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THEORY OF THE ANISOTROPIC HEISENBERG FERROMAGNET

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16. Abstract

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SUMMARY

The development of a formalism for the investigation of phase transitions of the anisotropic Heisenberg ferromagnet is presented. By the use of Green's function theory the magnetization is determined by several decoupling schemes. A method of calculating the generalized Watson sums is also formulated.

The thermodynamic quantity to be studied is the magnetization at and near the Curie point. By use of various decoupling schemes, different phase transitions are generated. An analytical formulation is developed to determine at what temperature the transition takes place.

INTRODUCTION

As the temperature of a ferromagnet is increased, the magnetization will decrease until, at a temperature known as the Curie temperature T_c the sample becomes paramagnetic. The process by which this change from ferromagnet to paramagnet occurs is referred to as the ferromagnetic phase transition. The fundamental problem in the theory of ferromagnetism is the theoretical description of the phase transition. The theory of this phase transition, as well as many other types of phase transitions occurring in nature, has been the subject of many investigations. These investigations have shown that electrical, mechanical, and many thermodynamic properties of a material are altered when the material undergoes a phase transition.

One way of describing the ferromagnetic phase transition is to look upon it as an order-disorder transition in the material. The property of order in a system describes the correlation between the properties of two atoms, even when the atoms are widely separated in space. The spontaneous magnetization present in a ferromagnet is due to the correlations between the spins of the atoms. Above the Curie temperature the long-range order is gone, and the system is paramagnetic. The description of this change from an ordered to a disordered state is the description of the thermodynamic phase transition.

Thermodynamic phase transitions can be classified by the discontinuities that occur in the Gibbs thermodynamic potential. From an experimental standpoint, it is not easy to decide what types of transition are present because of the rapid variation of a thermodynamic variable such as specific heat or entropy, near the critical temperature. It is often difficult to distinguish, for example, whether a transition in specific heat against temperature has a finite, infinite, or cusp discontinuity.

This report is concerned with the investigation of the thermodynamic properties of the anisotropic Heisenberg ferromagnet. The thermodynamic quantity studied was the magnetization at and near the Curie point. The statistical method used to determine the thermodynamics of the system was the double time thermodynamic Green's functions. The objectives of this report are threefold: One is to investigate the various decoupling schemes for the Green's function theory of the anisotropic Heisenberg model. The second purpose is the evaluation of the generalized Watson sums, which arise in the theory of magnetism and other order-disorder phenomena, in analytical form. These sums must be evaluated in order to calculate the thermodynamic quantities of interest as a function of temperature. Previous calculations of the generalized Watson sums have been mostly based on series expansions and are therefore valid only over limited temperature regions. The purpose here is to describe a method of evaluating the Watson sums without using series expansions or extensive computer summations. The third objective is to propose a new type of decoupling. This report shows that it is theoretically possible to have different orders of transitions for the anisotropic Heisenberg model.

The simplest way of treating correlations between atoms in a ferromagnetic crystal is to consider only one atom and replace its interaction with the rest of the crystal by an effective field. This theory, called the molecular field theory, was first advanced by Weiss (ref. 1), who assumed the effective field to be proportional to the magnetization. This theory gave a satisfactory qualitative picture of the main features of a ferromagnet, namely, the existence of a transition temperature, specific heat anomaly, and a spontaneous magnetization. It had weak points, however, such as its failure to predict the correct behavior of these quantities at very low temperatures and its underestimation of the transition temperature. It also failed to explain the origin of the molecular field.

Not until the advent of quantum mechanics could the Weiss molecular field be justified. Heisenberg (ref. 2) showed that this field is a result of a quantum-mechanical exchange interaction. The exchange interaction is a consequence of the Pauli principle that requires the wave function to be antisymmetric with an exchange of space and spin coordinates. This exchange interaction can be interpreted naively as an interaction which tends to orient the spin angular momenta and hence affect the magnetic moments of the atoms.

Dirac (ref. 3) formulated a Hamiltonian which displays the effect of coupling of spin angular momenta of localized particles. This Hamiltonian is often referred to as the Heisenberg model, the mathematical statement of which is

$$H = - \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \qquad (1)$$

where J_{ij} is the exchange interaction between the spins on sites i and j and the summation is over all sites. The vector spin of the i^{th} particle is S_i.

The exchange interaction is positive for ferromagnetism and in practice is regarded as a phenomenological constant, which is determined by fitting the theory with a set of experimental results.

In principle, all the thermodynamic and magnetic properties of a crystal that contains N lattice points can be determined by constructing the partition function for the Hamiltonian, and taking the appropriate derivatives. In practice, it has not been possible to solve this problem only for certain limiting cases. The only solutions that have been obtained for the Heisenberg model are for very high or very low temperatures. These solutions have been derived from series expansions of the free energy in powers of T (the spin wave solution) valid for $T << T_c$ and in powers of $1/T$ for $T >> T_c$. Each of these solutions is only valid far from the transition temperature and therefore various approximations have been proposed to study the behavior at intermediate temperatures.

The existence of a phase transition in a system with long-range coupling is a question for statistical mechanics. At the present this question cannot be answered mathematically for the full exchange interaction. But the known (high and low temperature) solutions will provide both physical guides of the choice of approximation to be applied and the criteria against which to judge these approximations.

Perhaps the most powerful technique in the study of ferromagnetism is the method of temperature-dependent Green's functions (refs. 4 and 5). With this method the thermodynamics as well as the correlations of the spins can be analyzed. Green's function theory when applied to ferromagnetism agrees with the spin wave theory at low temperatures and with the $1/T$ expansion at high temperatures.

Some of the complications of the quantum mechanical theory of ferromagnetism are avoided if the Ising (ref. 6) model is used rather than the Heisenberg model. If, in the Heisenberg model, one assumes that the instantaneous values of the neighboring spins may be replaced by their time averages, then one obtains an Ising model. The Ising model may, however, be considered the limiting case of the Heisenberg model, in which the exchange forces are extremely anisotropic in the z direction, and thus the Hamiltonian is just

$$H = -\sum_{ij} J_{ij} S_i^z S_j^z \tag{2}$$

The suppression of the x and y components of the spin in this model produces consequences that must be treated with caution. This model is incorrect at low temperatures because it excludes spin waves. The absence of spin waves or low-temperature elementary excitations occurs because the quadratic x and y dependence of the energy is neglected. The advantages of the Ising model is that calculations can often be carried out with rigor and it can be solved exactly in one and two (ref. 7) dimensions.

The exact solution of the two-dimensional Ising model shows a spontaneous magnetization proving that the system is ferromagnetic. In contrast, the two-dimensional Heisenberg model has no ferromagnetism. In three dimensions, by the use of various approximations (refs. 8 to 10), the thermodynamics of these models can be estimated. The results of these approximations show that both models appear to exhibit a ferromagnetic behavior.

Besides the contrasting behavior pattern of the Ising and Heisenberg models in two dimensions, there are other apparent differences in three dimensions. Thermodynamic quantities like magnetization and susceptibility behave differently below the transition temperature. The only place where both models show similar behavior is in the paramagnetic state.

Because of the dissimilar behavior of these models, Dalton and Wood (ref. 11) have considered an intermediate model. They have studied the critical behavior of this anisotropic model in two and three dimensions for intermediate values of an anisotropy parameter η, where $0 \leq \eta \leq 1$, by the Green function method and series expansion technique. The Ising and isotropic Heisenberg models are special cases with values of η equal to 0 and 1, respectively. The Dalton and Wood Hamiltonian is

$$H = -\sum_{i}\sum_{j} J_{ij} S_i^z S_j^z + \frac{\eta}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) \tag{3}$$

where

$$S^{\pm} = S_j^x \pm i S_j^y \tag{4}$$

In a physical sense, η can be interpreted as a strength parameter for an anisotropic exchange interaction. It is usually so interpreted for the case of ferromagnetic crystals where crystal field effects give rise to magnetic anisotropy. The magnetic anisotropy can have significant effects on the correlation and long-range order properties of the system.

The exact equations of motion for any order of the Green's functions for the anisotropic Heisenberg model involve higher order Green's functions. These higher order Green's functions thus necessitate a decoupling approximation in order to obtain a solvable closed system of equation. From these equations the correlation function and hence the thermodynamics of the system can be exposed. Various types of phase transitions are predicted, depending on the form of the decoupling parameter. This will involve a solution for the magnetization that will be valid for all temperature regions of interest without the use of any separate approximations for high or low temperature regions.

REVIEW OF MOLECULAR FIELD THEORY OF FERROMAGNETISM

A qualitative understanding of the Weiss molecular field theory can be obtained by examining the Ising Hamiltonian of equation (2). This equation may be considered to be the statement that a spin S_i^z feels an effective field

$$\mathcal{H}_i = \sum_j J_{ij} S_j^z \tag{5}$$

where the sum is over all nearest neighbor sites of the site i, such that the Hamiltonian is

$$H = - \sum_i \mathcal{H}_i S_i^z$$

It is assumed here that the exchange energy between nearest neighbor electrons of the same atom is constant and that all electrons have the same exchange energy. Only nearest neighbor interactions are included. The molecular field approximation consists of replacing equation (5) by

$$\langle \mathcal{H}_i \rangle = Jz \left\langle S_j^z \right\rangle \tag{6}$$

where z is the number of nearest neighbors. The process of replacing the spin operator S_j^z by its statistical average $\left\langle S_j^z \right\rangle$ is the essential approximation of this method. The replacement is equivalent to neglecting fluctuations of $\left\langle S_j^z \right\rangle$, if S_i^z is up, its neighbors will have more than average predilection for being up. The problem is then reduced essentially to treating a paramagnetic gas of noninteracting spins.

As all the magnetic atoms are identical and equivalent, $\left\langle S_j^z \right\rangle$ is related to the total magnetic moment of the crystal by

$$M = N\left\langle S_j^z \right\rangle \tag{7}$$

where N is the number of atoms and M is the magnetization. Equation (5) can then be written in the form

$$\langle \mathcal{H}_i \rangle = \frac{zJ}{N} M \tag{8}$$

The thermodynamic quantities can be determined directly from the partition function. It is a straightforward matter to calculate the average z component of spin

$$S_j^z = \frac{T_r\left[S_j^z \exp\left(\mathscr{B}\langle \mathcal{H}_i \rangle \sum_i S_i^z\right)\right]}{T_r\left[\exp\left(\mathscr{B}\langle \mathcal{H}_i \rangle \sum_i S_i^z\right)\right]}$$

where

$$\mathscr{B} = \frac{1}{KT}$$

Writing out the trace for spin 1/2 and setting $\left\langle S_j^z \right\rangle = \langle s^z \rangle$ yields

$$\langle S^z \rangle = \frac{1}{2} \frac{\left[\exp\left(\frac{\mathscr{B}}{2} \langle \mathcal{H}_i \rangle\right) - \exp\left(-\frac{\mathscr{B}}{2} \langle \mathcal{H}_i \rangle\right)\right]}{\left[\exp\left(\frac{\mathscr{B}}{2} \langle \mathcal{H}_i \rangle\right) + \exp\left(\frac{\mathscr{B}}{2} \langle \mathcal{H}_i \rangle\right)\right]}$$

or

$$\langle S^z \rangle = \frac{1}{2} \tanh\left(\frac{1}{2} \mathscr{B} Jz \langle S^z \rangle\right) \tag{9}$$

using $\langle \mathcal{H}_i \rangle = J\langle S^z \rangle$. Comparison with various experimental data gives a surprisingly good qualitative picture of the thermodynamic properties such as the temperature dependence of the magnetization, susceptibility, and specific heat. However, the molecular field theory does not describe accurately the exact behavior of a spin system near absolute zero or the Curie point.

There have been many extensions of and improvements to the Weiss theory for both ferromagnets and antiferromagnets. In the molecular-field theory approach, the exchange interactions in the crystal are replaced by an effective field, so that certain interactions arising from $\vec{S} \cdot \vec{S}$ are lost. If the exchange interaction were to be considered, the problem would become unmanageable. A compromise has been sought where a small section of the crystal is treated; the exchange interaction in this region can be solved exactly. The effect of the remainder of the crystal was then taken to be an effective field. The first detailed treatment of the exchange-coupled spin pair in an effective field was given by Oguchi (ref. 12). He considered the effective field to be a molecular field which is proportional to the average magnetization. This method was an improvement over the Weiss field theory in describing short-range order above the critical point, and it gave a nonvanishing specific heat. On the other hand, it failed for the temperature dependence of magnetization near absolute zero and the transition point. The Bethe-Peierls-Weiss method showed some improvements over the Oguchi technique as far as short-range order, but it could not be used for temperatures much below the Curie point because of the expansions used in the effective field. Thus, one of the major flaws in these techniques has been the use of expansions that either did not converge or gave very inaccurate results. The shortcomings of the effective field theories at low temperatures have been corrected by the spin-wave theories.

The effective field theories are also inaccurate at high temperatures where local correlations are important.

GREEN'S FUNCTION THEORY OF ANISOTROPIC HEISENBERG FERROMAGNET

In this section, the Green's function theory is applied to the anisotropic Heisenberg model, using some of the decoupling approximations previously applied to the isotropic Heisenberg model. The algebra of the Green's functions is presented in appendix A. The Hamiltonian for the anisotropic model is

$$H = -\sum_i \sum_j J_{ij} S_i^z S_j^z + \frac{\eta}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) \tag{10}$$

where

$$S_j^{\pm} = S_j^x \pm i S_j^y \tag{11}$$

η is the anisotropy parameter, J_{ij} is the exchange interaction between spins on sites i and j, and the sum is carried over all sites in the crystal. The exchange interaction is assumed to be a function only of the distance between sites. The self-exchange terms such as J_{ii} or J_{jj} vanish.

The anisotropic parameter η separates the interaction into an isotropic and anisotropic part and, in effect, takes into account any crystalline field or lattice distortions.

Since the thermodynamic quantity of interest is the magnetization of the system, one is interested in evaluating correlation functions of the form $\left\langle S_g^- S_m^+ \right\rangle$ and hence of the retarded Green's function $\left\langle\left\langle S_g^+ ; S_m^- \right\rangle\right\rangle$. The reason for this choice will be apparent in the section on magnetization.

Using the Hamiltonian in equation (10), together with the known spin commutation relations, results in

$$\left.\begin{aligned} \left[S_i^+ , S_j^-\right] &= 2S_j^z \delta_{ij} \\ \left[S_i^\pm , S_j^z\right] &= \mp S_j^\pm \delta_{ij} \end{aligned}\right\} \tag{12}$$

One can write the equation of motion (A29) in the form

$$E\left\langle\left\langle S_g^+ ; S_m^- \right\rangle\right\rangle = \left\langle S_g^z \right\rangle \frac{\delta_{gm}}{(\pi)} + 2\sum_f J_{gf}\left(\left\langle\left\langle S_f^z S_g^+ ; S_m^- \right\rangle\right\rangle - \eta\left\langle\left\langle S_g^z S_f^+ ; S_m^- \right\rangle\right\rangle\right) \tag{13}$$

For a system of interacting spins, the second and third terms on the right hand side of equation (13) contain Green's functions with three operators and are called higher order Green's functions. The equation of motion for one of these higher order Green's functions involves the next higher order Green's function. In this way an infinite hierarchy of equations is generated. Thus the exact treatment of the equations of motion involves the solution of an infinite set of coupled equations for an infinite number of Green's functions. To obtain a closed solution for a Green's function, this hierarchy of equations must be truncated at some point. The procedure usually adopted is to make a so-called decoupling approximation in which the higher order Green's functions on the right hand side of equation (13) are expressed in terms of lower order Green's functions. By doing this, equation (13) can be explicitly solved for $\left\langle\left\langle S_g^+ ; S_m^- \right\rangle\right\rangle$.

Random-Phase Approximation

One of the most commonly used decoupling schemes is the random-phase approximation (RPA; ref. 13). This technique ignores any fluctuations of $\left\langle S_g^z \right\rangle$, and the operator S_g^z is replaced by its average value

$$\left\langle\left\langle S_g^z S_f^+ ; S_m^- \right\rangle\right\rangle \xrightarrow[g\neq f]{} \left\langle S_g^z \right\rangle \left\langle\left\langle S_f^+ ; S_m^- \right\rangle\right\rangle \tag{14}$$

A physical justification of this decoupling procedure is plausible at low temperatures where the spins are nearly completely alined. It is here that any deviation of the z component of the spin at any one lattice site is very small; therefore, neglecting the fluctuation is valid for a first approximation. Although this approximation yields qualitatively correct results for the magnetization, it overestimates the transition point.

Because of translational symmetry of the lattice, the subscript can be dropped in $\langle S^z \rangle$. On substitution of equation (14) into equation (13),

$$\left[E - 2\langle S^z \rangle J(0)\right] A_{gm} = \frac{1}{\pi} \langle S^z \rangle \delta_{gm} - 2\eta \langle S^z \rangle \sum_f J_{gf} A_{fm} \tag{15}$$

results where, for brevity,

$$A_{gm} = \left\langle\left\langle S_g^+ ; S_m^- \right\rangle\right\rangle \tag{16}$$

and

$$J(\vec{k}) = \sum_f J_{gf} \exp\left[i\vec{k} \cdot (\vec{f} - \vec{g})\right]$$

The translational invariance dictates the use of Fourier transformation with respect to the inverse lattice, that is,

$$A_{gm} = \frac{1}{N} \sum_{\vec{k}} \exp\left[i\vec{k} \cdot (\vec{g} - \vec{m})\right] A_{\vec{k}} \tag{18}$$

where N is the total number of sites in the lattice and the sums are restricted to the first Brillouin zone. It is shown in appendix A that the Green's function for this model can be written in the following form

$$A_k = \frac{1}{\pi} \langle S^z \rangle \left[E - E(\vec{k})\right]^{-1} \tag{19}$$

where

$$E(\vec{k}) = 2\langle S^z \rangle J(0) \left[1 - \frac{\eta J(\vec{k})}{J(0)}\right] \tag{20}$$

the elementary excitation energy. It should be noted in contrast to the isotropic case that the ground-state energy E(0) has a gap of magnitude $2(1-\eta)\langle S^z \rangle J(0)$.

Symmetric Decoupling

Callen (ref. 14), using a heuristic argument based on physical grounds, suggested a decoupling that attempts to account for the spin correlation on one site with the spin on another. He proposed a symmetric method of decoupling the Green's function

$$\left\langle\left\langle S_g^- S_g^+ S_{fj}^+ S_m^- \right\rangle\right\rangle$$

such that

$$\left\langle\left\langle S_g^- S_g^+ S_{fj}^+ S_m^- \right\rangle\right\rangle \xrightarrow[g \neq f]{} \left\langle S_g^- S_g^+ \right\rangle \left\langle\left\langle S_{fj}^+ S_m^- \right\rangle\right\rangle + \left\langle S_g^- S_g^+ \right\rangle \left\langle\left\langle S_{gj}^+ S_m^- \right\rangle\right\rangle + \left\langle S_g^+ S_f^+ \right\rangle \left\langle\left\langle S_{gj}^- S_m^- \right\rangle\right\rangle \tag{21}$$

where the last term $\left\langle S_g^+ S_f^+ \right\rangle$ vanishes because it has no diagonal elements in the representation of the total z component of spin. The symmetric decoupling method is similar to the Wick-Bloch-de Dominicus theorem for statistical averages (ref. 15). For spin 1/2, S_g^z can be written exactly as

$$S_g^z = S - S_g^- S_g^+ , \left(S = \frac{1}{2}\right) \tag{22}$$

Furthermore, for any value of spin, from equation (12),

$$S_g^z = \frac{1}{2}\left(S_g^+ S_g^- - S_g^- S_g^+\right) \tag{23}$$

Multiplying equation (22) by α, equation (23) by $(1 - \alpha)$, and adding result in

$$S_g^z = \alpha S + \frac{(1 - \alpha) S_g^+ S_g^-}{2} - \frac{(1 + \alpha) S_g^- S_g^+}{2} \tag{24}$$

Substituting equation (24) into equation (14) and using the symmetric decoupling scheme (eq. (21)), one finds

$$\left\langle\left\langle S_g^z S_f^+ ; S_m^- \right\rangle\right\rangle \xrightarrow[g \neq f]{} \langle S^z \rangle \left\langle\left\langle S_f^+ ; S_m^- \right\rangle\right\rangle - \left\langle \alpha\ S_g^- S_f^+ \right\rangle \left\langle\left\langle S_g^+ ; S_m^- \right\rangle\right\rangle \tag{25}$$

Here, if $\alpha = 1$, the decoupling is on the basis of identity (22) and is strictly valid only for $S = 1/2$. If $\alpha = 0$, the decoupling is on the basis of identity (23), which holds for arbitrary spin. Actually equation (22) is valid for arbitrary spin, also, if it operates only on spin states that have $S_g^z = \pm S$, in effect neglecting deviations from spin-up and spin-down. Thus, the Callen decoupling scheme with a suitable choice of α may give a correction to the random-phase approximation by introducing deviations from spin-up and spin-down. A physical criterion is required to select the proper value of α.

The operator $S_g^- S_g^+$ in equation (22) represents the deviation of S^z from S. It therefore seems plausible to use equation (23) when $\langle S^z \rangle \sim S$, that is, at low temperatures. Thus $\alpha = 1$ corresponds to a low-temperature decoupling scheme. It should be noted that the random-phase approximation neglects these terms.

On the other hand, as seen from equation (22), the operator $1/2(S^+S^- - S^-S^+)$ represents the deviation of S^z from zero, and it is therefore reasonable to use this equation when $S^z = 0$. Thus, Callen chose $\alpha = 0$ to represent a high-temperature decoupling scheme.

For $S = 1/2$ all the preceding requirements are satisfied by the choice

$$\alpha = 2\langle S^z \rangle \tag{26}$$

When $\alpha = 0$, one obtains the same equations of motion as for the random-phase approximation. However, it should be emphasized again that this is not the only possible choice that can satisfy the physical boundary conditions. In other words, α is not unique. Inserting equation (25) into the equation of motion (eq. (13)) gives

$$EA_{gm} = \frac{\langle S^z \rangle \delta_{gm}}{\pi} + 2\langle S^z \rangle \sum_f J_{gf} \left(A_{gm} - \eta A_{fm}\right) + 2\alpha \sum_f J_{gf}\left(\eta \psi_{gf} A_{gm} - \psi_{fg} A_{fm}\right) \tag{27}$$

where again for brevity,

$$A_{gm} = \left\langle\left\langle S_g^+ ; S_m^- \right\rangle\right\rangle \tag{28}$$

and

$$\psi_{gf} = \left\langle S_g^- S^+ f \right\rangle \tag{29}$$

When it is assumed that the lattice is translationally invariant, a Fourier transform with respect to the reciprocal lattice can be used to obtain the following result (see appendix B):

$$A_k = \frac{\langle S^z \rangle}{\pi\left[E - E(k)\right]} \tag{30}$$

where, here, for the Callen decoupling scheme

$$E(\vec{k}) = 2\langle S^z\rangle \left[J(0) - \eta J(\vec{k})\right] + \frac{2\alpha}{N}\sum_{k'} \left[\eta J(\vec{k}') - J(\vec{k}' - \vec{k})\right]\psi_{\vec{k}'} \tag{31}$$

and

$$J(\vec{k}) = \sum_{f} J_{gf} \exp\left[-i\vec{k}\cdot(\vec{g} - \vec{f})\right] \tag{32}$$

The Curie temperature is defined as that temperature at which $\langle S^z\rangle$ vanishes. Then from equation (26) this is the temperature at which $\alpha = 0$. However, the form for α is by no means unique. In this report the decoupling parameter α will take on other forms which also meet the physical criteria. It will turn out that, not only is the Curie temperature sensitive to this parameter, but so is the type of phase transition.

MODIFICATIONS OF THE DECOUPLING PARAMETERS

As mentioned previously, for a second-order transition the long-range order parameter (magnetization for the anisotropic ferromagnet) changes continuously from the ordered to the disordered state but has a discontinuity in its first temperature derivative. In contrast, for a first-order transition, the long-range order parameter itself changes discontinuously at the transition point. Other types of transitions appear in which the long-range order decreases smoothly with a discontinuity in some higher order derivative. There is also the possibility of a transition with no discontinuities in any derivative. Such a process will be called a washed-out transition which is characterized by a tail in going from the normal to the condensed state. The washed-out behavior is believed to occur for the Ising model of solid orthohydrogen (refs. 16 and 17).

It will be shown that these transitions appear to be quite sensitive to the choice of α and β. In the case of the Callen decoupling, certain criteria were used which imply that α must be equal to 1 at $T = 0$ and must approach zero at $T = T_c$. Thus, to meet these conditions, the calculations were based on $\alpha = 2\langle S^z\rangle$ for spin 1/2. Copeland and Gersch (ref. 18) changed the parameter to the form

$$\alpha = \left(2\langle S^z\rangle\right)^p \tag{33}$$

where p is any power. Applying this parameter to the isotropic Heisenberg model, they reached the conclusion that this form with $p = 3$ gave better results near the Curie point than $p = 1$ and that the result still agreed with spin-wave theory at low temperatures and $1/T$ expansions at high temperatures. They also showed, with the use of a computer, that some powers of p gave a first-order transition and that others were ruled out because they do not produce a transition.

The anisotropic model is applicable not only to ferromagnetism but also to a host of other physical problems that involve phase transitions. One would like not only to investigate Callen's parameter, with or without various powers, but also to modify the decoupling scheme such that the critical point values can be improved as well as to yield other types of transitions.

Since there appears a logarithmic variation of the long-range order, a suitable modification which is used in this report has the form

$$\alpha = \left(2\langle S^z\rangle\right)^p - \left(2\langle S^z\rangle\right)^p \log\left(2\langle S^z\rangle\right)^p \tag{34}$$

When $\langle S^z\rangle = 1/2$, $\alpha = 1$ at low temperatures, and when $\langle S^z\rangle = 0$, $\alpha = 0$ above the critical point. This choice also meets Callen's physical criteria. The results of these modifications will be discussed in the next two sections.

The purpose in modifying the decoupling approximation is to determine what types of phase transition can be present. Conventionally, the ferromagnet is believed to undergo a second-order phase transition from the ordered ferromagnetic phase to the disordered paramagnetic phase at a critical temperature called the Curie temperature. However, because of intrinsic difficulties in measuring the thermodynamic anomalies at the critical point, the experimentalists are not able to determine what type of phase is present. The Heisenberg model has never been exactly solved, and thus there is no rigorous proof that the Heisenberg model predicts a phase transition. However, with the approximations discussed above the Heisenberg model does exhibit a phase transition. Thus, it is of interest to study, within these approximations, at what temperature and in what manner the spontaneous magnetization goes to zero.

SPONTANEOUS MAGNETIZATION AND CRITICAL BEHAVIOR:
RANDOM-PHASE APPROXIMATION

Spontaneous magnetization means the presence of a magnetic moment in the absence of an applied magnetic field. If there were such a field present, some of the spins in a paramagnetic system would line up parallel to it, and there would be long-range order. The average z component of the spin can be considered to be a measure of this long-range order. The thermal average $\langle S^z\rangle$ is proportional to the magnetization.

In order to calculate the spontaneous magnetization $\langle S^z\rangle$, one makes use of the commutation relations of equation (12) as well as

$$\vec{S}\cdot\vec{S} = S^-S^+ + S^z + \left(S^z\right)^2 \tag{35}$$

which fixes the magnitude of the spin. Thus the average value of the spin correlation is

$$\langle S^-S^+\rangle = S(S+1) - \langle S^z\rangle - \left\langle\left(S^z\right)^2\right\rangle \tag{36}$$

For spin 1/2 equation (36) reduces to

$$\langle S^-S^+\rangle = \frac{1}{2} - \langle S^z\rangle \tag{37}$$

The magnetization for the anisotropic Heisenberg ferromagnet is calculated explicitly using the decoupling schemes described previously.

The calculation of the correlation function follows directly from equation (A30) in the limit $t = t'$. Using the δ function representation,

$$\delta(x) = \underset{\epsilon\to 0}{\lim}\,\frac{1}{2\pi i}\left(\frac{1}{x - i\epsilon} - \frac{1}{x + i\epsilon}\right) \tag{38}$$

it follows that

$$\langle S^-S^+\rangle = 2\langle S^z\rangle\Phi \tag{39}$$

where

$$\Phi = \frac{1}{N}\sum_{\vec{k}}\frac{1}{\exp\left[E(\vec{k})\beta\right] - 1} \tag{40}$$

where $E(\vec{k})$ is given by equation (20).

Using equations (37) and (39) one finds that

$$\langle S^-S^+\rangle = 2\langle S^z\rangle\Phi = \frac{1}{2} - \langle S^z\rangle \tag{41}$$

The expression for $\langle S^z\rangle$ then becomes

$$\langle S^z\rangle = \frac{\frac{1}{2}}{1 + 2\Phi} \tag{42}$$

And it is easily shown that

$$\Phi = \frac{1}{2N} \sum_{\vec{k}} \left[\coth \frac{\beta E(\vec{k})}{2}\right] - \frac{1}{2} \tag{43}$$

The magnetization as a function of temperature is evaluated from the sum in equation (43) over all values of $\vec{k}$ in the first Brillouin zone of the appropriate lattice. Except in the low- and high-temperature limits numerical methods are generally used. But in general, numerical solutions are difficult. It is a purpose of this report to show that analytical solutions of equation (43) are possible.

Consider only crystals with cubic symmetry. For these lattices replace the sum in equation (39) by an integral

$$\frac{1}{N} \sum_{\vec{k}} \longrightarrow \frac{v}{(2\pi)^3} \int\int\int d\vec{k} \tag{44}$$

where v is the volume per site:

for the simple-cubic (sc) lattices

$$v = a^3$$

for body-centered-cubic (bcc) lattices

$$v = \frac{1}{2} a^3$$

for face-centered-cubic (fcc) lattices

$$v = \frac{1}{4} a^3$$

and the integration is over the first brillouin zone of the appropriate lattice. For the cubic lattices, equation (44) can be stated in the form

$$\frac{1}{N} \sum_{\vec{k}} \longrightarrow \frac{1}{\pi^3} \int_0^{\pi} \int_0^{\pi} \int_0^{\pi} dx\, dy\, dz \tag{45}$$

where for sc lattices

$$x = k_x a \qquad y = k_y a \qquad z = k_z a \tag{46}$$

for bcc lattices

$$x = \frac{1}{2} k_x a \qquad y = \frac{1}{2} k_y a \qquad z = \frac{1}{2} k_z a \tag{47}$$

and for fcc lattices

$$x = \frac{1}{2} k_x a \qquad y = \frac{1}{2} k_y a \qquad z = \frac{1}{2} k_z a \tag{48}$$

$$\coth(\pi t) = \frac{1}{\pi t} + \frac{2}{\pi} \sum_{R=1}^{\infty} \frac{t}{R^2 + t^2} \tag{49}$$

one may write equation (43) in the form

$$\Phi = -\frac{1}{2} + I_1 + I_2 \tag{50}$$

where

$$I_1 = \frac{v\tau}{(2\pi)^3\, 2\langle S^z \rangle} \iiint \frac{d^3\vec{k}}{1 - \eta \dfrac{J(k)}{J(0)}} \tag{51}$$

$$I_2 = \frac{v\tau}{(2\pi)^3\, 2\langle S^z \rangle} \sum_{R=1}^{\infty} \left[\iiint \frac{d^3\vec{k}}{1 - \eta \dfrac{J(k)}{J(0)} + i\Gamma(R)} + cc \right] \tag{52}$$

Here $\Gamma(R) = R\pi e/\langle S^z \rangle$; $\tau = kT/J(0)$, the reduced temperature; and cc indicates the complex conjugate.

Body-Centered-Cubic Lattice

Consider first the case of a bcc lattice, where (from eq. (32)) J(k) can be written as

$$\frac{J(k)}{J(0)} = \cos\frac{k_x a}{2}\cos\frac{k_y a}{2}\cos\frac{k_z a}{2} \tag{53}$$

From equation (47) it follows that equations (51) and (52) have the form

$$I_1(\mathrm{bcc}) = \frac{\tau}{(2\pi)^3\langle S^z\rangle}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\frac{dx\,dy\,dz}{1 - \eta\cos x\cos y\cos z} \tag{54}$$

$$I_2(\mathrm{bcc}) = \frac{\tau}{(2\pi)^3\langle S^z\rangle}\sum_{R=1}^{\infty}\left[\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\frac{dx\,dy\,dz}{1 + i\Gamma(R) - \eta\cos x\cos y\cos z} + cc\right] \tag{55}$$

The integrals appearing in equations (54) and (55) are evaluated in appendix C. The summation in equation (55) is evaluated by the use of Laplace transforms, and this method is shown in appendix D. The results are

$$I_1(\mathrm{bcc}) = \frac{\tau}{2\langle S^z\rangle}\left[\frac{2}{\pi}K(\kappa)\right]^2 \tag{56}$$

$$I_2(\mathrm{bcc}) = \frac{1}{(2Q)}\left[Q\coth(Q) - 1 - \frac{\eta^2}{8} + \left(\frac{Q}{2}\right)^3\eta^2\operatorname{csch}^2(Q)\coth(Q)\right] \tag{57}$$

where $K(\kappa)$ is a complete elliptic integral of the first kind,

$$\kappa^2 = \frac{1}{2}\left(1 - \sqrt{1 - \eta^2}\right) \tag{58}$$

and $Q = \langle S^z\rangle/\tau$. On substitution of equations (56) and (57) into equation (50), the magnetization is obtained from equation (42).

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. 21) are used. In fact, by setting $\eta = 0$ in equation (42), a result equivalent to the familiar Ising result for magnetization (eq. (9)) is obtained,

$$\langle S^z\rangle = \frac{1}{2}\tanh Q \tag{59}$$

Face-Centered-Cubic Lattice

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

$$I_1(\mathrm{fcc}) = \frac{1}{\pi^2 gQ} \int_0^{\pi} K(\kappa_1)dx \tag{60}$$

$$I_2(\mathrm{fcc}) = \frac{1}{Q^2 \langle S^z \rangle g} \left[gQ \coth(gQ) + \frac{g}{3} Q^2 \operatorname{csch}^2(gQ) - \frac{\eta}{3g} + \left(2g^2\right)^{-1} \left(\frac{\eta}{3}\right)^2 - \frac{g\eta^2 Q^3}{18} \operatorname{csch}^2(gQ)\coth(gQ) \right] \tag{61}$$

where

$$\kappa_1^2 = \frac{4\eta(3 + \eta)\cos^2(x)}{(3 + \eta)^2} \tag{62}$$

$$g = \frac{3 + \eta}{3} \tag{63}$$

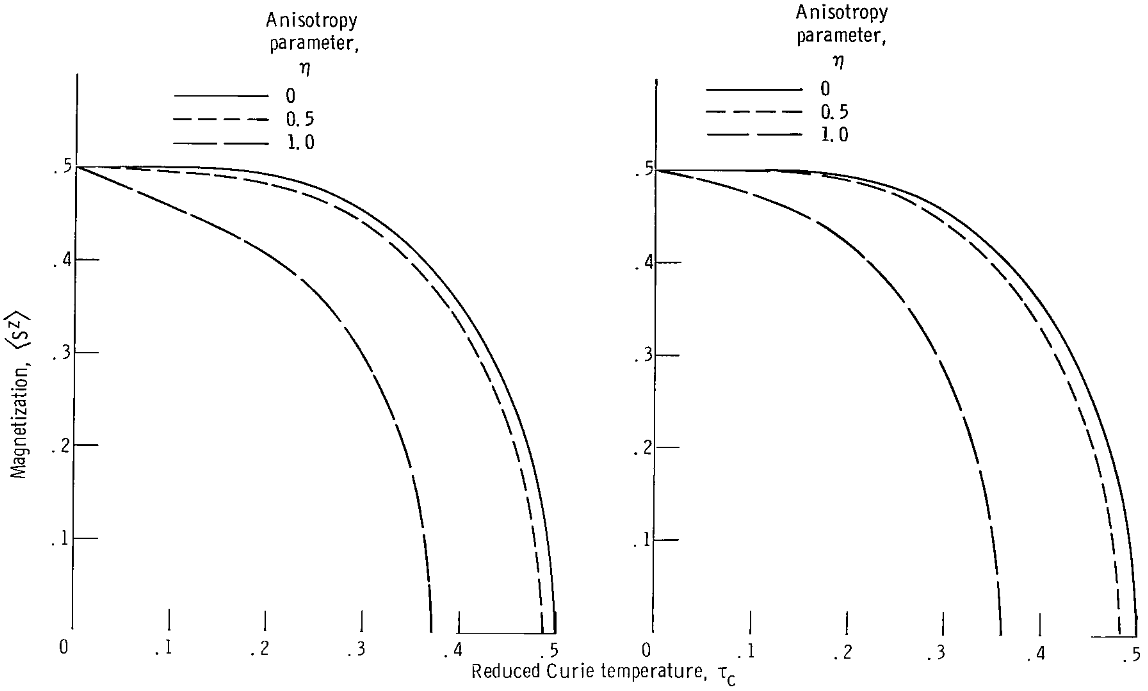
and

$$\frac{3J(k)}{J(0)} = \cos\frac{k_x a}{2} \cos\frac{k_y a}{2} + \cos\frac{k_y a}{2} \cos\frac{k_z a}{2} + \cos\frac{k_z a}{2} \cos\frac{k_x a}{2} \tag{64}$$

Simple-Cubic Lattice

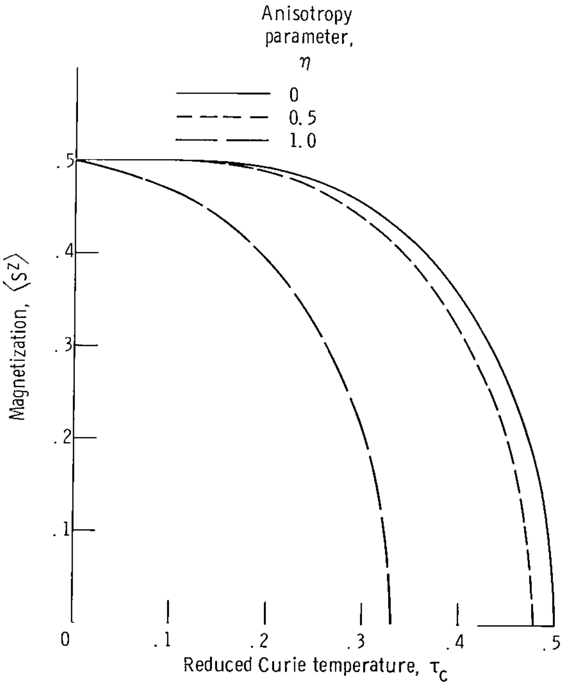
The results for the simple-cubic lattice are obtained in a similar fashion:

$$I_1(\mathrm{sc}) = \frac{3}{\pi^2 Q} \int_0^{\pi} \frac{K(\kappa_2)dx}{3 - \eta \cos(x)} \tag{65}$$



(a) For body-centered-cubic lattice.

(b) For face-centered-cubic lattice.



(c) For simple cubic lattice.

Figure 1. - Magnetization as function of reduced Curie temperature.

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

$$- \frac{3}{2Q}\left(9 - \eta^2\right)^{-1/2} \frac{1 + \eta^2\left(18 + \eta^2\right)\left(9 - \eta^2\right)^{-3/2}}{2} \tag{66}$$

where

$$\kappa_2^2 = \left[\frac{2\eta}{3 - \eta\cos(x)}\right]^2 \tag{67}$$

$$p = \frac{3 - \eta\cos(x)}{3} \tag{68}$$

and

$$\frac{3J(k)}{J(0)} = \left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right] \tag{69}$$

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 (42) for several values of η.

Critical Behavior in Random-Phase Approximation

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 Curie temperature. The Curie temperature decreases smoothly as η increases. Physically, this decrease 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 vanished because of spin waves. These physical (intuitive) arguments are supported by the numerical calculations presented in this report.

The Curie temperature is easily obtained from the derived results. For example, consider the bcc lattice. By substituting equations (56) and (57) into equation (42), one finds

$$2\tau = \left\{\left[\frac{2}{\pi} K(\kappa)\right]^2 + Q \coth(Q) - 1 + \frac{\eta^2 Q^3 \operatorname{csch}^2(Q)\coth(Q)}{8} - \frac{\eta^2}{8}\right\}^{-1} \tag{70}$$

where

$$\tau = \frac{kT}{J(0)}$$

and

$$Q = \frac{\langle S^z \rangle}{\tau}$$

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

$$\lim_{Q \to 0} Q \coth(Q) = 1 \tag{71}$$

$$\lim_{Q \to 0} Q^3 \coth(Q)\operatorname{csch}^2(Q) = 1 \tag{72}$$

and

$$2\tau_c = \left[\frac{2K(\kappa)}{\pi}\right]^{-2} \tag{73}$$

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 the values of the reduced Curie temperature τ_c are given for various values of η for the three cubic lattices. Also shown are results for τ_c calculated from other approximations. The results for $\eta = 1$ agree with the Curie temperature of a Heisenberg ferromagnet calculated in reference 13 which also uses the random-phase approximation.

The preceding calculations were limited to positive values of η. However, for these calculations the thermodynamic quantities are independent of the sign of η. Perhaps, if next nearest neighbors were taken into account, different results would be obtained.

Of particular interest is the behavior of the magnetization as η varies from the Ising to the Heisenberg limit. No singularity or nonconvergence problems arise for $0 \leq \eta \leq 1$ in the analytical expressions derived, which are valid for the total temperature range. Previously, different approximations had to be made for different tempera-

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

Lattice	Anisotropy parameter, η	Brown and Buttinger (ref. 29)	Tahir-Kheli and ter Haar (ref. 13)	Callen (ref. 14)	This report
		Reduced Curie temperature, τ_c			
Body centered cubic	0	0.2987	0.3588	0.4625	0.5000
	.5				.4830
	1.0				.3588
Face centered cubic	0	0.3500	0.3718	0.4666	0.5000
	.5				.4869
	1.0				.3718
Simple cubic	0	0.3166	0.3296	0.4500	0.5000
	.5				.4776
	1.0				.3297

ture regions of interest. In fact, as shown in reference 11 $\eta << 1$ produces series convergence problems.

The data in table I shows that the reduced Curie temperatures in the present calculation are lower than the results Callen (ref. 14) obtained using a symmetric decoupling scheme and are slightly larger than the Brown and Luttinger (ref. 19) results, which are based on extrapolation of the high-temperature series expansion. The low-temperature expansions for spin 1/2 tend to be in agreement with Brown and Luttinger. The Callen case will be discussed in the next section. The anisotropic Heisenberg ferromagnet has been described in references 20 and 21.

At $\eta = 0$, τ_c is given by the Ising model values which, as shown in the figures 1 to 3 and table I, are independent of the lattice structure.

SPONTANEOUS MAGNETIZATION AND CRITICAL BEHAVIOR IN THE SYMMETRIC DECOUPLING APPROXIMATION

For the symmetric or Callen decoupling approximation one finds that

$$E(k) = 2\langle S^z \rangle \left\{ \left[J(0) - \eta J(\vec{k})\right] + \frac{2\alpha}{N} \sum_{k'} \left[\eta J(\vec{k}) - J(\vec{k}' - \vec{k})\right] \varphi_{\vec{k}'} \right\} \tag{74}$$

and

$$J(k) = \sum_{f} J_{gf} \exp\left[-i\vec{k} \cdot (\vec{g} - \vec{f})\right] \tag{75}$$

By use of equations (A30) and (38), an elementary integration yields the following relation for the correlation function:

$$\psi_{k'} = 2\langle S^{z}\rangle \Phi \tag{76}$$

where

$$\Phi = \frac{1}{N} \sum_{k} \frac{1}{\exp\left[\beta E(k)\right] - 1} = \sum_{k} \varphi_{k'} \tag{77}$$

Thus equation (74) can be replaced by

$$E(k) = 2\langle S^{z}\rangle \left\{\left[J(0) - \eta J(\vec{k})\right] + \frac{2\alpha}{N} \sum_{\vec{k}'} \left[\eta J(\vec{k}) - J(\vec{k}' - \vec{k})\right]\varphi_{k'}\right\} \tag{78}$$

For the nearest neighbor approximation and constant J,

$$J(k) = J \sum_{\vec{\delta}} \exp(i\vec{k} \cdot \vec{\delta}) \tag{79}$$

where $\vec{\delta}$ is a nearest neighbor vector. It is shown in appendix E that the term

$$\left[J(\vec{k}') - J(\vec{k}' - \vec{k})\right]\varphi_{k'} \tag{80}$$

which appeared in equation (74), can be replaced by

$$\left[J(0)\right]^{-1}\left\{\left[J(0) - J(\vec{k})\right]\sum_{k'} J(\vec{k}')\varphi_{\vec{k}'}\right\} \tag{81}$$

Hence,

$$E(k) = 2\langle S^{z}\rangle J(0) \frac{1 + 2\alpha\eta f - J(\vec{k})}{J(0)(\eta + 2\alpha f)} \tag{82}$$

where

$$f = \frac{1}{N} \sum_{k'} \frac{J(\vec{k}')}{J(0)} \varphi_{k'} \tag{83}$$

The definition of $E(\vec{k})$ as given by equation (82) together with equation (79) are the basic equations of the theory; $\varphi_{k'}$ is determined by the requirement that these equations be self-consistent.

The calculation of the spontaneous magnetization $\langle S^z \rangle$ for the Callen decoupling follows in the same manner as in the random-phase approximation. The expression for $\langle S^z \rangle$ is given by

$$\left\langle S_g^z \right\rangle = \frac{\frac{1}{2}}{1 + 2\Phi} \tag{84}$$

where from equations (77), (82), and (83), one finds

$$\Phi = \frac{1}{N} \sum \varphi_k = \frac{1}{N} \sum_{\vec{k}} \frac{1}{\exp \beta E(\vec{k}) - 1} = \frac{1}{2N} \sum_{\vec{k}} \coth \frac{\beta E(\vec{k})}{2} - 1 \tag{85}$$

where $E(k)$ is given by equation (82).

Inserting equations (44), (48), and (81) into equations (83) and (85), one obtains

$$\Phi = -\frac{1}{2} + I_3 + I_4 \tag{86}$$

where

$$I_3 = \frac{\tau}{2\pi^3 \langle S^z \rangle A} \int_0^\pi \int_0^\pi \int_0^\pi \frac{dx\, dy\, dz}{1 - G \frac{J(x,y,z)}{J(0)}} \tag{87}$$

$$I_4 = \frac{\tau}{2\pi^3 \langle S^z \rangle A} \sum \left[\int_0^\pi \int_0^\pi \int_0^\pi \frac{dx\, dy\, dz}{1 - G \frac{J(x,y,z)}{J(0)} + i\Gamma(R)} + cc \right] \tag{88}$$

$$I_5 = \frac{\tau}{2\pi^3\langle S^z\rangle AG}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi} dx\,dy\,dz\,\frac{G\,\dfrac{J(x,y,z)}{J(0)}}{1 - G\,\dfrac{J(x,y,z)}{J(0)}} \tag{89}$$

$$I_6 = \frac{\tau}{2\pi^3\langle S^z\rangle A}\sum\left[\int_0^{\pi}\int_0^{\pi}\int_0^{\pi} dx\,dy\,dz\,\frac{\dfrac{J(x,y,z)}{J(0)}}{1 - \dfrac{J(x,y,z)}{J(0)} + i\Gamma(R)} + cc\right] \tag{90}$$

and

$$A = 1 + \alpha(2f\eta) \tag{91}$$

$$B = \eta + \alpha(2f) \tag{92}$$

$$G = \frac{B}{A} \tag{93}$$

where

$$f = I_5 + I_6 \tag{94}$$

From this point on only the bcc lattice will be considered. In appendixes C and D, it is shown that the solution of equations (87) to (94) in the nearest neighbor approximation is

$$I_3 = \frac{\tau}{2\langle S^z\rangle A}\left[\frac{2}{\pi}K(\kappa)\right]^2 \tag{95}$$

$$I_4 = \frac{\tau}{2\langle S^z\rangle A}\left[Q\coth(Q) - 1 + \frac{Q^3G^2}{8}\operatorname{csch}^2 Q\,\frac{\coth(Q) - G^2}{8}\right] \tag{96}$$

$$I_5 = -\frac{1}{2QAG}\left\{1 - \left[\frac{2}{\pi K(\kappa)}\right]^2\right\} \tag{97}$$

$$I_6 = \frac{G}{Q8A}\left[Q^2\operatorname{csch}^2(Q) = \frac{1}{2}\right] \tag{98}$$

where K is a complete elliptic integral and

$$\kappa^2 = \frac{1}{2}\left(1 - \sqrt{1 - G^2}\right) \tag{99}$$

Equations (94) to (99) must now be solved simultaneously for f and E(k). The resulting value of f is then substituted in equations (84) and (86) to yield the magnetization.

Figure 2 shows a plot of $\langle S^z \rangle$ as a function of reduced temperature for several values of η for the bcc lattice using $\alpha = 2\langle S^z \rangle$. For $\eta = 0$, the Callen decoupling approximation gives no solutions for $\alpha \neq 0$. The only solution in this case is for $\alpha \equiv 0$.

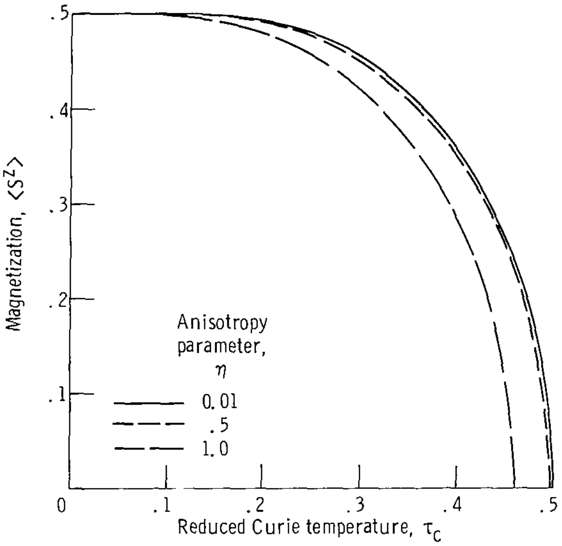


Figure 2. - Magnetization as function of reduced temperature for the body-centered-cubic lattice (Callen approximations). Decoupling parameter, $\alpha = 2\langle S^z \rangle$.

TABLE II. - CURIE TEMPERATURES FOR BODY-CENTERED-CUBIC LATTICE WITH NEAREST NEIGHBOR INTERACTION FOR SPIN 1/2 AND $\alpha = 2\langle S^z \rangle$

Anisotropy parameter, η	Callen	This report
	Curie temperature, τ_c, K	
0.01	Not calculable	0.5
.5	Not calculable	.4970
1.0	0.4625	.4601

In table II, the values of $kT_c/J(0)$ as calculated from equation (86) are listed for several values of η using the Callen parameter $\alpha = 2\langle S^z \rangle$ (but not the Callen method, which yields only the $\eta = 1$ result).

MODIFICATIONS OF CALLEN DECOUPLING PARAMETER

The formalism for the investigation of the anisotropic Heisenberg model has now been developed for an arbitrary α. A choice of the decoupling parameter to be of the form proposed by Copeland and Gersch (ref. 18)

$$\alpha = \left(\langle 2S^z \rangle\right)^p \tag{100}$$

makes it possible to investigate the effect of this parameter on the types of transitions and Curie points for various positive powers p. The case $p = 1$ is just the ordinary Callen decoupling which has already been discussed.

All $p \geq 3$ give a second-order phase transition at the same Curie point. The Curie point value becomes nearly identical to those obtained by the random-phase approximation. Figures 3 and 4, which show the reduced-temperature dependence of the magnetization for the bcc lattice, indicate this effect. In contrast to figure 1 for the random-phase approximation, the low-temperature behaviors are identical.

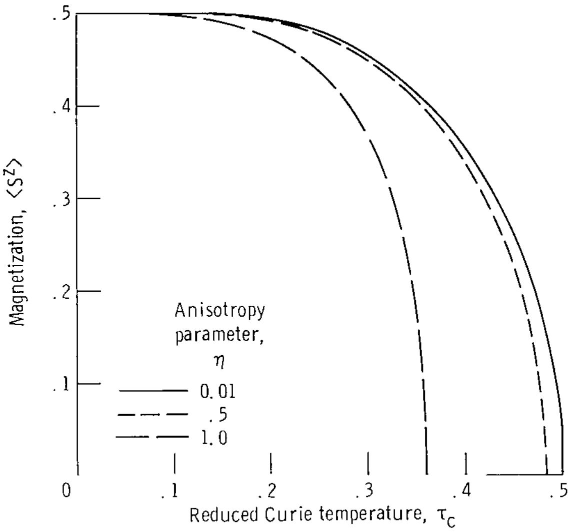


Figure 3. - Magnetization as function of reduced temperature for a body-centered-cubic lattice. Decoupling parameter, $\alpha = (2\langle S^z \rangle)^3$.

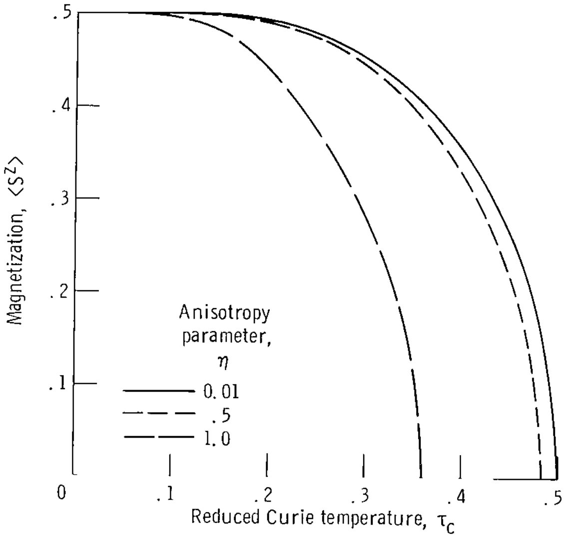


Figure 4. - Magnetization as function of reduced temperature for a body-centered-cubic lattice. Decoupling parameter, $\alpha = (2\langle S^z \rangle)^{10}$.

With α given by equation (100) for $1 < p \leq 3$, one finds a first-order transition for the isotropic Heisenberg ferromagnet ($\eta = 1$) in agreement with the Copeland and Gersch computer solution. However, for the anisotropic case, a first-order transition results for $\eta \geq 0.5$, as evidenced by double valuedness of $\langle S^z \rangle$. In figure 5 the $\eta = 1$ curve shows this first-order transition. This has the consequence that the order of the ferromagnetic transition is not only affected by the decoupling parameters, but also is quite sensitive to the value of η.

In table III the Curie temperature as calculated by equation (84) is listed for several values of η and p. It should be noted that there is no simple Curie temperature that can be obtained from these curves for a first-order phase transition. A transition temperature for the phase transition must be obtained from a Maxwell construction of the free energy for the system. The Curie temperature values in table III for such cases

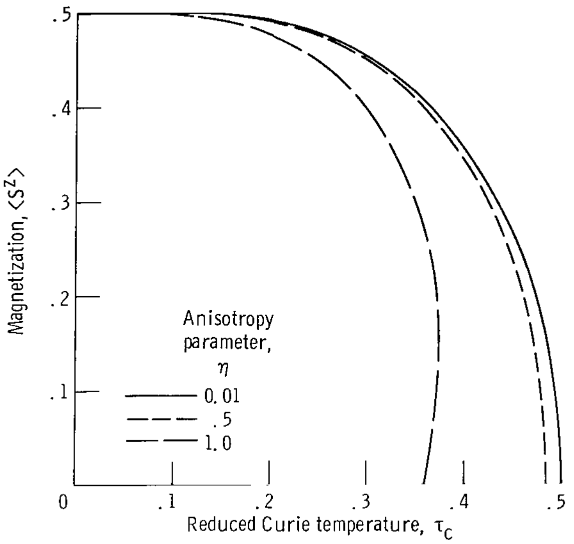


Figure 5. - Magnetization as function of reduced temperature for body-centered-cubic lattice. Decoupling parameter, $\alpha = (2\,S^z\,)^2$.

TABLE III. - REDUCED CURIE TEMPERATURE CALCULATED USING $\alpha = (2\langle S^2 \rangle)^p$ FOR BODY-CENTERED-CUBIC LATTICE AND NEAREST NEIGHBOR INTERACTIONS

Exponent in decoupling equation, p	Anisotropy parameter, η	Data from ref. 7	Data from this study	Type of phase transition
		Curie temperature, T_C, K		
2	0.01	(a)	0.5000	2
	.5	(a)	.4831	2
	1.0	(a)	.3597	1
3	0.01	(a)	0.5000	2
	.5	(a)	.4830	2
	1.0	0.3625	.3589	2
10	0.01	(a)	0.5000	2
	.5	(a)	.4830	2
	1.0	0.3625	.3589	2

[a] Not calculated.

are the intercepts of the $\langle S^z \rangle$ curve on the temperature axis.

The formalism has been developed up to this point for an arbitrary functional form for α. There is no unique way to determine α within the Green's function formalism, and thus one must rely on experimental observations for this information.

Structural characteristics of the material have strong effects on the nature of the ferromagnetic transition. Inhomogeneity of the concentration, that is, nonuniform distribution, of impurities may lead to the appearance of a tail on the curve of the spontaneous magnetization. The ferromagnetic transition can occur, therefore, not at a single temperature but over a range of temperatures. Thus, the transition is smeared out. One possible reason for this tail is that the inhomogeneity of the concentration leads to regions in the material which have different Curie temperatures. In those regions of the specimen having a higher Curie temperature, the spontaneous magnetization is still retained when a part of the ferromagnetic material has gone over into the paramagnetic phase (ref. 22). It is suggested, therefore, that the anisotropy parameter can, in effect, serve as a measure of inhomogeneity.

In the section MODIFICATIONS OF THE DECOUPLING PARAMETERS a model was developed that had the form

$$\alpha = \left(2\langle S^z \rangle\right)^p + \left(2\langle S^z \rangle\right)^p \log\left(2\langle S^z \rangle\right)^p \tag{101}$$

If equation (101) is used in conjunction with equation (74), one finds the following results:

For $p = 1$ (fig. 6), a washed-out transition is obtained.

For $p = 2$ (fig. 7) the isotropic Heisenberg model ($\eta = 1.0$) gives a first-order transition; whereas, for small η one obtains a second-order transition. This corresponds closely to the $p = 2$ case for the Callen exponential decoupling.

For $p = 3$ an important effect comes into play. Previously the exponential Callen decoupling parameter (eq. (100)) gave only a second-order phase transition for $\eta \geq 0$, as well as the same Curie temperature independent of the p. For the present decoupling approximation, the order of the phase transition depends on p. For $p = 3$ (fig. 8) the isotropic Heisenberg model ($\eta = 1.0$) produces a first-order transition; whereas for small η a second-order transition results. However, for $p = 10$ (fig. 9) only a second-order transition is present. For $\eta = 0$ there is no change in the Ising model value for the Curie temperature. Figures 8 and 9 illustrate that various transitions occur when the decoupling scheme (eq. (101)) is used.

Table IV gives the reduced Curie temperatures for this decoupling parameter for the bcc lattice. The W means that a washed-out transition occurs. Experimentally, it is difficult to distinguish between a higher order and a truly washed-out transition.

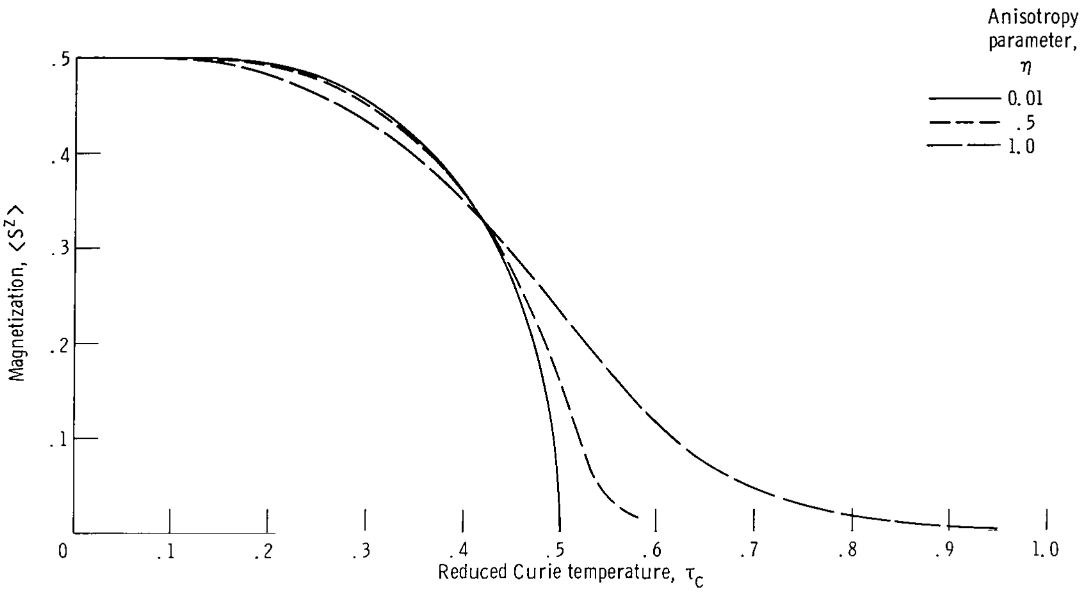


Figure 6. - Magnetization as function of reduced temperature for body-centered-cubic lattice. Decoupling parameter, $\alpha = 2\langle S^z\rangle - 2\langle S^z\rangle \ln(2\langle S^z\rangle)$.

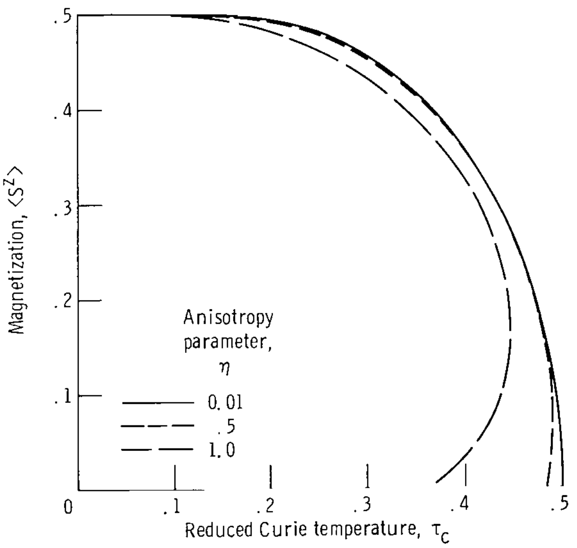


Figure 7. - Magnetization as function of reduced temperature for body-centered-cubic lattice. Decoupling parameter, $\alpha = (2\langle S^z\rangle)^2 - (2\langle S^z\rangle)^2 \ln(2\langle S^z\rangle)^2$.

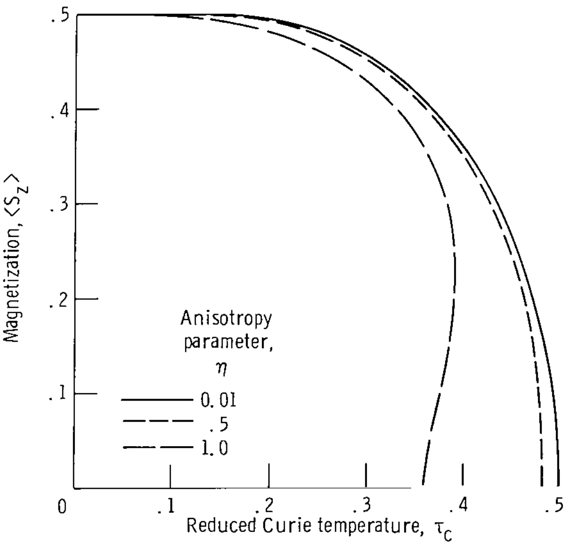


Figure 8. - Magnetization as function of reduced temperature for body-centered-cubic lattice. Decoupling parameter, $\alpha = (2\langle S^z\rangle)^3 - (2\langle S^z\rangle)^3 \ln(2\langle S^z\rangle)^3$.

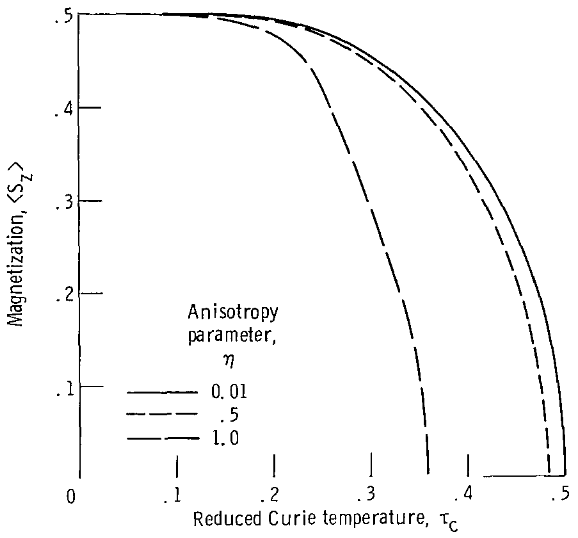


Figure 9. - Magnetization as function of reduced temperature for body-centered-cubic lattice. Decoupling parameter, $\alpha = (2\langle S^z \rangle)^{10} - (2\langle S^z \rangle)^{10} \ln(2\langle S^z \rangle)^{10}$.

TABLE IV. - REDUCED CURIE TEMPERATURE CALCULATED $\alpha = (2\langle S^z \rangle)^p - (2\langle S^z \rangle)^p \log(2\langle S^z \rangle)^p$ FOR BODY-CENTERED-CUBIC LATTICE AND THE NEAREST NEIGHBOR INTERACTIONS

Exponent in decoupling equation, p	Anisotropy parameter, η	Reduced Curie temperature, τ_c, K	Order of phase transition
1	0.01	0.5000	2
	.5	------	W[a]
	1.0	------	W
2	0.01	0.5000	2
	.5	.4841	2
	1.0	.3650	1
3	0.01	0.5000	2
	.5	.4830	2
	1.0	.3500	1
10	0.01	0.5000	2
	.5	.4830	2
	1.0	.3590	2

[a] Washed-out transition.

CONCLUSIONS

From the results obtained by the use of Green's functions and various decoupling schemes, certain conclusions can be stated:

1. A single analytical expression for magnetization, which is valid for all temperatures, was obtained. The demonstrated technique of evaluating certain Watson sums and integrals was employed without requiring various series approximations or extensive computer summations. Other thermodynamic quantities, such as specific heat, can be calculated from the magnetization.

2. The random-phase approximation predicts that the spontaneous magnetization shows a second-order phase transition at Curie temperature (a discontinuity in the slope of the magnetization and in the second derivative of the free energy) independent of the anisotropy. The effect of the anisotropy parameter is to shift the critical (Curie) temperature. The curie temperature decreases monotonically as the anisotropy parameter increases.

3. The Callen approximation for spontaneous magnetization produces self-consistent field equations that predict a second-order phase transition. The anisotropy parameter shifts the Curie temperature. The values of the reduced Curie temperature are higher than those obtained by the random phase approximation.

4. The exponential decoupling parameter for $1 < p < 3$ predicts, by the use of self-consistent field equations, a first-order transition for large values of anisotropy parameter η and a second-order phase transition for small values. The type of phase transition is sensitive to the value of the anisotropy parameter. For $p \geq 3$ (where p is any power), a second-order transition is obtained whose reduced Curie temperature is in close agreement with the random-phase approximation. The low-temperature dependence of magnetization is not the same as that predicted by the random-phase approximation.

5. The logarithmic decoupling parameter shows what type of transition is sensitive to the value of anisotropy parameter. For example, for $p = 10$ a washed-out transition is obtained. But for $p = 3$ the Heisenberg model gives a first-order transition for large values of η and a second-order transition for small values. In contrast, $p = 2$ shows the reverse situation. For $p = 1$ and $n = 1$, a washed-out transition is obtained. For $\eta < 1$, the behavior is that of either a washed-out or higher order phase transition.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, June 30, 1970,
129-02.

APPENDIX A

REVIEW OF GREEN'S FUNCTION

The Green's function method allows one to focus attention on the quantity of interest and to determine from the complete Hamiltonian the exact coupled equations of motion for the associated Green's function. In order to solve these equations they must be truncated or uncoupled by a suitable decoupling approximation. Although the usual decoupling approximations are not now well understood, this method is a convenient technique for the calculation of various thermodynamic quantities as a function of temperature.

In this review, the properties of the temperature-dependent double-time Green's function are studied in relation to the work presented in this report. More standard treatments of the problems may be found in general review articles and books, such as those by Zubarev (ref. 4), Bonch-Bruevich and Tyablikov (ref. 23), Kadanoff and Baym (ref. 24), and Perry and Turner (ref. 25).

Causal Retarded and Advanced Green's Function

For a system with a time independent Hamiltonian H, the causal retarded and advanced Green's function for a pair of operators A and B are defined as follows:

$$G_C(t, t') = \langle\langle A(t) ; B(t')\rangle\rangle = -i\langle TA(t)B(t')\rangle \tag{A1}$$

$$G_R(t, t') = \langle\langle A(t) ; B(t')\rangle\rangle = i\theta(t - t')\Big\langle [A(t), B(t')]\Big\rangle \tag{A2}$$

$$G_A(t, t') = \langle\langle A(t) ; B(t')\rangle\rangle = i\theta(t' - t)\Big\langle [A(t), B(t')]\Big\rangle \tag{A3}$$

where A(t) is the Heisenberg representation for the operator A,

$$A(t) = \exp(\lambda Ht)A \exp(-\lambda Ht) \tag{A4}$$

and T is the time ordering operator of Dyson, which is defined in the usual way so that

$$TA(t)B(t') = \theta(t)A(t)B(t') + \theta(-t)B(t')A(t) \tag{A5}$$

with $\theta(t)$ as the step function,

$$\theta(t) = \begin{Bmatrix} 1, & t > 0 \\ & \\ 0, & t < 0 \end{Bmatrix} \tag{A6}$$

$$[A, B] = AB - \sigma BA: \qquad \sigma = \begin{matrix} +1 \\ \\ -1 \end{matrix} \tag{A7}$$

Note that A and B are not restricted to be either Bose or Fermi operators and that the choice of σ is arbitrary. For the case of Bose operators that are used herein, $\sigma = 1$ and the singular angular bracket denotes the average with respect to the canonical density matrix of the system

$$\langle O \rangle = \mathrm{Tr}\,\zeta O \tag{A8}$$

where

$$\zeta = \frac{\exp(-\beta H)}{\mathrm{Tr}\,\exp(-\beta H)} \tag{A9}$$

and

$$\beta = \frac{1}{kT} \tag{A10}$$

Using the equation of motion

$$\frac{idA}{dt} = [A, H] = AH - HA \tag{A11}$$

and the property of the step function

$$\frac{d\theta(t)}{dt} = \frac{d}{dt}\left[\int_{-\infty}^{t} \delta(t')dt'\right] = \delta(t) \tag{A12}$$

results in

$$\frac{id}{dt} G_R(t, t') = \delta(t - t')\langle [A(t), B(t')] \rangle + \langle\langle [A(t), H(t)]; B(t') \rangle\rangle \tag{A13}$$

and similarly for the causal and advanced Green's function. Note that the Green's function on the right side of the equation can be of higher order than on the left. Writing down the equations of motion for the higher order functions, a set of coupled equations for the complete hierarchy of Green's function can be obtained. It is easily shown that the Green's function $G(t, t')$ can be written in the form $G(t - t')$, and thus depends only on the time difference.

The time correlation function plays an important role in statistical mechanics and is usually the quantity of direct physical interest. It is written as

$$\left.\begin{aligned} F_{AB}(t, t') &= \langle A(t)B(t')\rangle \\ F_{BA}(t, t') &= \langle B(t')A(t)\rangle \end{aligned}\right\} \tag{A14}$$

which can be calculated from equations (15), (16), and the cyclic property of the trace.

SPECTRAL REPRESENTATION

To obtain the spectral representation of the time correlation functions the eigenfunction m and eigenvalues E_m of the Hamiltonian must be considered. Thus

$$H|m\rangle = E_m|m\rangle \tag{A15}$$

From equation (A14), the correlation function can be written

$$\begin{aligned} F_{BA}(t't) &= \langle B(t')A(t)\rangle \\ &= \frac{\mathrm{Tr}\left[\exp(-\beta H)\exp(-iHt')B\,\exp(iHt)A\right]}{\mathrm{Tr}\,\exp(-\beta H)} \\ &= Z^{-1}\sum_{m,n}\langle m|B|n\rangle\langle n|A|m\rangle\exp(-E_m\beta)\exp - \left[i(E_m - E_n)(t' - t)\right] \end{aligned} \tag{A17}$$

with

$$Z = \sum_m \exp(-\beta E_m) \tag{A17}$$

the partition function for the canonical ensemble. Equation (23) can be rewritten in the following manner:

$$\langle B(t')A(t)\rangle = \int_{-\infty}^{\infty} J(\omega)\exp[-i\omega(t - t')]d\omega \tag{A18}$$

where

$$J(\omega) = Z^{-1} \sum_{m,n} \langle m|A|n\rangle\langle n|B|m\rangle \exp(-\beta E_m)\delta(E_n - E_m - \omega) \tag{A19}$$

In a similar manner

$$\langle A(t)B(t')\rangle = \int_{-\infty}^{\infty} J(\omega)\exp(\omega B)\exp[-i\omega(t - t')]d\omega \tag{A20}$$

Equations (A18) and (A20) are the spectral representation for the time correlation function, and $J(\omega)$ is the spectral density.

The rest of the discussion will be limited to the retarded Green's function, thus the subscript R will be omitted. The Fourier transform of $G(t - t')$ is

$$G(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} G(t - t')\exp(iEt)dt \tag{A21}$$

Using equations (A2) and (A20) and integrating equation (A21) yields

$$G(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} [\exp(\omega\beta) - \sigma] \frac{J(\omega)d\omega}{(E - \omega + i\epsilon)} \tag{A22}$$

where $E \to 0^+$.

Using the symbolic identity

$$\frac{1}{(\omega - \omega' \pm i\epsilon)} = P\left[\frac{1}{(\omega - \omega') \pm i\pi\delta(\omega - \omega')}\right] \tag{A23}$$

where $E \to 0$ and P denotes Cauch's principal value of the integral, equation (A20) can be written alternatively as

$$G(E) = \left(\frac{1}{2\pi}\right) P \int_{-\infty}^{\infty} [\exp(\beta\omega) - \sigma]J(\omega) \frac{d\omega}{E - \omega} - \frac{1}{2} [\exp(\beta E) - \sigma]J(E) \tag{A24}$$

It follows from equation (A23) that

$$\operatorname{Re} G(E) = \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{\operatorname{Im} G(\omega)}{\omega - E}\, d\omega \tag{A25}$$

If the function G(E) is known so the spectral intensity $J(\omega)$ of equation (A20) can be found by taking the difference of the two expressions of equation (A22), then

$$G(\omega + i\epsilon) - G(\omega - i\epsilon) = \frac{1}{2} \int_{-\infty}^{\infty} [\exp(\beta E) - \sigma] J(E) \left[\frac{1}{(\omega - E + i\epsilon)} - \frac{1}{(\omega - E - i\epsilon)} \right] dE \tag{A26}$$

If the δ function representation

$$\delta(x) = \underset{\substack{\lim \\ \epsilon \to 0}}{\frac{1}{(2\pi i)}} \left[\frac{1}{(x - i\epsilon)} - \frac{1}{(x + i\epsilon)} \right] \tag{A27}$$

is used, then

$$G(\omega + i\epsilon) - G(\omega - i\epsilon) = -i[\exp(\omega\beta) - \sigma] J(\omega) \tag{A28}$$

The equation of motion for the Green's function can be obtained by the Fourier transform of equation (20) as

$$E\langle\langle A\, ;\, B\rangle\rangle = \frac{1}{2\pi} \langle [A\, ,\, B] \rangle + \langle\langle [A\, ,\, H]\, ;\, B \rangle\rangle \tag{A29}$$

Except for the simplest cases, an infinite number of coupled equations are necessary to solve for the correlation function $\langle B A \rangle$. Thus, these equations must be reduced to a finite number by applying an appropriate decoupling scheme.

The time correlation function is found from

$$\langle B(t')A(t) \rangle = \lim_{\epsilon \to 0} i \int_{-\infty}^{\infty} G(\omega + \epsilon) - G(\omega - \epsilon) \exp \frac{[i\omega(t - t')] d\omega}{\exp(\beta\omega) - \sigma} \tag{A30}$$

APPENDIX B

FOURIER TRANSFORM OF THE GREEN'S FUNCTION

Consider the equation of motion for the Green's function A_{gm} (eq. (27)), which has the form

$$EA_{gm} = \langle S^z\rangle \frac{\delta_{gm}}{\pi} + 2\langle S^z\rangle \sum_{f} J_{gf}(A_{gm} - \eta A_{fm}) + 2\alpha \sum_{f} J_{gf}(\eta\psi_{gf}A_{gm} - \psi_{fg}A_{fm}) \qquad \text{(B1)}$$

Defining the Fourier transforms of the Green's function by

$$A_{gm} = \frac{1}{N} \sum_{k} \exp\left[i\vec{k}\cdot(\vec{g} - \vec{m})\right]A_{\vec{k}} \qquad \text{(B2)}$$

and of the correlation function by

$$\psi_{gf} = \frac{1}{N} \sum_{\vec{k}} \exp\left[-i\vec{k}\cdot(\vec{g} - \vec{m})\right]\psi_{k} \qquad \text{(B3)}$$

one obtains from equation (A1)

$$\frac{E}{N} \sum_{\vec{k}} \exp\left[i\vec{k}\cdot(\vec{g} - \vec{m})\right]A_{\vec{k}} = \langle S^z\rangle \frac{\delta_{gm}}{\pi}$$

$$+ \frac{2\langle S^z\rangle}{N} \sum_{f} \sum_{\vec{k}} J_{gf}\left\{\exp\left[i\vec{k}\cdot(\vec{g} - \vec{m})\right]A_{k} - \eta \exp\left[i\vec{k}\cdot(\vec{f} - \vec{m})\right]A_{k}\right\}$$

$$+ \frac{2\alpha}{N^2} \sum_{f} \sum_{\vec{k}} \sum_{\vec{k}'} \left\{\eta \exp\left[i\vec{k}\cdot(\vec{g} - \vec{m})\right]\exp -\vec{k}'\cdot(\vec{g} - \vec{m})\right]A_{k}\right.$$

$$\left. - \exp\left[-i\vec{k}'\cdot(\vec{f} - \vec{g})\right]\exp\left[i\vec{k}\cdot(\vec{f} - \vec{m})\right]\psi_{\vec{k}'}A_{\vec{k}}\right\} \qquad \text{(B4)}$$

If equation (B4) is multiplied by

$$\sum_{g} \exp\left[-i\vec{k}'' \cdot (\vec{g} - \vec{m})\right] \tag{B5}$$

and if the following relations are used

$$\frac{1}{N} \sum_{\vec{k}} \sum_{\vec{g}} \exp\left[i(\vec{k} - \vec{k}') \cdot (\vec{g} - \vec{m})\right] A_{\vec{k}} = \sum_{\vec{k}} \delta_{\vec{k}\vec{k}''} A_{\vec{k}} = A_{\vec{k}''} \tag{B6}$$

$$\sum_{g} \delta_{gm} \exp\left[-i\vec{k}'' \cdot (\vec{g} - \vec{m})\right] = 1 \tag{B7}$$

$$\frac{1}{N} \sum_{f} \sum_{k} \sum_{g} J_{gf} \exp\left[i\vec{k} \cdot (\vec{g} - \vec{m})\right] \exp\left[-i\vec{k}'' \cdot (\vec{g} - \vec{m})\right] A_{\vec{k}} = \sum_{f} J_{gf} A_{\vec{k}''} = A_{\vec{k}''} J(0) \tag{B8}$$

$$\frac{1}{N} \sum_{f} \sum_{k} \sum_{g} J_{gf} \exp\left[ik(\vec{f} - \vec{m})\right] \exp\left[-i\vec{k}''(\vec{g} - \vec{m})\right] A_{\vec{k}} = \sum_{f} J_{gf} \exp\left[i\vec{k}(\vec{g} - \vec{f})\right] A_{\vec{k}''} = J(\vec{k}'') A_{\vec{k}''} \tag{B9}$$

$$\begin{aligned} &\frac{1}{N^2} \sum_{f} \sum_{k} \sum_{k'} \sum_{g} \exp\left[i\vec{k} \cdot (\vec{g} - \vec{m})\right] \exp\left[i\vec{k}' \cdot (\vec{g} - \vec{f})\right] \exp\left[-i\vec{k}'' \cdot (g - \vec{m})\right] A_{k} \psi_{k'} \\ &\qquad = \frac{1}{N} \sum_{f} \sum_{k} \sum_{k'} \exp\left[-ik' \cdot (\vec{g} - \vec{f})\right] A_{\vec{k}} \psi_{\vec{k}'} \delta_{\vec{k}\vec{k}''} \\ &\qquad = \frac{1}{N} \sum_{k'} J(\vec{k}') \psi_{\vec{k}'} A_{\vec{k}''} \end{aligned} \tag{B10}$$

$$\frac{1}{N^2}\sum_{f}\sum_{k}\sum_{k'}\sum_{g} J_{gf} \exp\left[i\vec{k}\cdot(\vec{f} - \vec{m})\right]\exp\left[-i\vec{k}'\cdot(\vec{f} - \vec{g})\right] \exp\left[-i\vec{k}''\cdot(\vec{g} - \vec{m})\right]A_{\vec{k}}\psi_{\vec{k}'}$$

$$= \frac{1}{N}\sum_{\vec{k}'} J(\vec{k}'' - \vec{k}')\psi_{\vec{k}}A_{\vec{k}'} \qquad \text{(B11)}$$

then

$$EA_{\vec{k}} = \frac{\langle S^z\rangle}{\pi} + 2\langle S^z\rangle A_{\vec{k}}\left[J(0) - \eta J(\vec{k})\right] + \frac{2\alpha}{N} A_{\vec{k}}\sum_{\vec{k}'} \eta\left[J(\vec{k}) - J(\vec{k} - \vec{k}'')\right]\psi_{\vec{k}} \qquad \text{(B12)}$$

is obtained by substituting into equation (B1). Finally, collecting terms of $A_{\vec{k}}$ gives equation (30).

APPENDIX C

EVALUATION OF INTEGRALS I_1

Body-Centered-Cubic Lattice

It follows from equation (54) that the integral I_1(bcc) is written as

$$I_1(\text{bcc}) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi dx\,dy\,dz\Big[(1 - \eta)\cos(x)\cos(y)\cos(z)\Big]^{1/2} \tag{C1}$$

Performing the integration on x results in

$$I_1(\text{bcc}) = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi dy\,dx\Big[(1 - \eta^2)\cos^2(y)\cos^2(z)\Big]^{1/2} \tag{C2}$$

The integrand is expanded in ascending powers of $\cos^2(y)\cos^2(z)$ and then integrated term by term to obtain

$$I_1(\text{bcc}) = \frac{1}{\pi^2}\sum_{n=}^{\infty}\int_0^\pi\int_0^\pi \eta^2 \cos^{2n}(x)\cos^{2n}(y)dy\,dz$$

$$= \sum_{n=}^{\infty} a_n^3\eta^{2n} \tag{C3}$$

where

$$a_n = \frac{1\cdot 3\cdot 5\ .\ .\ .\ (2n - 1)}{2\cdot 4\cdot 6\ .\ .\ .\ 2n} \tag{C4}$$

where $a_0 = 1$.

Watson (ref. 26) has shown that the square of the complete elliptic integral of the first kind can be written as

$$K^2(k) = \frac{1}{4}\pi^2\sum_{m=}^{\infty} a_n^3(2kk')^{2n} \tag{C5}$$

where

$$k' = \left(1 - k^2\right)^{1/2} \tag{C6}$$

Equating equations (C5) and (C3), thus,

$$\eta^{2n} = (2kk')^{2n} \tag{C7}$$

it is easily shown that

$$k^2 = \frac{1}{2}\left[1 - \left(1 - \eta^2\right)^{1/2}\right] \tag{C8}$$

This gives

$$I_1(\mathrm{bcc}) = \left[\frac{2K(k)}{\pi}\right]^2 \tag{C9}$$

in agreement with equation (56).

Face-Centered-Cubic Lattice

The fcc case can be investigated by the triple integral

$$I_1(\mathrm{fcc}) = \left(\frac{1}{\pi}\right)^3 \int_0^{\pi}\int_0^{\pi}\int_0^{\pi} 1 - \frac{\eta}{3}\left[\cos(x)\cos(y) + \cos(y)\cos(z) + \cos(z)\cos(x)\right]^{-1} dx\, dy\, dz \tag{C10}$$

On integrating with respect to x the result is

$$I_1(\mathrm{fcc}) = \frac{1}{\pi^2\eta}\int_0^{\pi}\int_0^{\pi}\left(a_0 + a_1 \cos y + a_5 \sin^2 y\right)^{-1/2} dy\, dz \tag{C11}$$

where

$$\left.\begin{aligned} a_o &= \left(\frac{3}{\eta}\right)^2 - 1 \\ a_I &= \frac{-2(1 + 3)}{\eta}\cos(z) \\ a_5 &= \sin^2(z) \end{aligned}\right\} \tag{C12}$$

Let

$$t = \tan\left(\frac{y}{2}\right) \tag{C13}$$

Then,

$$2\ dt = \sec^2\left(\frac{y}{2}\right)dy = (1 + t^2)dy \tag{C14}$$

$$\cos(y) = \frac{1 - \tan^2\left(\frac{y}{2}\right)}{1 + \tan^2\left(\frac{y}{2}\right)} = \frac{1 - t^2}{1 + t^2} \tag{C15}$$

$$\sin(y) = 2\ \tan\left(\frac{y}{2}\right)\ 1 + \tan^2\left(\frac{y}{2}\right) = \frac{2t}{1 + t^2} \tag{C16}$$

If these relations are substituted into equation (C11), then

$$I_1(fcc) = 2\left[(\pi^2\eta)\right] \int_0^{\pi}\int_0^{\infty} \left(b_o\right)^{-1/2}\left(A + Bt^2 + t^4\right)^{-1/2}\ dt\ dz \tag{C17}$$

where

$$b_o = (a_o - a_1) \tag{C18}$$

$$A = \frac{a_o + a_1}{b_o} \tag{C19}$$

and

$$B = \frac{2(a_o + 2a_5)}{b_o} \tag{C20}$$

If

$$\zeta_+^2 = B\ 2 + \sqrt{\frac{B^2 - 4A}{2}} \tag{C21}$$

$$\zeta_-^2 = B\ 2 - \sqrt{\frac{B^2 - 4A}{2}} \tag{C22}$$

then

$$I_1(fcc) = \left[2(\pi^2\eta)\right] \int_0^{\pi} \int_0^{\infty} \left(b_o\right)^{-1/2} \left[\left(t^2 + \zeta_+^2\right)\left(t^2 + \zeta_-^2\right)\right]^{-1/2} dt\ dz \tag{C23}$$

Once the radical has been expressed in this factored form as the product of sums or differences of squares, the integral can be reduced to Jacobian or elliptical form. The integral of (C23) is finite everywhere and leads to the integral of the first kind. Thus, from elementary tables

$$I_1(fcc) = \frac{2}{\pi^2\eta} \int_0^{\pi} \left(b_o\right)^{-1/2} \left(\zeta_+\right)^{-1} K(k_1) dz \tag{C24}$$

where

$$k_1^2 = \frac{\left(\zeta_+^2 - \zeta_-^2\right)}{\zeta_+^2} = \frac{4\eta\left[3 + \eta \cos^2(z)\right]}{(3 + \eta)^2} \tag{C25}$$

Some algebraic manipulation gives

$$I_1(fcc) = \frac{6}{\pi^2} \int_0^{\pi} \frac{K(k_1)}{3 + \eta} dz \tag{C26}$$

which is the same as equation (60).

Simple-Cubic Lattice

The integral for the sc lattice in three dimensions can be written as

$$I_1(sc) = \frac{1}{\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi} dx\,dy\,dz\left\{1 - \frac{\eta}{3}\left[\cos(x) + \cos(y) + \cos(z)\right]\right\}^{-1} \tag{C27}$$

The same procedure that was outlined in the previous section gives for the fcc case:

$$I_1(sc) = \frac{6}{\pi^2}\int_0^{\pi} \zeta\left[3 - \eta\cos(z)\right]K(k_2)dz \tag{C28}$$

where

$$k_2^2 = \left[\frac{2\eta}{3 - \eta\cos(z)}\right]^2 \tag{C29}$$

which is of the same form as in equation (65).

APPENDIX D

SUMMATION AND THE LAPLACE TRANSFORM

The calculation of the integral I_2 involves the summation of an infinite series. A direct approach to the problem of the summation of infinite series has been given by several authors (refs. 27 and 28). Some of these techniques will be used and extended to evaluate I_2.

As an example of the technique used, consider the fcc lattice. (The calculation for the other two cubic lattices follow in the same manner): the fcc lattice integral is written as

$$I_2(\mathrm{fcc}) = \frac{3}{\pi^3 Q} \sum_{R=1}^{\infty} \int_0^{\pi}\int_0^{\pi}\int_0^{\pi} dx\, dy\, dz \frac{\dfrac{1 - \eta J(x, y, z)}{J(0)}}{\left[\dfrac{1 - \eta J(k)}{J(0)}\right]^2} \tag{D1}$$

where

$$\frac{3J(x, y, z)}{J(0)} = \cos(x)\cos(y) + \cos(y)\cos(z) + \cos(z)\cos(x) \tag{D2}$$

The triple integration and the summation exist and are real. However, they can be written as the difference of two complex integrals as was done in equation (52). Integrating on x and y (appendix D) gives

$$I_2(\mathrm{fcc}) = \frac{3}{2\pi^2 Q} \sum_{R=1} \int_0^{\pi} \left[K\left(k_1'\right) \frac{dz}{3 + \eta + 3i\Gamma(R)} + cc\right] \tag{D3}$$

where

$$k_1'^2 = \frac{4\eta\left[3 + \eta \cos^2(z) + 3i\Gamma(R)\right]}{\left[3 + \eta + 3i\Gamma(R)\right]^2} \tag{D4}$$

$$Q = \frac{S^z}{\tau} \tag{D5}$$

$$\Gamma(R) = \frac{R\pi}{Q} \tag{D6}$$

and cc indicates the complex conjugate.

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

$$K(k) = \frac{\pi}{2} \sum_{n} a_n^2 k^{2n} \qquad |k| < 1 \tag{D7}$$

where

$$a_n = \frac{1 \cdot 3 \cdot 5 \;.\;.\;.\; (2n - 1)}{2 \cdot 4 \cdot 6 \;.\;.\;.\; 2n} \qquad a_o = 1 \tag{D8}$$

Only the first two terms of the series in equation (D7) are necessary for four place accuracy. There is no difficulty in extending it to as many terms as needed.

Taking the first two terms in equation (D3) and integrating the complex function with respect to z, the terms can be rearranged to show that

$$I_2(fcc) = I_2^a + I_2^b + I_2^c \tag{D9}$$

where

$$I_2^a = (1\pi) \sum_{R=1}^{\infty} \frac{y}{y^2 + R^2} \tag{D10}$$

$$I_2^b = \frac{\eta}{\pi G} \sum_{R=1}^{\infty} \left[\frac{1}{y^2 + R^2} - \frac{2R^2}{\left(y^2 + R^2\right)^2} \right] \tag{D11}$$

$$I_2^c = \frac{\eta^2 y}{2\pi G^2} \sum_{R=1}^{\infty} \left[\frac{1}{\left(y^2 + R^2\right)^2} - \frac{4R^2}{\left(y^2 + R^2\right)^3} \right] \tag{D12}$$

$$G = \frac{3\pi}{Q} \qquad y = \frac{3 + \eta}{G} \tag{D13}$$

The following Laplace transforms are used

$$\frac{1}{y^2 + R^2} = \mathscr{L}\frac{1}{y}\sin(yt) \tag{D14}$$

$$\frac{R^2}{\left(y^2 + R^2\right)^2} = \mathscr{L}\left\{\frac{1}{2y}\left[\sin(yt) + yt\cos(yt)\right]\right\} \tag{D15}$$

$$\frac{R^2}{\left(y^2 + R^2\right)^3} = \mathscr{L}\left\{\frac{1}{8y^3}\left[(1 + y^2t^2)\sin(yt) - yt\cos(yt)\right]\right\} \tag{D16}$$

Equation (D14) can be written as

$$\frac{1}{y^2 + R^2} = \frac{1}{y}\int_0^\infty \sin(yt)\left[\exp(-tR)\right]dt \tag{D17}$$

and similarly for the other terms.

The summation then becomes

$$\sum_{R=1} \frac{1}{y^2 + R^2} = \frac{1}{y}\int_0^\infty \sin(yt)\frac{dt}{\exp(t) - 1} = \frac{1}{2}\frac{\pi}{y}\coth(y\pi) - \frac{1}{2y} \tag{D18}$$

Using the general form of integration such that

$$\int_0^{t^{2m}} \sin(yt)\frac{dt}{\exp(t) - 1} = (-1)^m \frac{\partial^{2m}}{\partial y^{2m}}\frac{\pi}{2}\coth(y\pi) - \frac{1}{2y} \tag{D19}$$

$$\int_0^{t^{2m+1}} \cos(yt)\frac{dt}{\exp(t) - 1} = (-1)^m \frac{\partial^{2m+1}}{\partial y^{2m+1}}\frac{\frac{\pi}{2}\coth(y\pi) - 1}{2y} \tag{D20}$$

results in a closed form solution as was done in SPONTANEOUS MAGNETIZATION AND CRITICAL BEHAVIOR: RANDOM-PHASE APPROXIMATION.

APPENDIX E

NEAREST NEIGHBOR INTERACTIONS

Consider the sum

$$K' = \sum_{\vec{k}'} \left[J(\vec{k}') - J(\vec{k}' - \vec{k})\right]\varphi_{\vec{k}'} \tag{E1}$$

which appears in equation (78). For lattice with cubic symmetry and with nearest neighbor interactions,

$$J_{ij} = J$$

if i and j are nearest neighbors, and

$$J_{ij} = 0$$

otherwise. Thus

$$J(\vec{k}) = J \sum_{\vec{\delta}} \exp(i\vec{k} \cdot \vec{\delta}) \tag{E2}$$

can be written where $\vec{\delta}$ is a nearest neighbor vector. Then equation (E1) can be written as

$$K' = J\sum_{\vec{\delta}} \left[1 - \exp(-i\vec{k} \cdot \vec{\delta})\right] \sum_{\vec{k}'} \exp(i\vec{k}' \cdot \vec{\delta})\varphi_{\vec{k}} \tag{E3}$$

By symmetry, the sum over $\vec{k}'$ is clearly independent of δ, so that it can be replaced by

$$(1z) \sum_{\vec{\delta}'} \exp(i\vec{k} \cdot \vec{\delta}') \tag{E4}$$

where z is the number of nearest neighbors. Hence, equation (E3) yields

$$K' = \frac{J}{Z} \sum_{\vec{\delta}} \left[1 - \exp(-i\vec{k} \cdot \vec{\delta})\right] \sum_{\vec{\delta}'} \sum_{\vec{k}'} \exp(i\vec{k}' \cdot \vec{\delta}')\varphi_{\vec{k}'}$$

$$= J \sum_{\delta} \left[1 - \exp(-i\vec{k} \cdot \vec{\delta})\right] \sum_{k'} \frac{J(\vec{k}')}{Jz\varphi_{\vec{k}'}}$$

$$= \frac{1}{J(0)} \left[J(0) - J(\vec{k})\right] \sum_{\vec{k}'} J(\vec{k}')\varphi_{\vec{k}'} \qquad \text{(E5)}$$

since for cubic lattices

$$J(\vec{k}) = J(-\vec{k}) \qquad \text{(E6)}$$

and

$$J(0) = Jz \qquad \text{(E7)}$$

Equation (82) is obtained by substituting equation (E5) into equation (81).

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