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Theory of the Effects of Anisotropy on Spiral Spin-Configurations with Application to Rare Earth Metals

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Some effects of anisotropy on spirals are studied by considering a spin-hamiltonian that includes exchange forces, crystal field and dipolar forces. It is shown that the ferromagnetic spiral (FS) observed in Er at low temperatures by the Oak Ridge diffraction group can be the ground state provided terms of at least fourth order in the spin variables are present in the hamiltonian. Furthermore, the observed cone angles (which imply large deviations from configurations possible with exchange forces alone) can be realized with anisotropy forces much smaller than the exchange forces. The spin wave spectrum for the FS has the properties that $\omega(k)$ is linear in k for small k (even though the net spin is not zero), and there are two distinct branches, as contrasted with the case of simple spirals. For high temperatures, calculations are made on the basis of the molecular field approximation. It is shown that a small easy axis anisotropy implies that at the highest transition temperature, T_c, the ordered spin configuration is a static longitudinal spin wave as observed in Er. As T decreases below T_c, the amplitude of this wave grows in order $(T_c-T)^{1/2}$, with odd harmonics appearing in order $(T_c-T)^{3/2}$. The transverse components remain zero until a second transition temperature is reached, below which they begin to order. The observed thermal variation in wavelength (of the fundamental harmonic) can be accounted for in Er specifically by the dipolar forces.

Since spirals were discovered theoretically[1,2,3], they and related configurations have been found experimentally in a number of materials. Some of the most interesting examples of spiral-like states have been obtained in rare earth metals by Wilkinson, Koehler, Wollan and Cable[4], using neutron diffraction. A striking aspect of these results is the large deviation, in some cases, from what would be allowed by exchange interactions alone. (The reason that this is striking is that one expects anisotropy forces to be only of the order of 10% of the exchange forces, as in the case of dysprosium.)[5] It can be shown[6] that if the only forces are exchange type, then the classical ground state for the hcp lattice must be a simple spiral (SS), that is, a spiral of the type discussed previously[1,2,3], in which all spins are parallel to one fixed plane[7]. But this coplanarity is not a property of the low temperature configuration of erbium[4], in which the spins all lie on the surface of a cone, the transverse, x-y components forming a simple spiral, the longitudinal, z-components being constant. We have called this configuration a ferromagnetic spiral (FS)[8]. Furthermore, the cone half-angle, $\theta\sim 30$ degrees[4], showing a large deviation from coplanarity. Hence anisotropy forces must play an important role in determining the magnetic ordering[9]. In the high temperature phase of erbium[4], which we call a longitudinal spin wave (LSW), the average spins are collinear, their lengths varying sinusoidally as one moves along the c-axis—the transverse components are completely disordered to within the accuracy of experiment. This configuration is, of course, quite unlike anything discussed previously.

Because of these features of erbium—large deviation in the ground state from what is possible by exchange forces only, and apparent intuitive opaqueness as to the reason for the high temperature state—we have concentrated on this type of behavior. We shall see that the simple energy function.

$$E=-\sum J_{ij}S_i\cdot S_j-\sum K_{ij}S_{iz}S_{jz}+\frac{1}{2}K'\sum(S_{iz})^4\,, \tag{1}$$

with costant values of the parameters J_{ij}, etc., (following Yosida and Miwa[10]), can

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reasonably account for much of this behavior. (S_{iz} is the component of S_i along the c-axis.)

The minimum of E over the class of ferromagnetic spirals (with cone axis in the z-direction) is obtained by choosing the propagation vector, $k=k_0$, where $\mathscr{J}(k_0)$ is the maximum over k of the Fourier transform, $\mathscr{J}(k)$, or J_{ij}, and $\theta=\theta_0$ given by $\cos^2\theta_0=[\kappa(0)-\mathscr{J}(k_0)+\mathscr{J}(0)]/K'S^2$, where $\kappa(k)$ is the transform of K_{ij}, provided $0<\cos^2\theta_0<1$ and $K'>0$. Thus we must have $\kappa(0)>\mathscr{J}(k_0)-\mathscr{J}(0)$; hence the second order terms must provide an easy axis and the fourth order terms must give an easy plane in order to obtain a FS. To get an idea of the required orders of magnitude, we have assumed first and second neighbor J_{ij} only (for the linear chain model); then, using the wavelength of roughly 8 layers found in erbium[4], we find that $[\mathscr{J}(k_0)-\mathscr{J}(0)]/|\mathscr{J}(k_0)|\sim 10\%$, which is the expected order of magnitude of κ.

We have examined further the question of whether the FS can minimize Eq. (1) by a local stability calculation[6]. We found that the FS locally stable for a considerable range of parameters.

The spin wave spectrum (assuming the FS to be the ground state) shows the interesting properties, **1** the spectrum is linear in k for small k, despite the fact that the net moment is not zero and **2** there are two distinct acoustic branches, as contrasted with the case of a simple spiral[1,10].

Concerning high temperatures, we have investigated the molecular field approximation (MFA) to the statistical mechanics associated with Eq. (1). The average spins $\boldsymbol{\sigma}_i$ are given by the minimum free energy solution of equations

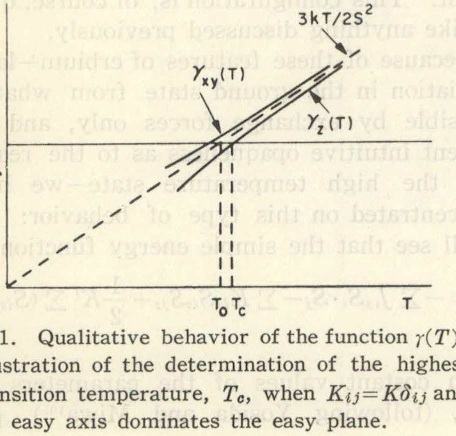

Fig. 1. Qualitative behavior of the function $\gamma(T)$; illustration of the determination of the highest transition temperature, T_c, when $K_{ij}=K\delta_{ij}$ and the easy axis dominates the easy plane.

$\boldsymbol{\sigma}_i=S\mathscr{L}_a(\ldots\boldsymbol{\sigma}_i\ldots)$, where $\mathscr{L}_a$ is like the Langevin (or Brillouin) function, but modified by the anisotropy. At high temperature, $\mathscr{L}_a$ is expanded (as usual) to lowest order in the σ_i, giving a set of linear equation. For the case $K_{ij}=K\delta_{ij}$, these are $\sum J_{ij}\sigma_{ju}=\gamma_u(T)\sigma_{iu}$, where $u=x, y, z$, $\gamma_x=\gamma_y$, and the γ's are shown in Fig. 1, for the case in which the easy axis dominates the easy plane. The highest transition temperature T_c is easily seen to occur when the lowest γ crosses $\mathscr{J}(k_0)$; furthermore, when γ_z lies lowest, the solution just below T_c is precisely the longitudinal spin wave with wave vector k_0. The "reason" for this is the removal of the degeneracy ($\gamma_x=\gamma_z$) by the anisotropy. Putting back the dipolar force (K_{ij} for $i\neq j$) then allows thermal variation of wavelength (in agreement with experiment[4]). Many other characteristics observed in Er also result when this approach is pushed to lower temperatures, for example, the ordering of the transverse components a finite interval below T_c, and the appearance of odd higher harmonics.

The unsatisfactory feature of this theory for high T is that the MFA can be shown to give qualitatively incorrect results[6,10] for a spin-hamiltonian like (1) with the second order terms giving a hard axis.

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