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## MAGNETIC EXCITATIONS AND QUASIELASTIC LINEWIDTHS IN $\text{YbBe}_{13}$ FROM NEUTRON SCATTERING

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Inelastic magnetic neutron spectra were taken on polycrystalline  $\text{YbBe}_{13}$  between 1.2 and 300 K. At low temperatures the formation of a magnon corroborates the existence of a magnetic phase transition observed also by static susceptibility. At higher temperatures two distinct CF-transition lines are observed, which lead to the cubic CF-parameters  $x = 0.911$  and  $W = 0.1543$  meV. The magnetic quasielastic linewidth increases linearly with temperature and is anomalous large compared to  $\text{TbBe}_{13}$  but small everywhere compared to  $k_{\text{B}}T$ .

### 1. Introduction

Magnetic susceptibility measurements of  $\text{YbBe}_{13}$  [1] have established an effective magnetic moment of  $\mu_{\text{eff}} = 4.54\mu_{\text{B}}$  of the 4f-shell in Yb, which is exactly the theoretical value of the stable trivalent 4f<sup>13</sup> configuration in the Hund's rule groundstate. Until recently, this compound was the only intermetallic compound with Yb known to order magnetically. This singular case is in contrast to the large number of magnetically ordering Ce-compounds on the other end of the rare earth series. The reason for the rare occurrence of the magnetic ordering for Yb is expected to lie in the instability of the 4f-shell. Actually, one expects more symmetry in the behaviour between Ce and Yb. Indeed, three more magnetically ordering Yb-compounds have been found recently, namely  $\text{YbPd}$  [2],  $\text{Yb}_3\text{Pd}_4$  [3] and  $\text{YbIr}_2$  [4]. When Yb does actually order magnetically in a metal, its properties should carry some memory of the valence instability, which would lead to the kind of interplay between valence instability and magnetic order, which has attracted so much attention in the magnetic ordering of Ce-compounds, e.g.  $\text{CeAl}_2$  and  $\text{CeAg}$ , in the past. Indeed, recent measurements of the magnetic quasielastic (QE)-linewidth of  $\text{YbPd}$  and  $\text{Yb}_3\text{Pd}_4$  [5] show qualitatively the same behaviour as  $\text{CeAl}_2$  and  $\text{CeAg}$ . In the work we present here, we have investigated the magnetic neutron spectrum of  $\text{YbBe}_{13}$  to find out whether we here also have a case of magnetic order at the verge of valence instability.

### 2. Experimental and discussion

$\text{YbBe}_{13}$  crystallizes in the cubic  $\text{NaZn}_{13}$  structure (Fm3c). While 8 Yb-ions are placed at equivalent cubic sites 104 Be-ions occupy two different types of sites (monoclinic, cubic) thus forming a kind of cage around the Yb-ions.

We have prepared polycrystalline  $\text{YbBe}_{13}$  with lattice parameter  $a_0 = 10.195$  Å and have measured its inelastic neutron spectrum at the time-of-flight spectrometer IN6 (ILL, Grenoble,  $E_0 = 3.1$  meV) in the temperature region between 1.2 and 300 K.

Fig. 1 shows the scattering function as measured from  $\text{YbBe}_{13}$  at low temperatures. At  $T = 1.2$  K the full line is a fit to the measured spectrum (open circles) with only one inelastic line centred at about 0.13 meV. Since this inelastic line becomes quasielastic above 1.5 K, we interpret it as a magnon. Support is given to this assumption by the fact that *only* a Gaussian line shape can be fitted to those data. The existence of a magnon at 1.2 K is in agreement with the existence of an antiferromagnetic phase transition at  $T_{\text{N}} = 1.28$  K observed by magnetic susceptibility [1]. However, it should be pointed out that the spin fluctuations (SF) associated with the magnon at 1.2 K do not die out quickly above  $T_{\text{N}}$  as expected. Instead, they survive as critical spin fluctuations up to temperatures at least ten times  $T_{\text{N}}$  as a large additional QE-SF-line (see fig. 4) with a typical Gaussian lineshape (for  $T = 10$  K (fig. 1) only a fit with Gaussian lineshape gives satisfactory results). For example at  $T = 10$  K the QE-SF-intensity turns out to be 2.8 barn, whereas the standard QE-CF-intensity is 1.6 barn. (The latter could be determined by the CF-parameters

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extracted from higher temperatures (see below) with the restriction that the inelastic (IN) CF-lines at  $T = 10$  K (not shown here) imply that the magnetic moment is reduced by a factor of 3 at that temperature). At higher

temperatures (fig. 2,  $T = 40$  K) two distinct inelastic transitions can be observed at about 1.2 and 3.2 meV. If we take these lines as CF-transitions and interpret the QE-scattering as CF-like, too, we only get consistent fits

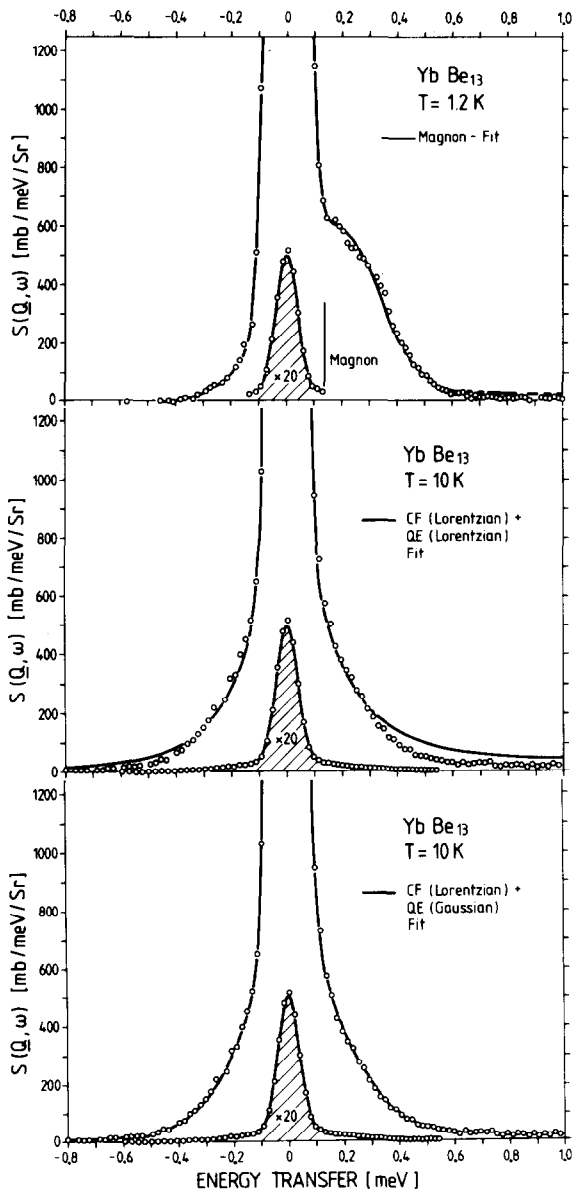


Fig. 1. Scattering function (open circles) of  $\text{YbBe}_{13}$  at 1.2 and 10 K at  $\theta = 60^\circ$  mean scattering angle and  $E_0 = 3.1$  meV. The solid line is a fit to the spectra with one magnon line at  $T = 1.2$  K and one QE-CF-line plus one additional QE-SF-line for  $T = 10$  K.

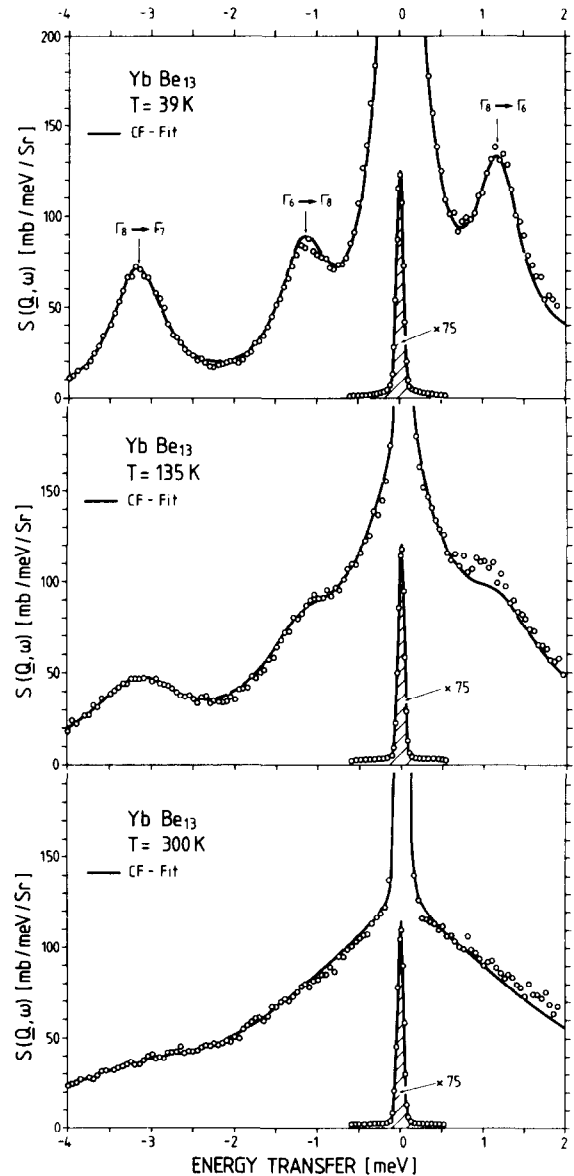


Fig. 2. Scattering function (open circles) of  $\text{YbBe}_{13}$  between 40 and 300 K at  $\theta = 30^\circ$  mean scattering angle and  $E_0 = 3.1$  meV. The solid line is a fit to the spectra with  $x = 0.911$  and  $W = 0.1543$  meV (Lorentzian lines) as direct CF-fit parameters and one additional QE-CF-line (Lorentzian; see text). Shaded area indicates elastic incoherent nuclear scattering.

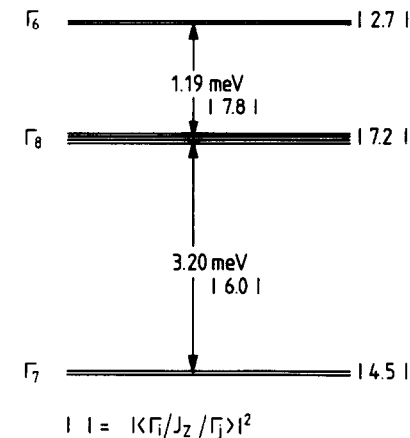
for all temperatures above 40 K, if we assume

$$W = 0.1543 \pm 0.001 \text{ meV}$$

$$x = 0.911 \pm 0.003$$

( $x$  and  $W$  were treated as direct fit parameters). The corresponding CF-splitting is shown in fig. 3. It conflicts with the values extracted from ESR and magnetization measurements [1,6], which however recognize also a  $\Gamma_7$  CF-ground state.

The CF-lineshapes could only be fitted with a Lorentzian shape function as usual with a single generating QE-linewidth for *all* QE- and IN-lines. The dependence of this QE-linewidth is shown in fig. 4 by the full circles. It is important to mention that for temperatures above 40 K the fits require an additional QE-intensity analogous to  $T < 40$  K described above. However, in contrast to the former case this additional QE-intensity is of Lorentzian type and thus will be interpreted as additional QE-CF-scattering, i.e. in addition to the scattering which occurs in the limit of very small linewidths compared to the CF-splitting (standard QE-CF-scattering). This additional QE-CF-intensity increases rapidly with increasing temperatures and at 300 K becomes the same order of magnitude as the standard QE-CF-scattering. The growth of the additional QE-CF-intensity goes hand in hand with a decrease of the inelastic intensity, such that the total magnetic cross section remains constant at the value corresponding to the trivalent Yb-ion. This feature can be attributed to the renormalization of the CF-eigen-



**Yb Be<sub>13</sub>**  $W = 0.1543 \pm 0.001 \text{ meV}$   
 $X = 0.911 \pm 0.003$

Fig. 3. CF-splitting, transition energies and transition matrix elements  $|\langle \Gamma_i | J_z | \Gamma_j \rangle|^2$  of trivalent Yb ( $J = 7/2$ ) in YbBe<sub>13</sub>.

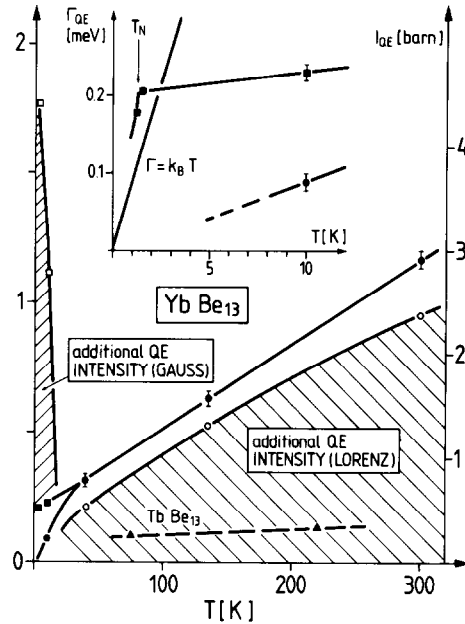


Fig. 4. Magnetic scattering intensities (open symbols) and QE-linewidths (HWHM; full symbols) of YbBe<sub>13</sub> at different temperatures. Discussion for additional QE-intensities with Lorentzian shape functions (circles) and Gaussian shape functions (squares) see text.

states, if their linewidths become comparable or greater than the CF-splitting. Indeed the application of the BFK-theory [7] by a program written by Keller, which takes this renormalization effect into account (in this theory this effect is induced by the exchange or Coulomb scattering of the conduction electrons at the 4f-shell) leads to the requested additional QE-CF-intensity. However, a fit with that theory fails for the calculation of the inelastic transitions. Here it generates wrong relative linewidths both in the case of pure exchange and Coulomb scattering. In addition, the best BFK-fit leads to an exchange constant  $N(0)J_{\text{ex}} = 0.17$ , which is very large compared to the expected value of about 0.01, which is a typical value in metallic RE-compounds [8], e.g. REAL<sub>2</sub>. This anomalous large constant which implies an anomalous large QE-linewidth can also be compared with the linewidth of the reference sample TbBe<sub>13</sub>, which has also been measured [9] and which is indicated by full triangles in fig. 4.

### 3. Conclusion

The conclusion from this is that the anomalous large linewidth *cannot* be interpreted as the *usual* (Korringa)

exchange scattering between the conduction electrons and the 4f electrons but should originate from another scattering effect such as the hybridization of 4f with 5d electrons as in the case of intermediate valence or of the Kondo effect. However, we believe that the occurrence of the additional QE-intensities should be understood at low temperatures from the classical theory of critical phenomena near magnetic phase transitions for stable ions with long range (metallic) interactions.

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