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THEORY OF THE TWO-SUBLATTICE HEISENBERG ANTIFERROMAGNET

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16. Abstract

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SUMMARY

Thermodynamic properties of the two-sublattice anisotropic Heisenberg antiferromagnet are calculated by the Green function method in the random-phase (Tyablikov) and Callen approximations for spin 1/2. Analytic expressions for the sublattice magnetization and internal energy are obtained which are valid over the whole temperature range up to the Néel temperature for the body-centered cubic lattice.

INTRODUCTION

Antiferromagnetism, like ferromagnetism, is a cooperative phenomenon with an ordered state below a well-defined critical temperature. For the antiferromagnet, however, the exchange energy is negative, and neighboring spins tend to aline antiparallel.

The simplest and most often used model for the antiferromagnet is the two-sublattice model wherein the lattice of magnetic atoms is subdivided into two equivalent interpenetrating sublattices. If only nearest-neighbor interactions are considered, the spins on one sublattice interact only with the nearest spins on the adjacent sublattice. A negative exchange interaction energy results in the two sublattices being spontaneously magnetized in opposite directions. This is the model originally proposed by Néel and has been much used in subsequent theoretical studies of the antiferromagnet. At absolute zero the spins on each sublattice are completely alined antiparallel, and with increasing temperature the spontaneous magnetitization of each sublattice decreases and finally disappears, in zero applied field, at a critical temperature called the Néel temperature. Because of the equivalence of the two sublattices, the net magnetization is zero. The two-sublattice model, which is considered in this report, is compatible only with simple cubic and body-centered cubic crystal structures. More complicated models must be used for antiferromagnetic materials with the face-centered cubic or other crystal structures. Further discussion of the two-sublattice and other models, as well as the experimental properties of antiferromagnets, can be found in the books on magnetism by Morrish (ref. 1) and Smart (ref. 2).

The theory of antiferromagnetism has been much investigated in recent years. The Green function technique is now well established as one of the most useful statistical methods in the theory of magnetism and has been applied many times already to the study of antiferromagnetism (ref. 3 and references cited therein). Earlier methods, especially the molecular field theory, are discussed in detail in references 1 and 2. A useful feature of the Green function method is its applicability over the whole temperature range. Calculations of thermodynamic properties using Green functions have been found to be in good agreement with the results of noninteracting spin wave approximations at low temperatures and with the results of other statistical methods near the Néel temperature (ref. 3).

In this report the Green function technique is applied to the anisotropic Heisenberg exchange model of a two-sublattice antiferromagnet to obtain the correlations between spins, from which the thermodynamic properties can be calculated.

The Heisenberg model is considered reasonably valid for insulators and semiconductors. The sublattice magnetization and other thermodynamic quantities involve complicated lattice sums which, generally, have been evaluated by means of series expansions at the high- and low-temperature limits. In a few cases numerical calculations have been made at a limited number of intermediate points (ref. 3). Flax and Raich have developed a method for evaluating the lattice sums and successfully applied it to the ferromagnet to obtain analytic expressions for the spontaneous magnetization valid over the whole temperature range (refs. 4 to 6). In this report, their method is applied to the antiferromagnet with spin 1/2 to obtain analytic expressions for the sublattice magnetization and internal energy for the body-centered cubic (bcc) structure. The calculations are made for two Green function decoupling schemes, the random-phase approximation (RPA), which is the Tyablikov approximation, (ref. 7), and the Callen approximation. The random-phase approximation is justifiable at low temperatures, where the spins are nearly completely alined and fluctuations are indeed small. However, near the critical point, fluctuations in S^z become significant, and the RPA gives an overestimate of the transition temperature. The Callen approximation takes these fluctuations into account and, for spin greater than 1/2, gives better results near the critical point. The Néel temperatures are also calculated and compared with previous results.

GREEN FUNCTION METHOD

As stated previously, the model used in the present study is a cubic, two-sublattice anisotropic Heisenberg antiferromagnet with nearest-neighbor interactions. The Hamiltonian is

$$H = \sum_{\alpha,\beta} \sum_{l,m} J_{\alpha l,\beta m}\left[S^z_{\alpha l} S^z_{\beta m} + \frac{\eta}{2}\left(S^+_{\alpha l} S^-_{\beta m} + S^-_{\alpha l} S^+_{\beta m}\right)\right] \tag{1}$$

where $J_{\alpha l, \beta m}$ is the exchange energy, S^z and $S^\pm$ are spin operators, and αl and βm refer to lattice sites l and m in sublattices α and β, respectively. Here $\alpha, \beta = 1, 2$ with $N/2$ sites in each sublattice; η is an anisotropy factor where $\eta = 0$ corresponds to the Ising model and $\eta = 1$ to the isotropic Heisenberg model. In the Green function method, the sublattice magnetization $\left\langle S^z_\alpha \right\rangle$ and internal energy $\langle H \rangle$ are calculated from correlation functions involving pairs of spin operators, for example, $\left\langle S^-_{\beta m} S^+_{\alpha l} \right\rangle$. For a general description of the double-time temperature dependent Green function method, see Zubarev (ref. 8 and references cited therein). (Symbols are defined in appendix A.)

The equation of motion in the energy (E) representation for the Green function $\left\langle\left\langle S^+_{\alpha l} ; S^-_{\beta m} \right\rangle\right\rangle$ is

$$E\left\langle\left\langle S^+_{\alpha l} ; S^-_{\beta m} \right\rangle\right\rangle = \frac{1}{2\pi}\left\langle\left[S^+_{\alpha l}, S^-_{\beta m}\right]\right\rangle + \left\langle\left\langle\left[S^+_{\alpha l}, H\right] ; S^-_{\beta m}\right\rangle\right\rangle \tag{2}$$

The commutators for spin operators

$$\left[S^\pm_{\alpha l}, S^z_{\beta m}\right] = \mp S^\pm_{\alpha l}\, \delta_{\alpha\beta} \delta_{l m}$$

and

$$\left[S^+_{\alpha l}, S^-_{\beta m}\right] = 2S^z_{\alpha l}\, \delta_{\alpha\beta} \delta_{l m} \tag{3}$$

where $\delta_{\alpha\beta}$ and $\delta_{l m}$ are Kronecker deltas, are used to evaluate $\left[S^+_{\alpha l}, H\right]$. The equation of motion is then

$$E\left\langle\left\langle S^+_{\alpha l}; S^-_{\beta m}\right\rangle\right\rangle = \frac{1}{\pi}\left\langle S^z_{\alpha l}\right\rangle \delta_{\alpha\beta}\delta_{lm} - 2\sum_{\mu}\sum_{g} J_{\alpha l,\mu g}\left[\left\langle\left\langle S^z_{\mu g}S^+_{\alpha l}; S^-_{\beta m}\right\rangle\right\rangle - \eta\left\langle\left\langle S^z_{\alpha l}S^+_{\mu g}; S^-_{\beta m}\right\rangle\right\rangle\right] \tag{4}$$

Equation (4) represents an infinite hierarchy of coupled equations since each Green function on the right side is of higher order and satisfies a similar equation of motion. To solve this system of coupled equations some decoupling approximation must be made to limit the number of equations. We treat the two decoupling schemes most commonly used in the theory of ferro- and antiferromagnetism, the random-phase and Callen approximations.

Decoupling the equations of motion enables one to solve for the Green function in terms of the energy and excitation energy spectrum. The corresponding correlation functions are related to the Green functions by the following equation:

$$\langle B(t')A(t)\rangle = \lim_{\epsilon\to 0} i\int_{-\infty}^{\infty}\left[\langle\langle A; B\rangle\rangle_{E+i\epsilon} - \langle\langle A; B\rangle\rangle_{E-i\epsilon}\right]\frac{e^{-iE(t-t')}}{e^{\beta E} - 1}\, dE \tag{5}$$

where A and B are the appropriate spin operators, t and t' are times, $\beta = 1/kT$, k is Boltzmann's constant, and T is absolute temperature. Thermodynamic quantities of interest, for example, sublattice magnetization and internal energy, are obtained from these correlation functions.

SUBLATTICE MAGNETIZATION

Random-Phase Approximation

In the RPA, the fluctuations in S^z are ignored and the operator is replaced by its average value. Then

$$\left\langle\left\langle S^z_{\mu g}S^+_{\alpha l}; S^-_{\beta m}\right\rangle\right\rangle \xrightarrow[\mu g\neq\beta m]{} \left\langle S^z_{\mu g}\right\rangle \left\langle\left\langle S^+_{\alpha l}; S^-_{\beta m}\right\rangle\right\rangle \tag{6}$$

The equation of motion becomes

$$EA_{\alpha l,\beta m} = \frac{1}{\pi}\left\langle S^z_{\alpha l}\right\rangle \delta_{\alpha\beta}\delta_{l m} - 2\sum_{\mu}\sum_{g} J_{\alpha l,\mu g}\left(\left\langle S^z_{\mu g}\right\rangle A_{\alpha l,\beta m} - \eta\left\langle S^z_{\alpha l}\right\rangle A_{\mu g,\beta m}\right) \tag{7}$$

where

$$A_{\alpha l,\beta m} \equiv \left\langle\left\langle S^+_{\alpha l}; S^-_{\beta m}\right\rangle\right\rangle \tag{8}$$

Assuming translational invariance of the direct lattice, we Fourier transform to the reciprocal lattice. Let

$$A_{\alpha l,\beta m} = \frac{2}{N}\sum_{k} A_{\alpha\beta}(\vec{k})e^{i\vec{k}\cdot(\vec{R}_{\alpha l} - \vec{R}_{\beta m})} \tag{9}$$

$$J_{\alpha l,\mu g} = \frac{2}{N}\sum_{k} J_{\alpha\mu}(\vec{k})e^{i\vec{k}\cdot(\vec{R}_{\alpha l} - \vec{R}_{\mu g})} \tag{10}$$

where $\vec{k}$ is a vector in the reciprocal lattice, and $\vec{R}_{\alpha l}$ is a vector in the direct lattice for lattice site l in sublattice α. Furthermore, we make the nearest-neighbor approximation in which the spins on sublattice 1 interact only with spins on sublattice 2. Let

$$\vec{\Delta} \equiv \vec{R}_{\alpha l} - \vec{R}_{\mu g} \tag{11}$$

denote a nearest-neighbor vector. Then

$$J_{\alpha l,\mu g} = J\delta_{\alpha,\mu\pm 1}\delta_{g,l\pm\Delta} \tag{12}$$

Therefore,

$$
\begin{aligned}
J_{\alpha\mu}(\vec{k}) &= \sum_{g} J_{\alpha l,\mu g}\, e^{-i\vec{k}\cdot(\vec{R}_{\alpha l}-\vec{R}_{\mu g})} \\
&= J \sum_{\Delta} e^{-i\vec{k}\cdot\vec{\Delta}}\, \delta_{\alpha,\mu\pm 1} \\
&= J(0)\gamma(\vec{k})\,\delta_{\alpha,\mu\pm 1} \\
&= J(\vec{k})\,\delta_{\alpha,\mu\pm 1} \qquad (13)
\end{aligned}
$$

where $J(0) = Jz$,

$$\gamma(\vec{k}) = \frac{1}{z}\sum_{\Delta} e^{\pm i\vec{k}\cdot\vec{\Delta}} \qquad (14)$$

is the structure factor, and z is the number of nearest neighbors. The equation of motion becomes

$$\left[E + 2\left\langle S^{z}_{\mu}\right\rangle J(0)\right] A_{\alpha\beta}(\vec{k}) = \frac{1}{\pi}\left\langle S^{z}_{\alpha}\right\rangle \delta_{\alpha\beta} + 2\eta\left\langle S^{z}_{\alpha}\right\rangle J(0)\gamma(\vec{k})A_{\mu\beta}(\vec{k}) \;\; (\mu = \alpha \pm 1) \qquad (15)$$

or

$$\left[E + K_1\left\langle S^{z}_{\mu}\right\rangle\right] A_{\alpha\beta}(\vec{k}) = \frac{1}{\pi}\left\langle S^{z}_{\alpha}\right\rangle \delta_{\alpha\beta} + K_2\left\langle S^{z}_{\alpha}\right\rangle \gamma(\vec{k})A_{\mu\beta}(\vec{k}) \qquad (16)$$

where $K_1 = 2J(0)$ and $K_2 = 2J(0)\eta$. For $S = 1/2$ the sublattice magnetization can be written as $m = \left\langle S^{z}_{1}\right\rangle = -\left\langle S^{z}_{2}\right\rangle$.

Substitution into the equation of motion yields two pairs of simultaneous linear equations. One pair gives the Green functions

$$A_{11} = \frac{m}{\pi} \frac{E + mK_1}{E^2 - E_k^2} \tag{17}$$

and

$$A_{21} = -\frac{m^2}{\pi} \frac{K_2\gamma(\vec{k})}{E^2 - E_k^2} \tag{18}$$

where

$$E_k = m\left[K_1^2 - K_2^2\gamma(\vec{k})\right]^{1/2} \tag{19}$$

is the excitation energy spectrum. The Green functions A_{22} and A_{12} are similarly obtained but are not needed in the calculation of the thermodynamic quantities.

The corresponding correlation functions are

$$\psi_{11}(\vec{k}) = m\left(-1 + \frac{mK_1}{E_k} \coth \frac{\beta E_k}{2}\right) \tag{20}$$

and

$$\psi_{12}(\vec{k}) = \frac{-m^2K_2\gamma(\vec{k})}{E_k} \coth \frac{\beta E_k}{2} \tag{21}$$

Transforming back to spin operators, we get

$$\left\langle S_1^- S_1^+ \right\rangle = m\left(-1 + \frac{2mK_1}{N} \sum_k \frac{1}{E_k} \coth \frac{\beta E_k}{2}\right) \tag{22}$$

and

$$\left\langle S_1^- S_2^+ \right\rangle = \frac{-2m^2 K_2}{N} \sum_k \frac{\gamma^2(k)}{E_k} \coth \frac{\beta E_k}{2} \tag{23}$$

The lattice sums appearing in equations (22) and (23) are taken over the first Brillouin zone and can be evaluated analytically by the Flax-Raich method. The results are expressions for the correlation functions which are valid over the whole temperature range up to the Néel temperature.

The series expansion

$$\coth(\pi t) = \frac{1}{\pi t} + \frac{2}{\pi} \sum_{R=1}^{\infty} \frac{t}{R^2 + t^2} \tag{24}$$

is used where $\pi t = \beta E_k/2$. For a cubic two-sublattice model

$$\frac{2}{N} \sum_k \rightarrow \frac{1}{\pi^3} \int_0^{\pi} \int_0^{\pi} \int_0^{\pi} \ . \ . \ . \ dx\, dy\, dz$$

The correlation functions can then be written as the sums of integrals:

$$\left\langle S_1^- S_1^+ \right\rangle = m(-1 + I_1 + I_2) \tag{25}$$

and

$$\left\langle S_1^- S_2^+ \right\rangle = -(II_1 + II_2) \tag{26}$$

where the integrals I_1, I_2, and II_2 are given in appendix B by equations (B1) to (B4). When evaluated for the bcc lattice, the integrals become

$$I_1 = \frac{1}{Q} \left[\frac{2}{\pi} K(\kappa) \right]^2 \tag{27}$$

$$I_2 = -\frac{1}{Q}\left(1 + \frac{\xi^2}{8}\right) + \left(1 + \frac{\xi^2}{16}\right)\coth Q + \frac{\xi^2 Q}{16}\,\mathrm{csch}^2\, Q \tag{28}$$

$$II_1 = \frac{m}{\xi Q}\left\{\left[\frac{2}{\pi}K(\kappa)\right]^2 - 1\right\} \tag{29}$$

$$II_2 = \frac{m\xi}{8}\left[-\frac{1}{Q}\left(1 + \frac{27\xi^2}{64}\right) + \left(1 + \frac{27\xi^2}{128}\right)\coth Q + \frac{27\xi^2 Q}{128}\,\mathrm{csch}^2\, Q\right] \tag{30}$$

where

$$\tau = \frac{1}{\beta J(0)} \tag{31}$$

$$Q = \frac{m}{\tau} \tag{32}$$

$$\xi = \eta \tag{33}$$

$$\kappa^2 = \frac{1}{2}\left(1 - \sqrt{1 - \eta^2}\right) \tag{34}$$

and $K(\kappa)$ is a complete elliptic integral of the first kind. For spin $S = 1/2$ the sublattice magnetization is

$$m = \left\langle S_1^z \right\rangle = \frac{1}{2} - \left\langle S_1^- S_1^+ \right\rangle \tag{35}$$

Then

$$m = \frac{1}{2(I_1 + I_2)} \tag{36}$$

The RPA sublattice magnetization m is plotted as a function of reduced temperature

$\tau = kT/J(0)$ in figure 1 for $\eta = 0,\ 0.5$, and 1. In the RPA, the correlation function $\langle S_1^- S_2^+\rangle$ is not needed in the calculation of the sublattice magnetization but is used later for the internal energy.

Callen Approximation

The Callen approximation is a symmetric decoupling scheme which attempts to take into account the fluctuations of S^z around its average value and was first proposed for the ferromagnet (ref. 9) and subsequently applied to the antiferromagnet (refs. 3 and 10). For the antiferromagnet,

$$\langle\langle S^z_{\mu g} S^+_{\alpha l}; S^-_{\beta m}\rangle\rangle \xrightarrow[\mu g \neq \alpha l]{} \langle S^z_{\mu g}\rangle \langle\langle S^+_{\alpha l}; S^-_{\beta m}\rangle\rangle - a\langle S^-_{\mu g} S^+_{\alpha l}\rangle \langle\langle S^+_{\mu g}; S^-_{\beta m}\rangle\rangle \tag{37}$$

In the case of the ferromagnet, the empirical factor a is chosen to be $\langle S^z\rangle / 2S^2$. For the antiferromagnet, two choices for a are possible because of the existence of the two sublattices, namely $\langle S^z_{1g}\rangle / 2S^2$ and $-\langle S^z_{2g}\rangle / 2S^2$. In the absence of an applied field both choices lead to identical results. In the present calculation, we will use

$$a_{\mu g} = -\frac{\langle S^z_{\alpha l}\rangle}{2S^2}$$

$$a_{\alpha l} = -\frac{\langle S^z_{\mu g}\rangle}{2S^2}$$

After decoupling and Fourier transforming to reciprocal space, the equation of motion is

$$EA_{\alpha\beta}(\vec{k}) = \frac{1}{\pi}\langle S^z_\alpha\rangle \delta_{\alpha\beta} - 2A_{\alpha\beta}(\vec{k}) \sum_\mu \langle S^z_\mu\rangle \left[J_{\alpha\mu}(0) - \frac{\eta}{NS^2}\sum_{k'} J_{\alpha\mu}(\vec{k}')\psi_{\alpha\mu}(\vec{k}')\right] + 2\langle S^z_\alpha\rangle$$

$$\times \sum_\mu A_{\mu\beta}(\vec{k})\left[\eta J_{\alpha\mu}(\vec{k}) - \frac{1}{NS^2}\sum_{k'} J_{\alpha\mu}(\vec{k} - \vec{k}')\psi_{\mu\alpha}(\vec{k}')\right] (\mu \neq \alpha) \tag{38}$$

Applying the same nearest-neighbor approximation used in the RPA calculation gives

$$EA_{\alpha\beta}(\vec{k}) = \frac{1}{\pi}\left\langle S_{\alpha}^{z}\right\rangle \delta_{\alpha\beta} - 2\left\langle S_{\mu}^{z}\right\rangle J(0)\left[1 - \frac{\eta}{NS^2}\sum_{k'} \gamma(\vec{k}')\psi_{\alpha\mu}(\vec{k}')\right]A_{\alpha\beta}(\vec{k}) + 2\left\langle S_{\alpha}^{z}\right\rangle J(0)\gamma(\vec{k})$$

$$\times\left[\eta - \frac{1}{NS^2}\sum_{k'} \gamma(\vec{k}')\psi_{\mu\alpha}(\vec{k}')\right]A_{\mu\beta}(\vec{k})(\mu = \alpha \pm 1) \tag{39}$$

where (ref. 6)

$$\sum_{k'} J(\vec{k} - \vec{k}')\psi_{\mu\alpha}(\vec{k}') = J(0)\gamma(\vec{k})\sum_{k'} \gamma(\vec{k}')\psi_{\alpha\mu}(\vec{k}') \tag{40}$$

By symmetry,

$$\psi_{12}(\vec{k}) = \psi_{21}(\vec{k}) \tag{41}$$

Let

$$K_1 = 2J(0)(1 - 2\eta F) \tag{42}$$

$$K_2 = 2J(0)(\eta - 2F) \tag{43}$$

where

$$F = \frac{2}{N}\sum_{k'} \gamma(\vec{k}')\psi_{12}(\vec{k}') \tag{44}$$

and $S = 1/2$. Then

$$\left(E + K_1\left\langle S_{\mu}^{z}\right\rangle\right) A_{\alpha\beta}(\vec{k}) = \frac{1}{\pi}\left\langle S_{\alpha}^{z}\right\rangle \delta_{\alpha\beta} + K_2\left\langle S_{\alpha}^{z}\right\rangle \gamma(\vec{k})A_{\mu\beta}(\vec{k})(\mu \neq \alpha) \tag{45}$$

The equation of motion for the Callen approximation has the same general form as for the RPA and leads to a similar set of coupled equations for the Green functions. The correlation functions are given by equations (20) and (21).

The difference is that for the Callen approximation K_1 and K_2 are defined by equations (42) and (43), respectively. The second correlation function $\left\langle S_1^- S_2^+ \right\rangle$ is identical to the sum F which appears in K_1 and K_2 and is given by equation (47). In the same way as for the RPA, the correlation functions in the Callen approximation can be written as the sums of integrals as in equations (25) and (26). The integrals have the same form for both the RPA and Callen approximations and are given in appendix B by equations (B1) to (B4). The results are given by equations (27) to (30) with K_1 and K_2 defined by equations (41) and (42). Also,

$$\kappa^2 = \frac{1}{2}\left(1 - \sqrt{1 - \xi^2}\right) \tag{46}$$

where

$$\xi = \frac{K_2}{K_1} \tag{47}$$

$$Q = \frac{m}{\tau}(1 - 2\eta F) \tag{48}$$

and τ is defined by equation (31). The sublattice magnetization m for the Callen approximation is plotted against τ in figure 2 for $\eta = 0$, 0.5, and 1. A comparison with previous theoretical calculations (ref. 3) shows that for spin 1/2 the RPA gives a better approximation of the sublattice magnetization.

INTERNAL ENERGY

The internal energy is a useful thermodynamic function for the calculation of many other properties. For a system of interacting spins, differentiation with respect to temperature gives the specific heat due to spin disorder. The entropy and other properties may then be calculated. In previous studies of the antiferromagnet, the internal energy has been derived only for very low temperatures or for the paramagnetic state above the Néel temperature. In this section an exact expression is derived for the internal energy of a two-sublattice anisotropic Heisenberg antiferromagnet with spin $S = 1/2$. This expression for the internal energy is then evaluated in the random-phase and Callen approximations for the bcc lattice by means of the same method used for evaluating the lattice sums in calculating the magnetization. The result is an analytic expression for the internal energy valid over the whole temperature range up to the Néel temperature. The calculation is made for zero applied magnetic field, but the method is equally useful for nonzero fields.

The internal energy U is obtained from the average value of the interacting spin Hamiltonian:

$$U = \langle H \rangle = 2 \sum_{f,g} J_{1f,2g} \left(\left\langle S^z_{1f} S^z_{2g} \right\rangle + \eta \left\langle S^-_{1f} S^+_{2g} \right\rangle \right) \tag{49}$$

The correlation function $F = \left\langle S^-_1 S^+_2 \right\rangle$ has already been calculated, and

$$2 \sum_{f,g} J_{1f,2g} \left\langle S^-_{1f} S^+_{2g} \right\rangle = NJ(0)F \tag{50}$$

The term $2 \sum_{f,g} J_{1f,2g} \left\langle S^z_{1f} S^z_{2g} \right\rangle$ is calculated exactly for spin 1/2 in appendix C and is given by

$$2 \sum_{f,g} J_{1f,2g} \left\langle S^z_{1f} S^z_{2g} \right\rangle = -\frac{NJ(0)}{2} \left[m + \eta F + \frac{m^2 K_1}{J(0)} \right] + m \sum_k E_k \coth \frac{\beta E_k}{2} \tag{C17}$$

An exact expression for the internal energy of the two-sublattice anisotropic Heisenberg antiferromagnet for spin 1/2 is then

$$U = \langle H \rangle = -\frac{NJ(0)}{2} \left[m - \eta F + \frac{m^2 K_1}{J(0)} \right] + m \sum_k E_k \coth \frac{\beta E_k}{2} \tag{51}$$

where K_1 is defined by equation (B5) or (B6). The sum $\sum_k E_k \coth(\beta E_k/2)$ can be evaluated with the help of the integrals of appendix B. Using equation (24) and converting from a sum to integrals give

$$\frac{m}{NJ(0)}\sum_{k} E_k \coth\frac{\beta E_k}{2} = \frac{m}{\beta J(0)} + \frac{2m}{\beta J(0)}\frac{1}{\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\left[\sum_{R=1}^{\infty}\frac{\left(\frac{\beta E_k}{2\pi}\right)^2}{R^2 + \left(\frac{\beta E_k}{2\pi}\right)^2}\right] dx\, dy\, dz$$

$$= \frac{m}{\beta J(0)} + \frac{m^2 K_1}{2J(0)} I_2 - \frac{mK_2}{2J(0)} II_2 \tag{52}$$

where I_2 and II_2 are given by equations (B2) and (B4), respectively, and K_2 is defined by equation (B5) or (B6). Substituting

$$I_2 = \frac{1}{2m} - I_1$$

and

$$II_2 = -\frac{m}{\xi}\left(I_1 - \frac{2}{\beta m K_1}\right) - F$$

into equation (51) and simplifying result in

$$\frac{m}{NJ(0)}\sum_{k} E_k \coth\frac{\beta E_k}{2} = \frac{mK_1}{4J(0)} + \frac{mK_2 F}{2J(0)} \tag{53}$$

Defining a reduced energy by $u = U/NJ(0)$ gives

$$u = -\frac{1}{2}(m - \eta F) - \frac{mK_1}{2J(0)}\left(m - \frac{1}{2}\right) + \frac{mK_2 F}{2J(0)} \tag{54}$$

Specifically,

Specifically,

$$u = -m^2 + \eta F\left(m + \frac{1}{2}\right) \qquad \text{(RPA)} \tag{55}$$

and

$$u = -m^2 + \eta F\left(2m^2 + \frac{1}{2}\right) - 2mF^2 \qquad \text{(Callen)} \tag{56}$$

The quantity u is plotted against the reduced temperature τ in figures 3 and 4 for the RPA and Callen approximations, respectively, for $\eta = 0$, 0.5, and 1.

For both decoupling approximations and $\eta = 0$, $u = 0$ at T_C. This confirms the persistence of some order even above T_C due to the transverse coupling of spins. The intersections of the curves for the RPA appear to result primarily from the lesser weight given to the transverse coupling of spins. For the zero-field case it is not possible to determine from u alone which decoupling scheme gives a more accurate description of the internal energy. A calculation and comparison of the specific heats is more suitable for this purpose.

Values of u at the Néel temperature are presented in table I. The ground-state energy u_0 is the value of the internal energy at 0 K. These values are given in table II, together with the values for the sublattice magnetization at 0 K. The ground-state energy for the isotropic case ($\eta = 1$) in the Callen approximation agrees exactly with the value of -0.293 obtained by Lee and Liu. They use a somewhat different and more complicated method to evaluate the longitudinal correlation function $\left\langle S_1^z S_2^z \right\rangle$ which appears in $\langle H \rangle$ (ref. 3).

NÉEL TEMPERATURE

The transition temperature for an antiferromagnet (Néel temperature) is defined as that temperature at which the sublattice magnetization vanishes. With $Q = Q'A$ and $Q' = m/\tau$, the reduced Néel temperature τ_N is determined from equations (27), (28), and (36) as

$$\tau_N^{-1} = \lim_{m \to 0} \frac{1}{2A}\left\{\left[\frac{2}{\pi} K(\kappa)\right]^2 - \left(1 + \frac{\xi^2}{8}\right) + \left(1 + \frac{\xi^2}{16}\right) Q'A \coth(Q'A) + \frac{\xi^2}{16}(Q'A)^2 \operatorname{csch}^2(Q'A)\right\} \tag{57}$$

where A = 1 for the random phase and $1 - 2\eta F$ for the Callen approximations. It is easily shown that

$$\left.\begin{aligned} &\lim_{Q'A \to 0} (Q'A) \coth (Q'A) = 1 \\ &\lim_{Q'A \to 0} (Q'A) \operatorname{csch} (Q'A) = 1 \end{aligned}\right\} \tag{58}$$

Then

$$\tau_N^{-1} = \lim_{m \to 0} \frac{1}{2A} \left[\frac{2}{\pi} K(\kappa)\right]^2 \tag{59}$$

The calculation τ_N for the Callen approximation also requires

$$\begin{aligned} F_N &= \lim_{m \to 0} F \\ &= \lim_{m \to 0} (-II_1 - II_2) \\ &= \frac{\tau_N}{\eta - 2F_N} \left\{\left[\frac{2}{\pi} K(\kappa_N)\right]^2 - 1\right\} \end{aligned} \tag{60}$$

Then equations (58) and (59) are used to determine τ_N.

The calculated values of τ_N for $\eta = 0$, 0.5, and 1 are presented in table III. For $\eta = 1$, both the RPA and the Callen Néel temperature values agree exactly with those obtained previously for the antiferromagnet (refs. 3 and 11). The value of $\tau_N = 0.5$ for $\eta = 0$ is the well-known value for the Ising model. It is noted that the reduced Néel temperatures for the antiferromagnet are identical to the reduced Curie temperatures for the ferromagnet for both the random-phase and Callen approximations.

CONCLUDING REMARKS

Our results for the sublattice magnetization and the Néel temperatures agree with results obtained previously from high- and low-temperature expansions. This suggests that the method for evaluating the lattice sums which was successfully applied to the study of the anisotropic Heisenberg ferromagnet can be applied with equal validity to the two-sublattice anisotropic Heisenberg antiferromagnet. The result is an analytic expression for the sublattice magnetization that depends on the decoupling scheme. This expression is valid over the whole temperature range.

For spin 1/2, an exact expression for the internal energy due to the ordering of spins (eq. (51)) has been derived for the two-sublattice antiferromagnet and is independent of any decoupling scheme or approximation. This expression was then evaluated for the bcc lattice using the Flax-Raich method, for both the RPA and Callen decoupling schemes. The result is an analytic expression for the internal energy valid over the whole temperature range. In the Callen approximation, the value of the ground-state energy for the isotropic model ($\eta = 1$) agrees exactly with the value obtained previously from a low-temperature expansion. The internal energy in the presence of an applied field can be obtained by essentially the same methods. The analytic expression for the internal energy can then be used to calculate the specific heat and many other thermodynamic quantities and hence is a starting point for formulating the thermodynamics of the two-sublattice antiferromagnet.

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National Aeronautics and Space Administration,
Cleveland, Ohio, July 8, 1971,
129-02.

APPENDIX A

SYMBOLS

E_k	excitation energy
H	Hamiltonian
$J_{\alpha l,\beta m}$	exchange energy
$K(\kappa)$	complete elliptic integral of first kind
k	Boltzmann's constant
m	sublattice magnetization
N	total number of lattice sites
$S^z, S^{\pm}$	spin operators
T	temperature
U	internal energy
β	$1/kT$
$\gamma(\vec{k})$	structure factor
$\vec{\Delta}$	nearest-neighbor vector
η	anisotropy parameter
τ	reduced temperature
$\langle\ \rangle$	correlation function
$\langle\langle\ \rangle\rangle$	Green function

APPENDIX B

EVALUATION OF INTEGRALS FOR BODY-CENTERED CUBIC LATTICE

The method for evaluating the integrals which appear in the calculations of the correlation functions in the random-phase and Callen approximations are outlined in this appendix. The methods are similar to those applied to the ferromagnet (refs. 4 to 6). The integrals are

$$I_1 = \frac{2mK_1}{\beta\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{1}{E_k^2}\, dx\, dy\, dz \tag{B1}$$

$$I_2 = \frac{m\beta K_1}{\pi^5} \int_0^\pi \int_0^\pi \int_0^\pi \left[\sum_{R=1}^{\infty} \frac{1}{R^2 + \left(\frac{\beta E_k}{2\pi}\right)^2} \right] dx\, dy\, dz \tag{B2}$$

$$II_1 = \frac{2m^2K_2}{\beta\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{\gamma^2(k)}{E_k^2}\, dx\, dy\, dz \tag{B3}$$

$$II_2 = \frac{m^2\beta K_2}{\pi^5} \int_0^\pi \int_0^\pi \int_0^\pi \left[\sum_{R=1}^{\infty} \frac{\gamma^2(k)}{R^2 + \left(\frac{\beta E_k}{2\pi}\right)^2} \right] dx\, dy\, dz \tag{B4}$$

where

$$\left.\begin{aligned} K_1 &= 2J(0) \\ & \qquad\qquad (\text{RPA}) \\ K_2 &= 2\eta J(0) \end{aligned}\right\} \tag{B5}$$

$$\left.\begin{aligned} K_1 &= 2J(0)(1 - 2\eta F) \\ & \qquad\qquad (\text{Callen}) \\ K_2 &= 2J(0)(\eta - 2F) \end{aligned}\right\} \tag{B6}$$

and

$$\begin{aligned} E_k^2 &= m^2\left[K_1^2 - \gamma^2(\vec{k})K_2^2\right] \\ &= m^2K_1^2\left[1 - \xi^2\gamma^2(k)\right] \end{aligned} \tag{B7}$$

with $\xi = K_2/K_1$. For the bcc lattice, the structure factor is

$$\gamma(\vec{k}) = \cos x \cos y \cos z \tag{B8}$$

Then

$$\begin{aligned} I_1 &= \frac{2}{\beta m K_1 \pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \left(\frac{1}{1 - \xi^2 \cos^2 x \cos^2 y \cos^2 z}\right) dx\, dy\, dz \\ &= \frac{2}{\beta m K_1 \pi^3} \int_0^\pi \int_0^\pi \frac{1}{(1 - \xi^2 \cos^2 x \cos^2 y)^{1/2}}\ dx\, dy\, dz \end{aligned} \tag{B9}$$

The denominator can be expanded as

$$(1 - \xi^2 \cos^2 x \cos^2 y)^{1/2} = \sum_{n=0}^{\infty} a_n \xi^{2n} \cos^{2n} x \cos^{2n} y \tag{B10}$$

where

$$a_n = \frac{(2n)!}{2^{2n}(n!)^2} \tag{B11}$$

Also,

$$\int_0^{\pi} \cos^{2n} x \, dx = a_n \pi \tag{B12}$$

Therefore,

$$I_1 = \frac{2}{\beta m K_1} \sum_{n=0}^{\infty} a_n^3 \xi^{2n} \tag{B13}$$

The series corresponds to a complete elliptic integral of the first kind (ref. 4):

$$K^2(\kappa_1) = \frac{\pi^2}{4} \sum_{n=0}^{\infty} a_n^3 (2\kappa_1 \kappa_1')^{2n} \tag{B14}$$

where

$$\kappa_1^2 = \frac{1}{2}\left(1 - \sqrt{1 - \xi^2}\right) \tag{B15}$$

and κ_1 and κ_1' are conjugates. Then

$$I_1 = \frac{2}{\beta m K_1}\left[\frac{2}{\pi} K(\kappa_1)\right]^2 \tag{B16}$$

The integral II_1 can be written in terms of I_1 as

$$II_1 = \frac{m}{\xi}\left(I_1 - \frac{2}{\beta m K_1}\right) \tag{B17}$$

and is thereby easily evaluated. The evaluation of I_2 proceeds as follows:

$$I_2 = \frac{4}{\beta m K_1} \sum_{R=1}^{\infty} \frac{1}{\Gamma^2} \left[\frac{1}{\pi^3} \int_0^{\pi}\int_0^{\pi}\int_0^{\pi} \frac{dx\,dy\,dz}{1 - \left(\frac{\xi}{\Gamma}\right)^2 \cos^2 x \cos^2 y \cos^2 z} \right] \tag{B18}$$

where

$$\Gamma^2 = \left(\frac{2\pi R}{\beta m K_1}\right)^2 + 1 \tag{B19}$$

Then

$$I_2 = \frac{4}{\beta m K_1} \sum_{R=1}^{\infty} \frac{1}{\Gamma^2} \left[\frac{2}{\pi} K(\kappa_2)\right]^2 \tag{B20}$$

where

$$\kappa_2^2 = \frac{1}{2}\left[1 - \sqrt{1 - \left(\frac{\xi}{\Gamma}\right)^2}\right] \tag{B21}$$

Using the same expansion as in the evaluation of I_1,

$$\left[\frac{2}{\pi} K(\kappa_2)\right]^2 = \sum_{n=0}^{\infty} a_n^3 \left(\frac{\xi}{\Gamma}\right)^{2n}$$

$$= 1 + \frac{1}{8}\left(\frac{\xi}{\Gamma}\right)^2 + \frac{27}{512}\left(\frac{\xi}{\Gamma}\right)^4 + \ldots \tag{B22}$$

gives

$$I_2 = \frac{4}{\beta m K_1} \sum_{R=1}^{\infty} \left(\frac{1}{\Gamma^2} + \frac{\xi^2}{8\Gamma^4} + \frac{27\xi^4}{512\Gamma^6} + \ldots \right) \tag{B23}$$

Substituting $1/\Gamma^2 = S^2/(R^2 + S^2)$, where $S = \beta m K_1/2\pi$, gives

$$I_2 = \frac{2}{\pi S} \left[S^2 \sum_{R=1}^{\infty} \left(\frac{1}{R^2 + S^2} \right) + \frac{\xi^2 S^4}{8} \sum_{R=1}^{\infty} \frac{1}{(R^2 + S^2)^2} + \frac{27\xi^4 S^6}{512} \sum_{R=1}^{\infty} \frac{1}{(R^2 + S^2)^6} + \ldots \right] \tag{B24}$$

The sums over R are evaluated by the method of Laplace transforms (see refs. 4 to 6 and references cited therein). Sufficiently accurate results are obtained by keeping only the first few terms in the sum over n. Specifically, the sums over R needed to calculate I_2 and II_2 are

$$\sum_{R=1}^{\infty} \frac{1}{R^2 + S^2} = -\frac{1}{2S^2} + \frac{\Pi}{2S} \coth(\pi S) \tag{B25}$$

$$\sum_{R=1}^{\infty} \frac{1}{(R^2 + S^2)^2} = -\frac{1}{2S^4} + \frac{\Pi}{4S^3} \coth(\pi S) + \frac{\Pi^2}{4S^2} \operatorname{csch}^2(\pi S) \tag{B26}$$

Finally,

$$I_2 = -\frac{1}{\pi S}\left(1 + \frac{\xi^2}{8}\right) + \left(1 + \frac{\xi^2}{16}\right) \coth(\pi S) + \frac{\xi^2 (\pi S)}{16} \operatorname{csch}^2(\pi S) \tag{B27}$$

The integral II_2 is evaluated in a similar way. For the RPA, $\pi S = m/\tau$ and $\xi = \eta$. For the Callen approximation, $\pi S = m(1 - 2\eta F)/\tau$ and $\xi = (\eta - 2F)/(1 - 2\eta F)$.

APPENDIX C

EVALUATION OF THE TERM $2\sum_{f,g} J_{1f,2g}\left\langle S^z_{1f}S^z_{2g}\right\rangle$

For spin 1/2, the term $2\sum_{f,g} J_{1f,2g}\left\langle S^z_{1f}S^z_{2g}\right\rangle$ can be evaluated exactly. The operator S^z can be written as

$$\left.\begin{aligned} S^z_1 &= \frac{1}{2} - S^-_1S^+_1 \\ S^z_2 &= -\frac{1}{2} - S^-_2S^+_2 \end{aligned}\right\} \tag{C1}$$

Then

$$\left\langle S^z_{1f}S^z_{2g}\right\rangle = -\frac{1}{4} + \frac{1}{2}\left(\left\langle S^-_{1f}S^+_{1f}\right\rangle - \left\langle S^-_{2g}S^+_{2g}\right\rangle\right) + \left\langle S^-_{1f}S^+_{1f}S^-_{2g}S^+_{2g}\right\rangle = -\frac{1}{4} + \left\langle S^-_{1f}S^+_{1f}\right\rangle$$

$$+ \left\langle S^-_{1f}S^+_{1f}S^-_{2g}S^+_{2g}\right\rangle \tag{C2}$$

since

$$\left\langle S^-_2S^+_2\right\rangle = -\left\langle S^-_1S^+_1\right\rangle$$

The correlation function $\left\langle S^-_{1f}S^+_{1f}S^-_{2g}S^+_{2g}\right\rangle$ can be evaluated by using the Green function equation of motion given by equation (2) for $\alpha, \beta = 1$:

$$EA_{1l,1m} = \frac{1}{\pi}\left\langle S^z_{1l}\right\rangle \delta_{lm} - 2\sum_g J_{1l,2g}\left[\left\langle\left\langle S^z_{2g}S^+_{1l}; S^-_{1m}\right\rangle\right\rangle - \eta\left\langle\left\langle S^z_{1l}S^+_{2g}; S^-_{1m}\right\rangle\right\rangle\right] \tag{C3}$$

Substituting equations (C1) on the right side for S^z gives

$$EA_{1l,1m} = \frac{1}{\pi}\left\langle S^z_{1l}\right\rangle \delta_{lm} + \sum_g J_{1l,2g}(A_{1l,1m} + \eta A_{2g,1m}) + 2\sum_g J_{1l,2g}$$

$$\times (A_{2g2g1l,1m} - \eta A_{1l1l2g,1m}) \tag{C4}$$

where $A_{2g2g1l,1m} \equiv \left\langle\left\langle S^-_{2g}S^+_{2g}S^+_{1l}; S^-_{1m}\right\rangle\right\rangle$ is a Green function of higher order.

To simplify the calculation, the spectral density ρ for a Green function is introduced. It is defined in reference 7 by

$$\rho(A,B;E) = i \lim_{\epsilon\to0}\left[\left\langle\left\langle A;B\right\rangle\right\rangle_{E+i\epsilon} - \left\langle\left\langle A;B\right\rangle\right\rangle_{E-i\epsilon}\right] \tag{C5}$$

The corresponding correlation functions are calculated from equation (5). For $t = t'$ equation (5) can be written as

$$\langle BA\rangle = \int_{-\infty}^{\infty}\left(e^{\beta E} - 1\right)^{-1}\rho(A,B;E)dE \tag{C6}$$

Equation (C4) can be written in terms of spectral densities. Setting $1 = m = f$ results in

$$E\rho(1f,1f;E) = \sum_g J_{1f,2g}\left[\rho(1f,1f;E) + \eta\rho(2g,1f;E)\right] + 2\sum_g J_{1f,2g}$$

$$\times\left[\rho(2g2g1f,1f;E) - \eta\rho(1f1f2g,1f;E)\right] \tag{C7}$$

where

$$\rho(1f,1f;E) = i\lim_{\epsilon\to0}\left[A_{1f,1f}(E+i\epsilon) - A_{1f,1f}(E-i\epsilon)\right] \tag{C8}$$

$$\rho(2g2g1f,1f;E) = i\lim_{\epsilon\to0}\left[A_{2g2g1f,1f}(E+i\epsilon) - A_{2g2g1f,1f}(E-i\epsilon)\right] \tag{C9}$$

Multiplying equation (C7) by $(e^{\beta E} - 1)^{-1}$, integrating over E from $-\infty$ to $+\infty$, and summing over f give

$$\sum_{f} \int_{-\infty}^{\infty} (e^{\beta E} - 1)^{-1} E\rho(1f, 1f; E)dE = \sum_{f,g} J_{1f,2g} \left(\left\langle S_{1f}^{-} S_{1f}^{+} \right\rangle + \eta \left\langle S_{1f}^{-} S_{2g}^{+} \right\rangle \right) + 2 \sum_{f,g} J_{1f,2g}$$

$$\times \left(\left\langle S_{1f}^{-} S_{2g}^{-} S_{2g}^{+} S_{1f}^{+} \right\rangle - \eta \left\langle S_{1f}^{-} S_{1f}^{-} S_{1f}^{+} S_{2g}^{+} \right\rangle \right) \qquad \text{(C10)}$$

On the right side, $\left\langle S_{1f}^{-} S_{1f}^{-} S_{1f}^{+} S_{2g}^{+} \right\rangle = 0$, because for $S = 1/2$, $(S^{-})^{2} \left| \right\rangle = 0$ for any state $\left| \right\rangle$. Fourier transforming $\rho(1f, 1f; E)$ to reciprocal space yields

$$\sum_{f} \rho(1f, 1f; E) = \sum_{k} \rho_{11}(\vec{k}; E)$$

$$= \sum_{k} i \lim_{\epsilon \to 0} \left[A_{11}(\vec{k}; E + i\epsilon) - A_{11}(\vec{k}; E - i\epsilon) \right] \qquad \text{(C11)}$$

Rearranging equation (C10) gives

$$2 \sum_{f,g} J_{1f,2g} \left\langle S_{1f}^{-} S_{1f}^{+} S_{2g}^{-} S_{2g}^{+} \right\rangle = \sum_{k} \int_{-\infty}^{\infty} (e^{\beta E} - 1)^{-1} E\rho_{11}(\vec{k}; E)dE - \sum_{f,g} J_{1f,2g}$$

$$\times \left(\left\langle S_{1f}^{-} S_{1f}^{+} \right\rangle + \eta \left\langle S_{1f}^{-} S_{2g}^{+} \right\rangle \right) \qquad \text{(C12)}$$

Then from equations (C2) and (C12),

$$2 \sum_{f,g} J_{1f,2g} \left\langle S_{1f}^{z} S_{2g}^{z} \right\rangle = \frac{-NJ(0)}{4} + \sum_{f,g} J_{1f,2g} \left(\left\langle S_{1f}^{-} S_{1f}^{+} \right\rangle - \eta \left\langle S_{1f}^{-} S_{2g}^{+} \right\rangle \right) + \sum_{k} \int_{-\infty}^{\infty} (e^{\beta E} - 1)^{-1}$$

$$\times E\rho_{11}(\vec{k}; E)dE \qquad \text{(C13)}$$

Also,

$$\sum_{f,g} J_{1f,2g}\left\langle S_{1f}^{-}S_{1f}^{+}\right\rangle = \frac{NJ(0)}{2}\left\langle S_{1}^{-}S_{1}^{+}\right\rangle$$

$$= \frac{NJ(0)}{2}\left(\frac{1}{2} - m\right) \tag{C14}$$

and

$$\sum_{f,g} J_{1f,2g}\left\langle S_{1f}^{-}S_{2g}^{+}\right\rangle = \frac{NJ(0)F}{2} \tag{C15}$$

The integral over E is evaluated by using the Green function of equation (17) in the spectral density $\rho_{11}(k;E)$. The result is

$$\sum_{k} \int_{-\infty}^{\infty} \left(e^{\beta E} - 1\right)^{-1} E\rho_{11}(\vec{k};E)dE = m\sum_{k} E_k \coth\frac{\beta E_k}{2} - \frac{Nm^2}{2}K_1 \tag{C16}$$

Substituting equations (C14), (C15), and (C16) into (C13) gives

$$2\sum_{f,g} J_{1f,2g}\left\langle S_{1f}^{z}S_{2g}^{z}\right\rangle = -\frac{NJ(0)}{2}\left[m + \eta F + \frac{m^2K_1}{J(0)}\right]\sum_{k} E_k \coth\frac{\beta E_k}{2} \tag{C17}$$

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TABLE I. - REDUCED INTERNAL ENERGY EVALUATED AT NÉEL TEMPERATURE FOR SPIN 1/2 ANTIFERROMAGNET WITH BODY-CENTERED CUBIC LATTICE

Anisotropy factor, η	Approximation	
	Random phase	Callen
	Reduced internal energy, $u = \langle H \rangle /NJ(0)$	
0	0	0
.5	-.0043	-.0097
1.0	-.0706	-.0706

TABLE II. - REDUCED INTERNAL ENERGY AND SUBLATTICE MAGNETIZATION EVALUATED AT T = 0 K FOR SPIN 1/2 ANTIFERROMAGNET WITH BODY-CENTERED CUBIC LATTICE

Anisotropy factor, η	Approximation			
	Random phase		Callen	
	Sublattice magnetization, m_0	Reduced internal energy, $u_0 = \langle H \rangle /NJ(0)$	Sublattice magnetization, m_0	Reduced internal energy, $u_0 = \langle H \rangle /NJ(0)$
0	0.5000	-0.2500	0.5000	-0.2500
.5	.4293	-.2584	.4907	-.2597
1.0	.4706	-.2906	.4706	-.2934

TABLE III. - REDUCED NÉEL TEMPERATURE FOR SPIN 1/2, TWO-SUBLATTICE, ANISOTROPIC HEISENBERG ANTIFERROMAGNET WITH BODY-CENTERED CUBIC LATTICE

Anisotropy factor, η	Approximation	
	Random phase	Callen
	Reduced Néel temperature	
0	0.5000	0.5000
.5	.4830	.4970
1	.3589	.4601

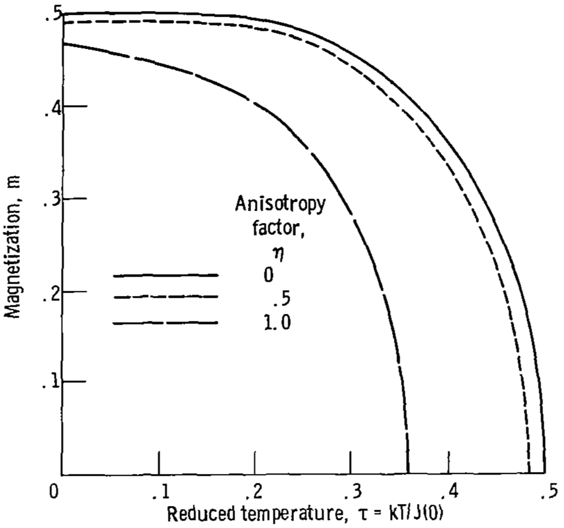

Figure 1. - Magnetization as function of reduced temperature for random-phase approximation.

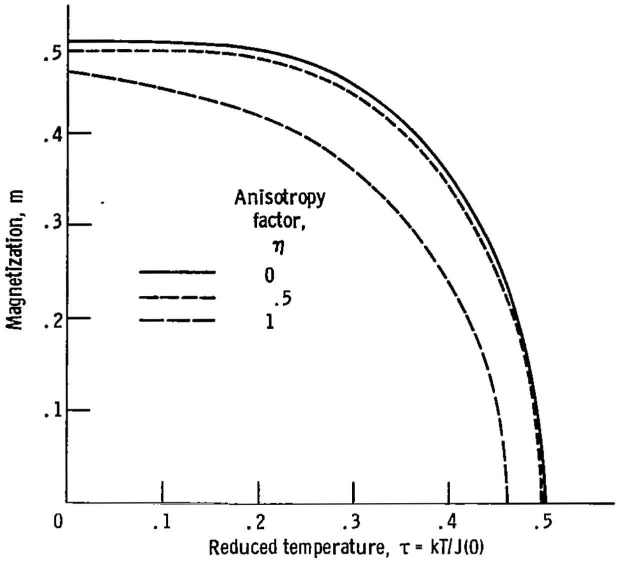

Figure 2. - Magnetization as function of reduced temperature for Callen approximation.

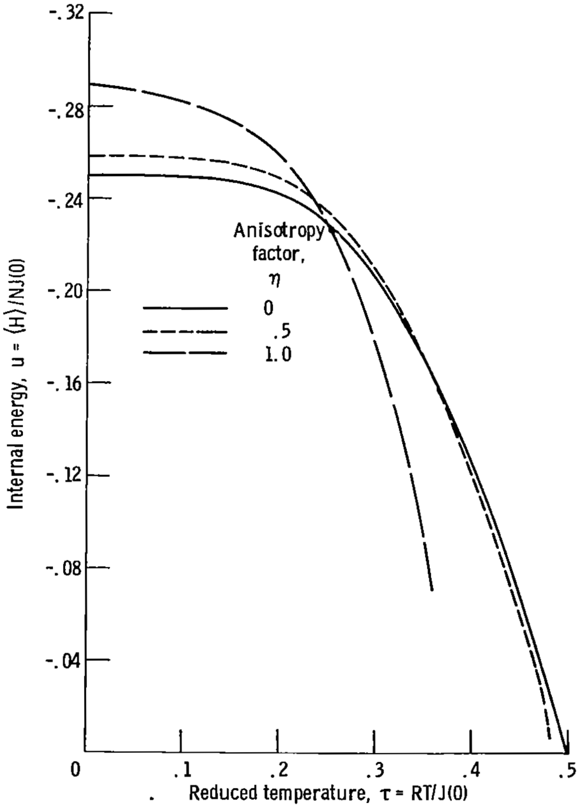

Figure 3. - Internal energy as function of reduced temperature for random-phase approximation.

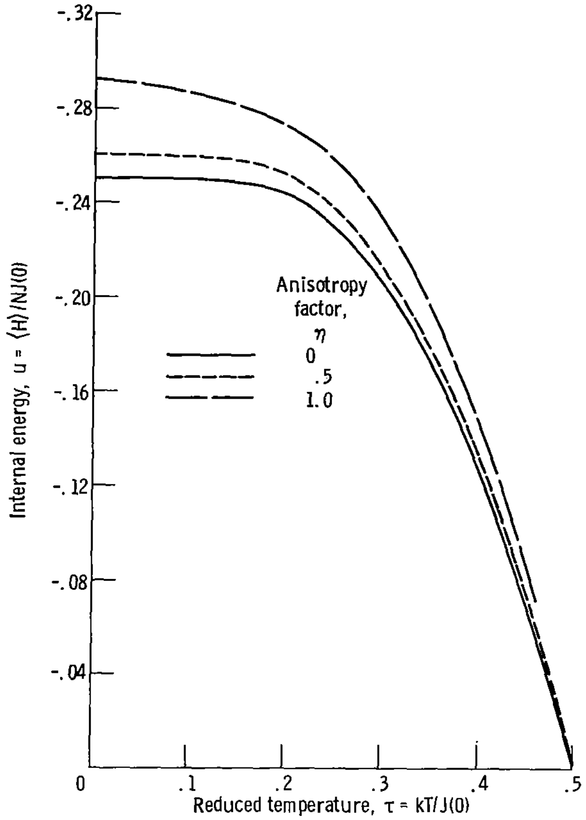

Figure 4. - Internal energy as function of reduced temperature for Callen approximation.

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