Exchange Interaction Model of Ferromagnetism
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Citation: J. Math. Phys. 13, 725 (1972); doi: 10.1063/1.1666044
View online: http://dx.doi.org/10.1063/1.1666044
View Table of Contents: http://jmp.aip.org/resource/1/JMAPAQ/v13/i5
Published by the American Institute of Physics.

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Since $D_1D_2 \geq 0$, it follows immediately from the minmax principle for the eigenvalues of a Hermitian operator that $H + D_1D_2$ has at least as many positive eigenvalues as $H$ and at least as many nonnegative eigenvalues as $H$; since $P^{1/2}$ is Hermitian positive definite, the number of positive eigenvalues as well as the number of zero eigenvalues of the operators $H + D_1D_2$ and $P^{1/2}(H + D_1D_2)P^{-1/2}$ are identical. Therefore $P^{1/2}(H + D_1D_2)P^{-1/2}$ has at least $J$ positive eigenvalues and at least $J + M$ nonnegative eigenvalues. Similarly, since $D_1D_2 \geq 0$, $-P^{1/2}(H + D_1D_2)P^{-1/2}$ has at least $J$ negative eigenvalues and at least $J + M$ nonpositive eigenvalues.

**Theorem 5:** Let $N (< n = \dim E)$ be the number of negative eigenvalues of $H$ counted according to their multiplicity. Suppose the system (1) admits a Liapunov operator of the form $LP(T)$, where $p(x)$ is a real polynomial in $x$ (i.e., suppose the system is structurally stable). Then the degree of $p(x)$ need not exceed $4N + 1$, i.e., there exists a real polynomial $f(x)$ of degree less than or equal to $4N + 1$ such that $LF(T)$ is a Liapunov operator.

**Proof:** Let $N (< n)$ be the number of negative eigenvalues of $H$ and let $p(x)$ be a complete $L$-canonical set of eigenvectors satisfying Eqs. (15) and (18) with real eigenvalues $\lambda_n$ enumerated so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. If $0$ is not an eigenvalue of $H$, we conclude from Theorem 4, with $J = n - N$, that $\lambda_{n+N+1} < 0 < \lambda_{n-N}$. If $0$ is an eigenvalue of $H$, then $0$ is an eigenvalue of $T$ if $|\eta| = 0$ implies $T(\eta) = 0$. By assumption, the system is structurally stable, so that the sets $Q = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ and $Q_0 = \{\lambda_{n+1}, \ldots, \lambda_{2n}\}$ are disjoint, and therefore either $0 \in Q_0$ or $0 \in Q$, but not both. If $0 \in Q$, then we conclude from Theorem 4 (with $J = M = n - N$) that $\lambda_{n+N+1} \leq 0 < \lambda_{n-N}$, while if $0 \in Q_0$, Theorem 4 implies that $\lambda_{n-N+1} \leq 0 < \lambda_{n+N}$. Thus, in any case, $\lambda_{n+N+1} < \lambda_{n-N}$. Let $y$ be the greatest integer $\leq n$ such that $\lambda_y \geq \lambda_n$, and let $u$ be the least integer $\geq n + 1$ such that $\lambda_u \leq \lambda_n$. Then $n - N \leq y \leq n$, $n + 1 \leq u \leq n + N + 1$, $\lambda_y \leq \lambda_u$, and $\lambda_u \leq \lambda_n$ for $r + 1 \leq k \leq u$, and $\lambda_n \leq \lambda_u$ for $n + 1 \leq k \leq n - u$. Let $\lambda_u < \lambda_n$, and define $p_n(x) = x - \lambda_n$. If $p_n(\lambda_u) < 0$ for $1 < k < u$ and $u \leq 2m$. Let $\Omega_1, \ldots, \Omega_N$ denote the distinct elements of the set $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$, and let $\Omega_{n+1}, \ldots, \Omega_{2n}$ denote the distinct elements of the set $\{\lambda_{n+1}, \ldots, \lambda_{2n+1}\}$, then $q = n - r \leq N$ and $y < n - u \leq n - N$. Since $\Omega_n \in Q$, and $\Omega_n \cap Q_0 = \phi$, there exists $\epsilon > 0$ such that the $q$ closed intervals $I_k = [\Omega_k - \epsilon, \Omega_k + \epsilon]$ are all disjoint and satisfy $I_k \cap Q = \phi, k = 1, \ldots, q$. Similarly, there exists $\delta > 0$ such that the $N$ closed intervals $I_k = [\Omega_k - \delta, \Omega_k + \delta]$ are all disjoint and satisfy $I_k \cap Q_0 = \phi, k = 1, \ldots, N$. We define

$$p(x) = p_n(x) \prod_{\lambda \in \Omega} (x - \lambda) + p_m(x) \prod_{\lambda \in \Omega_m} (x - \lambda)$$

Then by construction, Eq. (19) holds, so that $LP(T) > 0$ and is therefore a Liapunov operator. The degree of $p(x)$ is given by $1 + 2q + 2y \leq 1 + 2N + 2N = 1 + 4N$, and the proof is complete.

**ACKNOWLEDGMENT**

The work presented here was sponsored by the Air Force Office of Scientific Research, under Research Grant No. AFOSR 71-2053.

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**Exchange Interaction Model of Ferromagnetism**

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(Received 4 January 1971)

The Schrödinger exchange operator for arbitrary spin has been used to form an interaction Hamiltonian for a nearest-neighbor model of ferromagnetism. Through use of the cluster expansion method and new group theoretic results in conjunction with the diagrammatic method, eight terms in the high temperature series for the zero-field partition function and the low-field susceptibility are obtained for arbitrary spin and general crystal lattice. Critical parameters are estimated from these series by means of various ratio tests and Padé approximants. For the cubic lattices the Curie temperature $T_C$ and the critical index $\gamma$ are given by

$$k_B T_C / J = 0.547 (q - 1.6) (r^{-1} + 0.21)$$

and

$$\gamma = 0.48 + 2.16 Y^{-1}$$

for $S > \frac{1}{2}$;

$$\gamma = 1.41 \pm 0.02$$

for $S = \frac{1}{2}$, respectively, where $Y = 2S + 1$. Comparison of these results with those appropriate to the Heisenberg model as well as to experimental values is made. The concept of multipolar ordering is also discussed. It is shown that for the present model all of the $2S$ "independent" multipolar phase transitions are exactly degenerate with the usual dipolar transition.

1.**Introduction**

For the Heisenberg model of ferromagnetism, high temperature series for various thermodynamic quantities have been extensively studied and used to investigate critical properties of ferromagnetic systems. If we consider a ferromagnetic system containing
ing $N$ particles of spin $S$ with isotropic nearest-
neighbor exchange interactions, the Heisenberg Hamiltonian is given by

$$\mathcal{H} = - J \sum_{i < j} S_i \cdot S_j - g \mu_B H \sum_{i} S_i z,$$

(1)

where $J$ is the nearest-neighbor exchange constant, $S_i$ is the spin operator of an atom at the lattice site labeled $i$, $g$ is the gyromagnetic ratio, $\mu$ the Bohr magneton, $H$ the external magnetic field, and $S_i z$ is the $z$ component of $S_i$. The first term in the Hamiltonian represents the exchange energy and the summation is taken over all nearest-neighbor pairs of atoms, denoted $(ij)$; the sum in the second term is over all atoms and is the Zeeman energy of the system.

The Heisenberg Hamiltonian linear in $S_i \cdot S_j$, which arises from a consideration of the Coulomb interaction together with the Pauli principle is in fact only the lowest-order significant term in a perturbation expansion which when carried further leads to terms nonlinear in $S_i \cdot S_j$.

In order to study the properties of systems containing nonlinear terms, such as $\sum S_i \cdot S_j S_k \cdot S_l$, in the Hamiltonian, the Schrödinger exchange operator has been used to form an interaction Hamiltonian for a nearest-neighbor model of ferromagnetism:

$$\mathcal{H} = - J \sum_{i < j} P_{ij} - g \mu_B H \sum_{i} S_i z,$$

(2)

Here $P_{ij}$ is the Schrödinger exchange operator and is a polynomial of degree $2S$ in $S_i \cdot S_j$:

$$P_{ij} = \sum_{n=0}^{2S} A_n (S_i \cdot S_j)^n, \quad i \neq j,$$

(3)

The coefficients $A_n$ are determined from the property that $P_{ij}$ exchanges, or permutes, the spin coordinates of two atoms labeled $i$ and $j$:

$$P_{ij} | m_{ij} \rangle | m'_{ij} \rangle = | m'_{ij} \rangle | m_{ij} \rangle$$

(4)

or

$$P_{ij} O(i,j) = O(i,j) P_{ij},$$

(5)

where $O(i,j)$ is any operator which contains the spins of operators $i$ and $j$ and $| m_{ij} \rangle$ and $| m'_{ij} \rangle$ are eigenstates of $S_i$ and $S_j$, respectively. Schrödinger$^4$ has explicitly shown that

$$P_{ij} = (-1)^{2S} \left( 1 + \sum_{\rho=1}^{2S} \frac{(-1)^{\rho}}{(\rho)!} \prod_{\rho} [M - q(\rho - 1)] \right),$$

(6)

where $M \geq 2 |S(S+1) + S_i \cdot S_j|$. The coefficients $A_n$ typically have the values

$$A_0 = \frac{1}{2}, \quad A_1 = \frac{1}{2}, \quad A_2 = 1,$$

$$S = 1: \quad A_0 = -\frac{1}{2}, \quad A_1 = 1, \quad A_2 = 1,$$

$$S = \frac{3}{2}: \quad A_0 = -\frac{3}{8}, \quad A_1 = -\frac{5}{8}, \quad A_2 = \frac{11}{16},$$

$$A_3 = \frac{3}{8}, \quad A_4 = \frac{5}{8},$$

etc.

Inclusion of these special combinations of nonlinear terms in the Hamiltonian may not be realized in nature. However, a study of this model gives detailed information about what effect such nonlinear terms should have on the critical properties of the system.

Due to the permutation property of the Schrödinger exchange operator (5), the high temperature series can be extended further with less effort for the present Hamiltonian than for the Heisenberg Hamiltonian. For the case $S = \frac{1}{2}$, the present Hamiltonian is identical to that of the Heisenberg model; Baker et al.$^5$ obtained terms through $T^{-9}$ for the close-packed lattices and $T^{-10}$ for the loose-packed lattices for the zero-field partition function series and the low-field susceptibility series. For $S = 1$, Allan and Betts$^6$ obtained eight terms in these series for the face-centered cubic lattice. Such a large number of terms was obtained through the use of the cluster expansion method in conjunction with a technique making use of "Branching diagrams"; this is practicable only for the case of $S$ equal to $\frac{1}{2}$ or 1. We have developed a new method which can be applied to the case of arbitrary spin directly and hence obtained eight terms in the high temperature series for general crystal lattices.

High temperature series expansions and the cluster expansion method are discussed in Secs. II and III, respectively; these ideas can be applied to any of the spin Hamiltonians usually studied. Sections IV and V contain group theoretical considerations and the diagrammatic method required to calculate the series coefficients for the present model. Details of the calculations are given in Sec. VI and the explicit series results are presented in Sec. VII. Several checking procedures on the results are considered in Sec. VIII. In Sec. IX these high temperature series are used to estimate various critical properties by means of ratio tests and the method of Padé approximants. The significance of the results as well as the concept of multipolar ordering is found in Sec. X.

II. HIGH TEMPERATURE SERIES EXPANSIONS

A. Preliminary Remarks

For any spin Hamiltonian $\mathcal{H}$, the high temperature series expansion method introduced by Kramers$^6$ and Opecchowski$^7$ makes use of a result of the form

$$Z = \text{tr} e^{-\beta \mathcal{H}} = \text{tr} [1 - \beta (\mathcal{H}) + (\beta^2/2!)(\mathcal{H}^2) - \cdots],$$

(8)

where $Z$ is the partition function, $\beta = (k_B T)^{-1}$, $k_B$ is Boltzmann’s constant, $(\mathcal{H}^n) = \text{tr} \mathcal{H}^n$, and $I$ is the unit matrix. Related thermodynamic functions can then be expressed as ascending series in powers of $1/T$ by evaluating the leading coefficients in the series for various crystal lattices. The first few terms of these series provide a good approximation to each thermodynamic quantity at high temperatures. Furthermore, extrapolations from such truncated expansion series are considered to be the most powerful theoretical approach yet developed for obtaining estimates of the various critical parameters.

B. Zero-Field Partition Function and Related Thermodynamic Functions

Since the various thermodynamic functions are re-

lated to the expression of the partition function by \( \ln Z \), it is convenient to express the partition function in the form \( \ln Z \). Moreover, since \( \ln Z \) is an extensive quantity, considerable simplification can be made in the derivation of high temperature series by means of the cluster expansion method, as will be discussed in the next section. We introduce the following convenient notations: \( Y = 2S + 1 \), \( X = S(S + 1) \), \( \alpha = g_{\mu}H/J \), \( K = J/\hbar_bT \), and

\[
Q = \sum_{i=1}^{N} S_i, \tag{9}
\]

\[
\Phi = \sum_{\langle ij \rangle} P_{ij}, \quad \text{for the exchange interaction model,} \tag{10}
\]

\[
= 2 \sum_{\langle ij \rangle} S_i S_j, \quad \text{for the Heisenberg model,} \tag{11}
\]

\[
= 2 \sum_{\langle ij \rangle} S_i S_j, \quad \text{for the Ising model.} \tag{12}
\]

Then,

\[
\mathcal{Z} = -J(\Phi + \alpha Q) = \mathcal{Z}_0 - J\alpha Q. \tag{13}
\]

For a system which consists of \( N \) particles of spin \( S \), in zero external field,

\[
Z = Y^N \left( 1 + \sum_{n=1}^{\infty} \frac{K^n}{n!} (\phi^n) \right), \tag{14}
\]

and

\[
\ln Z = N \ln Y + \sum_{n=1}^{\infty} \frac{\zeta_n K^n}{n!}, \tag{15}
\]

with

\[
e = \sum \frac{(-1)^{p+q+r+\cdots+n} (a_1 + a_2 + \cdots + a_p - 1)!}{a_1! a_2! \cdots a_p!} \langle \phi^{a_1} \rangle \langle \phi^{a_2} \rangle \cdots \langle \phi^{a_p} \rangle \phi^{p+q+r+\cdots+n} \tag{16}
\]

The summation is taken over all partitions of the integer \( n \), namely, all sets of positive integers \( a_1, a_2, \ldots, a_p, a_1, a_2, \ldots, a_r \) which satisfy the conditions

\[
a_1 a_1 + a_2 a_2 + \cdots + a_r a_r = n \tag{18}
\]

and

\[
a_1 < a_2 < \cdots < a_r. \tag{19}
\]

Each thermodynamic function series can now be directly obtained from Eq. (14):

\[
\text{internal energy:} \quad E = k_b T \frac{\partial}{\partial \phi} \left( \ln Z \right) = -J \frac{\partial}{\partial \phi} \left( \ln Z \right), \tag{20}
\]

\[
\text{entropy:} \quad S = k_b \frac{\partial}{\partial T} \left( T \ln Z \right) = k_b K \frac{\partial}{\partial T} \left( T \ln Z \right), \tag{21}
\]

\[
\text{specific heat:} \quad C_v = k_b \frac{\partial}{\partial T} \left( \frac{T^2}{2} \frac{\partial}{\partial T} \ln Z \right) = k_b K \frac{\partial}{\partial T} \left( \frac{T^2}{2} \frac{\partial}{\partial T} \ln Z \right), \tag{22}
\]

C. Low-Field Susceptibility

The low-field susceptibility is defined as

\[
\chi = \frac{1}{N} \frac{\mu_{\text{B}}^2}{\hbar_b T^2} \frac{\partial^2}{\partial \phi^2} \ln Z = \frac{1}{N} \frac{\mu_{\text{B}}^2}{\hbar_b T^2} \frac{\partial^2}{\partial \phi^2} \ln Z, \tag{23}
\]

Since \( \Phi \) and \( Q \) commute, \( (\partial / \partial \phi) \langle \Phi + \alpha Q \rangle = \alpha \langle \Phi \rangle + \alpha \langle Q \rangle \langle Q \rangle \). It is then straightforward to show that

\[
\chi = \left( \frac{\mu_{\text{B}}^2}{\hbar_b T} \right) \langle \Phi \rangle, \tag{24}
\]

where \( \langle \Phi \rangle = \langle \phi^n \rangle \) is the zero-field thermal fluctuation of \( \Phi \) and, for any operator \( A \),

\[
\langle A \rangle = \frac{\text{tr} e^{-\beta H_0} \langle \phi^{n A} \rangle}{\text{tr} e^{-\beta H_0}} = \sum_{n=0}^{\infty} \frac{K^n}{n!} \langle \phi^n A \rangle / \sum_{n=0}^{\infty} \frac{K^n}{n!}. \tag{25}
\]

As a consequence of the fact that \( \ln Z \) is an even function of the external field, \( \text{tr} \Phi Q = 0 \) for all \( n \); hence, \( \langle \Phi \rangle = 0 \), so that we can rewrite \( \chi \) in the form

\[
\chi = \left( \frac{\mu_{\text{B}}^2}{\hbar_b T} \right) N \left( n + \sum_{n=1}^{\infty} \frac{K^n}{n!} \right) \tag{26}
\]

It is easy to show that the coefficients \( \zeta_n \) satisfy the recursion relation

\[
\zeta_n = \frac{3}{N} \left( \langle \phi^n \rangle^2 \right) - \sum_{k=0}^{\infty} \frac{1}{(n-k)!} \frac{1}{k!} \langle \phi^{n-k} \rangle \langle \phi^{n-k} \rangle, \tag{27}
\]

with \( a_0 = N \). In order to obtain the terms \( \zeta_n \) and \( \zeta_k \), we must calculate the quantities \( \langle \phi^n \rangle \) and \( \langle \phi^n \rangle^2 \) for \( n < k \). Here the matrices \( \Phi \) and \( Q \) are of order \( (2S + 1)^N \). For real crystals, \( N \to \infty \), and direct computation of the required traces is impossible. However, there are two alternative methods of handling the calculation. In the next section we discuss the cluster expansion method, while the diagrammatic method is considered in Sec. V.

III. CLUSTER EXPANSION METHOD

A. Preliminary Remarks

The use of the cluster expansion method in deriving series expansions for magnetic systems was first suggested by Domb. It was pointed out that high temperature series for extensive quantities for infinite lattices \( (N \to \infty) \) can be obtained simply by calculating the corresponding series for clusters of finite sites. One advantage of this method as compared to the diagrammatic method is that the number of configurations that one has to consider is considerably smaller than that required in the diagrammatic method. More important, however, is the fact that most of the calculations called for in the cluster expansion method can easily be done on a fast computer.

The general method of the cluster expansion has been developed by many authors and derived in a number of different ways. In this section we introduce a new proof of an essential theorem of this method (Theorem I), which can be applied directly to the calculation of the high temperature series for any spin Hamiltonian.

B. General Concepts

A (linear) graph is a collection of points with lines joining certain pairs of points. If a subset of points

are joined successively by lines, the assembly of these lines is called a path connecting the initial and the final points. A graph is said to be connected if any two points in the graph are connected by a path. Otherwise, the graph is said to be disconnected.

Clearly, any graph consists of connected graphs, and each connected graph is called a component. If the initial point and the final point of a path coincide, we speak of a cycle. A set of different cycles is said to be independent if none of the cycles can be made up of parts of other cycles. The maximum number of independent cycles in a graph is called the cyclo-matic number of the graph.

If \( g_i \) and \( g_s \) are two graphs having no points in common, the union of these two graphs, denoted \( g_i \cup g_s \), is the collection of all points and lines of \( g_i \) and \( g_s \). A graph \( g \) is a subgraph of \( G \) if any point in \( g \) is a point in \( G \) and any line in \( g \) is a line in \( G \). A graph \( G' \) is said to be isomorphic with \( G \) if there is a one-to-one correspondence between their points such that pairs of points are joined by lines in \( G' \) if and only if the corresponding pairs of points are joined in \( G \). The lattice constant \( \phi \) of a graph \( G \) is the number of subgraphs of \( G \) isomorphic with \( g_i \), denoted \( \phi(g_i; G) \). A graph \( G \) is sometimes abbreviated as \( [g] \) if \( G \) is not specified. Lattice constants of disconnected graphs can be expressed in terms of lattice constants of connected graphs. For example, consider the equation shown in Fig. 1. The first term on the right-hand side is of second order while the others are of first order in the lattice constants of connected graphs. In general, lattice constants of disconnected graphs having \( n \) connected components will consist of terms from the first order to the \( n \)th order in lattice constants of connected graphs.

C. New Derivation of the Cluster Expansions

Let \( \phi(g) \) be any quantity associated with the graph \( g \). \( \phi \) is said to be extensive if, for any graphs \( g_i \) and \( g_s \) having no points in common,

\[
\phi(g_i \cup g_s) = \phi(g_i) + \phi(g_s); \tag{28}
\]

that is, the quantity \( \phi \) of two graphs considered together is the sum of the quantities of the two graphs considered separately. The number of lines and the number of points in a graph are obviously extensive. \( \phi(g_i; G) \) is also an extensive quantity of \( G \), i.e.,

\[
(\phi; g_i; G) = (\phi; g_i; g_s) \quad \text{if} \quad g_i \cap g_s = \emptyset.
\]

Let \( \epsilon = c - p + 1 \),

\[
c = \ell - p + 1, \tag{26}
\]

where \( c \) is the cyclo-matic number, \( \ell \) the number of lines, and \( p \) the number of points in a graph. In general, if we denote the number of connected components in a graph by \( n \), then

\[
c = \ell - p + n. \tag{27}
\]

A connected graph is said to be closed if any point in the graph has at least two lines connected to it. Otherwise, it is said to be open.

If \( g_i \) and \( g_s \) are two graphs having no points in common, the union of these two graphs, denoted \( g_i \cup g_s \), is the collection of all points and lines of \( g_i \) and \( g_s \). A graph \( g \) is a subgraph of \( G \) if any point in \( g \) is a point in \( G \) and any line in \( g \) is a line in \( G \). A graph \( G' \) is said to be isomorphic with \( G \) if there is a one-to-one correspondence between their points such that pairs of points are joined by lines in \( G' \) if and only if the corresponding pairs of points are joined in \( G \). The lattice constant \( \phi \) of a graph \( G \) is the number of subgraphs of \( G \) isomorphic with \( g_i \), denoted \( \phi(g_i; G) \). A graph \( G \) is sometimes abbreviated as \( [g] \) if \( G \) is not specified. Lattice constants of disconnected graphs can be expressed in terms of lattice constants of connected graphs. For example, consider the equation shown in Fig. 1. The first term on the right-hand side is of second order while the others are of first order in the lattice constants of connected graphs. In general, lattice constants of disconnected graphs having \( n \) connected components will consist of terms from the first order to the \( n \)th order in lattice constants of connected graphs.

\[
(\phi; g_i; G) = (\phi; g_i; g_s) \quad \text{if} \quad g_i \cap g_s = \emptyset. \tag{29}
\]

Suppose that a graph \( G \) consists of the number \( \pi_i \) of connected graphs \( g_i \), \( i = 1, 2, 3, \cdots \). Let \( \phi(G; t) \) be an extensive quantity of \( G \) and \( t \) be a set of parameters independent of graphs. By the extensive property of \( \phi \),

\[
\phi(G; t) = \sum_i \phi(g_i; t)\pi_i. \tag{30}
\]

Using the extensive property of the lattice constant as expressed by Eq. (29), set \( g = g_i \) for \( j = 1, 2, 3, \cdots \).

We then have a set of linear equations

\[
(\phi; g_j; g_i) = \sum_j (\phi; g_j; g_i)\pi_j, \quad j = 1, 2, 3, \cdots. \tag{31}
\]

If the graphs are labeled in the graph dictionary order such that

\[
l_j < l_i, \quad \text{for} \quad i < j, \tag{32}
\]

where \( l_j \) and \( l_i \) are the numbers of lines of graphs \( g_i \) and \( g_j \), respectively, it is then obvious that

\[
(\phi; g_j; g_i) = 0, \quad \text{for} \quad j > i, \tag{33}
\]

\[
= 1, \quad \text{for} \quad j = i. \tag{34}
\]

Define a matrix \( A \) with elements \( A_{ij} = (\phi; g_i; g_j) \). Equation (33) then means that \( A \) is a triangular matrix with the lower triangular elements equal to zero. Furthermore, all the diagonal elements are unity.

Therefore, \( A \) is nonsingular and its inverse exists.

From Eq. (31), we get

\[
\pi_j = \sum_j (A^{-1})_{ij}, \quad i = 1, 2, 3, \cdots. \tag{34}
\]

where \( (A^{-1})_{ij} \) are elements of the inverse matrix of \( A \).

Substituting Eq. (34) into Eq. (30) yields

\[
\phi(G; t) = \sum_i \phi(g_i; t)(A^{-1})_{ij}(g_i; G) \quad \text{if} \quad \pi_j = 1, \quad j = 1, 2, 3, \cdots. \tag{35}
\]

where \( F_i(t) = \sum_j (g_i; g_j) \pi_j \) is independent of \( G \). Since \( G \) may be any graph, let \( G' = g_i \). Equation (35) yields

\[
\phi(g_i; t) = \sum_j F_j(t)(g_i; g_j). \tag{36}
\]

On substituting Eq. (33) into Eq. (36) and rearranging terms, we obtain an important theorem formulated by Sykes et al.\(^{10}\)

Theorem 1: If \( \phi(G; t) \) satisfies the extensive property, then \( \phi \) can be expressed by Eq. (35) in which \( F_i(t) \) are given by the recursion formula

\[
F_i(t) = \phi(g_i; t) - \sum_{j=1}^{i-1} (g_i; g_j) F_j(t). \tag{37}
\]

and

\[
F_i(t) = \phi(g_i; t). \tag{38}
\]

D. Application to Magnetic Systems

In a nearest-neighbor model of any of the spin Hamiltonians, if spin sites are represented by points and interactions between nearest-neighbor sites are repre-
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sented by lines joining the corresponding pairs of points, then systems represented by graphs isomorphic to each other will have the same physical properties and systems which consist of a number of independent subsystems will be represented by disconnected graphs. Let \( \phi(G) \) be any quantity of a magnetic system represented by a graph \( G \). It is clear then that \( \ln Z(G) \) and \( \chi(G) \) satisfy Eq. (28) since \( \ln Z \) and \( \chi \) are extensive thermodynamic quantities. We can then use Theorem 1 to calculate \( \ln Z(G; t) \) and \( \chi(G; t) \) for any cluster or crystal lattice \( G \) and for a set of parameters \( t \), such as temperature \( T \), spin values \( S \), external magnetic field \( H \), exchange constant \( J \), etc. In high temperature series expansions, we express \( F_j \) [in Eq. (35)] in powers of \( kT/J \kappa \).

\[
F_j = \sum_{\kappa} f_j(\kappa)k^\kappa \quad (39)
\]

Theorem 1 is useful because in most cases \( f_j(\kappa) = 0 \) for \( n < \kappa \). This will be explicitly shown in Sec. V for the present Hamiltonian when \( \phi = \ln Z \) or \( \chi \). Therefore, if we want to obtain series up to the \( \kappa \)th power in \( K \) for \( \phi(G) \), we need only calculate \( \phi_j(\kappa) \) and hence \( F_j \) for connected graphs having up to \( k \) lines. Thus, instead of considering infinite lattices, we have reduced the problem to clusters of finite size.

IV. APPLICATION OF GROUP THEORY

A. Symmetric Group

A rearrangement of the order of \( N \) symbols is called a permutation. There are \( N! \) number of possible permutations on \( N \) symbols. The set of all these permutations forms a group called the symmetric group of degree \( N \), denoted \( S_N \). Each element in \( S_N \) can be written as a product of independent cycles. For example, the permutation by which \( \{a, b, c, d, e, f, g\} \) is replaced by \( \{b, f, c, e, d, a, g\} \) can be written as \( (ab)(cfedag) \). Each cycle in \( ( \) is the order of the cycle. In writing a permutation as the product of cycles, cycles of order 1 need not be mentioned. Furthermore, the sequence of appearance of the cycles as well as the first symbol in each cycle is arbitrary.

Cycles having no symbols in common are said to be independent. A cycle of order 2 is called an interchange. Any cycle of higher order can be expressed as a product of interchanges (having symbols in common). For example,

\[
(abc \cdots de) = (ac)(ad)(bc)(bd)(cd) \quad (40)
\]

Permutations which are products of an even number of interchanges are called even permutations. Otherwise, they are called odd permutations. It is straightforward to show that

\[
(fg)(ab) = (af)(bg) \quad (41)
\]

and

\[
(fg)(ab)(cd) = (ac)(bd)(fg) \quad (42)
\]

Equations (41) and (42) imply that for any group element, say \( P \), multiplied by an interchange \( (fg) \), \( (fg)P \) has one more cycle than \( P \) if \( f, g \) belong to the same cycle in \( P \) and has one less cycle than \( P \) if \( f, g \) belong to different independent cycles in \( P \).

Elements in \( S_N \) are divided into classes. Elements which have the same cycle structure are transforms of one another by elements in \( S_N \) and belong to the same class. Elements which belong to the class \( (a_1^1 a_2^2 \cdots a_p^p) \) have \( a_1 \) cycles of order \( a_1 \), \( a_2 \) cycles of order \( a_2 \), \ldots, and \( a_p \) cycles of order \( a_p \). The number of classes in \( S_N \) is equal to the number of partitions of the integer \( N \), and each class is labeled by a partition of \( N \). The number of group elements in a class is called the order of the class. For the class \( k = (a_1^1 a_2^2 \cdots a_p^p) \), its order \( h_k \) is

\[
h_k = N!/a_1!a_2!\cdots a_p! a_1^{a_1} a_2^{a_2} \cdots a_p^{a_p} \quad (43)
\]

Associated with \( S_N \) there is a finite number of inequivalent representations, called irreducible representations. Each irreducible representation is also labeled by a partition of \( N \). Since elements of a class are transforms of one another, their matrices in any representation, say \( \nu \), have the same trace. This value is referred to as the character of the class \( k \) in the representation \( \nu \), denoted \( \chi_k^{(\nu)} \).

Below we summarize some group theoretic results which will be useful in deriving high temperature series for the present Hamiltonian.

For the irreducible representations \( \nu \) and \( \nu' \), we have the orthogonality relations

\[
\sum_k \chi^{(\nu)}_k \chi^{(\nu')}_k = \delta_{\nu\nu'} \quad (44)
\]

and

\[
\sum_k \chi^{(\nu)}_k \chi^{(\nu')}_k = \delta_{\nu
u'} \quad (45)
\]

where \( \chi_k \) is the order of the class \( k \), \( \delta \) is the order of \( S_N \), and the summations \( \sum_k \) and \( \sum \) are taken over all classes \( k \) and all irreducible representations \( \nu \) respectively.

Let \( P^{(\nu)} \) be any matrix representation of an element \( P \) in \( S_N \). \( P^{(\nu)} \) can be resolved into a direct sum of \( n_\nu \) irreducible representations, i.e., the matrix \( P^{(\nu)} \) now takes the form of a series of blocks, the irreducible representations, placed along the principal diagonal, which can be written as

\[
P^{(\nu)} = \sum \chi^{(\nu)}_k P_k \quad (46)
\]

From Eq. (44), we get

\[
\sum \chi^{(\nu)}_k = \delta \quad (47)
\]

For two irreducible representations labeled by a pair of conjugate partitions \( \nu \) and \( \nu' \), we have

\[
\chi^{(\nu)}_k = \pm \chi^{(\nu')}_{k'} \quad (48)
\]

with the plus sign applying for even classes and the minus sign for odd classes of permutations.

If we sum the matrices of an irreducible representation \( \nu \) for all elements of a class \( k \), we obtain a multiple of the unit matrix:

\[
\sum P^{(\nu)} = \delta \chi^{(\nu)}_k \quad (49)
\]

where \( \chi^{(\nu)}_k \) is the matrix dimension of the irreducible representation \( \nu \).

Using these equations, we now prove several useful new theorems.

B. New Theorems

Theorem 2: If $R$ is any matrix which commutes with all elements of $S_N$ in a matrix representation $\Gamma$, then

$$\text{tr}(\Phi^\Gamma R) = \sum_{\nu} \text{tr}(\Phi^{\nu}) R_k^k = \sum_{\nu} \chi_{\nu}^\Gamma \text{tr}(P^{\nu} R),$$

(50)

where $\Phi^\Gamma$ and $\Phi^{\nu}$ are sums of elements in $S_N$ in the $\Gamma$ and $\nu$ representations, respectively, $P_k$ is any element in the class $k$, and the summations are taken over all irreducible representations $\nu$ and all classes $k$.

**Proof:** The condition that $R$ commutes with all elements of $S_N$ in a matrix representation $\Gamma$ and the fact that elements of a class are transforms of one another imply that $\text{tr}(P^{\nu} R)$ have the same value for all elements $P$ which belong to the same class. Since products of elements in $S_N$ are also elements in $S_N$, as well as $\Phi$ is a sum of elements in $S_N$. It is then sufficient to show that for any element, say $P$, in $S_N$,

$$\text{tr}P^\Gamma R = \sum_k \sum_k \chi_k^\Gamma R_k^k P_k.$$

(51)

Let $P$ belong to the class $k'$; $\text{tr}(P^{\nu} R) = \chi_{k'}^\Gamma$. By Eq. (45),

$$\sum_{\nu} \sum_k \chi_{\nu}^\Gamma R_k^k P_k = \sum_k \delta_{k, k'} \chi^\Gamma P_k = \text{tr}P^\Gamma R.$$

(52)

Equation (51) and hence Eq. (50) then follow.

**Theorem 3:** If $\nu$ and $\delta$ are two irreducible representations labeled by a pair of conjugate partitions of $N$ and $\Phi$ is a sum of odd permutations in $S_N$, then

$$\text{tr}(\Phi^\nu \Phi^\delta) = (-1)^{\text{tr}(\Phi^\nu \Phi^\delta)}.$$

(53)

**Proof:** Since a product of $n$ odd permutations is an even permutation if $n$ is an even number and is an odd permutation if $n$ is odd, Eq. (53) follows from Eq. (48).

C. The $(2S + 1)^N$-Dimensional Representation of $S_N$

For a system containing $N$ particles of spin $S$, it is clear that matrices of the Schrödinger exchange operators $P_{ij}$ and their products form a $(2S + 1)^N$-dimensional representation of $S_N$. It is convenient to choose the basis of the $(2S + 1)^N$-dimensional vector space as the eigenstates of the $z$ component of the spins of the $N$ particles, $|m_1, m_2, \ldots, m_N\rangle$. In this section we restrict our attention to this representation. Unless otherwise specified, matrix representation of operators will be in this representation. We first prove the following results:

$$\text{tr}(ijk \cdots l) = \sum_{m_1} \sum_{m_2} \cdots \sum_{m_N} (\delta_{m_1 m_2} \delta_{m_3 m_4} \cdots \delta_{m_{N-1} m_N})$$

$$= \sum_{m} (1) = Y.$$

(54)

All sums in this equation, and those following directly after, range from $-S$ to $+S$. Similarly,

$$\text{tr}S_{2N}(ijk \cdots l) = \sum_{m_1} \sum_{m_2} \cdots \sum_{m_N} (\delta_{m_1 m_2} \delta_{m_3 m_4} \cdots \delta_{m_{N-1} m_N} r_{m_1 m_2} r_{m_3 m_4} \cdots r_{m_{N-1} m_N})$$

$$= \sum_{m} (m^2) = Y W_n,$$

(55)

where $W_n = Y^{-1} \sum_m (m^2)$.

(56)

and

$$\text{tr}S_{2N}(ijk \cdots l) = \sum_{m_1} \sum_{m_2} \cdots \sum_{m_N} (\delta_{m_1 m_2} \delta_{m_3 m_4} \cdots \delta_{m_{N-1} m_N} r_{m_1 m_2} r_{m_3 m_4} \cdots r_{m_{N-1} m_N})$$

$$= \sum_{m} (m^2) = Y W_{2n}.$$

(57)

Let us express any element in $S_N$, say $P$, as a product of independent cycles:

$$P = (a b c \cdots d)(ijk \cdots l) \cdots (x y \cdots z).$$

(58)

$P$ may be considered as a direct product of each cycle,

$$P = (a b c \cdots d) \times (ijk \cdots l) \times \cdots \times (x y \cdots z).$$

(59)

By the trace property of the direct product,

$$\text{tr}(A \times B) = \text{tr}(A) \text{tr}(B),$$

(60)

and

$$\text{tr}S_{2N}(ijk \cdots l) = \sum_{m} (m^2) = Y W_{2n}.$$

(61)

Then follow from Eqs. (54), (55), and (57) that

$$\text{tr}S_{2N}(ijk \cdots l) = \sum_{m} (m^2) = Y W_{2n}.$$

(62)

For the case $n = 1$, $W_1 = 0$ and $W_2 = X/3$. If the element $P$ belongs to the class $k = (a_1^2 a_2^2 \cdots a_p^2)$, then, from Eqs. (54), (60), and (62),

$$\text{tr}P = \sum_{i=1}^{a_1^2} \sum_{j=1}^{a_2^2} \cdots \sum_{p=1}^{a_p^2} Y_{ij} = \sum_{i=1}^{a_1^2} \sum_{j=1}^{a_2^2} \cdots \sum_{p=1}^{a_p^2} Y_{ij}.$$

(63)

and

$$\text{tr}P = \sum_{i} \sum_{j} \sum_{p} S_{2N} P_{ij} = \sum_{i} \sum_{j} \sum_{p} S_{2N} P_{ij} = (X/3)(a_1^2 + a_2^2 + \cdots + a_p^2).$$

(64)

where the summations are from 1 to $N$.

It also follows from Eqs. (41), (42) and Eqs. (54), (60) that

$$\text{tr}P_i^j P = Y \text{tr}P,$$

(65)

if $i, j$ belong to the same cycle in $P$,

$$= Y^{-1} \text{tr}P,$$

if $i, j$ belong to different independent cycles in $P$.

V. DIAGRAMMATIC METHOD

A. Preliminary Remarks

The diagrammatic method has been extensively used in deriving high temperature series for various spin Hamiltonians. In this section, the procedure previously used for the Heisenberg Hamiltonian by Rushbrooke and Wood will be modified for the exchange interaction Hamiltonian. The labor of evaluating series
coefficients by this method is much greater than the labor involved in the previously described cluster expansion method. However, there are a number of important results that can be directly proved by the diagrammatic technique which are not at all obvious from a consideration of the cluster expansion method.

B. Zero-Field Partition Function

For the exchange interaction model \(\sigma^x\) in Eq. (12) is a sum of products \(\Pi P_{ij}\) and each product contains \(n\) factors \(P_{ij}\). There is a correspondence between products in \(\sigma^x\) and diagrams of \(n\) lines on the lattice. For each of the \(n\) factors \(P_{ij}\) in the product, when we draw a straight line connecting lattice sites \(i\) and \(j\), we obtain a diagram of \(n\) lines. The diagrams may be connected or disconnected, and may have more than one line joining a pair of points.

Following Rushbrooke and Wood,\(^1\) we can write

\[
(\sigma^x) = \sum_{D_i} \langle D_i \rangle,
\]

where \(\sum_{D_i}\) sums over all diagrams \(D_i\) of \(n\) lines, \(\langle D_i \rangle\) is the number of times that the diagram \(D_i\) will occur on the lattice. \(\langle D_i \rangle\) is the weighting factor, or the contribution of the diagram \(D_i\) to \(\sigma^x\). For a diagram \(D\) having \(n\) lines between \(p\) points, following Rushbrooke and Wood,

\[
(D) = Y^p \sum_{\text{perm}} \text{tr}(P) \cdots (P),
\]

where each bracket is a Schrödinger exchange operator \(P_{ij}\) which corresponds to the line joining points \(i\) and \(j\) in the diagram \(D\) and \(\sum_{\text{perm}}\) sums over all different permutations in the order of appearance of the brackets.

The occurrence factor of a diagram on a lattice has the same meaning as the lattice constant of a graph. The only difference is that for graphs we speak of diagrams which have at most one line connecting a pair of points. Some typical examples of the relation between the occurrence factors of diagrams and lattice constants of graphs are shown in Fig. 2. As mentioned in Sec. III, lattice constants of disconnected graphs can be expressed in terms of lattice constants of connected graphs. Let \(\Lambda_n\) signify that part of \(\Lambda\) which is of \(n\)th order in the lattice constants of connected graphs. We can then write

\[
(\sigma^x) = \Lambda_1(\sigma^x) + \Lambda_2(\sigma^x) + \cdots.
\]

As shown in the section on the cluster expansion method, Eq. (35), any extensive quantity, such as \(\ln Z\) or \(\chi\) is of first order in lattice constants of connected graphs. Hence by Eq. (12),

\[
\ln Z = N\ln Y + \sum_{n=1}^\infty K^n \Lambda_n(\sigma^x).
\]

Those parts of higher order in lattice constants of connected graphs will cancel exactly when transformed from \(Z\) to \(\ln Z\). Comparing Eqs. (14) and (69), we have

\[
e_n = \Lambda_1(\sigma^x) = \sum_{i=1}^n \Lambda_i[D_i](D_i).
\]

In the limit \(N \to \infty\), lattice constants of connected graphs will be directly proportional to \(N\). \(\Lambda_1\) then means nothing more than "the part proportional to \(N\".

C. Low-Field Susceptibility

When a finite external magnetic field is applied, the partition function can be written in the form

\[
\ln Z = N\ln Y + K \Lambda_1(\sigma^x + \alpha Q)^x.
\]

Since \(\sigma^x\) and \(Q\) commute and \(\langle \sigma^x Q \rangle = 0\), it is easy to show that

\[
\chi = \lim_{B \to 0} k_B T \frac{\partial^2}{\partial H^2} \ln Z
\]

\[
= \frac{k_B^2}{2} \sum_{n=0}^\infty K^n \Lambda_n(\sigma^x Q^2).
\]

For \(n = 0, \langle Q^2 \rangle = 3X/3\). Comparing Eqs. (24) and (72) yields

\[
a_0 = (3X/3) \Lambda_0(\sigma^x Q^2).
\]

The situation in calculating \(\langle \sigma^x Q^2 \rangle\) is similar to that involved in \(\sigma^x\). We again have a correspondence between terms \(P_{ij}\) produced on expanding \(\sigma^x\) and diagrams of \(n\) lines on the lattice, but now, besides the \(n\) lines, a diagram will contain two crosses. Those are denoted +, and are placed on those sites from which we have extracted terms like \(S_d S_d\) from \(Q^2\). When two crosses coincide, we speak of a double cross, denoted *.

There are five kinds of ways in which two crosses may be added to a diagram \(D\):

(a) \(D^x\), a double cross superposed on \(D\),

(b) \(D^{xx}\), two crosses superposed on different sites of \(D\),

(c) \(D^+^*\), one cross superposed on \(D\), another not on \(D\),

(d) \(D^+\), a double cross not superposed on \(D\),

(e) \(D^+^*\), two separated crosses not superposed on \(D\).

Since \(\langle S_d \rangle = 0\) and \(\langle S_d^2 \rangle = X/3\), by the trace property of the direct product, we immediately find that diagrams (c) and (e) have zero contributions to \(\langle \sigma^x Q^2 \rangle\). That is, diagram (d) contributes an amount \((X/3)(D)\) to \(\langle \sigma^x Q^2 \rangle\). Let \(p\) be the number of points contained in the diagram \(D\). Then we have that the occurrence factor for diagram (d), \([D]\) contributes an amount \((X/3)(D)\) to \(\langle \sigma^x Q^2 \rangle\). Therefore, as far as terms of first order in lattice constants of connected graphs are concerned, it is equivalent to say that the diagram (d) has occurrence factor \([D]\) associated with the weighting factor \(-[\sigma^x]\).

For diagram (a) the double cross can be superposed on any of the \(p\) points. For diagram (b) there are \(p(p - 1)\) ways to superpose the two crosses on \(D\). If

\[
[D] = \begin{bmatrix} \sigma^x \end{bmatrix},
\]

\[
[D^+^*] = \begin{bmatrix} \sigma^x \end{bmatrix}^2 = [2[D]]
\]

\[
[D^+^*] = \begin{bmatrix} \sigma^x \end{bmatrix},
\]

\[
[D^{xx}] = \begin{bmatrix} \sigma^x \sigma^x \end{bmatrix}
\]


FIG. 2. Examples of the relation between the occurrence factors of diagrams and lattice constants of graphs.
we sum up these $p^2$ diagrams, with occurrence factor $[D]$, their contributions to $\langle p^n Q^2 \rangle$, denoted $\langle DQ^2 \rangle$, will be

$$\langle DQ^2 \rangle = Y \sum_{\text{perm}} \text{tr}(\gamma_1(\cdots(\gamma_3 \gamma_5 \cdots \gamma_{p-1} \gamma_p))^{2}).$$  \hspace{1cm} (74)

Therefore, including all five kinds of diagrams, with occurrence factor $[D]$, the weighting factor of the diagram $D$ to $\langle DQ^2 \rangle$, denoted $\langle DQ^2 \rangle$, will be

$$\langle DQ^2 \rangle = (pX/3)(D).$$  \hspace{1cm} (75)

Hence

$$a_n = (3/X) \sum_{i=1}^{n} a_i [D_i] [\langle DQ^2 \rangle] - p/3/[D_i].$$  \hspace{1cm} (76)

where $p_i$ is the number of points in $D_i$. By rewriting the products $\langle DQ^2 \rangle$, as products of independent cycles, the traces in Eqs. (67) and (74) can be obtained from Eqs. (65) and (64). $\langle D \rangle$ and $\langle DQ^2 \rangle$ are then determined. Note that for the present Hamiltonian these five kinds of diagrams can be considered together and the calculation of the coefficients $\alpha_n$ is greatly simplified.

D. Further Theorems

If we express $\lambda \langle D \rangle$ in terms of lattice constants of connected graphs, denoted $[g_i]$, we can rewrite $\alpha_n$ and $a_n$ as follows:

$$e_n = \sum_i [g_i] e_i(g_i)$$

and

$$a_n = \sum_i [g_i] a_i(g_i),$$

where $\sum_i$ sums over all connected graphs $g_i$. We then prove the following:

Theorem 4:

$$e_n(g_i) = \alpha_n(g_i) = 0, \text{ if } n < \xi.$$  \hspace{1cm} (79)

Proof: This is obvious since those diagrams with occurrence factor containing $[g_i]$ must have $\xi$ lines or more, and they contribute to $e_n$ and $a_n$ for $n \geq \xi$.

Theorem 5: If we define cycles of diagrams similar to those for graphs presented in Sec. III, then for diagrams containing $n$ lines and $c$ independent cycles their contributions to $e_n$ and $a_n$ contain terms $Y^{-c}$, where $Y$ ranges from 0 to $c$, but $2n > n$.

Proof: As mentioned in Sec. IV, for any group element $P$, if $f, g$ both belong to the same cycle in $P$ and has one less than $n$ if $f, g$ belong to different independent cycles in $P$. Assume that the diagram contains $p$ points. The identity element will have $p$ independent cycles, namely, (1) (2) \cdots (p). Consider one of the products $\langle \gamma_1 \gamma_2 \cdots \gamma_n \rangle$.

\hspace{1cm} FIG. 3. Let the first graph be $\gamma_1$. All diagrams of five lines with occurrence factors containing $[g_i]$ are shown. This illustrates the fact that diagrams of $\xi$ lines with occurrence factors containing $[g_i]$ consist of subgraphs of $g_i$. Of $n$ factors $(ij)$ occurring in Eqs. (67) and (74), and multiply successively to the identity element, first, the $n$th factor, then the $(n-1)$th factor, etc., and finally the first factor. Since each multiplication either decrease or increase the number of different independent cycles by 1, the resultant product will contain $p - n + 2k$ different independent cycles. Here $k$ is the number of times that $ij$ happen to occur in the same cycle in the product which is to be multiplied by $(ij)$. This can happen only when $ij$ are joined by paths other than the line $ji$, or $ij$ must be a line of a cycle. Therefore, $k < c$. Also, the number of independent cycles may not be greater than $p$, $2k < n$. Equation (63) says that for any permutation containing $l$ different independent cycles its trace in the $(2n + 1)^{\text{st}}$-dimensional matrix representation is $\gamma^i$. Theorem 5 then follows from a consideration of Eqs. (63), (67), (70) and Eqs. (64), (74), and (76).

A consequence of this theorem is that $e_n(g_i)$ and $a_n(g_i)$ contain terms $Y^{-c}$, $Y^{-c+2}$, \cdots, where we can write as

$$e_n(g_i) = \gamma^{c} g_i Y^{n} + \gamma^{c+2} g_i Y^{n+2} + \cdots + \gamma^{c+4} g_i Y^{n+4} \gamma^{-1} \left[ \text{or } \gamma^{c+4} g_i \right]$$

and

$$a_n(g_i) = \gamma^{c} g_i Y^{n} + \gamma^{c+2} g_i Y^{n+2} + \cdots + \gamma^{c+4} g_i Y^{n+4} \gamma^{-1} \left[ \text{or } \gamma^{c+4} g_i \right].$$

Theorem 6:

$$\gamma^{c+2k} g_i = \alpha^{c+2k} g_i = 0, \text{ for } k > c_i + n - \xi,$$

where $c_i$ is the number of independent cycles and $\xi$ is the number of lines in the connected graph $g_i$.

Proof: Consider first the case that $n = \xi$. Diagrams of $\xi$ lines which have an occurrence factor containing $[g_i]$ are those which consist of subgraphs of $g_i$, and hence cannot have more cycles than $g_i$. For example, let $g_i$ be the connected graph in Fig. 3. Other diagrams of five lines with occurrence factor containing $[g_i]$ are those disconnected graphs shown in the figure. Hence from Theorem 5, Theorem 6 is proved for the case $n = \xi$. When $n > \xi$, we can superspose the additional $n - \xi$ lines on $g_i$. Each line supersposed on $g_i$ is equivalent to forming an additional cycle in the resultant diagram, and the maximum number of independent cycles will be $c_i + n - \xi$, in some of the $n$ diagrams which have occurrence factors containing $[g_i]$. This then completes the proof of Theorem 6.

Theorem 7:

$$\alpha^{c+2k} g_i = 0 \text{ for all } g_i.$$  \hspace{1cm} (83)

Proof: Consider a diagram $D$ of $p$ points and $n$ lines which has occurrence factor containing $[g_i]$. Those products $\lambda \langle D \rangle$ in Eqs. (67) and (74) which contribute to $\alpha^{c+2k}$ must be equal to the identity operator. Since $\text{tr}Q^2 = pX/3$, Eq. (83) follows from Eq. (75).

Theorem 8:

$$\alpha^{c+2k} g_i = \frac{1}{2} \alpha^{c+2k} g_i = \text{for all } g_i.$$  \hspace{1cm} (84)
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Proof: Those products in Eqs. (67) and (74) which contribute to $d(j)^2$ and $d(j)^3$ must contain $p-1$ cycles, or belong to the class $1^p-3^2$. From Eqs. (63) and (64), for permutations $P$ belonging to the class $1^p-3^2$,

$$\text{tr}P \left( \sum_{i=1}^{p} S_i \right) = \frac{N}{3} (p+2) Y^{p-1}$$

and

$$\text{tr}P = Y^{p-1}. \quad (85)$$

From Eqs. (67), (74), and (75), the contributions of these products to $(d_j^2)$ and $(3/X)(d_j^2)$ will be $Y^{-1}$ and $2Y^{-1}$, respectively. Theorem 8 then follows.

VI. CALCULATIONS OF SERIES COEFFICIENTS

A. Clusters Up to Seven Sites

From the discussion in Sec. III we know that in order to obtain the high temperature series for general lattices up to the seventh power in $K=J/k_B T$, we must calculate the corresponding series for clusters having up to seven lines. For computational convenience we group these clusters into two categories, those having up to seven points and those containing eight points. Consider first clusters with up to seven points and seven lines. They are labeled in the graph dictionary order such that Eq. (33) is satisfied.12

To calculate the coefficients in the zero-field partition function and the low-field susceptibility series for finite clusters we make use of Eqs. (15) and (25), in which the quantities $\text{tr}0^n$ and $\text{tr}0^n Q^2$ for $n \leq 7$ are obtained from Theorem 2 by setting $R$ equal to the unit matrix and $Q^2$, respectively. Now $(d_j^0)$ in Eq. (50) is a sum of Schrödinger exchange operators which correspond to the lines in each cluster, $h_k$ and $\chi_k^2$ are available in a number of texts which deal specifically with the symmetric group.13 The values of $\text{tr}P_j$ and $\text{tr}P_j Q^2$ can be calculated by Eqs. (63) and (64). Corresponding to $0^{(1)(p0)}$ is a sum of interchanges in the irreducible representation $\nu$. The explicit form of the permutation matrices in any irreducible representation can be obtained by the technique introduced by Yamanouchi.14

For two conjugate representations $\text{tr}0^n$ are related to each other by Eq. (53) and hence only one of the traces need be calculated. The quantities $\text{tr}((d_j^0)+n)$ are calculated on a computer for all required clusters with up to seven points. The size of the greatest matrix involved in the calculation is of dimension $35 \times 35$.

B. Clusters Containing Eight Sites

For clusters with seven lines and eight sites, we can still evaluate the high temperature series following the procedure just described. However, for the symmetric group of degree eight some of the irreducible representations are of dimension $70 \times 70$ and the trace calculation on a computer would have been too expensive for us. From Eq. (26) we have that clusters with eight lines and eight points contain no cycles. It then follows immediately from Theorem 4 that for these clusters $e_5(g_j^4) = e_5(g_j^5) = 0$. For $n \leq 6$ and from Theorem 6 that $e_7(g_j^6)$ and $e_7(g_j^6)$ can be written in the form

$$e_7(g_j^6) = e_7(g_j^6) Y^{-7} \quad (87)$$

and

$$a_4(g_j^6) = a_4(g_j^6) Y^{-7}. \quad (88)$$

For $S = \frac{1}{2}$ the exchange interaction Hamiltonian is identical to the Heisenberg Hamiltonian, and the high temperature series for these two models are the same. It is known that for the Heisenberg model graphs with $n$ lines containing no cycles will not contribute to $e_n$ and the only graph with $n$ lines containing no cycles which contributes to $a_n$ is the simple chain.15 Therefore, $e_7(g_j^6) = a_4(g_j^6) = 0$ for all clusters of eight points with the exception that for the simple chain $a_4(g_j^6) = 10 080 Y^{-7}$. This value was obtained from Eq. (88) together with the results of Domb and Wood15; for the case of spin $\frac{1}{2}$ and for the simple chain of eight points they obtained $a_4(g_j^6) = 10 080 \times 2^{-7}$.

VII. SERIES RESULTS

The simplest way to represent the series coefficients $e_n$ and $a_n$ [see Eqs. (14) and (24)] for any finite cluster or crystal lattice is in the form of Eqs. (77) and (78) together with Eqs. (80) and (81). The number of graphs which contribute to $e_n = a_n$ are 1, 1, 2, 4, 7, 15, and 29, respectively, while the numbers of graphs that contribute to $a_1 - a_n$ are 1, 2, 4, 8, 16, 32, respectively. The values of $e_n(g_j^1)$ and $a_n(g_j^1)$ for these graphs are given in Appendix D of Ref. 12.

For regular lattices, e.g., body-centered cubic and face-centered cubic lattices with $N \rightarrow \infty$, the lattice constants of connected graphs are proportional to $N$, and lattice constants of open graphs can be expressed in terms of the lattice constants of closed graphs and the coordination number of the lattice. We rewrite Eqs. (14) and (24) in the form

$$\ln Z/N = \ln Y + \sum_{n=2}^{\infty} e_n Y^n, \quad (89)$$

and

$$X = \frac{C}{T} \left( 1 + \sum_{n=1}^{\infty} a_n K^n \right), \quad (90)$$

where $C = N(gj)^2 X/3k_B$. Note that the numbers $n$ do not appear in these expressions and that $e_1$ has been set equal to zero by adjusting the zero of energy such that the internal energy is equal to zero at infinite temperature, that is, the constant $Y^{-1}$ is subtracted from $F(T)$ to make $X$ traceless. The coefficients $e_n$ and $a_n$ will be written in the form

$$e_n = e_n^{(a)} Y^{-n} + e_n^{(s=2)} Y^{-n-2} + \cdots$$

and

$$a_n = a_n^{(a)} Y^{-n} + a_n^{(s=2)} Y^{-n-2} + \cdots$$

The various quantities $e_n^{(a)}$ and $a_n^{(a)}$ are then given below:

$$e_0^{(a)} = \frac{1}{2}(a + 1), \quad e_0^{(s=2)} = -\frac{1}{2}(a + 1),$$

$$e_1^{(a)} = -\frac{1}{2}[(a + 1) - 6p_g],$$

$$e_2^{(a)} = \frac{1}{2}[(a + 1) - 6p_g], \quad e_2^{(s=2)} = -\frac{1}{12}[(a + 1)^2 - 12p_g],$$

$$e_0^{(s=2)} = \frac{1}{4}(a + 1)(a + 4) - 84p_g + 24p_4,$$


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\[
e^{(0)}_4 = - \frac{1}{4} [(a + 1) - 24 p_3 + 4 p_4],
\]
\[
e^{(1)}_5 = \frac{1}{6} [(a + 1)(5a + 7) - 15 p_2(2a + 7) + 40 p_4 + 30 p_{5a}],
\]
\[
e^{(0)}_5 = - \frac{1}{15} [(a + 1)(a + 2) - 3 p_3(2a + 31) + 50 p_4 + 12 p_5 + 30 p_{5a}],
\]
\[
e^{(1)}_6 = \frac{1}{6} [(a + 1) - 60 p_3 + 40 p_4 - 10 p_5 + 20 p_{5a}],
\]
\[
e^{(0)}_6 = \frac{1}{120} [(a + 1)(110^2 + 20a + 8) + 36 p_3(7a + 4)
+ 72 p_4 + 132 p_{5a} + 96 p_{6a}],
\]
\[
e^{(1)}_7 = - \frac{1}{720} [(a + 1)(110^2 + 110a + 68) - 108 p_3
\times (19a + 23) + 24 p_4(20a + 93) - 600 p_5 + 3132 p_{5a} - 360 p_{6a} - 240 p_{6c}
+ 1536 p_{6d}],
\]
\[
e^{(0)}_8 = \frac{1}{4} [(a + 1)(3a + 4) + 6 p_3(10a + 51) + 8 p_4
\times (2a + 39) - 140 p_5 + 364 p_{5a} + 24 p_{6a} - 60 p_{6c} + 8 p_{6d} + 192 p_{6e}],
\]
\[
e^{(1)}_9 = - \frac{1}{1440} [(a + 1)(110^2 + 2356 + 385c + 136) - 422 p_3
\times (37a^2 + 280 b + 18) + 560 p_4(50a + 6) - 910 p_5 + 28 p_{5a}(77c + 310) - 1260 p_{6a} - 1456 p_{6b} + 2352 p_{6c} + 3864 p_{6d} - 798 p_{7e} - 840 p_{7f}
- 644 p_{7g}],
\]
\[
e^{(0)}_{10} = \frac{1}{1440} [(a + 1)(35a^2 + 175c + 88) - 6 p_3
\times (37a^2 + 1128 a + 348) + 80 p_4(421 a + 78)
- 10 p_{5a}(600a + 343) + 532 p_{5a}(280 a + 234) + 720 p_5 + 2060 p_{6a} - 380 p_{6b} + 2256 p_{6c} + 912 p_{6d} + 360 p_{7a} + 360 p_{7b} - 1314 p_{7c} - 240 p_{7d} + 360 p_{7e} - 1000 p_{7f} - 1532 p_{7g}],
\]
\[
e^{(1)}_{11} = - \frac{1}{103080} [(a + 1)(20 + 1)^2 - 3 p_3(30a + 59) + 48 p_4(a + 7)
- 5 p_{5a}(2a + 47) + 10 p_{5a}(2a + 59) + 84 p_{6d}
- 192 p_{6e} - 216 p_{6f} + 352 p_{6g} + 576 p_{6h} - 12 p_{7a} + 30 p_{7b} + 30 p_{7c} + 68 p_{7d} - 4 p_{7e} + 30 p_{7f}
- 120 p_{7g} - 96 p_{7h}],
\]
\[
e^{(2)}_{12} = \frac{1}{6} [(a + 1) - 162 p_3 + 280 p_4 - 210 p_5 + 476 p_{5a}
+ 84 p_{6a} - 168 p_{6b} - 182 p_{6c} + 504 p_{6d} - 14 p_{7b}
+ 28 p_{7c} + 28 p_{7d} - 56 p_{7e} + 28 p_{7f} - 84 p_{7g}
- 84 p_{7h}],
\]
\[
e^{(0)}_{13} = (a + 1), \quad a^{(0)}_1 = (a + 1)(a - 1),
\]
\[
e^{(1)}_{14} = - \frac{1}{6} [(a + 1) - 6 p_{3a}],
\]
\[
e^{(2)}_{15} = [(a + 1)(a - 1) - 18 p_{3a}], \quad a^{(2)}_1 = - \frac{1}{3} [(a + 1)(3a - 8) - 48 p_3(a - 5) - 56 p_{3a}],
\]
\[
e^{(3)}_4 = [(a + 1)(a - 1)^3 - 18 p_{3a}(2a - 5) - 32 p_{3a}],
\]
\[
e^{(4)}_5 = \frac{1}{6} [(a + 1)(5a + 4) - 15 p_3(2a + 7) + 40 p_4
+ 30 p_{5a}],
\]
\[
e^{(5)}_6 = - \frac{1}{15} [(a + 1)(a + 2)^2 - 6 p_{3a}(6 a + 34) - 60 p_{3b} + 120 p_{3c} - 360 p_{3d} - 840 p_{3e} + 180 p_{3f} + 240 p_{3g}
+ 720 p_{3h} - 1260 p_{4a} - 1456 p_{4b} + 2352 p_{4c} + 3864 p_{4d} - 798 p_{5e} - 840 p_{5f}
- 644 p_{5g}],
\]
\[
e^{(6)}_7 = - \frac{1}{1530} [(a + 1)(40a^2 + 200 + 18) + 560 p_4(50a + 6) - 910 p_5 + 28 p_{5a}(77c + 312) - 1260 p_{6a} - 1456 p_{6b} + 2352 p_{6c} + 3864 p_{6d} - 798 p_{7e} - 840 p_{7f}
- 644 p_{7g}],
\]
\[
e^{(7)}_8 = - \frac{1}{10308} [(a + 1)(400a + 205a^2 + 3470 + 264)
- 6 p_3(180a + 2 + 210a + 18) + 560 p_4(50a + 6) - 910 p_5 + 28 p_{5a}(77c + 312) - 1260 p_{6a} - 1456 p_{6b} + 2352 p_{6c} + 3864 p_{6d} - 798 p_{7e} - 840 p_{7f}
- 644 p_{7g}],
\]
\[
e^{(8)}_9 = \frac{1}{6} [(a + 1)(a - 1) - 6 p_{3a}],
\]

EXCHANGE INTERACTION MODEL OF FERROMAGNETISM

\[ a q^4 = [(0 + 1)(0 - 1)^3 - 18p_3(50^4 - 320^2 + 840^2) - 1100 + 62] \]
\[ - 128p_q(a^3 - 6c^2 + 14o - 14) - 50p_a \]
\[ \times (3o^2 - 16o + 28) + 4p_{sa}(990^2 - 540^2 + 971) \]
\[ - 144p_q(a^4 - 4) + 384p_q(a^4 - 4) + 2p_{gq} \]
\[ \times (188o - 777) + 144p_{sa}(a^4 - 4) - 1248p_{ad} \]
\[ \times (a - 4) - 98p_q + 525p_{7c} + 252p_{7c} - 506p_{7c} \]
\[ + 72p_{7d} + 96p_{7c} + 260p_{7j} - 58p_{7e} - 34p_{7b} \].

(94)

Here the \( p_{sa} \) are lattice constants for closed graphs per lattice site and \( q = \sigma + 1 \) is the coordination number of the lattice. The values \( p_{sa} \) and \( q \) for various crystal lattices are well known. For convenience, the coefficients \( e_n \) for the cubic lattices and for several spin values are shown in Appendix A, and values of \( a_n \) for the cubic lattices and for a number of two dimensional lattices are given in Appendix B. It is generally found that, similarly to the Heisenberg model, \( ^{11} \) the coefficients in these series expansions increase in smoothness as \( q \) increase. However, the series coefficients for the present model are much more irregular than those of the Heisenberg model, especially for large values of spin.

VIII. CHECKING PROCEDURES

Since there are numerous possibilities for errors to be made in the computations, it is important to be able to check the general expressions for the coefficients \( e_n \) before using them to estimate critical parameters. We have considered a large number of finite clusters of eight lines. For these clusters we can calculate the zero-field partition function and the low-field susceptibility series from Eqs. (93) and (94) by substituting the appropriate lattice constants. Comparing the results with those obtained from a direct machine calculation as described in Section VI yields full agreement up to \( c_\gamma \) and \( a_2 \) in all cases.

By observing the general expressions for \( e_n^{(a)} \) and \( a_n^{(a)} \) that we obtained [Eqs. (93) and (94)], we see that

\[ \sum_n e_n^{(a)} = 0, \quad m = n, n - 2, n - 4, \ldots, 1 \quad \text{(or 0)}, \quad (95) \]

and

\[ e_1^{(a)} = \tfrac{1}{2}a_1^{(a)}. \quad (96) \]

These two equations hold for all \( n \) and provide an additional check on our results. Equation (96) has been proved in Theorem 8, while Eq. (95) is a necessary consequence of the fact that, for \( S = 0 \), \( \ln z = 0 \).

As a final check, we see that when we set \( S \) equal to \( \frac{1}{2} \) and \( 1 \), respectively, our general results for \( e_\gamma \) and \( a_2 \) reduce exactly to those obtained previously by Domb and Wood 15 and by Allan and Betts, 16 respectively.

IX. ANALYSIS OF SERIES

A. Estimates of Curie Temperatures and Critical Indices

The Curie temperature \( T_\gamma \) and the critical index \( \gamma \) for the susceptibility series are defined by

\[ \chi \sim (T - T_\gamma)^{\gamma}, \quad \text{for} \quad T \rightarrow T_\gamma^+. \quad (97) \]

or

\[ \sim (K_C - K)^{-\gamma}, \quad \text{for} \quad K \rightarrow K_C, \quad (98) \]

where \( K_C \) is \( J/\hbar g T_C \). For the face-centered cubic lattice \( T_C \) and \( \gamma \) were first estimated by means of the ratio method. From Eq. (98) the coefficients \( a_n \) in Eq. (96) have the property that for large \( n \)

\[ \frac{a_n}{a_{n-1}} = \left( \frac{a_n}{a_{n-2}} \right)^{1/2} \frac{1}{K_C \left( 1 + \gamma - \frac{1}{n} \right)}. \quad (99) \]

If we plot the two sets of values \( a_n/a_{n-1} \) and \( (a_n/a_{n-2})^{1/2} \) vs \( 1/n \), each of the plots tends to a straight line as \( n \) increases and intersects with \( 1/n = 0 \) at \( K_C \) with slope \( (\gamma - 1)/2 \). If we plot \( a_n \) vs \( 1/n \), the plot also intersects with \( 1/n = 0 \) at \( K_C \) but does not approach the intersection in a simple linear fashion for large \( n \). Figure 4 illustrates these plots for the face-centered cubic lattice and for \( S = 1 \). The Curie temperature and the critical index can also be estimated by the method of Padé approximants. 17 The \([M, N] \) Padé approximant to a polynomial \( f(z) \) is given by \( P(z)/Q(z) \), where \( P(z) \) and \( Q(z) \) are polynomials of degree \( N \) and \( M \), respectively, such that \( f(0) = 1 \) and \( f(1) \) agrees with the expansion of \( P(z)/Q(z) \) for the first \( M + N + 1 \) terms.

If the divergence of \( \chi \) at \( K_C \) is in the form shown in Eq. (98), then

\[ \chi^{(a)}/\chi = (K_C - K)^{-1}, \quad (100) \]

and

\[ \chi^{(a)}/\chi = (K_C - K)^{-1}, \quad (101) \]

and

\[ \chi^{(a)}/\chi = \frac{d}{dz} \left( \frac{d}{dz} \right) \frac{1}{\phi_{\text{lin}}(\ln x)} = 1 + \frac{1}{\gamma}. \quad (102) \]

These equations suggest four methods of determining \( K \) and/or \( \gamma \) from \( \chi^i \):

FIG. 4. Plots of \( (a_n/a_{n-1})^{1/2}, (a_n/a_{n-2})^{1/2} \), and \( (a_n/a_{n-1})^{-1} \) for the face-centered cubic lattice, \( S = 1 \).
(a) Choosing \( \gamma, K_C \) can be presented by appropriate poles of the Padé approximants to \((1/y)^{1/y}\).

(b) Choosing \( K_C, \gamma \) can be obtained by evaluating Padé approximants to \((K_C - K)/\chi^2\) at \( K = K_C \).

(c) For a Padé approximant to \( \chi^2/\chi \) the appropriate pole gives \( K_C \) and the residue at this pole gives \(-y\).

(d) Evaluating Padé approximants to \( \chi^2/\chi \) at \( K = K_C \) gives \( 1 + 1/y \).

For the face-centered cubic lattice and for \( S = \frac{1}{2} \), we have estimated \( K_C \) and \( \gamma \) by all four methods. In method (a) instead of tabulating the various approximants in Padé table for several values of \( \gamma \) we have plotted the various approximants of \( K_C \) as functions of \( \gamma \) in the \( K_C - \gamma \) plane. The proper values of \( \gamma \) and \( K_C \) are easily obtained from these curves in the region in which the various approximants coalesce.

Figure 5 shows several of these curves for the face-centered cubic lattice and for \( S = 1 \). In method (b) the approximants of \( \gamma \) as functions of \( K_C \) are also plotted in the \( K_C - \gamma \) plane. These curves are roughly parallel to and close to curves obtained from method (a) in the region of interest. The various approximants in methods (c) and (d) are rather irregular. However, they are not inconsistent with what methods (a) and (b) yield. The estimates of \( K_C \) and \( \gamma \) from Padé analysis are also in agreement with estimates based on the various ratio tests. The final estimates of \( \gamma \) and \( T_C \) are given in Figures 6 and 7, respectively.

These results can be simply described by the equations

\[
k_B T_C/J = 1.19 + 5.70y^{-1} \tag{103}
\]

and

\[
\gamma = 0.48 + 2.16y^{-1}. \tag{104}
\]

Equations (103) and (104) hold for all \( S \) with the exception that \( \gamma = 1.41 \pm 0.02 \) for \( S = \frac{1}{2} \).

For the body-centered cubic lattice and the simple cubic lattice the series coefficients are in general too irregular to estimate both \( K_C \) and \( \gamma \) either by ratio tests or by the Padé approximant method. However, within our precision, \( \gamma \) seems to be the same for all of the cubic lattices for each \( S \). If the values of \( \gamma \) for the face-centered cubic and the simple cubic lattices are chosen to be the same as those of the face-centered cubic lattice, then an estimate of \( K_C \) from Padé approximants to \((1/y)^{1/y}\) suggests that for all of the cubic lattices \( T_C \) can be described to within a few percent by

\[
k_B T_C/J = 0.547(y - 1.6)(y^{-1} + 0.21). \tag{105}
\]

The estimates of \( T_C \) for the face-centered cubic and
the simple cubic lattices are also contained in Figure 7.

For the two-dimensional lattices no consistent results could be obtained since the series are erratic and consist of positive and negative terms.

We have also investigated the specific heat series. The scatter in the various series and the internal energy series obtained from Eq. (18) and (19) were also analyzed by the Padé approximant method. For the face-centered cubic lattice we found that

\[
\frac{(S_\infty - S_C)}{S_\infty} = 0.494 - 0.353 V^{-1}
\]

and

\[
\frac{(E_\infty - E_C)}{JN} = 3.98 - 5.04 V^{-1},
\]

for all \( S \) with the exception that, for \( S = \frac{1}{2} \), \( \frac{(E_\infty - E_C)}{JN} = 1.60 \). Here \( S_\infty = N g_\eta \ln \eta \) and \( E_C = 0 \) are the entropy and the internal energy, respectively, at infinite temperature. For the body-centered cubic and the simple cubic lattices the convergence of the Padé approximants is in general fairly poor. However, the critical change of the entropy for the body-centered cubic and the simple cubic lattices seem also to vary linearly in \( V^{-1} \) and for each spin value it is higher than that for the face-centered cubic lattice by an amount 0.025 and 0.055, respectively.

**B. Critical Energy and Critical Entropy**

Making use of the values of \( K_c \) in Eq. (105) the entropy series and the internal energy series obtained from Eq. (18) and (19) was also analyzed by the Padé approximant method. For the face-centered cubic lattice we found that

\[
\frac{(S_\infty - S_C)}{S_\infty} = 0.494 - 0.353 V^{-1}
\]

Here \( D_n(S) \) is a quantity which is independent of both lattice and temperature and \( W \) is given by Eq. (56). This means that for a given lattice, all of the \( x_n \to \infty \) at the same \( T_c \), in exactly the same way.

Since the (dipolar) susceptibility \( \chi \) can also be written in the form

\[
\chi = \frac{1}{2} g^2 \beta^2 \sum_{i \neq j} \langle S_i^z S_j^z \rangle, \tag{114}
\]

it is really necessary to investigate quantities of the form \( \sum_{i \neq j} \langle S_i^z S_j^z \rangle \) for \( 1 \leq n \leq 25 \). However, for both computational and theoretical reasons, we have restricted our attention to the single quantity \( \sum_{i \neq j} \langle S_i^z S_j^z \rangle \). Here the prime in the double sum over \( i \) and \( j \) means that terms for which \( i = j \) are to be excluded. The following theorem is also proved in Ref. 20.

**Theorem 10:**

\[
\sum_{i \neq j} \langle S_i^z S_j^z \rangle = \frac{3}{2} \chi_n \tag{115}
\]

where \( \chi_n \) is given by Eq. (47) and \( \chi_n^2 = \text{tr} P_n \) is given by Eq. (63). The labor required to derive \( \chi_n \) by this approach is about the same as the previous approach which made use of Theorem 2.

The numerical results for the critical properties of the exchange interaction model have been shown in the previous section. In order to study the possibility of such transitions we shall consider first the following modified Hamiltonian:

\[
\frac{1}{2} \sum_{i \neq j} \delta_{ij} \xi_{ij},
\]

where \( \xi_{ij} = -J \sum_{(\eta)} P_{ij} = -J \delta_{ij}, \)

\[
Q_n = \sum_{i=1}^{N} S_i^z, \quad n = 1, 2, \ldots, 2S_
\]

and \( \xi \) is some (fictitious) external magnetic field. We then define a generalized susceptibility \( x_n \) by

\[
x_n = \lim_{c \to 0} \frac{1}{c^2} \frac{\partial^2}{\partial \xi^2} \ln \text{tr} e^{-S_n \xi}. \tag{111}
\]

By definition \( x_1 \) is \( x_C \). Since \( \Phi \) and \( Q_n \) commute, as did \( \Phi \) and \( Q \), we have

\[
x_n = \beta \Delta(Q_n). \quad \tag{112}
\]

In Ref. 20 the following theorem is proved.

**Theorem 9:**

\[
x_n / x_1 = D_n(S) = (3/S)(W_{2n} - W_{2n}^2), \tag{113}
\]


\( S_d/S_o = 0.494 \quad O. \)

\( 7. \quad \)

\( 6. \quad \)

\( 5. \quad \)

\( 4. \quad \)

\( 3. \quad \)

\( 2. \quad \)

\( 1. \quad \)

\( 0. \quad \)
observed value of the critical index \( \gamma_{\text{obs}} \) is related to the theoretical value by

\[
\gamma_{\text{obs}} = \gamma / (1 - \alpha),
\]

where \( \alpha \) is the theoretical value of the critical exponent of the specific heat series defined by

\[
C_v \sim (T - T_c)^{-\alpha}, \quad \text{for } T \to T_c^+.
\]

For \( 0 < \alpha < 1, \gamma_{\text{obs}} > \gamma \). This then shows that the theoretical estimates of \( \gamma \) when renormalized by the factor \((1 - \alpha)^{-1}\) will be closer to the experimental values for the present model, while for the Heisenberg model the renormalized values of \( \gamma \) are in even further disagreement with the experimental values. This suggests that the present model may have more physical significance than originally thought.

(4) For the present model the fraction of the total entropy change occurring above \( T_c \) is higher than that of the Heisenberg model.

Hence we see that the inclusion of nonlinear terms in the Hamiltonian significantly affects the theoretical estimates of the critical parameters of magnetic systems.

The fact that \( T_c \) for the present model is lower than that of the Heisenberg model should be useful in a study of the possibility of a phase transition for the two-dimensional Heisenberg ferromagnet. If we can show that \( T_c > 0 \) for the two-dimensional exchange interaction model then there will be phase transitions for the two-dimensional Heisenberg model. However, as was previously mentioned, for large spin and/or for small coordination number, the series coefficients for the low-field susceptibility series are irregular and estimates of critical parameters from the high temperature series become quite inaccurate. It is then necessary that even more terms in the high temperature series be obtained.

**APPENDIX A: VALUES OF \( c_s \) FOR SEVERAL CRYSTAL LATTICES**

<table>
<thead>
<tr>
<th>Lattice Type</th>
<th>( S = \frac{1}{2} )</th>
<th>( S = 1 )</th>
<th>( S = \frac{3}{2} )</th>
<th>( S = 2 )</th>
<th>( S = \frac{3}{2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Face-centered cubic lattice</td>
<td>( c_2 ) 2.25</td>
<td>2.86667</td>
<td>2.8125</td>
<td>2.88</td>
<td>2.91667</td>
</tr>
<tr>
<td></td>
<td>( c_3 ) 2.25</td>
<td>2.86667</td>
<td>2.8125</td>
<td>2.88</td>
<td>2.91667</td>
</tr>
<tr>
<td></td>
<td>( c_4 ) 0.46875</td>
<td>-0.74074</td>
<td>-1.29976</td>
<td>-1.53696</td>
<td>-1.49089</td>
</tr>
<tr>
<td></td>
<td>( c_5 ) -1.3125</td>
<td>-1.48148</td>
<td>-1.29492</td>
<td>-1.10745</td>
<td>-0.95602</td>
</tr>
<tr>
<td></td>
<td>( c_6 ) 5.51542</td>
<td>4.34942</td>
<td>4.25171</td>
<td>4.12333</td>
<td>4.03917</td>
</tr>
<tr>
<td></td>
<td>( c_7 ) 22.57812</td>
<td>13.33333</td>
<td>8.65661</td>
<td>6.20234</td>
<td>4.9303</td>
</tr>
<tr>
<td>Body-centered cubic lattice</td>
<td>( c_2 ) 1.5</td>
<td>1.77778</td>
<td>1.875</td>
<td>1.92</td>
<td>1.94444</td>
</tr>
<tr>
<td></td>
<td>( c_3 ) -0.5</td>
<td>-0.39506</td>
<td>-0.3125</td>
<td>-0.256</td>
<td>-0.21605</td>
</tr>
<tr>
<td></td>
<td>( c_4 ) 0.4375</td>
<td>-1.08042</td>
<td>-1.73829</td>
<td>-2.0068</td>
<td>-2.24132</td>
</tr>
<tr>
<td></td>
<td>( c_5 ) 0.375</td>
<td>2.30453</td>
<td>2.37891</td>
<td>2.15962</td>
<td>1.91224</td>
</tr>
<tr>
<td></td>
<td>( c_6 ) 0.53125</td>
<td>1.28578</td>
<td>3.68896</td>
<td>5.25901</td>
<td>6.24193</td>
</tr>
<tr>
<td></td>
<td>( c_7 ) -0.46042</td>
<td>-6.28514</td>
<td>-9.35459</td>
<td>-9.96130</td>
<td>-9.68578</td>
</tr>
<tr>
<td>Simple cubic lattice</td>
<td>( c_2 ) 1.125</td>
<td>1.33333</td>
<td>1.40625</td>
<td>1.44</td>
<td>1.45833</td>
</tr>
<tr>
<td></td>
<td>( c_3 ) -0.375</td>
<td>-0.29629</td>
<td>-0.22437</td>
<td>-0.192</td>
<td>-0.12004</td>
</tr>
<tr>
<td></td>
<td>( c_4 ) -0.42187</td>
<td>-0.96396</td>
<td>-1.18652</td>
<td>-1.296</td>
<td>-1.35706</td>
</tr>
<tr>
<td></td>
<td>( c_5 ) 0.95025</td>
<td>1.03764</td>
<td>0.96387</td>
<td>0.84403</td>
<td>0.73737</td>
</tr>
<tr>
<td></td>
<td>( c_6 ) 0.72031</td>
<td>1.38354</td>
<td>2.10339</td>
<td>2.53984</td>
<td>2.80617</td>
</tr>
<tr>
<td></td>
<td>( c_7 ) -1.57969</td>
<td>-2.81536</td>
<td>-3.14886</td>
<td>-2.99927</td>
<td>-2.73934</td>
</tr>
</tbody>
</table>

**APPENDIX B: VALUES OF \( a_s \) FOR SEVERAL CRYSTAL LATTICES**

<table>
<thead>
<tr>
<th>Lattice Type</th>
<th>( S = \frac{1}{2} )</th>
<th>( S = 1 )</th>
<th>( S = \frac{3}{2} )</th>
<th>( S = 2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Face-centered cubic lattice</td>
<td>( a_2 ) 6.0</td>
<td>4.0</td>
<td>3.0</td>
<td>2.4</td>
</tr>
<tr>
<td></td>
<td>( a_3 ) 30.0</td>
<td>13.3333</td>
<td>7.5</td>
<td>4.8</td>
</tr>
<tr>
<td></td>
<td>( a_4 ) 158.0</td>
<td>45.1111</td>
<td>19.5</td>
<td>10.946</td>
</tr>
<tr>
<td></td>
<td>( a_5 ) 611.25</td>
<td>140.5555</td>
<td>53.25</td>
<td>26.4336</td>
</tr>
<tr>
<td></td>
<td>( a_6 ) 2658.55</td>
<td>456.03951</td>
<td>142.4</td>
<td>60.49024</td>
</tr>
<tr>
<td></td>
<td>( a_7 ) 11432.5125</td>
<td>1481.63621</td>
<td>372.44062</td>
<td>134.67033</td>
</tr>
<tr>
<td></td>
<td>( a_8 ) 40726.7262</td>
<td>4684.54243</td>
<td>988.30048</td>
<td>317.95349</td>
</tr>
<tr>
<td>Body-centered cubic lattice</td>
<td>( a_2 ) 4.0</td>
<td>2.66667</td>
<td>2.0</td>
<td>1.6</td>
</tr>
<tr>
<td></td>
<td>( a_3 ) 12.0</td>
<td>5.33333</td>
<td>3.0</td>
<td>1.92</td>
</tr>
<tr>
<td></td>
<td>( a_4 ) 34.66667</td>
<td>9.77778</td>
<td>3.83333</td>
<td>1.77066</td>
</tr>
<tr>
<td></td>
<td>( a_5 ) 95.83333</td>
<td>21.85185</td>
<td>8.20833</td>
<td>4.04373</td>
</tr>
<tr>
<td></td>
<td>( a_6 ) 268.7</td>
<td>45.19506</td>
<td>16.4125</td>
<td>8.99202</td>
</tr>
<tr>
<td></td>
<td>( a_7 ) 708.04166</td>
<td>93.46148</td>
<td>16.80729</td>
<td>3.55153</td>
</tr>
<tr>
<td></td>
<td>( a_8 ) 1893.28968</td>
<td>186.43935</td>
<td>24.68573</td>
<td>-3.13329</td>
</tr>
<tr>
<td>Simple cubic lattice</td>
<td>( a_2 ) 3.0</td>
<td>2.0</td>
<td>1.5</td>
<td>1.2</td>
</tr>
<tr>
<td></td>
<td>( a_3 ) 6.0</td>
<td>2.66667</td>
<td>1.5</td>
<td>0.96</td>
</tr>
<tr>
<td></td>
<td>( a_4 ) 11.0</td>
<td>2.88889</td>
<td>1.0</td>
<td>0.368</td>
</tr>
<tr>
<td></td>
<td>( a_5 ) 20.6250</td>
<td>4.72222</td>
<td>1.78125</td>
<td>0.80986</td>
</tr>
<tr>
<td></td>
<td>( a_6 ) 39.025</td>
<td>7.45185</td>
<td>3.34003</td>
<td>2.20864</td>
</tr>
<tr>
<td></td>
<td>( a_7 ) 68.77705</td>
<td>11.95037</td>
<td>6.61009</td>
<td>-0.48737</td>
</tr>
<tr>
<td></td>
<td>( a_8 ) 119.42976</td>
<td>19.01769</td>
<td>-1.84097</td>
<td>-3.98818</td>
</tr>
</tbody>
</table>


APPENDIX B: VALUES OF \( a_s \) FOR SEVERAL CRYSTAL LATTICES (Continued)

<table>
<thead>
<tr>
<th>Plane triangular</th>
<th>Plane square</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a_1 )</td>
<td>( a_1 )</td>
</tr>
<tr>
<td>( a_2 )</td>
<td>( 2.0 )</td>
</tr>
<tr>
<td>( a_3 )</td>
<td>( 1.3333 )</td>
</tr>
<tr>
<td>( a_4 )</td>
<td>( 1.8333 )</td>
</tr>
<tr>
<td>( a_5 )</td>
<td>( 0.50972 )</td>
</tr>
<tr>
<td>( a_6 )</td>
<td>( -4.82183 )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Plane triangular</th>
<th>Plane square</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a_1 )</td>
<td>( 3.0 )</td>
</tr>
<tr>
<td>( a_2 )</td>
<td>( 6.0 )</td>
</tr>
<tr>
<td>( a_3 )</td>
<td>( 8.5 )</td>
</tr>
<tr>
<td>( a_4 )</td>
<td>( 9.375 )</td>
</tr>
<tr>
<td>( a_5 )</td>
<td>( 11.025 )</td>
</tr>
<tr>
<td>( a_6 )</td>
<td>( 16.96458 )</td>
</tr>
</tbody>
</table>

\[ S = \sum a_s \]

Canonical Dynamics of Spinning Particles in Gravitational and Electromagnetic Fields*

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Department of Mathematics, University of Alberta, Edmonton, Canada

(Received 28 October 1971)

In terms of the canonical form and the connection form on the bundle of Lorentz frames \( F \) over a space–time manifold \( V \), a presymplectic form \( \omega \) is defined on \( F \), which induces a Poisson bracket on the set of real valued functions on the phase space of the system representing a spinning particle in an exterior gravitational and electromagnetic field. This structure coincides with the unique Poinsot invariant one for the free particle. Moreover, the projections into \( V \) of the integral manifolds of the kernel of \( \omega \) on \( F \) yield precisely the world lines of a spinning particle as observed for the dipole approximation of Dirac’s equations of motion for extended test bodies in general relativity.

1. INTRODUCTION

It is well known that if a classical system can be described by a Lagrangian \( L \), then not only the equations of motion are uniquely determined, but also a symplectic structure \( \omega \) on the set of all motions \( M \) (equivalent to the phase space) of the system. The 2-form \( \omega \) in turn induces a Lie algebra structure, the Poisson bracket, on the set of real valued functions on \( M \) (the “observables”). For several reasons it can be argued that, apart from the equations of motion, this symplectic structure is all that is needed (for the comparison with quantized systems) and it seems considerably more fundamental than the Lagrangian itself. For example, the Lagrangian is not quite unique for given equations of motion and given \( \omega \), and there are no Galilei or Poincaré invariant Lagrangians, but there are symplectic manifolds on which these groups act transitively. Moreover, to find a Lagrangian formulation it is necessary to separate phase space variables into position and momentum variables, a distinction which sometimes—e.g. in the case of a particle with spin—looks slightly artificial. One purpose of this paper is to illustrate, in the case of a test particle with spin in a curved space–time (a system described for fixed rest mass \( m \) and spin magnitude \( s \) at a given time \( t \) by initial data consisting of three position coordinates \( x \), the \( 4 \)-momentum \( p \), and the \( 4 \)-spin vector \( \sigma \), subject to the constraints \( d^\mu n = -m \), \( \sigma \cdot n = x^\mu n \), and \( d^\mu \sigma = 0 \), that it may be easier to guess a suitable form for the symplectic


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¶··· W. Opechowski, Physica 4, 181 (1937); 6, 1112 (1939).


¶····· The lattice constants defined here are the so-called high temperature lattice constant. See, for example, Ref. 8.


¶············ For \( S = 1 \) and the fcc lattice we get \( a_s = 4668.472 \). In private communication with Dr. Allan the mistake leading to the latter erroneous value has been discovered.


