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ABSTRACT

The theory of anisotropic Heisenberg ferromagnets is developed in the random phase and spin wave approximation. It is shown that thermodynamic quantities such as magnetization can be expressed in analytic form for all temperatures. To demonstrate the applicability of this technique the magnetization for body-centered, face-centered, and simple-cubic lattices was calculated.

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SUMMARY

The theory of anisotropic Heisenberg ferromagnets is developed in the random phase and spin wave approximation. It is shown that thermodynamic quantities such as magnetization can be expressed in analytic form for all temperatures. To demonstrate the applicability of this technique the magnetization for body-centered, face-centered, and simple-cubic lattices was calculated.

INTRODUCTION

The Ising and Heisenberg models of ferromagnetism have been the subject of intensive theoretical investigations for many years (ref. 1 and references contained therein). Because of the dissimilar behavior of these models, Dalton and Wood (ref. 1) have considered an intermediate approach. Using the Green's function method and series expansion techniques, they studied the critical behavior of their model in both two and three dimensions for intermediate values of the anisotropy parameter $\eta(0 < \eta < 1)$.

When treating the thermodynamic quantities of an anisotropic Heisenberg ferromagnet, it is usually necessary to use series expansions for the temperature regions of interest. A purpose of this report is to describe a method of evaluating certain temperature-dependent sums or (integrals) that occur in the theory of magnetism without necessitating the use of series approximations or extensive computer summations. A single analytical expression for the magnetization has been found which is valid for all temperatures. The expression, moreover, can easily be extended to include any magnitude of spin. It is hoped that the methods applied herein will be found useful in the evaluation of the thermodynamic quantities in the theory of magnetism and other cooperative phenomena.

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The method is applied to compute the temperature dependence of the magnetization for various values of η. The simple-cubic (sc), body-centered-cubic (bcc), and face-centered-cubic (fcc) lattices are considered.

The anisotropic model of Dalton and Wood is introduced in the random phase approximation, and an expression for the magnetization is formulated. The calculations for the bcc, fcc, and sc lattice cases are given. The critical temperature is determined, and the results are discussed. A detailed example of the evaluation of the integrals that occur in the lattice calculations is given in appendix A.

ANISOTROPIC FERROMAGNET

The nearest-neighbor exchange interaction model for the anisotropic ferromagnet in the absence of an external field, as described by Dalton and Wood, is specified by the Hamiltonian

$$H = -\sum_{i,j} J_{ij}\left[S_i^z S_j^z + \frac{\eta}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)\right] \tag{1}$$

where the sums extend over all sites in the lattice, $\underset{\sim}{S}_i$ is the spin operator for $S = 1/2$ for a spin at site i, and J_{ij} is the exchange integral. (All symbols are defined in appendix B.) The Ising and Heisenberg models are obtained by setting $\eta = 0$ and 1, respectively.

Starting with the Green's function $\left\langle\left\langle S_g^+; S_n^-\right\rangle\right\rangle$, Dalton and Wood derived the correlation function in the random phase approximation. Their results are

$$\left\langle S_n^- S_g^+\right\rangle = \frac{1}{N}\sum_{\underset{\sim}{k}} 2\left\langle S_g^z\right\rangle e^{i\underset{\sim}{k}\cdot(\underset{\sim}{g}-\underset{\sim}{m})}\left(e^{\beta E_{\underset{\sim}{k}}} - 1\right)^{-1} \tag{2}$$

where

$$\left.\begin{aligned} E_k &= 2\left\langle S_g^z\right\rangle J(0)\left[1 - \eta\frac{J(\underset{\sim}{k})}{J(0)}\right] \\ \text{and} \\ J(\underset{\sim}{k}) &= \sum_{\underset{\sim}{m}} J_{gm} e^{i\underset{\sim}{k}\cdot(\underset{\sim}{g}-\underset{\sim}{m})} \end{aligned}\right\} \tag{3}$$

The sum in equation (2) goes over all N lattice vectors in the first Brillouin zone.

To obtain the spontaneous magnetization $\langle S_g^z \rangle$, we make use of the relation

$$S_g^- S_g^+ = S(S+1) - S_g^z - \left(S_g^z\right)^2$$

For spin 1/2,

$$\left\langle \left(S_g^z\right)^2 \right\rangle = \frac{1}{4}$$

and, hence, the magnetization is given by

$$\langle S^z \rangle + \frac{1}{2}(1 + 2\Phi)^{-1} \tag{4}$$

where

$$\Phi = \frac{1}{N}\sum_{\underset{\sim}{k}} \left(e^{\beta E_{\underset{\sim}{k}}} - 1\right)^{-1} = \frac{1}{2N}\sum_{\underset{\sim}{k}} \left[\coth\left(\frac{\beta E_{\underset{\sim}{k}}}{2}\right) - 1\right] \tag{5}$$

To calculate the magnetization as a function of temperature the sums in equation (5) must be evaluated over all values of $\underset{\sim}{k}$ in the first Brillouin zone of the appropriate lattice. Except at the low and high temperature limits, numerical methods are usually used. However, it is shown below that these sums can be evaluated analytically over the entire temperature range.

Consider only crystals with cubic symmetry. For these lattices, one usually replaces the sum in equation (5) by an integral (ref. 2)

$$\frac{1}{N}\sum_{\underset{\sim}{k}} \frac{v}{(2\pi)^3} \int\int\int d\underset{\sim}{k} \tag{6}$$

where v is the volume per site: sc, $v = a^3$; bcc, $v = (1/2)a^3$; fcc, $v = (1/4)a^3$.

For the sc, bcc, and fcc lattices, equation (6) can be written in the form

$$\frac{1}{N}\sum_{\underset{\sim}{k}} \frac{1}{\pi^3} \int_0^{\pi}\int_0^{\pi}\int_0^{\pi} dx\, dy\, dz \tag{7}$$

where for sc,

$$x = k_x a,\ y = k_y a,\ z = k_z a \tag{8a}$$

for bcc,

$$x = \frac{1}{2} k_x a,\ y = \frac{1}{2} k_y a,\ z = \frac{1}{2} k_z a \tag{8b}$$

and for fcc,

$$x = \frac{1}{2} k_x a,\ y = \frac{1}{2} k_y a,\ z = \frac{1}{2} k_z a \tag{8c}$$

Using the identity

$$\coth(\pi t) = (\pi t)^{-1} + \frac{2}{\pi} \sum_{R=1}^{\infty} \frac{t}{R^2 + t^2}$$

Equation (5) is written in the form

$$\Phi = -\frac{1}{2} + I_1 + I_2 \tag{9}$$

where

$$I_1 = \frac{v\tau}{(2\pi)_2^3 \langle S^z \rangle} \iiint \frac{d^3 \underset{\sim}{k}}{1 - \eta \dfrac{J(\underset{\sim}{k})}{J(0)}} \tag{10}$$

$$I_2 = \frac{v\tau}{(2\pi)_2^3 \langle S^z \rangle} \sum_{R=1}^{\infty} \iiint \left[\frac{d^3k}{1 - \eta \frac{J(\underset{\sim}{k})}{J(0)} + i\Gamma} + \text{c.c.} \right] \tag{11}$$

Here $\Gamma = R\pi\tau/\langle S^z \rangle$, the reduced temperature $\tau = kT/zJ(0)$, z is the number of nearest neighbors, and c.c. indicates the complex conjugate.

BODY-CENTERED-CUBIC LATTICE

Consider first, the case of a bcc lattice, where $J(\underset{\sim}{k})$ can be written as

$$\frac{J(\underset{\sim}{k})}{J(0)} = \cos\left(k_x \frac{a}{2}\right)\cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right) \tag{12}$$

From equation (8b), it follows that equations (10) and (11) have the form

$$I_1(\text{bcc}) = \frac{\tau}{2\pi^3 \langle S^z \rangle} \int_0^{\pi}\int_0^{\pi}\int_0^{\pi} \frac{dx\, dy\, dz}{1 - \eta \cos(x)\cos(y)\cos(z)} \tag{13}$$

$$I_2(\text{bcc}) = \frac{\tau}{2\pi^3 \langle S^z \rangle} \sum_{R=1}^{\infty} \int_0^{\pi}\int_0^{\pi}\int_0^{\pi} \left[\frac{dx\, dy\, dz}{1 + \Gamma - \eta \cos(x)\cos(y)\cos(z)} + \text{c.c.} \right] \tag{14}$$

With the use of Laplace transforms, the summation in equation (14) can be reduced to integrals, and the method is outlined in appendix A. Integrating equations (13) and (14) yields the following

$$I_1(\text{bcc}) = \frac{\tau}{2 \langle S^z \rangle} \left[\frac{2}{\pi} K(k) \right]^2 \tag{15}$$

$$I_2(\text{bcc}) = \frac{1}{2Q}\left[Q\coth(Q) - 1 - \frac{\eta^2}{8} + \left(\frac{Q}{2}\right)^3 \eta^2 \operatorname{csch}^2(Q)\coth(Q)\right] \tag{16}$$

where K(k) is a complete elliptic integral of the first kind,

$$k^2 = \frac{1}{2}\left(1 - \sqrt{1 - \eta^2}\right) \tag{17}$$

and $Q = \langle S^z \rangle / \tau$. By substituting equations (15) and (16) into equation (9), the magnetization is obtained from equation (4).

No difficulty arises in the limiting case where $\eta = 0$, nor does it have to be considered separately as is the case when low and high temperature expansions (ref. 1) are used. By putting $\eta = 0$, the familiar Ising result for magnetization is obtained.

$$\langle S^z \rangle = \frac{1}{2}\tanh(Q) \tag{18}$$

FACE-CENTERED-CUBIC LATTICE

The treatment for the fcc case is analogous to the bcc calculation. The results are

$$I_1(\text{fcc}) = \frac{1}{\pi^2 gQ}\int_0^{\pi} K(k_1)dx \tag{19}$$

$$I_2(\text{fcc}) = \frac{1}{2Q\langle S^z \rangle g}\left[gQ\coth(gQ) + \frac{g}{3}Q^2\operatorname{csch}^2(gQ) - \frac{\eta}{3g} + \left(2g^2\right)^{-1}\left(\frac{\eta}{3}\right)^2 - \frac{g\eta^2 Q^3}{18}\right.$$

$$\left. \times \operatorname{csch}^2(gQ)\coth(gQ)\right] \tag{20}$$

where

$$k_1^2 = 4\eta\frac{3 + \eta\cos^2(x)}{(3 + \eta)^2} \tag{21a}$$

$$g = \frac{3 + \eta}{3} \tag{21b}$$

and

$$\frac{3J(k)}{J(0)} = \left[\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + \cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right) + \cos\left(\frac{k_z a}{2}\right)\cos\left(\frac{k_x a}{2}\right)\right] \tag{22}$$

SIMPLE-CUBIC LATTICE

The results for the simple-cubic lattice are obtained in a similar fashion:

$$I_1(sc) = \frac{3}{\pi^2 Q}\int_0^{\pi} \frac{K(k_2)dx}{3 - \eta\cos(x)} \tag{23}$$

$$I_2(sc) = \frac{1}{2\pi}\int_0^{\pi}\left[\coth(pQ) + \left(\frac{\eta Q}{3}\right)^2 \operatorname{csch}^2(pQ)\coth(pQ)\right]dx - \frac{3}{2Q}\left(9 - \eta^2\right)^{-1/2}$$

$$\times\left[1 + \eta^2\,\frac{\left(18 + \eta^2\right)\left(9 - \eta^2\right)^{-3/2}}{2}\right] \tag{24}$$

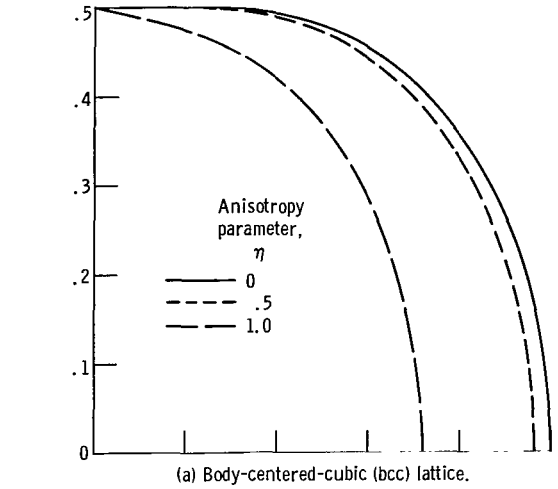
where

$$k_2^2 = \left(\frac{2\eta}{3p}\right)^2 \tag{25a}$$

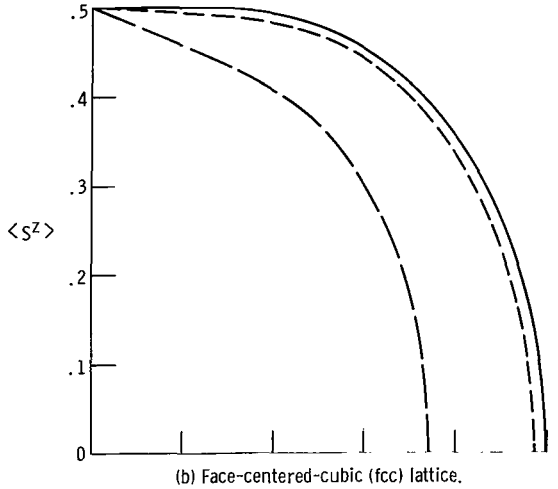
$$p = \frac{3 - \eta\cos(x)}{3} \tag{25b}$$

and

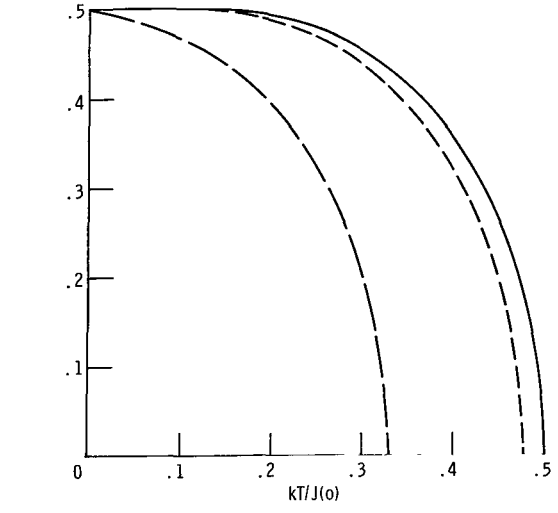
$$\frac{3J(k)}{J(0)} = \cos(k_x a) + \cos(k_y a) + \cos(k_z a) \tag{26}$$



(a) Body-centered-cubic (bcc) lattice.



(b) Face-centered-cubic (fcc) lattice.



(c) Simple-cubic (sc) lattice.

Figure 1. - Magnetization as function of reduced temperature.

Figure 1 shows the magnetization $\langle S^z \rangle$ for each of the cubic lattices plotted as a function of the reduced temperature τ. Numerical values were obtained from equation (4) for several values of the anisotropy parameter η.

CRITICAL REGION

The temperature at which $\langle S^z \rangle = 0$ is called the Curie temperature, and its value can be obtained from the preceding equations. For example, consider the bcc lattice. By substituting equations (15) and (16) into equation (4), one finds

$$2\tau = \left\{ \left[\left(\frac{2}{\pi} \right) K(k) \right]^2 + Q \coth(Q) - 1 + \frac{\eta^2 Q^3}{8} \operatorname{csch}^2(Q) \coth(Q) - \frac{\eta^2}{8} \right\}^{-1} \tag{27}$$

As $\langle S^z \rangle$ approaches zero, terms such as $Q \coth(Q)$ and $Q^3 \operatorname{csch}^2(Q) \coth(Q)$ became indeterminate. Use of L'Hospital's rule yields

$$\lim_{Q \to 0} Q \coth(Q) = 1 \tag{28}$$

$$\lim_{Q \to 0} Q^3 \coth(Q) \operatorname{csch}^2(Q) = 1 \tag{29}$$

and

$$2\tau_c = \left[\frac{2K(k)}{\pi} \right]^2 \tag{30}$$

Equation (30) is the same as obtained by Dalton and Wood by evaluating the sum over k-space at the critical temperature in the manner of Watson (ref. 3). Thus, the Curie temperature can be determined without the use of any expansions. The same procedure can be applied to the other cubic lattices.

In table I we give the values of the Curie temperature τ_c for various values of the parameter η. As expected, we find that our results for $\eta = 1$ agree with the Curie temperature of a Heisenberg ferromagnet calculated (ref. 2) in the random phase approximation.

The preceding calculations were limited to positive values of the anisotropy parameter η. If η were allowed to become negative, the model would then represent a

TABLE I. - REDUCED CURIE TEMPERATURE FOR CUBIC LATTICES, NEAREST-NEIGHBOR INTERACTIONS FOR SPIN 1/2

Lattice	Anisotropic parameter, η	Reduced Curie temperature, $kT_c/J(0)$
Body-centered-cubic (bcc)	0	0.5000
	.5	.4830
	1.0	.3589
Face-centered-cubic (fcc)	0	0.5000
	.5	.4869
	1.0	.3718
Simple-cubic (sc)	0	0.5000
	.5	.4776
	1.0	.3297

mixed ferromagnetic and antiferromagnetic system. However, the thermodynamic quantities are independent of the sign of η, in contrast to the anisotropic antiferromagnetic two-sublattice model which has been investigated by the present authors (unpublished data obtained by L. Flax and J.C. Raich of Lewis). The absence of the mixed state follows from the random phase approximation used for decoupling the Green's function equations of motion. Other decoupling schemes, such as Callen's (ref. 4), would give different results.

SPIN WAVE APPROXIMATION

The usual assumption in spin wave theory is that the spin waves are independent of each other. This supposition can be expected to be valid only as long as the number of reversed spins is small. According to Keffer and Loudon (ref. 3), Dyson (ref. 5), and Oguchi (ref. 6), the error in the magnetization when the spin wave interactions are neglected is less than 5 percent at the critical point.

The nearest-neighbor interaction model of the anisotropic ferromagnet is described by equation (1). The spin operators are expressed in the forms obtained by Mallev (ref. 7):

$$\left.\begin{aligned} S_f^- &= (2S)^{1/2}\left(b_f - \frac{b_f^+ b_f b_f}{2S}\right) \\ S_f^+ &= (2S)^{1/2} b_f^+ \\ S_f^z &= -S + b_f^+ b_f \end{aligned}\right\} \tag{31}$$

where the operators b_f and b_f^+ are to be regarded as the creation and annihilation operators which satisfy Bose commutation rules.

The Fourier transforms of b_f^+ and b_f are introduced where

$$\left.\begin{aligned} b_f^+ &= \left(\frac{1}{N}\right)^{1/2} \sum_{\underset{\sim}{\lambda}} e^{-i(\underset{\sim}{\lambda}\cdot\underset{\sim}{f})} a_\lambda^+ \\ b_f &= \left(\frac{1}{N}\right)^{1/2} \sum_{\underset{\sim}{\lambda}} e^{i(\underset{\sim}{\lambda}\cdot\underset{\sim}{f})} a_\lambda \end{aligned}\right\} \tag{32}$$

where N is the total number of lattice sites and the sums are over the first Brillouin zone. In terms of these operators the transformed Hamiltonian becomes

$$H = -NJ(0)S^2 + 2J(0)S \sum_\lambda 1 - \eta \frac{J(\underset{\sim}{\lambda})}{J(0)} a_\lambda^+ a_\lambda + \frac{1}{N} \sum_{\underset{\sim}{\lambda},\underset{\sim}{k},\underset{\sim}{r}} \left[\eta J(\underset{\sim}{\lambda}) - J(\underset{\sim}{\lambda} - \underset{\sim}{r})\right] a_\lambda^+ a_\mu^+ a_r a_{\lambda+\mu-r} \tag{33}$$

where

$$J(\underset{\sim}{\lambda}) = \sum_{\underset{\sim}{l}} J(\underset{\sim}{l}) e^{-i\underset{\sim}{l}\cdot\underset{\sim}{\lambda}} \tag{34}$$

We now construct the Fourier-type Green's function where there are no interactions.

Following reference 4, we need the equation of motion for the single spin wave Green's function $\langle\langle a_k; a_k^+ \rangle\rangle$, where the double brackets $\langle\langle\ \rangle\rangle$ indicate Fourier transforms of the Green's function, and the single brackets $\langle\ \rangle$ indicate averages over the canonical ensemble at temperature T. Hence, the equation of motion for the single spin wave is

$$E\langle\langle a_k; a_k^+ \rangle\rangle = \left\langle \frac{[a_k, a_k^+]}{2\pi} \right\rangle + \langle\langle (a_k, H); a_k^+ \rangle\rangle \tag{35}$$

Neglecting the interacting terms, we obtain

$$\langle\langle a_k; a_k^+ \rangle\rangle = \frac{1}{2\pi (E - E_{\underset{\sim}{k}})} \tag{36}$$

where

$$E_{\underset{\sim}{k}} = 2SJ(0)\left[1 - \eta \frac{J(\underset{\sim}{k})}{J(0)}\right] \tag{37}$$

is the energy of a noninteracting spin wave with wave vector $\underset{\sim}{k}$.

In order to determine the thermodynamic properties, we must solve for the correlation function, which is given by

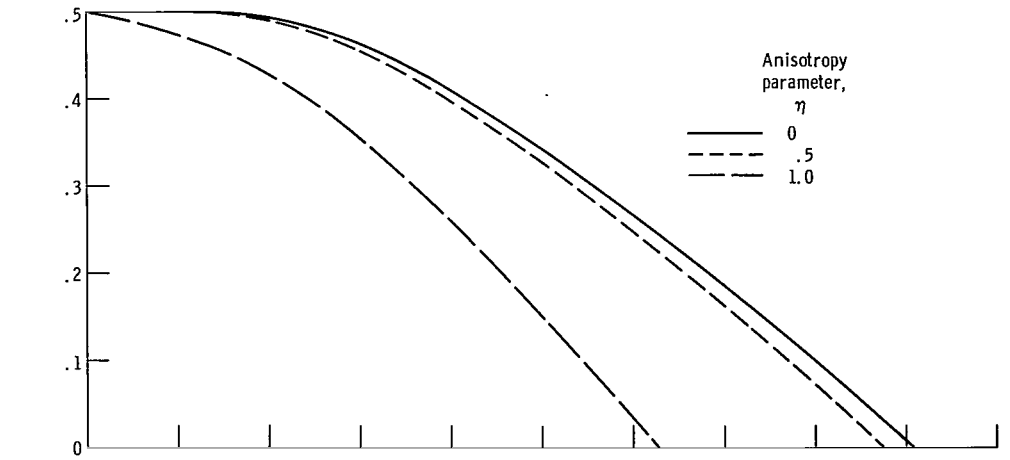
$$\langle B; A \rangle = \lim_{\epsilon \to 0} \frac{i}{} \int_{-\infty}^{\infty} \left(\langle\langle A; B \rangle\rangle_{E+i\epsilon} - \langle\langle A; B \rangle\rangle_{E-i\epsilon} \right) \frac{dE}{e^{\beta E} - 1} e^{iE(t-t')} \tag{38}$$

for the case $t = t'$. The result is

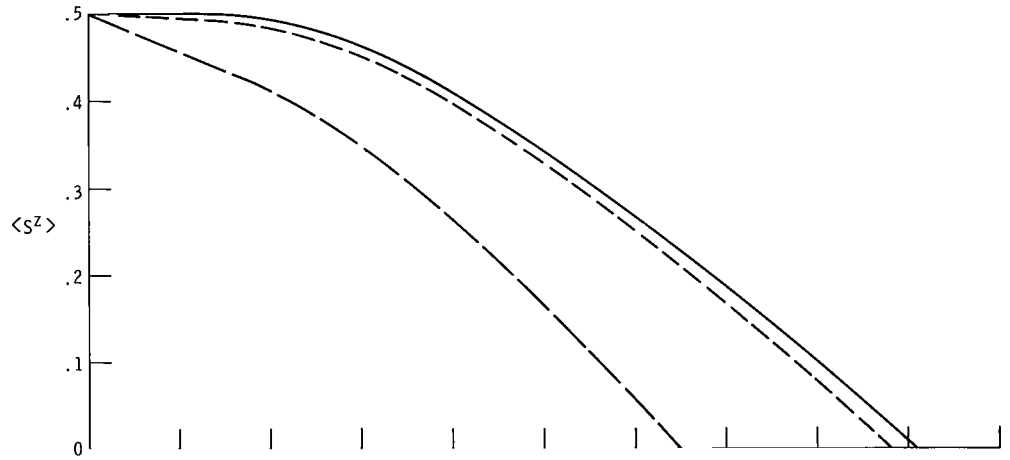
$$\langle a_k^+; a_k \rangle = \frac{1}{E e^{\beta E_k} - 1} \tag{39}$$

The average value of $\langle S^Z \rangle$ can be obtained from equation (31). As is expected, it is identical to the Bloch expression. For spin 1/2 it can be written as

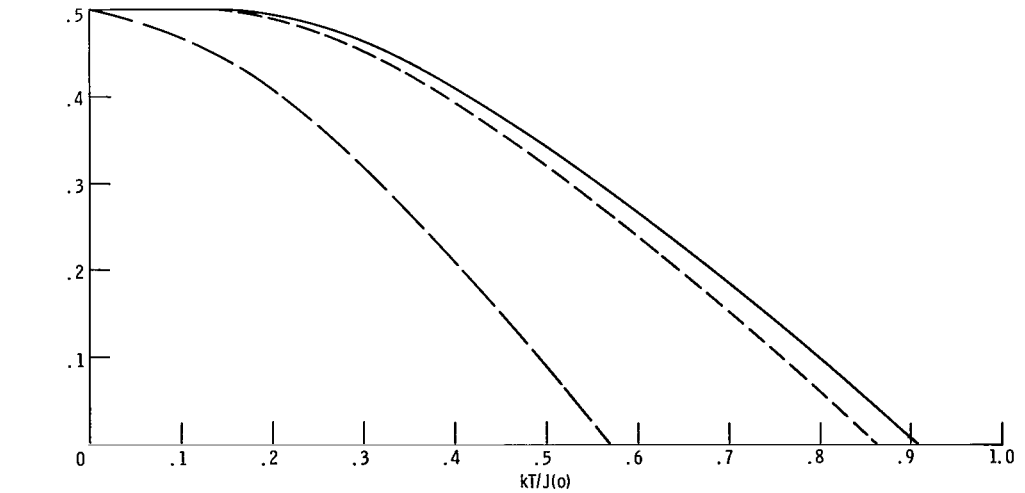
$$\langle S^Z \rangle = \frac{1}{2} - \frac{1}{N} \sum_{\underset{\sim}{K}} \langle a_k^+ a_k \rangle = \frac{1}{2} - \Phi \tag{40}$$



(a) Body-centered-cubic (bcc) lattice.



(b) Face-centered-cubic (fcc) lattice.



(c) Simple-cubic (sc) lattice.

Figure 2. - Magnetization as function of reduced temperature in spin wave approximation.

The solutions for Φ can be obtained from substituting equation (37) into equation (39) and using the same procedures as for the random phase approximation. Figure 2 shows plots of $\langle S^z \rangle$ as a function of the reduced temperature for each of the cubic lattices. It can be shown that for $\eta = 1$, the Bloch $T^{3/2}$ law for magnetization (ref. 8) is obtained at low temperatures for the behavior of $\langle S^z \rangle$ with temperature. In the extreme anisotropic case $\eta = 0$, one can obtain the familiar $e^{-1/T}$ law at low temperatures.

CONCLUDING REMARKS

An analytical procedure has been outlined for the calculation of the magnetization for an anisotropic ferromagnet in the random phase and spin wave approximation over the entire temperature range of interest. It is hoped that this technique is found useful for other applications also.

The random phase approximation predicts that the spontaneous magnetization shows a second-order phase transition independent of the anisotropy. The effect of the anisotropy parameter is to shift the critical temperature. The critical temperature decreases smoothly as η increases. Physically this is due to the energy it takes to reverse a spin. For the Ising model, since there is only one component present, an energy gap of magnitude $2J(0)$ is needed to create an excitation. In the isotropic model, the gap vanishes due to spin waves. These physical (intutive) arguments are supported by numerical calculations presented in this report.

The spin wave approximation gives information regarding the temperature behavior of the magnetization for the Heisenberg and Ising models. The results are in agreement with the random phase approximation for the appropriate limiting cases.

A comparison of the analytical technique with the direct numerical summation over the first Brillouin zone was made. The results agreed to four places. In addition, problems of convergence are avoided by the analytical method.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, March 6, 1969,
129-02-05-14-22.

APPENDIX A

EVALUATION OF I_2

The calculation of the integral I_2 involves the summation of an infinite series. These summation procedures are discussed by several authors (refs. 9 and 10). Here we shall employ some of these techniques and extend them to evaluate I_2.

As an example of the technique used, consider the face-centered-cubic (fcc) lattice. The calculations for the other two cubic lattices follow in the same manner. For the fcc lattice we can write

$$I_2(\text{fcc}) = \frac{3\tau}{\pi^2 \langle S^z \rangle} \sum_{R=1}^{\infty} \left[\int_0^{\pi} \frac{K(k_1)}{(3 + \eta) + 3i\Gamma} dx + \text{c. c.} \right] \tag{A1}$$

$$k_1^2 = 4\eta \left[\frac{(3 + \eta \cos^2 x) + 3i\Gamma}{(3 + \eta + 3i\Gamma)^2} \right] \tag{A2}$$

The complete elliptic integral of the first kind can be represented in series form as

$$K(k) = \left(\frac{\pi}{2}\right) \sum_{\eta} a_n^2 k^{2n} \quad |k| < 1 \tag{A3}$$

where

$$a_n = \frac{[1 \cdot 3 \cdot 5 \ldots (2n - 1)]}{[2 \cdot 4 \cdot 6 \ldots (2n)]} \tag{A4}$$

$$a_o = 1$$

Only the first two terms of the series (eq. (A3)) are necessary for four-place accuracy. There is no difficulty in extending it to as many terms as needed.

Taking the first two terms of equation (A3) into equation (A1), integrating the complex function with respect to x, and rearranging terms we find that

$$I_2 = I_2^a + I_2^b + I_2^c \tag{A5}$$

where

$$I_2^a = \frac{3\tau}{\langle S^z \rangle (3 + \eta)} \sum_{R=1}^{\infty} \frac{y^2}{y^2 + R^2} \tag{A6}$$

$$I_2^b = \left(\frac{\eta}{\pi C}\right) \sum_{R=1}^{\infty} \left[\frac{1}{y^2 + R^2} - \frac{2R^2}{(y^2 + R^2)^2} \right] \tag{A7}$$

$$I_2^c = \left(\frac{-\eta^2 y}{2\pi C^2}\right) \sum_{R=1}^{\infty} \left[\frac{1}{(y^2 + R^2)^2} - \frac{4R^2}{(y^2 + R^2)^3} \right] \tag{A8}$$

and

$$\left.\begin{aligned} C &= \frac{3\pi\tau}{\langle S^z \rangle} \\ y &= \frac{3 + \eta}{C} \end{aligned}\right\} \tag{A9}$$

The following Laplace transforms are used:

$$\frac{1}{y^2 + R^2} = \mathcal{L}\left[\left(\frac{1}{y}\right) \sin(yt)\right] \tag{A10}$$

$$\frac{R^2}{(y^2 + R^2)^2} = \mathcal{L}\left\{\left(\frac{1}{2y}\right) [\sin(yt) + yt \cos(yt)]\right\} \tag{A11}$$

$$\frac{R^2}{(y^2 + R^2)^3} = \mathcal{L}\left\{\left(\frac{1}{8y^3}\right)\left[(1 + y^2t^2)\sin(yt) - yt\cos(yt)\right]\right\} \tag{A12}$$

The summation for I_2^b becomes

$$\sum_{R=1}^{\infty} \frac{1}{R^2 + y^2} = \left(\frac{1}{y}\right)\int_0^{\infty} \frac{\sin(yt)dt}{e^t - 1} \tag{A13}$$

The other sums in I_2^a and I_2^c are obtained in a similar way. Integrating equation (A13) and its counterparts for the other sums leads to equation (20).

APPENDIX B

SYMBOLS

bcc	body centered cubic
b_f, a_λ	creation operators
b_f^+, a_λ^+	annihilation operator
E_k	excitation energy
fcc	face centered cubic
g, p	defined in the text
H	Hamiltonian
i, j	lattice sites
J(k)	defined in the text
J_{ij}	exchange interaction
K(k)	elliptic integral of the first kind
k	Boltzmann's constant
$\mathscr{L}$	Laplace transform
Q	$\langle S^z \rangle / \tau$
R	sum index
S_i	spin operator at site i
$\langle S^z \rangle$	magnetization
sc	simple cubic
T	temperature
v	volume per cit
y, c	defined in the text
z	number of nearest neighbors
β	1/kT
Γ	defined in the text
η	anisotropy parameter
τ	reduced temperature
$\langle\langle \ \rangle\rangle$	Fourier transform of the Green's function
$\langle \ \rangle$	conical average of the operator

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