SPIN WAVES IN THE MAGNETIC STRUCTURES OF HOLMIUM

J. Jensen

Physics Laboratory, H. C. Oersted Institute DK-2100 Copenhagen, Denmark

Abstract. — The MF-RPA model for Ho$_{90}$Tb$_{10}$, developed previously, is utilized for calculating the $c$-axis spin-wave energies of Ho. The low-temperature spin waves in the conical and helical phases agree well with the experiments of Stringfellow et al. At higher temperatures the calculations indicate that the hexagonal anisotropy still has appreciable effects on the spin waves, studied experimentally by Nicklow.

From their neutron scattering studies of the spin waves in Ho$_{90}$Tb$_{10}$ at low temperatures, Larsen et al. [1] deduced the effective interplanar exchange coupling of hcp Ho. They also derived a set of crystal-field parameters which account for the magnetic anisotropy observed at 4.2 K. The model is defined by

$$H = \sum_i \sum_{lm} B_i^m O_i^m (J_i) - \frac{1}{2} \sum_{ij} \sum_{\alpha \beta} J^{\alpha \beta} (ij) J_{\alpha i} J_{\beta j}$$

(1)

where, in Ho, $B_i^m = 0.024$ meV and $B_{ij}^m = 0$ are relatively small while $B_{ij}^{00} = -0.956 \times 10^{-6}$ meV and $B_{ij}^{0} = 9.21 \times 10^{-6}$ meV are very important. The two-ion coupling is assumed to comprise an isotropic Heisenberg exchange and the dipole-dipole interaction. Its Fourier transform is diagonal if $q$ is along the $c$-axis and the aa- and bb-components are equal the value $J_\perp (q)$, from which the cc-component may be obtained to a good approximation, by the subtraction of $4\pi (g_{\mu B})^2 / V \simeq 0.035$ meV when $q \neq 0$ [1].

The magnetic moments in Ho [2] order in a $c$-axis helix at $T_N \approx 133$ K. The interlayer turn-angle varies from about 50$^\circ$ at $T_N$ to 30$^\circ$ at 4.2 K. Below $T_C \approx 20$ K the structure is a shallow cone with an opening angle of about 80$^\circ$ at 4.2 K. At low temperatures the large hexagonal anisotropy causes a bunching of the moments in successive planes in pairs round the easy $b$-axes, with a small angle 2$\phi$ between the moments in each pair ($\phi \approx 5.8^\circ$ at 4.2 K). The angle between the moments in neighbouring planes belonging to different pairs is then 60$^\circ$ - 2$\phi$, giving an average turn angle of 30$^\circ$. Recently Gibbs et al. [3] have made magnetic X-ray diffraction studies on Ho showing that (at least) some of the helical structures, occurring at higher temperatures, are commensurate with the lattice. The larger value of the ordering wave vector $Q$ is due to the presence of "spin slips" , i.e. single planes with the moments along an easy axis between the pair of planes. At increasing temperatures $\langle O_i^0 \rangle$ rapidly decreases and $2\phi$ approaches the average turn angle. Above $\approx 50$ K the effects of $B_i^0$ on the magnetic structure apparently disappear.

The magnetic excitation spectrum in Ho has been calculated at different temperatures. First the stable structure is established within the MF-approximation, assuming its periodicity to be commensurate with the lattice. $J_\perp (Q)$ is set equal to 0.475 meV as estimated from $T_N$. Next the total MF-susceptibility tensor, $\chi^0 (i, \omega)$ is calculated [4] for an ion in each different layer of the periodic structure. The RPA-susceptibility tensor is determined by:

$$\tilde{\chi} (ij, \omega) = \chi^0 (i, \omega) + \sum_{j'} \chi^0 (i, \omega) J (ij') \tilde{\chi} (j', \omega)$$

(2)

These equations are transformed to a coordinate system where the axes in the basal plane rotate uniformly with the wave vector $Q$. In the structure with no spin-slips considered by Larsen et al., the subsequent Fourier transformation leads to two coupled 3 x 3-matrix equations determining the scattering cross-section, proportional to $\text{Im} \left\langle \chi (q, \omega) \right\rangle$, which may be readily solved. In the presence of spin slips there are, in general, still as many coupled equations as layers in the commensurable period. However, by replacing $\omega$ with $\omega + i\eta$ and $\eta = 0.1 - 0.2$ meV, these equations could be solved by a straightforward iteration (without the coordinate transformation the iteration did not converge). $B_i^0$ has the effect that the directions of the moments do not coincide with the associated directions of the molecular field. This leads to a mixing of the transverse spin-wave response with the longitudinal one. In RPA the longitudinal single-ion part includes a pure elastic response which, through higher-order effects, is changed into a diffusive peak with a width of the order of the spin-wave band-width. In anticipation of this we replaced the elastic single-ion response by a Lorentzian with width 2$\Gamma$ of 6 meV. The results are shown in figures 1, 2, and are compared with the neutron scattering results of Stringfellow et al. [5] and Nicklow [6]. Figure 3 shows the two-ion couplings, $J_\perp (q) - J_\perp (0)$, used at the different temperatures.

In the one spin-slip structures at 4.6 and 25 K, energy gaps are expected whenever the "unhybridized" spin-wave energies at $q$ and $q + nQ$ are equal ($n$ is an integer). However, only the one with $n = 6 (5)$ and $q \cdot Q$ positive (negative) has survived the resolution of
Fig. 1. – The spin-wave dispersion relation in the $c$-direction of Ho at low temperatures. The experimental results are taken from Stringfellow et al. [5], and the solid lines are the calculated energies. Because of the ferromagnetic component in the cone structure at 4.6 K there are both a $+q$ and a $-q$ branch referring to whether $q \cdot Q$ is positive or negative. The (upper) lower line is the $+q$ branch when $Q$ is (anti-)parallel to the ferromagnetic moment. At 25 K, just above $T_C$, the ferromagnetic component has disappeared and there is only one spin-wave branch. In both cases the basal-plane moments are ordered helically with a wave vector $Q$ along the $c$-axis close to 0.182 corresponding to 11 hexagonal layers per period (one spin-slip per period). The bunching of the basal plane moments gives rise to the energy gap near $q = 0.5$. Energy gaps smaller than about 0.2 meV are not resolved in the calculations. The energies calculated at long wavelengths in the basal plane are shown by the short heavy lines to the right of the ordinate axes. The discontinuities at $q = 0$ are due to the dipolar coupling (see [1]).

Fig. 2. – High temperature energies of the spin waves propagating along the $c$-axis in the helical phase of Ho. The experimental points are measured by Nicklow [6]. The solid lines indicate the positions of the main peaks in the calculated spectrum, whereas the dashed extensions designate peaks of relatively lower intensities. Apart from the change in temperature, the only difference between the two cases is that the length of the ordering wave vector is changed from 0.21 at 50 K to about 0.225 at 78 K. These values correspond quite nearly to the commensurate structures with 19 layers per double period and 9 layers per period, respectively, assumed in the calculations. The upper straight dashed lines in the two figures indicates the calculated positions of additional molecular-field excitations, which in reality might be strongly damped and thus difficult to detect.

Fig. 3. – The exchange coupling between the basal-plane moments as a function of wave vector along the $c$-axis. The exchange coupling below 30 K, used in figure 1, is the same as derived by Larsen et al. [1] (the dashed line is for the ferromagnetic phase). About 0.2 meV used in the calculations. This energy gap is about twice the one predicted at $q = 0.5$ in the structure without spin-slips [1] and it should probably be observable in a more precise experiment. The coupling to the longitudinal response is not important at low temperatures, but it is quite essential in the high temperature cases shown in figure 2 for the (near) suppression of the energy gap in the long-wavelength limit (also in the incommensurate case!). Most unexpectedly the high temperature spectra are split into many branches by $B_0^2$, although this coupling ceases to influence the structure itself significantly. The high temperature spin-waves indicate a more pronounced maximum in $J_1 (q)$ (depending somewhat on the value chosen for $\Gamma$), shifted to larger $q$, compared with the low temperature values.