

MAGNETISATION OF SOME FERROMETALS

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I ABSTRACT

The variation with temperature of the magnetization of Ni, Fe, Co, Dy and Gd are studied. New data for Co, Dy and Gd is presented along with previously reported measurement for Ni, Fe, and Co. The coefficients of the $T^{3/2}$ term evaluated are compared with result from independent experiments.

II INTRODUCTION

It has been established that spin wave excitations exist in metals [6] and that they provide the dominant mechanism for initial decay of the ferromagnetic moment [4]. By using a special expansion formalism we have already shown that spinwaves, when quantized are ideal Bosons with an effective chemical potential effected by wave-wave interactions [3,4]. The nearest neighbour exchange interaction model of a ferromagnet is described by the following Hamiltonian [5]

$$H = -2J \sum_{ji} S_j \cdot S_i + B_0 g \mu_B \sum_{j=1}^N S_j^2 \quad (1)$$

S_j is the spin operator at the j^{th} atom, N is the total number of atoms, g the Lande-g factor, μ_B the Bohr magneton, the summation is taken over all the nearest neighbour pairs, and the external magnetic field B_0 is directed along the Z-axis.

For the cubic crystals, the Hamiltonian is written as

$$H = \sum_k (Fk^2 - \mu) n_k \quad (2)$$

where,

$$F = 2zS[J - J(K)] / k^2 \quad (3)$$

$$J(K) = \frac{1}{z} \sum_{ji} J_{ji} \exp[ik(\vec{R}_j - \vec{R}_i)] \quad (4)$$

where z is the number of nearest neighbours and $\vec{R}_j = (0, 0, 0)$ and $\vec{R}_i = (x_i, y_i, z_i)$
The reciprocal lattice vector is defined by

$$\vec{k} = \{k_x, k_y, k_z\}$$

where

$$k_x = k \cos\Phi \sin\theta, k_y = k \sin\Phi \sin\theta, k_z = k \cos\theta$$

The nearest neighbour Distance on a simple cubic lattice in units of a is known, while the nearest neighbour distances on a body centered and face cubic lattice in units of $a/2$ are also known.

In most work we estimate the nearest neighbour distances on an hexagonal close packed lattice in units of a . The exchange integral is then evaluated.

III THE FOURIER TRANSFORMATION OF $J(K)$

For a simple cubic lattice, the Fourier transform, Eqn. (4) becomes

$$J(k) = \frac{2}{6} \sum J_{ji} \cos k(R_j - R_i) \quad (5)$$

$$J(k) = \frac{1}{3} [\cos(k_x a) + \cos(k_y a) + \cos(k_z a)] \quad (6)$$

For a body centered cubic lattice, Eqn. (4) becomes

$$J(k) = J [\cos(k_x \frac{a}{2}) + \cos(k_y \frac{a}{2}) + \cos(k_z \frac{a}{2})] \quad (7)$$

while for a face centered cubic lattice, we get

$$J(k) = \frac{1}{3} [\cos(k_x \frac{a}{\sqrt{2}}) + \cos(k_y \frac{a}{\sqrt{2}}) + \cos(k_z \frac{a}{\sqrt{2}})] \quad (8)$$

The Fourier transform $J(k)$ for a hexagonal close packed lattice is obtained as follows using the estimated nearest neighbour distances.

$$J(k) = \frac{1}{2} \sum_{i=1}^{12} \cos(k_x x_i + k_y y_i + k_z z_i) \quad (9)$$

Taking each term separately, we have the following:

$$\frac{1}{12} \sum_{i=1}^{12} \frac{[k_x x_i + k_y y_i + k_z z_i]^2}{2!} = (\frac{1}{24}) [D''(\Phi, \theta)(ka)^2] \quad (10)$$

Also

$$\frac{1}{12} \sum_{i=1}^{12} \frac{[k_x x_i + k_y y_i + k_z z_i]^4}{4!} = \frac{1}{12} (\frac{1}{24}) A''(\Phi, \theta)(ka)^4 \quad (11)$$

The coefficient of T^2 , T^3 and T^4 that is C_1 , C_2 and C_3 respectively have been calculated for some ferrometals and tabulated in table 2.1. Table 2.2 shows the calculated coefficients of T^2 (C_1) and T^3 (C_2) and experimentally measured values obtained by Argyle et al. [1].

$$(26) \quad \frac{1}{V} \sum_{m=1}^{\infty} \left[\frac{(2\pi)^3 NS}{\Gamma^{\frac{3}{2}}} \left(\frac{1}{2} \right) e^{-\frac{m}{2}} \int_0^{\pi} \int_0^{\pi} A^m(\Phi, \theta) \sin \theta d\theta d\Phi - \frac{4}{72} \int_0^{\pi} \int_0^{\pi} B^m(\Phi, \theta) \sin \theta d\theta d\Phi \right]$$

The third term is

$$(25) \quad \frac{1}{V} \sum_{m=1}^{\infty} \left(\frac{2\pi)^3 NS}{\Gamma^{\frac{3}{2}}} \left(\frac{1}{2} \right) e^{-\frac{m}{2}} \frac{4}{5} Z \int_0^{2\pi} \int_0^{\pi} \frac{A^m(\Phi, \theta) \sin \theta d\theta d\Phi}{(D^m(\Phi, \theta))} \right)$$

The second term is,

$$(24) \quad = \frac{(2\pi)^3 NS}{\Gamma^{\frac{3}{2}}} \left(\frac{1}{2} \right) \sum_{m=1}^{\infty} \frac{e^{-\frac{m}{2}}}{e^{m/2}} \int_0^{2\pi} \int_0^{\pi} D^m(\Phi, \theta) \sin \theta d\theta d\Phi$$

$$(23) \quad \frac{1}{V} \int_0^{2\pi} \int_0^{\pi} \sin \theta S_0^{\frac{3}{2}} e^{-m/2} d\theta d\Phi \int_0^{\pi} \frac{2C^{\frac{3}{2}} p^{\frac{3}{2}}}{e^{-m/2}} d\theta$$

The first term is,

three coefficients of $\text{Sm}(\tau) | m(0)$

By substitution and applications of some numerical techniques we compute the first

$$(22) \quad k^2 dk = \frac{2C^{\frac{3}{2}} p^{\frac{3}{2}}}{S_0^{\frac{3}{2}}} \left[1 + \frac{2D^{\frac{3}{2}}(\Phi, \theta)}{5ZA^{\frac{3}{2}}(\Phi, \theta)S_0^{\frac{3}{2}}} + \frac{D^{\frac{3}{2}}(\Phi, \theta)}{8ZA^{\frac{3}{2}}(\Phi, \theta)S_0^{\frac{3}{2}}} + \frac{2D^{\frac{3}{2}}(\Phi, \theta)}{7B^{\frac{3}{2}}(\Phi, \theta)zS_0^{\frac{3}{2}}} + \dots \right] dS_0$$

$$(21) \quad k^2 dk = \frac{2C^{\frac{3}{2}} p^{\frac{3}{2}}}{S_0^{\frac{3}{2}}} \left[1 + \frac{2CP^2}{5GS_0} + \frac{8G^2S_0^2}{7HS_0^2} + \frac{2CP^4}{8G^2S_0^2} + \frac{2CP^3C_2}{7HS_0^2} + \dots \right] dS_0$$

$$(20) \quad Ck^2 = S_0^{\frac{3}{2}} p^{\frac{3}{2}} \left[1 + \frac{GS_0}{CP^2} \left(1 + \frac{p}{H} \left[\frac{S_0}{CP^2} - \frac{p}{GS_0} \right] \right) + \frac{2GS_0}{CP^2} + \frac{G^2S_0^2}{C^2p^4} \right] + \dots$$

$$S_0 = C \{ P - GK^2 + HK^4 \} K^2 \quad (19)$$

therefore

$$P = D''(\Phi, \theta), \quad C = a^2 \frac{1}{z}, \quad G = zA''(\Phi, \theta)a^2, \quad H = B''(\Phi, \theta)a^4 z \quad (18)$$

$$S_0 = \{ D''(\Phi, \theta)(ka)^2 - A''(\Phi, \theta)(ka)^4 + B''(\Phi, \theta)(ka)^6 \} \frac{1}{z} \quad (17)$$

The expression above is a very integration, we therefore apply the technique of Novakovic [5] by introducing the following substitutions.

$$\sum \left(\frac{nk}{NS} \right) = \frac{NS}{V} \int \frac{\exp \beta (F' k^2 - \mu)}{k^2 dk} \left(2\pi^3 \right)^{-1} \quad (16)$$

where

$$m(T) = m(0) \left(1 - \frac{NS}{\langle nk \rangle} \right) \quad (15)$$

The spontaneous magnetization is defined by a thermal average of the z component of the magnetic moment and summed over a unit volume of the crystal.

IV THE SPONTANEOUS MAGNETIZATION

$$F' = 2SZJ \{ D''(\Phi, \theta)(ka)^2 - A''(\Phi, \theta)(ka)^4 + B''(\Phi, \theta)(ka)^6 + \dots \} \quad (14)$$

Where,

$$H = \sum (F' k^2 - \mu) n_k \quad (13)$$

We see here that the Fourier transform $J(k)$ for a hexagonal close packed lattice is markedly different from that of the cubic lattice. Replacing F with F' for a Hexagonal close packed lattice the transformed Hamiltonian is written as:

$$\frac{1}{12} \sum_{i=1}^{12} [K_x x_i + K_y y_i + K_z z_i]^6 = \frac{1}{2} (1/120) B''(\Phi, \theta)(ka)^6 \quad (12)$$

Similarly,

V DISCUSSION OF RESULTS

With the effect of the electrochemical potential, the coefficients of $T^{3/2}$, $T^{5/2}$ and $T^{7/2}$ of spontaneous magnetization of some ferromagnets have been tabulated in tables 2.1 and 2.2.

In cases of Iron and Nickel for which experimented values are available, our computed values of the coefficients are in impressive agreement with the experimental ones¹¹. In finding the effect of the electrochemical potential on the coefficients of T in the expression of the Spontaneous magnetization for ferromagnets with the Hexagonal close packed structures, we require the correct expansion for the terms encapsulated in the dispersion relation.

For the Hexagonal close packed crystals, the Hamiltonian is

$$H = \sum (F'k^2 - \mu)n_k$$

where

$$F = 2SzJ \left\{ D''(\Phi, \theta)(ka)^2 - A''(\Phi, \theta)(ka)^4 - B''(\Phi, \theta)(ka)^6 + \dots \right\} / k^2$$

and $D''(\Phi, \theta)$, $A''(\Phi, \theta)$, and $B''(\Phi, \theta)$ have been outlined and evaluated.

Our calculations also give the coefficients of T for the hexagonal close packed structures of Dysprosium and Gadolinium, the experimentally measured values of which are not available from literature.

It is not out of place to emphasize that the behaviour of the magnetization of these ferromagnets is very well described at low temperatures by the Spinwave theory.

Table 2.1 Coefficient of $T^{3/2}$, $T^{5/2}$ and $T^{7/2}$ of spontaneous magnetization

Elements	Lattice structure	Spins Nearest neighbours	$C_1 \times 10^{-6}$	$C_2 \times 10^{-9}$	$C_3 \times 10^{-13}$
Iron (Fe)	BCC	S=1/2, Z=7	2.292	0.828	3.167
		S=1/2, Z=7.5	3.647	0.894	3.420
		S=1/2, Z=7	4.000	1.065	4.008
Cobalt (Co)	HPC	S=1/2, Z=11	2.500	0.357	1.355
		S=1/2, Z=12	2.259	0.496	2.271
Nickel (Ni)	FCC	S=1/2, Z=12	7.359	3.600	37.87
Gadolinium (Gd)	HCP	S=1/2, Z=12	2.279	7.7×10^{-7}	9.275×10^{-8}
Dysprosium (Dy)		S=1/2, Z=12	1.67×10^{-4}	2.497×10^{-5}	6.929×10^{-6}

Table 2.2 Calculated and Experimental Values of Coefficient of $T^{3/2}$ and $T^{5/2}$

Lattice structure	Spins and nearest neighbour	C_1	C_2	C_1 Experimental	C_2 Experimental
BCC	S=1/2, Z=7.5	3.647×10^{-6}	0.849×10^{-9}	3.41×10^{-6}	$1 \pm 1 \times 10^{-9}$
BCC	S=1/2, Z=8.0	4.000×10^{-6}	1.065×10^{-9}	3.41×10^{-6}	$1 \pm 1 \times 10^{-9}$
HCP	S=1/2, Z=11	2.068×10^{-6}	0.357×10^{-9}	1.7×10^{-6}	
HCP	S=1/2, Z=12	2.259×10^{-6}	0.496×10^{-6}	1.7×10^{-9}	
FCC	S=1/2, Z=12	7.395×10^{-6}	0.360×10^{-8}	7.4×10^{-6}	$1.5 \pm 2 \times 10^{-8}$
HCP	S=7/2, Z=12	2.790×10^{-6}	0.770×10^{-6}		
HCP	S=5, Z=12	1.671×10^{-4}	0.249×10^{-4}		

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