

Fig. 3. Constant $\boldsymbol{Q}$ scans measured at IN14 (ILL) at different applied fields. All spectra correspond to the reduced wave vector $\boldsymbol{q} = (0.35\,0\,0)$. If $l = 0$ only half of the modes can be seen (see text)

cell (20 Nd atoms in AF1, 6 in F1, 32 in F2, and 2 in F3) produces a correspondingly large number of modes. However due to the structure factor along the (h 1 0) direction only half of 20, 6, 32, and 2 modes can be seen in AF1, F1, F2 and F3 . Similar to F3 [2] the data in AF1 and F1 exhibit a minimum in the excitation energy at about (2/3 1 0) associated with high scattering intensity. Note that this position is different from the magnetic propagation vector (in AF1: (0.6 0 0), in F1: (2/3 0 0), indicated by the arrows in Figs. 1 and 2). We take this as a proof of the strong anisotropy of the magnetic exchange interactions in all magnetic phases.

Further information for the identification of magnetic modes can be gained by measuring the detailed field dependence of the excitation spectra at a fixed $\boldsymbol{q}$ value. Figure 3 gives an example of such an analysis at the reduced wave vector $\boldsymbol{q} = (0.35\,0\,0)$. If $l = 0$ only half of the modes can be seen. Therefore the spectra at $\boldsymbol{Q} = (0.65\,1\,0)$ are shown. At equivalent points in reciprocal space other modes could additionally be identified, because the intensity varies strongly with $\boldsymbol{Q}$. In order to compare how the two modes in the phase F3 are resolved in spectra with $l \neq 0$, scans at $\boldsymbol{Q} = (0.35\,0\,2)$ are shown in Fig. 3.

After fitting the spectra by Gaussians, the data of the field dependence at the reduced wave vector $\boldsymbol{q} = (0.35\,0\,0)$ can be compared to the *McPhase* calculation in Fig. 4. The main features of the experimental data are well predicted by the numerical analysis. Some quantitative discrepancies such as the exact energy value of the lowest mode in AF1 are due to restrictions of the MF–RPA approach and additional terms in the Hamiltonian, which have not been considered.

In conclusion we emphasize that the identification of all magnetic modes in complex systems is not possible from inelastic neutron scattering data alone, because the intensity of the magnetic excitations varies rapidly and the resolution is limited. Therefore it is necessary to rely on a numerical model for the identification of the modes. The program package *McPhase* has been developed to address this problem. It provides an easy-to-use tool for the simulation of static and dynamic properties of complex magnetic systems.

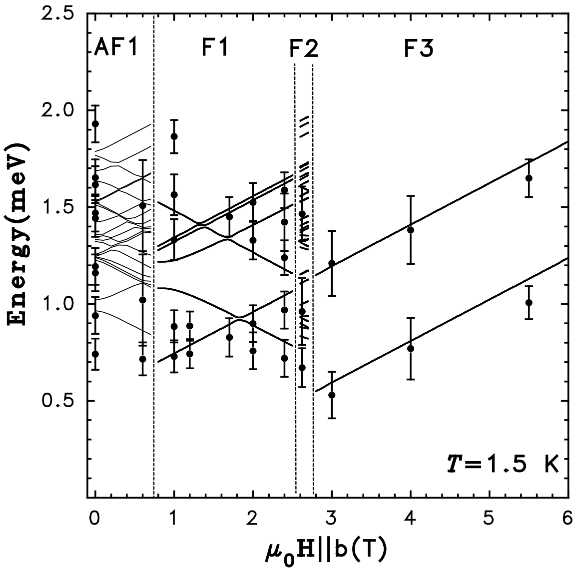

Fig. 4. Field dependence of the magnetic excitations at the reduced wave vector $\boldsymbol{q} = (0.35\,0\,0)$ as measured at IN14 and IN12 (ILL). The data were derived from spectra at several equivalent $\boldsymbol{Q}$ values. The *lines* indicate the results of the *McPhase* calculation

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