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EXCHANGE INTERACTION MODEL OF FERROMAGNETISM

by

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ABSTRACT

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 γ are given by

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

and

$$\gamma = 0.48 + 2.16\ Y^{-1} \quad \text{for } S > \frac{1}{2};$$

$$= 1.41 \pm 0.02 \quad \text{for } S = \frac{1}{2},$$

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.

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I. 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 N particles of spin S with isotropic nearest-neighbor exchange interactions the Heisenberg Hamiltonian is given by

$$\mathcal{H} = -2J \sum_{<ij>} \underset{\sim}{S}_i \cdot \underset{\sim}{S}_j - g\mu H \sum_{i=1}^{N} S_{zi}, \qquad (1)$$

where J is the nearest-neighbor exchange constant, $\underset{\sim}{S}_i$ is the spin operator of an atom located at the lattice site labelled i, g is the gyromagnetic ratio, μ the Bohr magneton, H the z directed external magnetic field, and S_{zi} is the z-component of $\underset{\sim}{S}_i$. 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 $\underset{\sim}{S}_i \cdot \underset{\sim}{S}_j$ 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 $\underset{\sim}{S}_i \cdot \underset{\sim}{S}_j$.[1]

In order to study the properties of systems containing nonlinear terms, $J_n(\underset{\sim}{S}_i \cdot \underset{\sim}{S}_j)^n$, in the Hamiltonian, the Schrödinger exchange operator has been used to form an interaction Hamiltonian for a nearest-neighbor model of ferromagnetism,[2,3]

$$\mathcal{H} = -J \sum_{<ij>} P_{ij} - g\mu H \sum_{i=1}^{N} S_{zi}. \tag{2}$$

Here P_{ij} is the Schrödinger exchange operator and is a polynomial of degree 2S in $\underset{\sim}{S}_i \cdot \underset{\sim}{S}_j$:

$$P_{ij} = \sum_{n=0}^{2S} A_n(S) \, (\underset{\sim}{S}_i \cdot \underset{\sim}{S}_j)^n; \qquad i \neq j. \tag{3}$$

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

$$P_{ij} |m\rangle_i |m'\rangle_j = |m'\rangle_i |m\rangle_j, \tag{4}$$

or

$$P_{ij} O(i,j) = O(j,i) \, P_{ij}, \tag{5}$$

where $O(i,j)$ is any operator which contains the spin

operators of atoms i and j, and $|m\rangle_i$ and $|m\rangle_j$ are eigenstates of S_{zi} and S_{zj}, respectively. Schrödinger[4] has explicitly shown that

$$P_{ij} = (-1)^{2S} \{ 1 + \sum_{p=1}^{2S} \frac{(-1)^p}{(p!)^2} \prod_{q=1}^{p} [M - q(q-1)] \}, \quad (6)$$

where $M \doteq 2 [S(S+1) + \underset{\sim}{S}_i \cdot \underset{\sim}{S}_j]$. The coefficients A_n typically have the values

$$\begin{aligned} S = \tfrac{1}{2}: &\quad A_0 = \tfrac{1}{2}, \ A_1 = 2, \quad (7) \\ S = 1: &\quad A_0 = -1, \ A_1 = 1, \ A_2 = 1, \\ S = \tfrac{3}{2}: &\quad A_0 = -\tfrac{67}{32}, \ A_1 = -\tfrac{9}{8}, \ A_2 = \tfrac{11}{18}, \ A_3 = \tfrac{2}{9}, \\ S = 2: &\quad A_0 = -1, \ A_1 = -\tfrac{5}{2}, \ A_2 = -\tfrac{13}{16}, \ A_3 = \tfrac{1}{6}, \ A_4 = \tfrac{1}{36}, \end{aligned}$$

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, Eq.(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[2] 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 Chapters II and III, respectively; these ideas can be applied to any of the spin Hamiltonians usually studied. Chapters 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 Chapter VI and the explicite series results are presented in Chapter VII. Several checking procedures on the results are considered in Chapter VIII. In Chapter 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 Chapter X.

II. High Temperature Series Expansions

II-A. Preliminary Remarks

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

$$Z = \mathrm{tr}\, e^{-\beta\mathcal{H}}$$

$$= \mathrm{tr}\, \underset{\sim}{I} \left[1 - \beta\langle\mathcal{H}\rangle + \frac{\beta^2}{2!}\langle\mathcal{H}^2\rangle - \frac{\beta^3}{3!}\langle\mathcal{H}^3\rangle + \ldots \right], \quad (8)$$

where Z is the partition function, $\beta = (k_B T)^{-1}$, k_B is Boltzmann's constant, $\langle\mathcal{H}^n\rangle = \mathrm{tr}\,\mathcal{H}^n / \mathrm{tr}\,\underset{\sim}{I}$, and $\underset{\sim}{I}$ is the unit matrix. Related thermodynamic functions can then be expressed as ascending series in powers of $\frac{1}{T}$ 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.

II-B. Zero-Field Partition Function And Related Thermodynamic Functions

Since the various thermodynamic functions are related to 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 chapter. We introduce the following convenient notations: $Y = 2S+1$, $X = S(S+1)$, $\alpha = g\mu H/J$, $K = J/k_B T$, and

$$Q = \sum_{i=1}^{N} S_{zi}, \tag{9}$$

$$\mathcal{P} = \sum_{<ij>} P_{ij}, \quad \text{for the exchange interaction model,} \tag{10}$$

$$= 2 \sum_{<ij>} \underset{\sim}{S}_i \cdot \underset{\sim}{S}_j, \quad \text{for the Heisenberg model,}$$

$$= 2 \sum_{<ij>} S_{zi} S_{zj}, \quad \text{for the Ising model.}$$

Then,

$$\mathcal{H} = -J(\mathcal{P} + \alpha Q) = \mathcal{H}_0 - J\alpha Q. \tag{11}$$

For a system which consists of N particles of spin S, $\mathrm{tr}\ \underset{\sim}{I} = Y^N$. In zero external field,

$$Z = Y^N \left[1 + \sum_{n=1}^{\infty} \frac{K^n}{n!} \langle \mathcal{P}^n \rangle \right], \tag{12}$$

and

$$\ln Z = N \ln Y + \ln \left[1 + \sum_{n=1}^{\infty} \frac{K^n}{n!} \langle \rho^n \rangle \right], \tag{13}$$

from which it follows on expanding the logarithm

$$\ln Z = N \ln Y + \sum_{n=1}^{\infty} e_n \frac{K^n}{n!}, \tag{14}$$

with

$$e_n = \sum \frac{(-1)^{\alpha_1+\alpha_2+\cdots+\alpha_p-1} (\alpha_1+\alpha_2+\cdots+\alpha_p-1)!}{\alpha_1!\alpha_2!\cdots\alpha_p!(a_1!)^{\alpha_1}(a_2!)^{\alpha_2}\cdots(a_p!)^{\alpha_p}}$$

$$\times \langle \rho^{a_1} \rangle^{\alpha_1} \langle \rho^{a_2} \rangle^{\alpha_2} \cdots \langle \rho^{a_p} \rangle^{\alpha_p}. \tag{15}$$

The summation is taken over all partitions of the integer n, namely, all sets of positive integers $(a_1, a_2, \ldots a_p; \alpha_1, \alpha_2, \ldots \alpha_p)$ which satisfy the conditions

$$a_1\alpha_1 + a_2\alpha_2 + \cdots + a_p\alpha_p = n, \tag{16}$$

and

$$a_1 < a_2 < \cdots < a_p. \tag{17}$$

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

internal energy: $$E = k_B T^2 \frac{\partial}{\partial T}(\ln Z) = - J \frac{\partial}{\partial K} (\ln Z), \tag{18}$$

entropy: $$S = k_B \frac{\partial}{\partial T}(T \ln Z) = - k_B K^2 \frac{\partial}{\partial K}(\ln Z)/K, \tag{19}$$

specific heat: $C_v = k_B \frac{\partial}{\partial T}(T^2 \frac{\partial}{\partial T} \ln Z) = k_B K^2 \frac{\partial^2}{\partial K^2}(\ln Z)$. (20)

II-C. Low-Field Susceptibility

The low-field susceptibility is defined as

$$\chi = \lim_{H \to 0} k_B T \frac{\partial^2}{\partial H^2} \ln Z = \lim_{\alpha \to 0} k_B T \left(\frac{g\mu}{J}\right)^2 \frac{\partial^2}{\partial \alpha^2} \ln Z. \quad (21)$$

Since $\mathcal{P}$ and Q commute, $\frac{\partial}{\partial \alpha}(\mathcal{P} + \alpha Q)^n = n (\mathcal{P} + \alpha Q)^{n-1} Q$. It is then straightforward to show that

$$\chi = \frac{(g\mu)^2}{k_B T} \Delta(Q), \quad (22)$$

where $\Delta(Q) = \langle Q^2 \rangle_\beta - \langle Q \rangle_\beta^2$ is the zero-field thermal fluctuation of Q, and for any operator A,

$$\langle A \rangle_\beta = \frac{\mathrm{tr}\, A\, e^{-\beta \mathcal{H}_0}}{\mathrm{tr}\, e^{-\beta \mathcal{H}_0}} = \frac{\sum_{n=0}^{\infty} \frac{K^n}{n!} \langle \mathcal{P}^n A \rangle}{\sum_{n=0}^{\infty} \frac{K^n}{n!} \langle \mathcal{P}^n \rangle}. \quad (23)$$

As a consequence of the fact that ln Z is an even function of the external field, $\mathrm{tr}\, \mathcal{P}^n Q = 0$ for all n; hence, $\langle Q \rangle_\beta = 0$, so that we can rewrite χ in the form

$$\chi = \frac{(g\mu)^2 \chi}{3 k_B T} \left[N + \sum_{n=1}^{\infty} a_n \frac{K^n}{n!} \right]. \quad (24)$$

It is easy to show that the coefficients a_n satisfy the recursion relation

$$a_n = \frac{3}{X}\langle \rho^n Q^2 \rangle - \sum_{k=0}^{n-1} \frac{n!}{k!(n-k)!} a_k \langle \rho^{n-k} \rangle, \qquad (25)$$

with $a_0 = N$. In order to obtain the terms e_k and a_k, we must calculate the quantities $\langle \rho^n \rangle$ and $\langle \rho^n Q^2 \rangle$ for $n \leq k$. Here the matrices ρ 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 chapter we discuss the cluster expansion method, while the diagrammatic method is considered in Chapter V.

III. Cluster Expansion Method

III-A. Preliminary Remarks

The use of the cluster expansion method in deriving series expansions for magnetic systems was first suggested by Domb.[8] 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 are considerably smaller than that required in the diagrammatic method.[11] 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 expansions has been developed by many authors and derived in a number of different ways. In this chapter 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. The proof given here is simpler than proofs given previously by others.

III-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 cyclomatic number of the graph. It is well known that for a connected graph

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

where c is the cyclomatic number, ℓ 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

* For relevant definitions see references 8 and 10.

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

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_r and g_s are two graphs having no points in common, the union of these two graphs, denoted $g_r \cup g_s$, is the collection of all points and lines of g_r 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[9] of a graph g on a graph G is the number of subgraphs of G isomorphic with g, denoted (g;G). (g;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 Figure 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

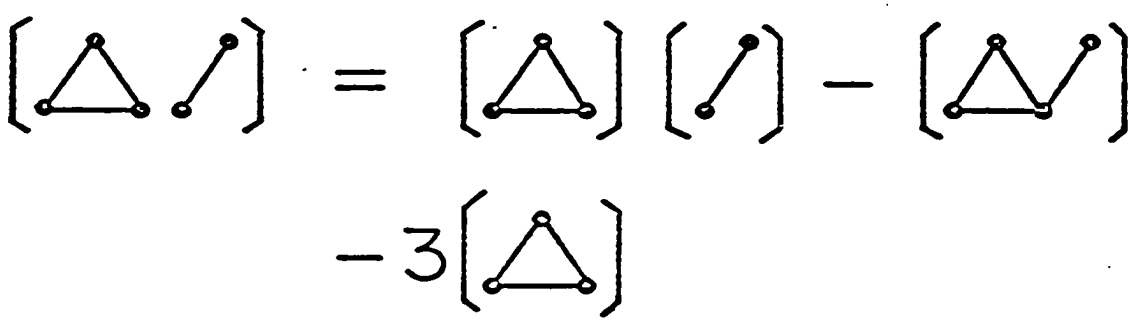


Figure 1. Example of expressing the lattice constant of a disconnected graph in terms of lattice constants of connected graphs.

components will consist of terms from the first order to the nth order in lattice constants of connected graphs.

III-C. New Derivation of the Cluster Expansions

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

$$\phi(g_r \cup g_s) = \phi(g_r) + \phi(g_s); \tag{28}$$

that is, the quantity ϕ 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. (g;G) is also an extensive quantity of G, i.e.,

$$(g;g_r \cup g_s) = (g;g_r) + (g;g_s). \tag{29}$$

Suppose that a graph G consists of the number π_i of connected graphs g_i, $i = 1, 2, 3, \ldots$. 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 ϕ,

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

Using the extensive property of the lattice constant as

expressed by Eq.(29), set $g=g_j$ for $j = 1, 2, 3, \ldots$. We then have a set of linear equations

$$(g_j;G) = \sum_i (g_j;g_i)\, \pi_i, \quad j = 1, 2, 3, \ldots . \tag{31}$$

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

$$\ell_i \leq \ell_j, \quad \text{for } i<j, \tag{32}$$

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

$$\begin{aligned} (g_j;g_i) &= 0, \quad \text{for } j>i, \\ &= 1, \quad \text{for } j=i. \end{aligned} \tag{33}$$

Define a matrix A with elements $A_{mn} = (g_m;g_n)$. Eq.(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

$$\pi_i = \sum_j (A^{-1})_{ij}(g_j;G), \quad i = 1, 2, 3, \ldots , \tag{34}$$

where $(A^{-1})_{ij}$ are elements of the inverse matrix of A. Substituting Eq.(34) into Eq.(30) yields

$$\phi(G;t) = \sum_i \sum_j \phi(g_i;t)(A^{-1})_{ij}(g_j;G)$$

$$= \sum_j F_j(t)(g_j;G), \qquad (35)$$

where $F_j(t) = \sum_i (g_i;t)(A^{-1})_{ij}$ is independent of G.

Since G may be any graph, let $G = g_i$. Eq.(35) yields

$$\phi(g_i;t) = \sum_j F_j(t)(g_j;g_i). \qquad (36)$$

On substituting Eq.(33) into Eq.(36) and rearranging terms we obtain an important theorem formulated by Sykes et al.[10]

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

$$F_j(t) = \phi(g_j;t) - \sum_{i=1}^{j-1} (g_i;g_j)\, F_i(t), \qquad (37)$$

and

$$F_1(t) = \phi(g_1;t). \qquad (38)$$

III-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 represented

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 χ are extensive thermodynamic quantities. We can then use Theorem I 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 value S, external magnetic field H, exchange constant J, etc. In high temperature series expansions, we express F_j (in Eq.(35)) in powers of K ($=J/k_BT$)

$$F_j = \sum_{n=0}^{\infty} f_n(g_j)\, K^n. \tag{39}$$

Theorem I is useful because in most cases $f_n(g_j) = 0$ for $n < \ell_j$. This will be explicitely shown in Chapter V for the present Hamiltonian when ϕ = ln Z or χ. Therefore if we want to obtain series up to the kth power in K for $\phi(G)$, we need only calculate $\phi(g_j)$ 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

IV-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 form a group called the symmetric group of degree N, denoted S_N. Each elements 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 (abf)(c)(de)(g). Each ( ) is called a cycle, and the number of symbols in ( ) is the order of the cycle. In writing a permutation as the product of cycles, cycles of order one need not be mentioned. Furthermore, the sequence of appearence 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 two is called an interchange. Any cycle of higher order can be expressed as a product of interchanges (having symbols in common). For example,

$$(abc \ldots de) = (ae)(ad) \ldots (ac)(ab). \qquad (40)$$

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

$$(fg)(fa \ldots bgc \ldots d) = (fa \ldots b)(gc \ldots d), \quad (41)$$

and

$$(fg)(fa \ldots b)(gc \ldots d) = (fa \ldots bgc \ldots d). \quad (42)$$

Eqs.(41) and (42) imply that for any group element, say P, when 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 $(a_1^{\alpha_1} a_2^{\alpha_2} \ldots a_p^{\alpha_p})$ have α_1 cycles of order a_1, α_2 cycles of order a_2, ... and α_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 labelled by a partition of N. The number of group elements in a class is called the order of the class. For the class $k = (a_1^{\alpha_1} a_2^{\alpha_2} \ldots a_p^{\alpha_p})$, its order h_k is

$$h_k = \frac{N!}{\alpha_1!\alpha_2! \ldots \alpha_p!\, a_1^{\alpha_1} a_2^{\alpha_2} \ldots a_p^{\alpha_p}} . \qquad (43)$$

Associated with S_N there is a finite number of inequivalent representations, called irreducible representations. Each irreducible representation is also labelled by a partition of N. Since elements of a class are transforms of one another, their matrices in any representation, say ν, have the same trace. This value is referred to as the character of the class k in the representation ν, 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 ν and ν', we have the orthogonality relations

$$\sum_k \frac{h_k}{h} \chi_k^{(\nu)} \chi_k^{(\nu')} = \delta_{\nu\nu'} , \qquad (44)$$

and

$$\sum_\nu \frac{h_k}{h} \chi_k^{(\nu)} \chi_{k'}^{(\nu)} = \delta_{kk'} , \qquad (45)$$

where h_k is the order of the class k, $h = N!$ is the order of S_N and the summations $\sum_k$ and $\sum_\nu$ are taken over all classes k and all irreducible representations ν,

respectively.

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

$$P^{(\Gamma)} = \sum_{\nu} n_\nu P^{(\nu)}. \tag{46}$$

From Eq.(44), we get

$$n_\nu = \sum_{k} \frac{h_k}{h} \chi_k^{(\nu)} \chi_k^{(\Gamma)}. \tag{47}$$

For two irreducible representations labelled by a pair of conjugate partitions ν and $\tilde{\nu}$, we have

$$\chi_k^{(\nu)} = \pm \chi_k^{(\tilde{\nu})}, \tag{48}$$

with the + sign applying for even classes and the - sign for odd classes of permutations.

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

$$\sum_{P\in k} P^{(\nu)} = \frac{h_k \chi_k^{(\nu)}}{\chi_{1N}^{(\nu)}} \underline{I}, \qquad (49)$$

where $\chi_{1N}^{(\nu)}$ is the matrix dimension of the irreducible representation ν.

Using these equations we now prove several useful new theorems.

IV-B. New Theorems

Theorem II. If R is any matrix which commutes with all elements of S_N in a matrix representation Γ, then

$$\mathrm{tr}\,[(\rho^{(\Gamma)})^n R] = \sum_{\nu}\sum_{k} \mathrm{tr}\,(\rho^{(\nu)})^n \frac{h_k}{h} \chi_k^{(\nu)} \mathrm{tr}\,[P_k^{(\Gamma)} R], \qquad (50)$$

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

Proof: The condition that R commutes with all elements of S_N in a matrix representation Γ and the fact that elements of a class are transforms of one another imply that $\mathrm{tr}\,P^{(\Gamma)}R$ 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, ρ^n as well as ρ is a sum

of elements in S_N. It is then sufficient to show that for any element, sat P, in S_N

$$\text{tr } P^{(\Gamma)}R = \sum_{\nu}\sum_{k} \text{tr } P^{(\nu)} \frac{h_k}{h} \chi^{(\nu)}_k \text{ tr } P^{(\Gamma)}_k R. \tag{51}$$

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

$$\begin{aligned} &\sum_{\nu}\sum_{k} \chi^{(\nu)}_{k'} \frac{h_k}{h} \chi^{(\nu)}_k \text{ tr } P^{(\Gamma)}_k R \\ &= \sum_{k} \delta_{kk'} \text{ tr } P^{(\Gamma)}_k R \\ &= \text{tr } P^{(\Gamma)}_{k'} R. \end{aligned} \tag{52}$$

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

Theorem III. If ν and $\tilde{\nu}$ are two irreducible representations labelled by a pair of conjugate partitions of N and $\mathcal{P}$ is a sum of odd permutations in S_N, then

$$\text{tr } (\mathcal{P}^{(\nu)})^n = (-1)^n \text{ tr } (\mathcal{P}^{(\tilde{\nu})})^n. \tag{53}$$

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).

IV-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 bases of the $(2S+1)^N$-dimensional vector space as the eigenstates of the z-component of the spins of the N particles, $|m_1\rangle|m_2\rangle \ldots |m_N\rangle$. 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:

$$\text{tr}\,(ijk \ldots l) = \sum_{m_i} \sum_{m_j} \ldots \sum_{m_k} \sum_{m_l} (\delta_{m_i,m_j}\, \delta_{m_i,m_k} \ldots \delta_{m_i,m_l})$$

$$= \sum_{m_i} (1) = Y. \tag{54}$$

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

$$\text{tr}\, S^n_{zi}(ijk \ldots l) = \sum_{m_i} \sum_{m_j} \ldots \sum_{m_k} \sum_{m_l} (m_i^n\, \delta_{m_i,m_j}\, \delta_{m_i,m_k} \ldots \delta_{m_i,m_l})$$

$$= \sum_{m_i} (m_i^n) = Y\, W_n, \tag{55}$$

where

$$W_n = Y^{-1} \sum_{m} (m^n), \tag{56}$$

and

$$\text{tr}\, S^n_{zi} S^n_{zj}(ik \ldots jl \ldots)$$

$$= \sum_{m_i} \sum_{m_k} \cdots \sum_{m_j} \sum_{m_l} \cdots (m_i^n m_j^n \delta_{m_i,m_k} \cdots \delta_{m_i,m_j} \delta_{m_i,m_l} \cdots)$$

$$= \sum_{m_i} (m_i^{2n}) = Y W_{2n}. \qquad (57)$$

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

$$P = (abc \ldots d)(ijk \ldots l) \ldots\ldots (xy \ldots z). \qquad (58)$$

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

$$P = (abc \ldots d)\times(ijk \ldots l)\times \ldots \times(xy \ldots z). \qquad (59)$$

By the trace propertity of the direct product

$$tr\ (A\times B) = (tr\ A)(tr\ B), \qquad (60)$$

it follows from Eqs(54), (55), and (57) that

$$tr\ S_{zi}^n P = W_n\ tr\ P, \qquad (61)$$

and

$$tr\ S_{zi}^n S_{zj}^n P = W_{2n} tr\ P, \quad \text{if } i=j \text{ or } i, j \text{ belong to the same cycle in P;} \qquad (62)$$

$$= W_n^2\ tr\ P, \quad \text{if } i, j \text{ belong to different independent cycles in P.}$$

For the case n=1, $W_1=0$, and $W_2=\frac{X}{3}$. If the element P

belongs to the class $k = (a_1^{\alpha_1} a_2^{\alpha_2} \ldots a_p^{\alpha_p})$, then, from Eqs. (54), (60), and (62),

$$\text{tr } P_k = Y^{\alpha_1+\alpha_2+ \ldots +\alpha_p}, \tag{63}$$

and

$$\begin{aligned} \text{tr } P_k Q^2 &= \sum_i \sum_j \text{tr } S_{zi} S_{zj} P_k \\ &= \frac{X}{3} (\alpha_1 a_1^2 + \alpha_2 a_2^2 + \ldots + \alpha_p a_p^2)\, Y^{\alpha_1+\alpha_2+\ldots+\alpha_p}, \end{aligned} \tag{64}$$

where the summations are from 1 to N.

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

$$\begin{aligned} \text{tr } P_{ij} P &= Y \text{ tr } P, && \text{if } i, j \text{ belong to the} \\ & && \text{same cycle in } P; \\ &= Y^{-1} \text{ tr } P, && \text{if } i, j \text{ belong to different} \\ & && \text{independent cycles in } P. \end{aligned} \tag{65}$$

V. Diagrammatic Method

V-A. Preliminary Remarks

The diagrammatic method has been extensively used in deriving high temperature series for various spin Hamiltonians. In this chapter, the procedure previously used for the Heisenberg Hamiltonian by Rushbrooke and Wood[11] 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.

V-B. Zero-Field Partition Function

For the exchange interaction model $\mathcal{P}^n$ in Eq.(12) is a sum of products ΠP_{ij} and each product contains n factors P_{ij}. There is a correspondence between products in $\mathcal{P}^n$ 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,[11] we can write

$$\langle \rho^n \rangle = \sum_{\ell_i=n} [D_i]\langle D_i \rangle, \tag{66}$$

where $\sum_{\ell_i=n}$ sums over all diagrams D_i of n lines. $[D_i]$ 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 $\langle \rho^n \rangle$. For a diagram D having n lines between ρ points, following Rushbrooke and Wood,

$$\langle D \rangle = Y^{-p} \sum_{\text{perm}} \text{tr}\,(\,)(\,)\ldots(\,), \tag{67}$$

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 appearence 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 Figure 2. As mentioned in Section III-B, lattice

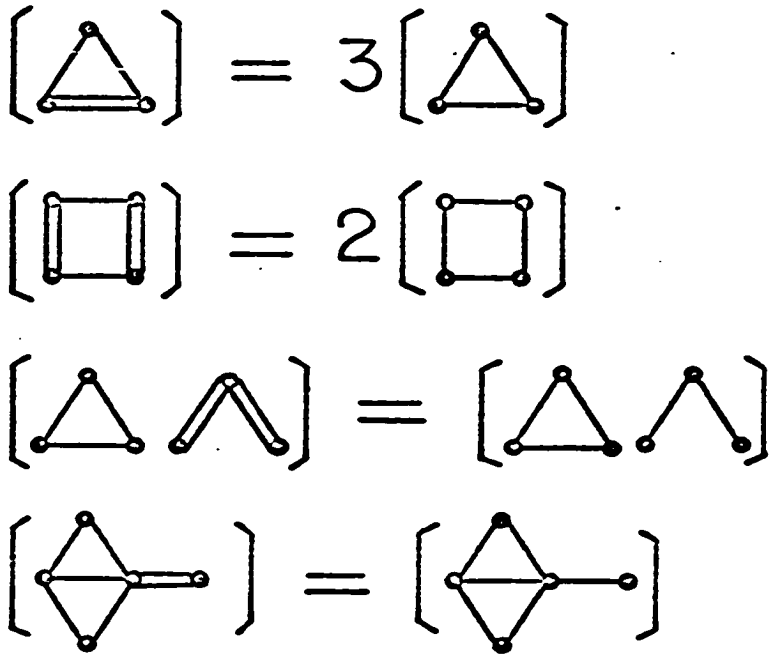


Figure 2. Examples of the relation between the occurrence factors of diagrams and lattice constants of graphs.

constants of disconnected graphs can be expressed in terms of lattice constants of connected graphs. Let $\Lambda_i\Phi$ signify that part of Φ which is of ith order in the lattice constants of connected graphs. We can then write

$$<\varphi^n> = \Lambda_1<\varphi^n> + \Lambda_2<\varphi^n> + \cdots \quad . \tag{68}$$

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

$$\ln Z = N \ln Y + \sum_{n=1}^{\infty} \frac{K^n}{n!} \Lambda_1<\varphi^n> . \tag{69}$$

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:

$$e_n = \Lambda_1<\varphi^n> = \sum_{\ell_i=n} \Lambda_1[D_i]<D_i> . \tag{70}$$

In the limit $N\to\infty$, lattice constants of connected graphs will be directly proportional to N. Λ_1 then means nothing more than "the part proportional to N".

V-C. Low-Field Susceptibility

When a finite external magnetic field is applied, the

partition function can be written in the form

$$\ln Z = N \ln Y + \sum_{n=1}^{\infty} \frac{K^n}{n!} \Lambda_1 \langle (\rho + \alpha Q)^n \rangle . \tag{71}$$

Since ρ and Q commute, and $\langle \rho^n Q \rangle = 0$, it is easy to show that

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

$$= \frac{g^2 \mu^2}{k_B T} \sum_{n=0}^{\infty} \frac{K^n}{n!} \Lambda_1 \langle \rho^n Q^2 \rangle . \tag{72}$$

For $n=0$, $\langle Q^2 \rangle = \frac{NX}{3}$. Comparing Eqs.(24) and (72), yields

$$a_n = \frac{3}{X} \Lambda_1 \langle \rho^n Q^2 \rangle . \tag{73}$$

The situation in calculating $\langle \rho^n Q^2 \rangle$ is similar to that involved in $\langle \rho^n \rangle$. We again have a correspondence between terms ΠP_{ij} produced on expanding ρ^n and diagrams of n lines on the lattice, but now, besides the n lines, a diagram will contain two crosses. These are denoted +, and are placed on those sites from which we have extracted terms like $S_{zi}S_{zj}$ 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^*, a double cross superposed on D,

(b) D^{++}, 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 $\langle S_{zi} \rangle = 0$ and $\langle S_{zi}^2 \rangle = \frac{X}{3}$, by the trace property of the direct product, we immediately find that diagrams (c) and (e) have zero contributions to $\langle \rho^n Q^2 \rangle$ and that diagram (d) contributes an amount $\frac{X}{3} \langle D \rangle$ to $\langle \rho^n Q^2 \rangle$. Let p be the number of points contained in the diagram D. Then the occurrance factor for diagram (d), [D *] = [D] [•] - p[D]. 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 occurrance factor [D] associated with the weighting factor $-\frac{pX}{3} \langle D \rangle$.

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 we sum up these p^2 diagrams, with occurrance factor [D], their contributions to $\langle \rho^n Q^2 \rangle$, denoted $\langle \overline{DQ}^2 \rangle$, will be

$$\langle \overline{DQ}^2 \rangle = Y^{-p} \sum_{\text{perm}} \text{tr} \, (\,)(\,) \ldots (\,)\Big(\sum_{i=1}^{p} S_{zi}\Big)^2. \qquad (74)$$

Therefore, including all five kinds of diagrams,

with occurrence factor [D], the weighting factor of the diagram D to $\Lambda_1 < \rho^n Q^2 >$, denoted $<DQ^2>$, will be

$$<DQ^2> = <\overline{DQ}^2> - \frac{pX}{3}<D>. \tag{75}$$

Hence

$$a_n = \frac{3}{X} \sum_{\ell_i = n} \Lambda_1[D_i](<\overline{D_i Q}^2> - p_i \frac{X}{3}<D_i>), \tag{76}$$

where p_i is the number of points in D_i. By rewriting the products ΠP_{ij} as products of independent cycles, the traces in Eqs.(67) and (74) can be obtained from Eqs.(63) and (64). $<D_i>$ and $<D_i Q^2>$ are then determined. Note that for the present Hamiltonian these five kinds of diagrams can be considered together and the calculation of the coefficients a_n is greatly simplified. For the Heisenberg Hamiltonian, weighting factors of these five kinds of diagrams have to be considered separately.

V-D. Further Theorems

If we express $\Lambda_1[D_i]$ in terms of lattice constants of connected graphs, denoted $[g_i]$, we can rewrite e_n and a_n as follows:

$$e_n = \sum_i [g_i]\, e_n(g_i), \tag{77}$$

and

$$a_n = \sum_i [g_i]\, a_n(g_i), \tag{78}$$

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

Theorem IV.

$$e_n(g_i) = a_n(g_i) = 0, \quad \text{if } n<\ell_i. \tag{79}$$

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

Theorem V. If we define cycles of diagrams similary to those for graphs presented in Chapter III, then for diagrams containing n lines and c independent cycles their contributions to e_n and a_n contain terms Y^{-n+2k}, where k ranges from 0 to c, but $2k \leq n$.

Proof: As mentioned in Section IV-A, for any group element P, (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. Assume that the diagram contains p points. The identity element will have p different independent cycles, namely, (1)(2) ... (p). Consider one of the products of n factors (ij) occuring

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 one, the resultant product will contain p-n+2k different independent cycles. Here k is the number of times that i, j happen to occur in the same cycle in the product which is to be multiplied by (ij). This can happen only when i, j are joined by paths other than the line ij, or, ij must be a line of a cycle. Therefore, $k \leq c$. Also, the number of independent cycles may not be greater than p, $2k \leq n$. Eq.(63) says that for any permutation containing t different independent cycles its trace in the $(2S+1)^p$-dimensional matrix representation is Y^t. Theorem V 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^{-n}, Y^{-n+2}, ... , which we can write as

$$e_n(g_i) = e_n^{(n)}(g_i)\, Y^{-n} + e_n^{(n-2)}(g_i)\, Y^{-n+2} + \ldots + e_n^{(1)}(g_i)\, Y^{-1} \quad [\text{or } e_n^{(0)}(g_i)], \qquad (80)$$

and

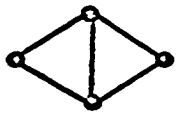
$$a_n(g_i) = a_n^{(n)}(g_i)\, Y^{-n} + a_n^{(n-2)}(g_i)\, Y^{-n+2} + \ldots + a_n^{(1)}(g_i)\, Y^{-1} \quad [\text{or } a_n^{(0)}(g_i)], \qquad (81)$$

Theorem VI.

$$e_n^{(-n+2k)}(g_i) = a_n^{(-n+2k)}(g_i) = 0, \text{ for } k > c_i + n - \ell_i, \qquad (82)$$

where c_i is the number of independent cycles and ℓ_i is the number of lines in the connected graph g_i.

Proof: Consider first the case that $n=\ell_i$. Diagrams of ℓ_i lines which have an occurrance 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 Figure 3. Other diagrams of five lines with occurrance factor containing $[g_i]$ are those disconnected graphs shown in the figure. Hence from Theorem V, Theorem VI is proved for the case $n=\ell_i$. When $n>\ell_i$, we can superpose the additional $n-\ell_i$ lines on g_i. Each line superposed on g_i is equivalent to forming an additional cycle in the resultant diagram, and the maximum number of independent cycles will be $c_i+n-\ell_i$ in some of the n line diagrams which have occurrance factors containing $[g_i]$. This then completes the proof of Theorem VI.

Graph g_i:  .

Diagrams of five lines with occurrence factors containing $[g_i]$:

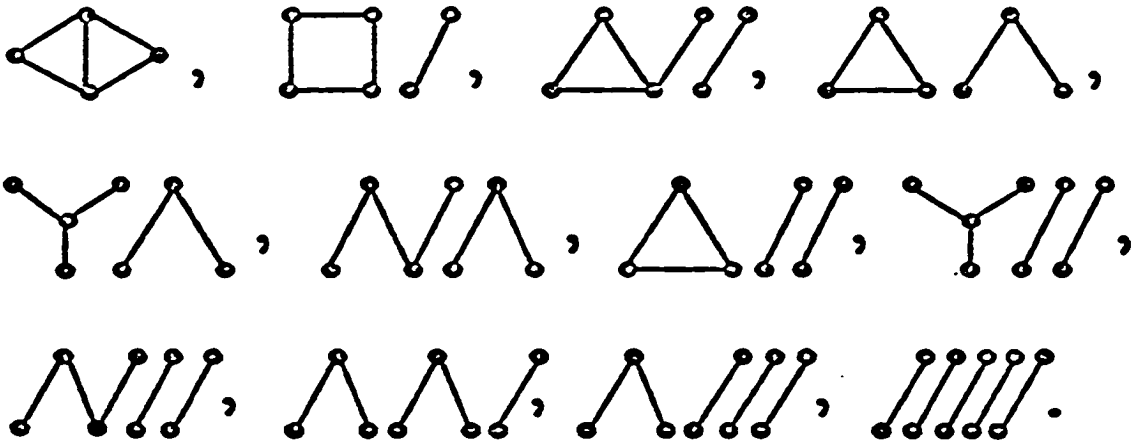


Figure 3. Example for illustrating the fact that diagrams of ℓ_i lines with occurrence factors containing $[g_i]$ consist of subgraphs of g_i.

Theorem VII.

$$a_n^{(0)}(g_i) = 0 \quad \text{for all } g_i. \tag{83}$$

Proof: Consider a diagram D of p points and n lines which has occurrance factor containing $[g_i]$. Those products ΠP_{ij} in Eqs.(67) and (74) which contribute to $a_n^{(0)}$ must be equal to the identity operator. Since $\text{tr } \underset{\sim}{I}Q^2 = \frac{pX}{3}$, Eq.(83) follows from Eq.(75).

Theorem VIII.

$$e_n^{(1)}(g_i) = \frac{1}{2} a_n^{(1)}(g_i) \quad \text{for all } g_i. \tag{84}$$

Proof: Those products in Eqs.(67) and (74) which contribute to $e_n^{(1)}$ and $a_n^{(1)}$ must contain p-1 cycles, or belong to the class $1^{p-2}2$. From Eqs.(63) and (64), for permutations P belonging to the class $1^{p-2}2$,

$$\text{tr } P\Big(\sum_{i=1}^{p} S_{zi}\Big)^2 = \frac{X}{3}(p+2)\, Y^{p-1}, \tag{85}$$

and

$$\text{tr } P = Y^{p-1}. \tag{86}$$

From Eqs.(67), (74), and (75), the contributions of these products to $\langle D \rangle$ and $\frac{3}{X}\langle DQ^2 \rangle$ will be Y^{-1} and $2Y^{-1}$, respectively. Theorem VIII then follows.

The theorems presented above (with the exception of Theorem IV)[11] have been developed by us. They will be applied to the derivation of the series coefficients in Chapter VI.

VI. Calculations of Series Coefficients

VI-A. Clusters With Up to Seven Sites

From the discussion in Chapter III we know that in order to obtain the high temperature series for general lattices up to the seventh power in K ($=J/k_BT$) 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 labelled in the graph dictionary order in Appendix A. Lattice constants $(g_i;g_j)$ for these clusters can readily be found and are also shown there.

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 tr ρ^n and tr $\rho^n Q^2$ for $n\leq 7$ are obtained from Theorem II by setting R equal to the unit matrix and Q^2, respectively. Now $\rho^{(\Gamma)}$ in Eq.(50) is a sum of Schrödinger exchange operators which correspond to the lines in each cluster. h_k and $\chi_k^{(\nu)}$

are available in a number of texts which deal specifically with the symmetric group[12] and are given in Appendix B for S_2 - S_7 together with the values of tr P_k and tr $P_k Q^2$ which are calculated by Eqs.(63) and (64). Corresponging to $\rho^{(\Gamma)}$, $\rho^{(\nu)}$ is a sum of interchanges in the irreducible representation ν. The explicit form of the permutation matrices in any irreducible representation can be obtained by the technique introduced by Yamanouchi [13] and is given in Appendix C. For two conjugate representations tr ρ^n are related to each other by Eq.(53) and hence only one of the two conjugate representations is given. The quantities tr $(\rho^{(\nu)})^n$ were 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 35×35. Computer programs for calculating tr $(\rho^{(\nu)})^n$ and hence tr ρ^n and tr $\rho^n Q^2$ for a finite cluster are given in Appendix I. Programs for computing the series coefficients $e_n^{(m)}(g_i)$ and $a_n^{(m)}(g_i)$ are also given in this appendix for clusters with up to seven points.

VI-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 70×70 and the trace calculation on a computer would have been too expensive for us. We have from Eq.(26) that clusters with seven lines and eight points contain no cycles. It then follows immediately from Theorem IV that for these clusters $e_n(g_i) = a_n(g_i) = 0$ for $n \leq 6$ and from Theorem VI that $e_7(g_i)$ and $a_7(g_i)$ can be written in the form

$$e_7(g_i) = e_7^{(7)}(g_i)\, Y^{-7}, \tag{87}$$

and

$$a_7(g_i) = a_7^{(7)}(g_i)\, Y^{-7}. \tag{88}$$

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.[14] Therefore $e_7(g_i) = a_7(g_i) = 0$ for all clusters of eight points with the exception that for the simple chain $a_7(g_i) = 10080\, Y^{-7}$. This value was

obtained from Eq.(88) together with the results of Domb and Wood[14]; for the case of spin $\frac{1}{2}$ and for the simple chain of eight points they obtained $a_7(g_i) = 10080 \times 2^{-7}$.

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 $e_1 - e_7$ are 1, 1, 2, 4, 7, 15, and 29, respectively, while the numbers of graphs that contribute to $a_1 - a_7$ are 1, 2, 4, 8, 16, 35, 82, respectively. The values of $e_n^{(m)}(g_i)$ and $a_n^{(m)}(g_i)$ for these graphs are given in Appendix D.

For regular lattices, e.g., body-centered cubic and face-centered cubic lattices with $N \to \infty$, 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

$$\ln Z/N = \ln Y + \sum_{n=2}^{\infty} e_n K^n, \tag{89}$$

and

$$\chi = \frac{C}{T}\left[1 + \sum_{n=1}^{\infty} a_n K^n\right], \tag{90}$$

where $C = N(g\mu)^2 X/3k_B$. 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 substracted from P_{ij} to make $\mathcal{H}$ traceless. The coefficients e_n and a_n will be written in the form

$$e_n = e_n^{(n)} Y^{-n} + e_n^{(n-2)} Y^{-n+2} + \ldots + e_n^{(1)} Y^{-1} \quad (\text{or } e_n^{(0)}), \tag{91}$$

$$a_n = a_n^{(n)} Y^{-n} + a_n^{(n-2)} Y^{-n+2} + \ldots + a_n^{(2)} Y^{-2} \quad (\text{or } a_n^{(1)} Y^{-1}). \tag{92}$$

The various quantities $e_n^{(m)}$ and $a_n^{(m)}$ for $n \leq 7$ are then given below:

$$e_2^{(0)} = \frac{1}{4}(\sigma+1), \tag{93}$$

$$e_2^{(2)} = \frac{-1}{4}(\sigma+1),$$

$$e_3^{(1)} = \frac{-1}{6}[(\sigma+1)-6p_3],$$

$$e_3^{(3)} = \frac{1}{6}[(\sigma+1)-6p_3],$$

$$e_4^{(0)} = \frac{-1}{24}[(\sigma+1)^2-12p_3],$$

$$e_4^{(2)} = \frac{1}{24}[(\sigma+1)(\sigma+4)-84p_3+24p_4],$$

$$e_4^{(4)} = \frac{-1}{8}[(\sigma+1)-24p_3+8p_4],$$

$$e_5^{(1)} = \frac{1}{60}[(\sigma+1)(5\sigma+4)-15p_3(2\sigma+7)+40p_4+30p_{5a}],$$

$$e_5^{(3)} = \frac{-1}{12}[(\sigma+1)(\sigma+2)-3p_3(2\sigma+31)+56p_4-12p_5+30p_{5a}],$$

$$e_5^{(5)} = \frac{1}{10}[(\sigma+1)-60p_3+40p_4-10p_5+20p_{5a}],$$

$$e_6^{(0)} = \frac{1}{720}[(\sigma+1)(11\sigma^2+20\sigma+8)-36p_3(7\sigma+4)+72p_4+132p_{5a}+96p_{6d}],$$

$$e_6^{(2)} = \frac{-1}{720}[(\sigma+1)(11\sigma^2+110\sigma+68)-108p_3(19\sigma+23)+24p_4(20\sigma+93)$$
$$-600p_5+3132p_{5a}-360p_{6a}-360p_{6b}+240p_{6c}+1536p_{6d}],$$

$$e_6^{(4)} = \frac{1}{24}[(\sigma+1)(3\sigma+4)-6p_3(10\sigma+51)+8p_4(2\sigma+39)-140p_5+364p_{5a}$$
$$+24p_6-60p_{6a}-60p_{6b}+8p_{6c}+192p_{6d}],$$

$$e_6^{(6)} = \frac{-1}{12}[(\sigma+1)-114p_3+120p_4-60p_5+132p_{5a}+12p_6-24p_{6a}-24p_{6b}+72p_{6d}],$$

$$e_7^{(1)} = \frac{-1}{5040}[(\sigma+1)(245\sigma^2+385\sigma+136)-42p_3(37\sigma^2+288\sigma+18)$$
$$+560p_4(5\sigma+6)-910p_5+28p_{5a}(77\sigma+312)-1260p_{6a}-1456p_{6b}$$
$$+2352p_{6c}+3864p_{6d}-798p_{7c}-840p_{7g}-644p_{7h}],$$

$$e_7^{(3)} = \frac{1}{720}[(\sigma+1)(35\sigma^2+175\sigma+88)-6p_3(37\sigma^2+1128\sigma+348)+80p_4(41\sigma+78)$$
$$-10p_5(60\sigma+343)+52p_{5a}(29\sigma+234)+720p_6-3060p_{6a}-3808p_{6b}$$
$$+2256p_{6c}+9192p_{6d}+360p_{7a}+360p_{7b}-1314p_{7c}-240p_{7e}+360p_{7f}$$
$$-3000p_{7g}-1532p_{7h}],$$

$$e_7^{(5)} = \frac{-1}{12}[2(\sigma+1)^2-3p_3(3\sigma\sigma+59)+48p_4(\sigma+7)-5p_5(2\sigma+47)+10p_{5a}(2\sigma+59)$$
$$+84p_6-192p_{6a}-216p_{6b}+32p_{6c}+576p_{6d}-12p_7+30p_{7a}+30p_{7b}-68p_{7c}$$
$$-4p_{7e}+30p_{7f}-120p_{7g}-96p_{7h}],$$

$$e_7^{(7)} = \frac{1}{14}[(\sigma+1)-168p_3+280p_4-210p_5+476p_{5a}+84p_6-168p_{6a}-182p_{6b}$$
$$+504p_{6d}-14p_7+28p_{7a}+28p_{7b}-56p_{7c}+28p_{7f}-84p_{7g}-84p_{7h}],$$

and

$$a_1^{(1)} = (\sigma+1), \qquad (94)$$

$$a_2^{(2)} = (\sigma+1)(\sigma-1),$$

$$a_3^{(1)} = \frac{-1}{3}[(\sigma+1)-6p_3],$$

$$a_3^{(3)} = [(\sigma+1)(\sigma-1)^2-18p_3],$$

$$a_4^{(2)} = \frac{-1}{12}[(\sigma+1)(3\sigma-8)-48p_3(\sigma-5)-56p_4],$$

$$a_4^{(4)} = [(\sigma+1)(\sigma-1)^3-18p_3(2\sigma-5)-32p_4],$$

$$a_5^{(1)} = \frac{1}{30}[(\sigma+1)(5\sigma+4)-15p_3(2\sigma+7)+40p_4+30p_{5a}],$$

$$a_5^{(3)} = \frac{-1}{6}[(\sigma+1)(\sigma^2-4\sigma+6)-6p_3(6\sigma^2-34\sigma+85)-8p_4(7\sigma-36)-50p_5+204p_{5a}],$$

$$a_5^{(5)} = [(\sigma+1)(\sigma-1)^4-54p_3(\sigma^2-4\sigma+5)-64p_4(\sigma-3)-50p_5+132p_{5a}],$$

$$a_6^{(2)} = \frac{1}{360}[(\sigma+1)(53\sigma^2-169\sigma-136)-18p_3(40\sigma^2-182\sigma-347)-48p_4(3\sigma+115)$$
$$+1380p_5+24p_{5a}(30\sigma-347)+756p_{6a}+828p_{6b}-216p_{6c}-4944p_{6d}],$$

$$a_6^{(4)} = \frac{-1}{12}[(\sigma+1)(\sigma^3-6\sigma^2+14\sigma-16)-12p_3(8\sigma^3-52\sigma^2+138\sigma-219)$$
$$-8p_4(21\sigma^2-124\sigma+344)-20p_5(10\sigma-57)+8p_{5a}(102\sigma-515)-156p_6$$
$$+636p_{6a}+636p_{6b}+64p_{6c}-2544p_{6d}],$$

$$a_6^{(6)} = [(\sigma+1)(\sigma-1)^5-18p_3(4\sigma^3-21\sigma^2+42\sigma-34)-32p_4(3\sigma^2-14\sigma+21)$$
$$-50p_5(2\sigma-7)+24p_{5a}(11\sigma-40)-72p_6+192p_{6a}+188p_{6b}+72p_{6c}-624p_{6d}],$$

$$a_7^{(1)} = \frac{-1}{2520}[(\sigma+1)(245\sigma^2+385\sigma+136)-42p_3(37\sigma^2+228\sigma+18)+560p_4(5\sigma+6)$$
$$-910p_5+28p_{5a}(77\sigma+312)-1260p_{6a}-1456p_{6b}+2352p_{6c}+3864p_{6d}$$
$$-798p_{7c}-840p_{7g}-644p_{7h}],$$

$$a_7^{(3)} = \frac{1}{360}[(\sigma+1)(46\sigma^3-205\sigma^2+347\sigma+264)-6p_3(180\sigma^3-1029\sigma^2+3411\sigma$$
$$+1292)-4p_4(192\sigma^2-1076\sigma-7012)+10p_5(28\sigma-1495)+4p_{5a}(270\sigma^2-$$
$$-1694\sigma+15589)+2976p_6+12p_{6a}(126\sigma-1243)+4p_{6b}(414\sigma-4531)$$
$$-16p_{6c}(27\sigma-406)-48p_{6d}(206\sigma-1135)+1388p_{7a}+1454p_{7b}-7820p_{7c}$$
$$+320p_{7d}-348p_{7e}+1292p_{7f}-12540p_{7g}-8272p_{7h}],$$

$$a_7^{(5)} = \frac{1}{6}[(\sigma+1)(\sigma^3-5\sigma^2+10\sigma-10)+6p_3(10\sigma^4-74\sigma^3+218\sigma^2-327\sigma+339)$$
$$+8p_4(14\sigma^3-95\sigma^2+279\sigma-554)+10p_5(15\sigma^2-98\sigma+307)-4p_{5a}(153\sigma^2$$
$$-962\sigma+2399)+12p_6(13\sigma-83)-12p_{6a}(53\sigma-267)-12p_{6b}(53\sigma-295)$$
$$-8p_{6c}(8\sigma-51)+48p_{6d}(53\sigma-228)+112p_7-456p_{7a}-456p_{7b}+1392p_{7c}$$
$$-96p_{7d}-52p_{7e}-456p_{7f}+1992p_{7g}+1796p_{7h}],$$

$$a_7^{(7)} = [(\sigma+1)(\sigma-1)^6-18p_3(5\sigma^4-32\sigma^3+84\sigma^2-110\sigma+62)-128p_4(\sigma^3-6\sigma^2+14\sigma$$
$$-14)-50p_5(3\sigma^2-16\sigma+28)+4p_{5a}(99\sigma^2-546\sigma+971)-144p_6(\sigma-4)$$

$$+384p_{6a}(\sigma-4)+2p_{6b}(188\sigma-777)+144p_{6c}(\sigma-4)-1248p_{6d}(\sigma-4)$$
$$-98p_{7}+256p_{7a}+252p_{7b}-580p_{7c}+72p_{7d}+96p_{7e}+260p_{7f}-588p_{7g}$$
$$-844p_{7h}].$$

Here the p_{nx} are lattice constants for closed graphs per lattice site and $q=\sigma+1$ is the coordination number of the lattice. The values of p_{nx} and q for various crystal lattices are well known[8] and are given in Appendix E. Numerical values of $e_n^{(m)}$ and $a_n^{(m)}$ for various crystal lattices can be found in pages 135 and 131 , respectivelv. For convenience, the coefficients e_n and a_n for the cubic lattices and a number of two-dimensional lattices and for several spin values are shown in Appendix F. 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 $e_n^{(m)}$ and $a_n^{(m)}$ before using them to estimate critical parameters. We have considered a large number of finite clusters of eight lines and several of them are shown in Appendix G. For these clusters we calculate the zero-field partition function and the low-field susceptibility series from the results of Appendix D by putting the appropriate lattice constants in Eqs.(77) and (78), respectively, and compare the results with those obtained from a direct machine calculation as described in Chapter VI. We have full agreement up to e_7 and a_7 in all cases. The lattice constants and the series coefficients $e_n^{(m)}$ and $a_n^{(m)}$ for these clusters are shown in Appendix G.

By observing the general expressions for $e_n^{(m)}$ and $a_n^{(m)}$ that we obtained (Eqs.(93) and (94)) we see that

$$\sum_m e_n^{(m)} = 0; \quad m = n, n-2, n-4, \ldots, 1 \text{ (or } 0), \tag{95}$$

and

$$e_n^{(1)} = \frac{1}{2} a_n^{(1)}. \tag{96}$$

These two equations hold for all n and provide an

additional check on our results. Eq.(96) has been proved in Theorem VIII, 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_n and a_n reduce exactly to those obtained previously by Domb and Wood,[14] and by Allan and Betts,[15] respectively.

IX. Analysis of Series

IX-A. Estimates of Curie Temperatures and Critical Indices

The Curie temperature T_C and the critical index γ in the susceptibility series are defined by

$$\chi \sim (T-T_C)^{-\gamma}; \quad \text{for } T \to T_C^+, \tag{97}$$

or

$$\sim (K_C-K)^{-\gamma}; \quad \text{for } K \to K_C^-, \tag{98}$$

where $K_C=J/k_BT_C$. For the face-centered cubic lattice T_C and γ were first estimated by means of the ratio method. From Eq.(98) the coefficients a_n in Eq.(90) have the properties that for large n

$$\frac{a_n}{a_{n-1}} = \left(\frac{a_n}{a_{n-2}}\right)^{1/2} \to \frac{1}{K_C}\left(1+\frac{\gamma-1}{n}\right). \tag{99}$$

If we plot the two sets of values a_n/a_{n-1} and $(a_n/a_{n-2})^{1/2}$ vresus $\frac{1}{n}$, each of the plots tends to a straight line as n increases and intersects with $\frac{1}{n}=0$ at K_C^{-1} with slope $(\gamma-1)K_C^{-1}$. If we plot $(a_n)^{1/n}$ versus $\frac{1}{n}$, the plot also intersects with $\frac{1}{n}=0$ at K_C^{-1} 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

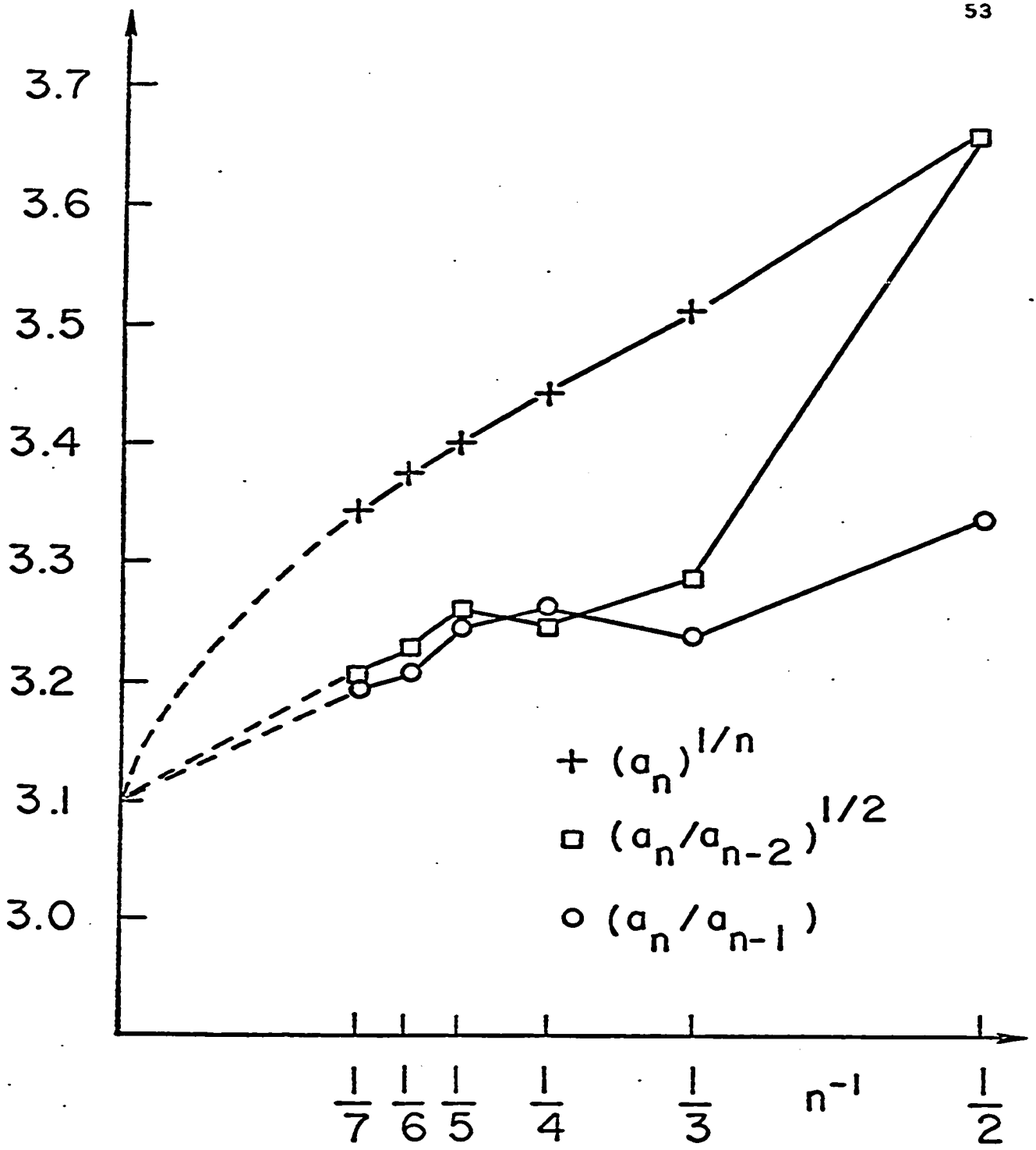


Figure 4. Plots of $(a_n)^{1/n}$, $(a_n/a_{n-2})^{1/2}$, and a_n/a_{n-1} versus n^{-1} for the face-centered cubic lattice, S=1.

of Padé approximants.[16] 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 Q(0)=1 and f(z) agrees with the expansion of P(z)/Q(z) for the first M+N+1 terms.

If the divergence of χ at K_c is in the form shown in Eq.(98) then

$$(\chi)^{1/\gamma} \sim (K_c-K)^{-1}, \tag{100}$$

$$\frac{\chi'}{\chi} = \frac{d}{dK} \ln \chi = \frac{\gamma}{K_c-K}, \tag{101}$$

and

$$\frac{\chi''\chi}{(\chi')^2} = \frac{\frac{d}{dK}(\ln \frac{d\gamma}{dK})}{\frac{d}{dK}(\ln \chi)} = 1 + \frac{1}{\gamma}. \tag{102}$$

These equations suggest four methods of determining K and/or γ from χ :

(a) Choosing γ, K_c can be presented by appropriate poles of the Padé approximants to $(\chi)^{1/\gamma}$;

(b) Choosing K_c, γ can be obtained by evaluating Padé approximants to $(K_c-K)\chi'/\chi$ at $K=K_c$;

(c) For a Padé approximant to χ'/χ the appropriate pole gives K_c and the residue at this pole gives $-\gamma$;

(d) Evaluating Padé approximants to $\chi''\chi/(\chi')^2$ at $K=K_c$ gives $1+\frac{1}{\gamma}$.

For the face-centered cubic lattice and for $S = \frac{1}{2} - 3$ we have estimated K_c and γ by all the four methods. In method (a) instead of tabulating the various approximants in Padé table for several values of γ we have plotted the various approximants of K_c as functions of γ in the K_c-γ plane. The proper values of γ 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 γ as functions of K_c are also plotted in the K_c-γ plane. These curves are roughly paralled 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 γ from Padé analysis are also in agreement with estimates based on the various ratio tests. The final estimates of γ and T_c are given in Figures 6 and 7, respectively. These results can be simply described by the equations

$$k_B T_c/J = 1.19 + 5.70\ \gamma^{-1}, \tag{103}$$

and

$$\gamma = 0.48 + 2.16\ \gamma^{-1}. \tag{104}$$

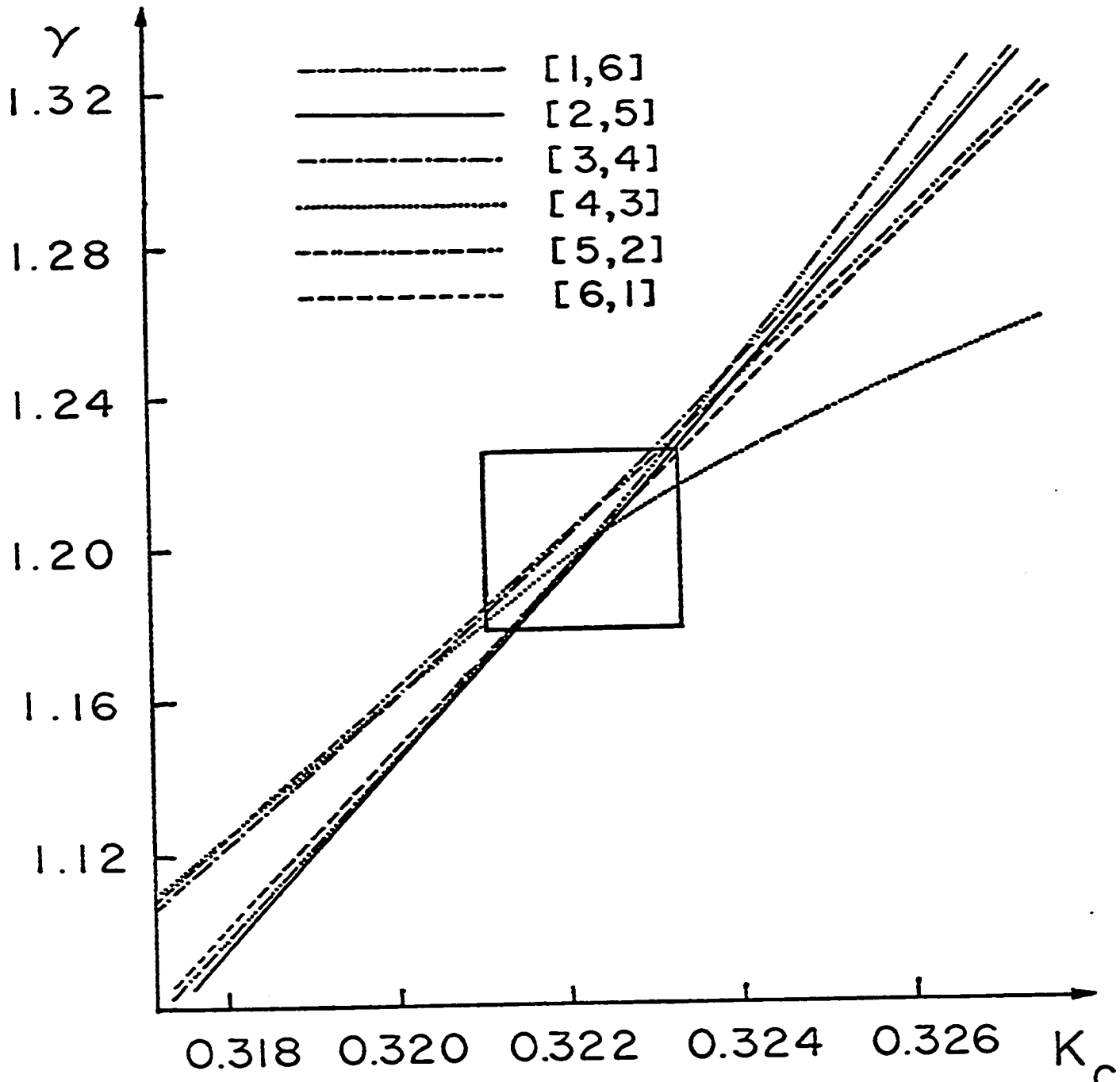


Figure 5. Plots of several Padé approximants of K_c as functions of γ for the f.c.c. lattice, S=1. The box in the figure indicates the region in which the various approximants coalesce.

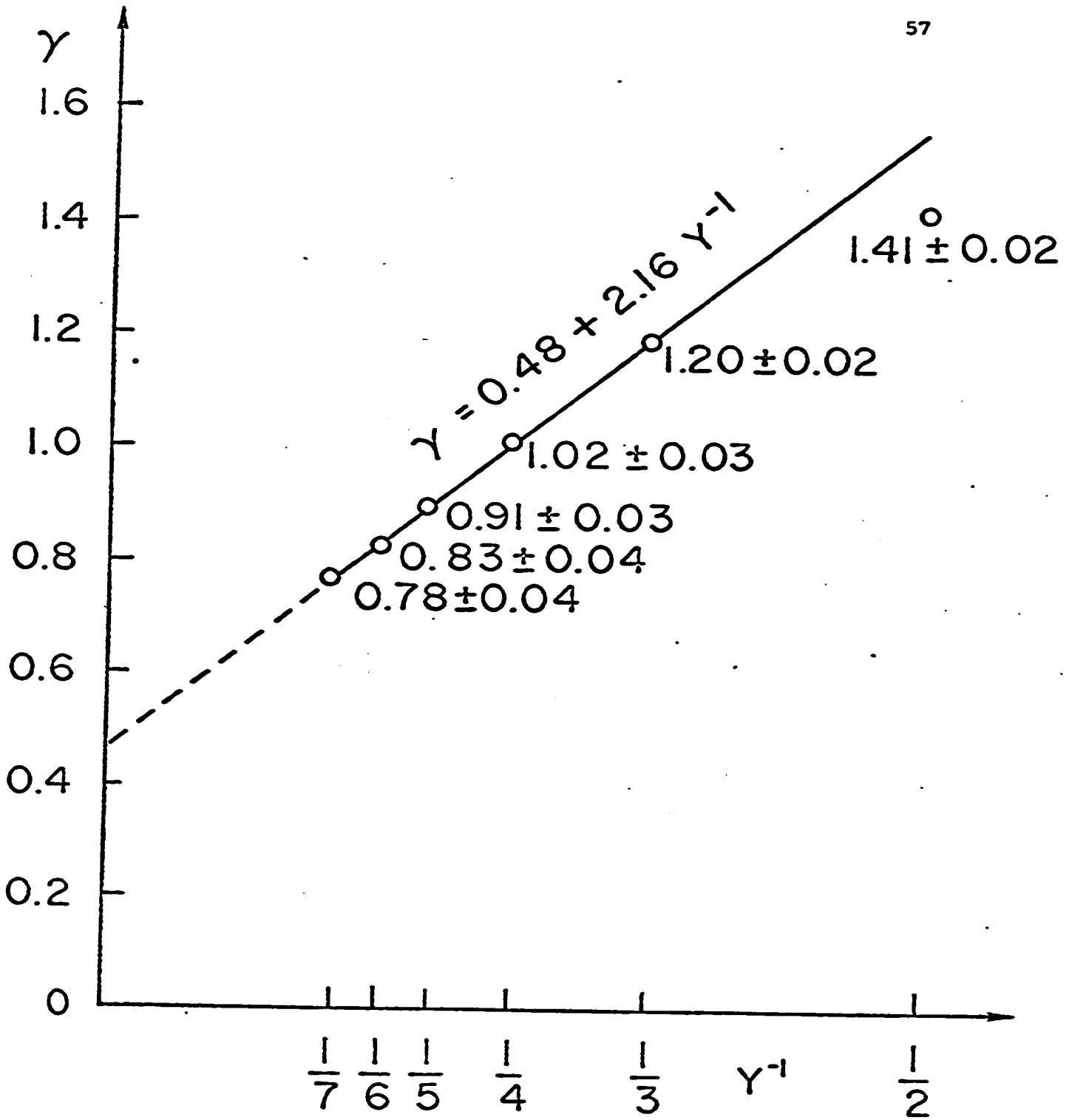


Figure 6. Critical indices, γ, for the cubic lattices plotted versus γ^{-1}.

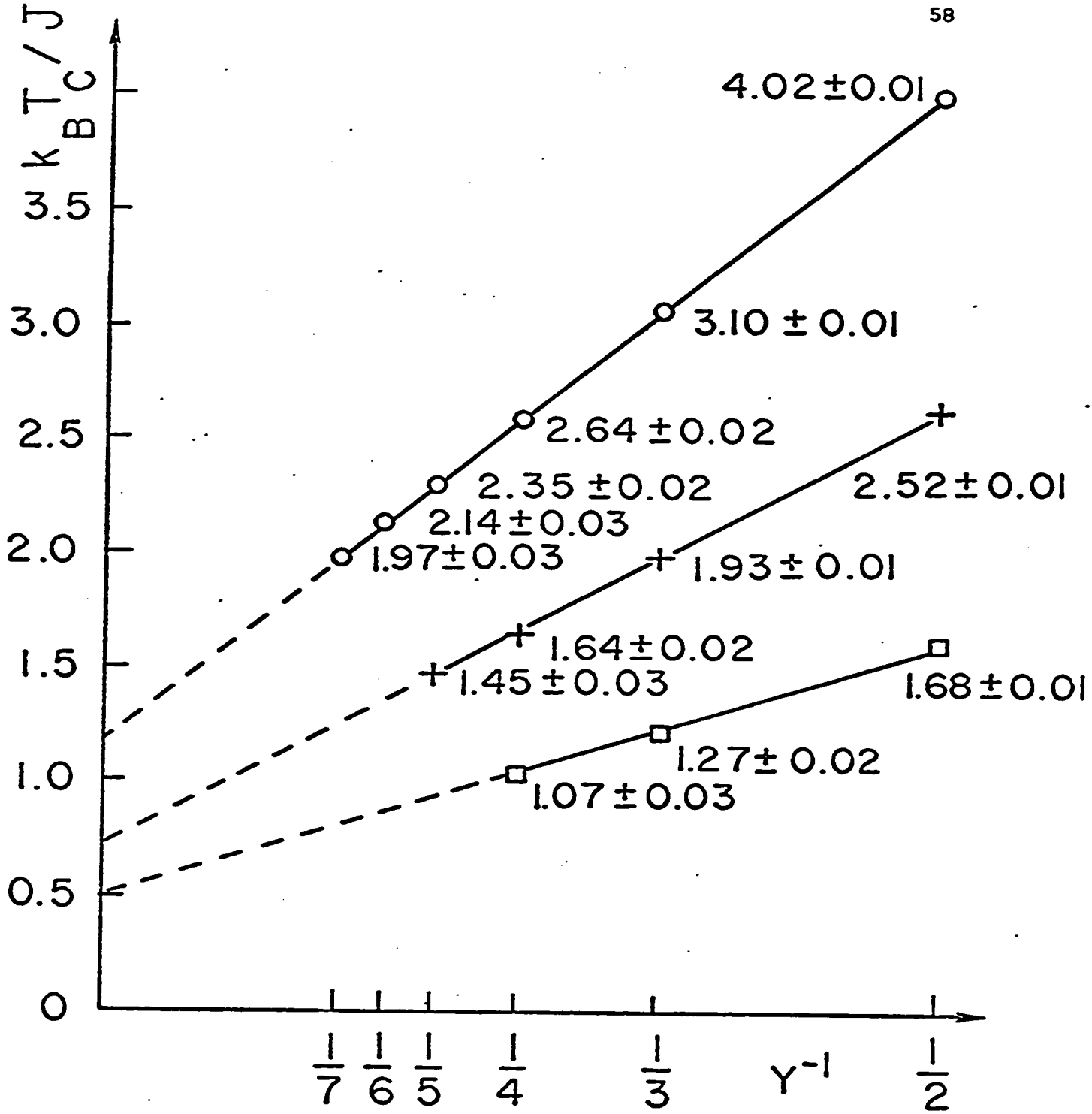


Figure 7. Curie temperatures, $k_B T_C/J$, for the cubic lattices plotted versus Y^{-1}. O, f.c.c. lattice; +, b.c.c. lattice; □, s.c. lattice.

Eqs.(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 γ either by ratio tests or by the Padé approximant method. However, within our precision, γ seems to be the same for all of the cubic lattices for each S. If the values of γ for the body-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 $(\chi)^{1/\gamma}$ suggests that for all of the cubic lattices T_c can be described to within a few percent by

$$k_B T_c/J = 0.547(q-1.6)(\gamma^{-1}+0.21). \qquad (105)$$

The estimates of T_c for the body-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 Padé approximants is too large to draw any conclusions concerning the critical temperature and the

nature of the divergence of the specific heat at T_c. Considerably longer series would be needed for this purpose.

IX-3. 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) were also analysed by the Padé approximant method. For the face-centered cubic lattice we found that

$$(S_\infty - S_c)/S_\infty = 0.494 - 0.353\ Y^{-1}, \tag{106}$$

and

$$(E_\infty - E_c)/JN = 3.98 - 5.04\ Y^{-1}, \tag{107}$$

for all S with the exception that for $S=\frac{1}{2}$, $(E_\infty - E_c)/JN = 1.60$. Here $S_\infty = Nk_B \ln Y$ and $E_\infty = 0$ 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 Y^{-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.

X. Discussion and Conclusions

Since there are 2S linearly independent isotropic interactions $(\underset{\sim}{S}_i \cdot \underset{\sim}{S}_j)^n$ $[1 \leq n \leq 2S]$ for spin S particles, there are other kinds of order parameters[17,18] besides $\sum_i S_{zi}$, with which phase transitions might be associated. In order to study the possibility of such transitions we shall consider first the following modified Hamiltonian:

$$\mathcal{H}_n = \mathcal{H}_0 - \zeta Q_n, \tag{108}$$

where

$$\mathcal{H}_0 = - J \sum_{<ij>} P_{ij} = - J \mathcal{P}, \tag{109}$$

$$Q_n = \sum_{i=1}^{N} S_{zi}^n; \quad n = 1, 2, \ldots 2S, \tag{110}$$

and ζ is some (fictitious) external magnetic field. We then define a generalized susceptibility χ_n by

$$\chi_n = \lim_{\zeta \to 0} \beta^{-1} \frac{\partial^2}{\partial \zeta^2} \ln \operatorname{tr} e^{-\beta \mathcal{H}_n} \tag{111}$$

By definition $\chi_1 = \chi$. Since $\mathcal{P}$ and Q_n commute, as did $\mathcal{P}$ and Q, we have

$$\chi_n = \beta \Delta(Q_n). \tag{112}$$

In Appendix H the following theorem is proved.

Theorem IX.

$$\chi_n/\chi_1 = D_n(S) = \frac{3}{X}(W_{2n}-W_n^2). \tag{113}$$

Here $D_n(S)$ is a quantity which is independent of both lattice and temperature. This means that for a given lattice, all of the $\chi_n \to \infty$ at the same T_C in exactly the same way.

Since the (dipolar) susceptibility, Eq.(21), can also be written in the form

$$\chi = \frac{1}{3} g^2\mu^2\beta \sum_{i,j} \langle \underset{\sim}{S}_i \cdot \underset{\sim}{S}_j \rangle_\beta, \tag{114}$$

it is really necessary to investigate quantities of the form $\sum_{i,j} \langle (\underset{\sim}{S}_i \cdot \underset{\sim}{S}_j)^n \rangle_\beta$ for $1 \leq n \leq 2S$. However, for both computional and theoretical reasons, we have restricted our attention to the single quantity $\sum_{i,j}' \langle P_{ij} \rangle_\beta$. 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 Appendix H .

Theorem X.

$$\sum_{i,j}' \langle P_{ij} - \frac{1}{Y} \underset{\sim}{I} \rangle_\beta = \frac{4}{Y} \sum_{i,j}' \langle \underset{\sim}{S}_i \cdot \underset{\sim}{S}_j \rangle_\beta. \tag{115}$$

Since $\langle \underset{\sim}{S}_i^2 \rangle_\beta = X$, it immediately follows from this result and Eq.(114) that the left hand side of Eq.(115) diverges at

the same T_C and in exactly the same way as χ. Hence we must conclude that for the exchange interaction model the 2S "independent" multipolar phase transitions are in fact exactly degenerate with the dipolar transition. This means that the values of T_C and γ predicted on the basis of analysis of the high temperature susceptibility series are completely characteristic of this model.

Theorem X also suggests another approach for the derivation of the susceptibility series. Since $\sum_{i,j}' \langle P_{ij} \rangle_\beta$ is equal to χ except for a constant, χ can be obtained by calculating the quantities $\mathrm{tr} \sum_{i,j}' P_{ij} \rho^n$ for each cluster. As was shown in Chapter IV, each Schrödinger exchange operator can be resolved into a direct sum of irreducible representations of the symmetric group. For a cluster of N sites it follows from Eqs.(46) and (49) that

$$\mathrm{tr} \sum_{i,j}' P_{ij} \rho^n = \sum_\nu n_\nu \left[N(N-1) \chi^{(\nu)}_{1^{N-2}2} / \chi^{(\nu)}_{1^N} \right] \mathrm{tr} \left(\rho^{(\nu)} \right)^n, \qquad (116)$$

where n_ν is given by Eq.(47) and $\chi^{(\Gamma)}_k = \mathrm{tr}\, P_k$ is given by Eq.(63). The labor required to derive χ by this approach is about the same as the previous approach which made use of Theorem II.

The numerical results for the critical properties of the exchange interaction model have been shown in the previous chapter. Comparison of these results to those appropriate to the Heisenberg model[19,20] then shows that for $S > \frac{1}{2}$:

(1) Both T_C and γ for the present model are lower than those of the Heisenberg model.

(2) For the present model T_C is a decreasing function of spin, while T_C is an increasing function of spin for the Heisenberg model.

(3) For the exchange interaction model γ depends strongly on S and even becomes less than unity for large enough spin. On the other hand, for the Heisenberg model γ is a weak function of spin and is greater than 1.33 for all spin. Experimental values of γ [21] appear to lie inbetween the estimated values for these two models. Fisher[22] has recently suggested that the observed value of the critical index γ_{obs} is related to the theoretical value by

$$\gamma_{obs} = \frac{\gamma}{1-\alpha} , \qquad (117)$$

where α is the theoretical value of the critical exponent of the specific heat series defined by

$$C_v \sim (T-T_C)^{-\alpha} \; ; \quad \text{for } T \to T_C^+ . \qquad (118)$$

For $0 < \alpha < 1$, $\gamma_{obs} > \gamma$. This then shows that the theoretical estimates of γ 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 γ 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 occuring 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. Lattice Constants $(g_i;g_j)$

In this appendix following each graph* g_j are the values $(g_1;g_j)$, $(g_2;g_j)$, $(g_3;g_j)$, ... , and $(g_k;g_j)$, respectively. For $i>k$ $(g_i;g_j) = 0$ with the exception that $(g_j;g_j) = 1$.

g_1  :

g_2  : 2.

g_3  : 3, 3.

g_4  : 3, 2.

g_5  : 3, 3.

g_6  : 4, 5, 1, 2, 1.

g_7  : 4, 4, 0, 4.

g_8  : 4, 3, 0, 2.

g_9  : 4, 4, 0, 2, 1.

g_{10}  : 4, 6, 0, 0, 4.

g_{11}  : 5, 8, 2, 6, 2, 4, 1.

g_{12}  : 5, 7, 1, 5, 2, 2, 0, 1, 2.

g_{13}  : 5, 8, 1, 4, 4, 2, 0, 0, 2, 1.

g_{14}  : 5, 6, 1, 4, 1, 1, 0, 2, 1.

* The simplest graph is that contains only a single point. Since it does not contribute to e_n and a_n for $n\geq 1$, we label the graphs begining from that of two points and one line.

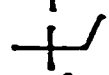
g_{15}  : 5, 6, 0, 6, 1, 0, 1, 2, 2,

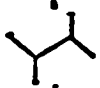
g_{16}  : 5, 5, 0, 5, 0, 0, 0, 5.

g_{17}  : 5, 4, 0, 3, 0, 0, 0, 2.

g_{18}  : 5, 5, 0, 3, 1, 0, 0, 2, 1.

g_{19}  : 5, 5, 0, 4, 1, 0, 0, 1, 2.

g_{20}  : 5, 7, 0, 3, 4, 0, 0, 0, 3, 1.

g_{21}  : 5, 6, 0, 4, 2, 0, 0, 0, 4.

g_{22}  : 5, 10, 0, 0, 10, 0, 0, 0, 0, 5.

g_{23}  : 6, 12, 4, 12, 4, 12, 3, 0, 0, 0, 6.

g_{24}  : 6, 10, 2, 10, 3, 5, 1, 4, 4, 0, 1, 2, 0, 2, 1.

g_{25}  : 6, 11, 2, 10, 5, 6, 1, 2, 5, 1, 1, 2, 2, 0, 1.

g_{26}  : 6, 10, 2, 8, 4, 4, 0, 4, 4, 1, 0, 0, 2, 4.

g_{27}  : 6, 9, 0, 12, 2, 0, 3, 6, 6, 0, 0, 0, 0, 0, 6.

g_{28}  : 6, 9, 1, 10, 2, 2, 1, 7, 4, 0, 0, 1, 0, 2, 2, 1.

g_{29}  : 6, 9, 1, 9, 3, 3, 0, 3, 6, 0, 0, 3, 0, 0, 0, 0, 0, 0, 3.

g_{30}  : 6, 8, 1, 7, 2, 2, 0, 4, 3, 0, 0, 1, 0, 1, 0, 0, 1, 1, 1.

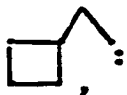
g_{31}  : 6, 10, 1, 8, 5, 3, 0, 2, 7, 1, 0, 2, 1, 0, 0, 0, 0, 1, 0, 1, 1.

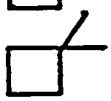
g_{32}  : 6, 7, 1, 5, 1, 1, 0, 4, 1, 0, 0, 0, 0, 1, 0, 0, 2, 1.

g_{33}  : 6, 8, 1, 6, 2, 1, 0, 4, 4, 0, 0, 0, 0, 2, 0, 0, 0, 2, 0, 0, 1.

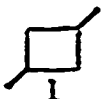
g_{34}  : 6, 9, 1, 7, 4, 2, 0, 2, 5, 1, 0, 0, 1, 1, 0, 0, 0, 0, 2, 1.

g_{35}  : 6, 12, 1, 6, 10, 3, 0, 0, 6, 5, 0, 0, 3, 0, 0, 0, 0, 0, 0, 2, 0, 1.

g_{36}  : 6, 7, 0, 8, 1, 0, 1, 4, 3, 0, 0, 0, 0, 0, 1, 0, 2, 0, 2.

g_{37}  : 6, 9, 0, 8, 4, 0, 1, 4, 6, 1, 0, 0, 0, 0, 2, 0, 0, 2, 0, 2.

g_{38}  : 6, 8, 0, 9, 2, 0, 1, 4, 6, 0, 0, 0, 0, 0, 2, 0, 1, 0, 2, 0, 1.

g_{39}  : 6, 8, 0, 8, 2, 0, 1, 6, 4, 0, 0, 0, 0, 0, 2, 0, 0, 4.

g_{40}  : 6, 7, 0, 7, 1, 0, 0, 7, 2, 0, 0, 0, 0, 0, 0, 1, 2, 2, 1.

g_{41}  : 6, 6, 0, 6, 0, 0, 0, 6, 0, 0, 0, 0, 0, 0, 0, 0, 6.

g_{42}  : 6, 5, 0, 4, 0, 0, 0, 3, 0, 0, 0, 0, 0, 0, 0, 0, 2.

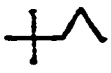
g_{43}  : 6, 6, 0, 4, 1, 0, 0, 3, 1, 0, 0, 0, 0, 0, 0, 0, 2, 1.

g_{44}  : 6, 6, 0, 5, 1, 0, 0, 3, 2, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1.

g_{45}  : 6, 6, 0, 6, 1, 0, 0, 3, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 3.

g_{46}  : 6, 7, 0, 4, 2, 0, 0, 4, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 4.

g_{47}  : 6, 7, 0, 6, 2, 0, 0, 2, 5, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 2, 0, 1.

g_{48}  : 6, 8, 0, 4, 4, 0, 0, 3, 3, 1, 0, 0, 0, 0, 0, 0, 0, 3, 0, 1.

g_{49}  : 6, 8, 0, 6, 4, 0, 0, 1, 6, 1, 0, 0, 0, 0, 0, 0, 0, 0, 2, 2.

g_{50}  : 6, 9, 0, 6, 5, 0, 0, 0, 9, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 3.

g_{51}  : 6, 11, 0, 4, 10, 0, 0, 0, 6, 5, 0, 0, 0, 0, 0, 0, 0, 0, 0, 4, 0, 1.

g_{52}  : 6, 15, 0, 0, 20, 0, 0, 0, 0, 15, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 6.

g_{53}  : 7, 15, 4, 18, 7, 15, 3, 6, 9, 1, 6, 6, 3, 3, 3, 0, 0, 0, 0, 0, 0, 0, 1, 3, 3.

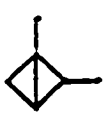
g_{54}  : 7, 14, 3, 17, 6, 10, 2, 10, 10, 1, 2, 5, 3, 6, 4, 1, 0, 0, 0, 0, 0, 0, 0, 2, 2, 1, 0, 2.

g_{55}  : 7, 13, 2, 18, 4, 6, 3, 14, 10, 0, 1, 4, 0, 6, 8, 2, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 1, 4.

g_{56}  : 7, 15, 3, 18, 8, 12, 3, 6, 12, 2, 3, 6, 6, 0, 6, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 6, 0, 1.

g_{57}  : 7, 12, 2, 14, 4, 6, 1, 10, 8, 0, 1, 4, 0, 4, 2, 0, 2, 4, 2, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 0, 1.

g_{58}  : 7, 14, 2, 15, 8, 8, 1, 6, 14, 2, 1, 6, 4, 0, 2, 0, 0, 4, 0, 2, 2, 0, 0, 0, 2, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0, 0, 0, 0, 1.

g_{59}  : 7, 13, 2, 15, 6, 7, 1, 7, 12, 1, 1, 5, 2, 2, 2, 0, 1, 1, 4, 1, 1, 0, 0, 1, 1, 0, 0, 0, 1, 1, 1, 0, 0, 1, 0, 0, 0, 1.

g_{60}  : 7, 11, 2, 12, 3, 5, 1, 8, 5, 0, 1, 2, 0, 3, 1, 0, 4, 2, 2, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 2, 0, 2, 0, 0, 0, 1.

g_{61}  : 7, 12, 2, 13, 5, 6, 1, 6, 8, 1, 1, 2, 2, 2, 1, 0, 2, 1, 4, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 2, 0, 0, 0, 2, 0, 1.

g_{62}  : 7, 15, 2, 14, 11, 8, 1, 4, 14, 5, 1, 4, 6, 0, 2, 0, 0, 2, 0, 4, 1, 1, 0, 0, 2, 0, 0, 0, 0, 0, 2, 0, 0, 0, 2, 0, 1.

g_{63}  : 7, 13, 2, 14, 6, 6, 1, 8, 12, 1, 1, 4, 1, 4, 2, 0, 0, 4, 0, 2, 2, 0, 0, 2, 0, 0, 0, 0, 0, 0, 2, 0, 2, 0, 0, 0, 1.

g_{64}  : 7, 14, 2, 12, 10, 6, 0, 4, 12, 5, 0, 0, 6, 4, 0, 0, 0, 0, 4, 4, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 4, 2.

g_{65}  : 7, 12, 2, 12, 5, 5, 0, 8, 9, 1, 0, 2, 2, 5, 0, 0, 2, 3, 2, 1, 1, 0, 0, 0, 0, 1, 0, 0, 0, 2, 1, 1, 1, 1.

g_{66}  : 7, 10, 2, 8, 2, 2, 0, 8, 4, 0, 0, 0, 0, 4, 0, 0, 4, 4, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 4, 2.

g_{67}  : 7, 11, 1, 14, 3, 3, 1, 11, 8, 0, 0, 3, 0, 2, 2, 1, 4, 2, 5, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 2, 0, 0, 0, 0, 0, 2, 0, 0, 0, 1.

g_{68}  : 7, 12, 1, 14, 5, 3, 1, 10, 11, 1, 0, 2, 1, 2, 3, 1, 2, 3, 3, 2, 1, 0, 0, 0, 0, 0, 0, 1, 0, 1, 1, 0, 0, 1, 0, 0, 1, 1, 0, 1.

g_{69}  : 7, 11, 1, 13, 3, 2, 1, 12, 8, 0, 0, 1, 0, 3, 3, 1, 3, 5, 2, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 1, 1, 0, 0, 0, 0, 1, 1, 1.

g_{70}  : 7, 11, 1, 12, 4, 2, 1, 8, 8, 1, 0, 0, 1, 2, 2, 0, 4, 2, 4, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 2, 0, 2, 1.

g_{71}  : 7, 10, 0, 14, 2, 0, 2, 10, 8, 0, 0, 0, 0, 0, 4, 0, 8, 0, 6, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 4, 0, 2, 0, 0, 1.

g_{72}  : 7, 10, 1, 11, 2, 2, 0, 12, 4, 0, 0, 1, 0, 2, 0, 1, 8, 4, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 2, 1.

g_{73}  : 7, 10, 0, 13, 2, 0, 1, 14, 6, 0, 0, 0, 0, 0, 2, 2, 6, 6, 4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 1, 4.

g_{74}  : 7, 12, 0, 15, 5, 0, 3, 12, 12, 1, 0, 0, 0, 0, 9, 0, 0, 9, 0, 3, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 3, 0, 3.

g_{75}  : 7, 11, 0, 16, 3, 0, 3, 10, 12, 0, 0, 0, 0, 0, 8, 0, 4, 0, 6, 0, 2, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 4.

g_{76}  : 7, 9, 1, 8, 2, 2, 0, 6, 3, 0, 0, 1, 0, 1, 0, 0, 4, 2, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1.

g_{77}  : 7, 9, 1, 9, 2, 2, 0, 7, 4, 0, 0, 1, 0, 2, 0, 0, 3, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0,

0, 0, 0, 0, 0, 0, 1, 0, 2.

g_{78}  : 7, 8, 1, 6, 1, 1, 0, 5, 1, 0, 0, 0, 0, 1, 0, 0, 4,
1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0,
0, 0, 0, 0, 0, 0, 2, 1.

g_{79}  : 7, 9, 1, 6, 2, 1, 0, 6, 2, 0, 0, 0, 0, 1, 0, 0, 4,
4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 1.

g_{80}  : 7, 9, 1, 8, 2, 1, 0, 6, 5, 0, 0, 0, 0, 2, 0, 0, 2,
3, 2, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 1.

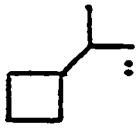
g_{81}  : 7, 10, 1, 10, 4, 2, 0, 5, 8, 1, 0, 0, 1, 2, 0, 0, 0,
0, 6, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 1.

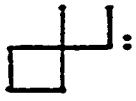
g_{82}  : 7, 10, 1, 8, 4, 2, 0, 5, 5, 1, 0, 0, 1, 1, 0, 0, 2,
3, 2, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0,
0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 1.

g_{83}  : 7, 9, 0, 10, 2, 0, 1, 8, 5, 0, 0, 0, 0, 0, 2, 0, 4,
4, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
1, 0, 0, 1, 0, 0, 0, 2, 2.

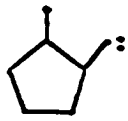
g_{84}  : 7, 9, 0, 11, 2, 0, 1, 7, 7, 0, 0, 0, 0, 0, 2, 0, 3,
1, 5, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
1, 0, 1, 0, 0, 0, 1, 0, 1, 1, 0, 1.

g_{85}  : 7, 8, 0, 9, 1, 0, 1, 6, 3, 0, 0, 0, 0, 0, 1, 0, 4,
1, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
1, 0, 0, 0, 0, 0, 2, 0, 2.

g_{86}  : 7, 9, 0, 10, 2, 0, 1, 6, 6, 0, 0, 0, 0, 0, 1, 0, 4,
2, 4, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
2, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 2.

g_{87}  : 7, 10, 0, 11, 4, 0, 1, 6, 9, 1, 0, 0, 0, 0, 2, 0, 2,
2, 4, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
1, 1, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 2.

g_{88}  : 7, 9, 0, 9, 2, 0, 0, 10, 4, 0, 0, 0, 0, 0, 0, 1, 5,
6, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 2, 0, 0, 2, 2, 0, 1.

g_{89}  : 7, 9, 0, 10, 2, 0, 0, 9, 6, 0, 0, 0, 0, 0, 0, 1, 4,
4, 4, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 2, 0, 1, 0, 2, 0, 0, 2.

g_{90}  : 7, 8, 0, 9, 1, 0, 0, 9, 3, 0, 0, 0, 0, 0, 0, 1, 4,
2, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 1, 0, 2, 0, 2, 1.

g_{91}  : 7, 10, 0, 9, 4, 0, 0, 9, 6, 1, 0, 0, 0, 0, 0, 1, 4,
6, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 2, 0, 0, 2, 0, 0, 0, 0, 2, 1.

g_{92}  : 7, 8, 0, 8, 1, 0, 0, 8, 2, 0, 0, 0, 0, 0, 0, 0, 8, 2, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 2, 2, 2.

g_{93}  : 7, 7, 0, 7, 0, 0, 0, 7, 0, 0, 0, 0, 0, 0, 0, 0, 7, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 7.

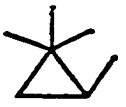
g_{94}  : 7, 10, 1, 11, 3, 3, 0, 7, 7, 0, 0, 3, 0, 1, 0, 0, 2, 2, 5, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 1.

g_{95}  : 7, 12, 1, 13, 6, 4, 0, 5, 14, 1, 0, 5, 1, 0, 0, 0, 0, 2, 6, 2, 2, 0, 0, 0, 0, 0, 0, 0, 2, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 1.

g_{96}  : 7, 10, 1, 9, 3, 2, 0, 7, 6, 0, 0, 1, 0, 2, 0, 0, 2, 5, 2, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 1.

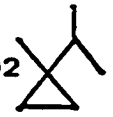
g_{97}  : 7, 11, 1, 11, 5, 3, 0, 5, 10, 1, 0, 2, 1, 1, 0, 0, 1, 2, 4, 2, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 1.

g_{98}  : 7, 11, 1, 10, 5, 3, 0, 6, 8, 1, 0, 2, 1, 1, 0, 0, 2, 4, 2, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 2, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 1.

g_{99}  : 7, 14, 1, 11, 11, 4, 0, 3, 15, 5, 0, 3, 3, 0, 0, 0, 0,
3, 0, 6, 3, 1, 0, 0, 0, 0, 0, 0, 0, 0, 3, 0, 0, 0, 1,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 1.

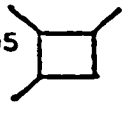
g_{100}  : 7, 13, 1, 12, 8, 4, 0, 4, 16, 2, 0, 4, 2, 0, 0, 0, 0,
4, 0, 4, 5, 0, 0, 0, 0, 0, 0, 0, 0, 0, 4, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 2.

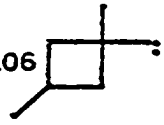
g_{101}  : 7, 11, 1, 8, 5, 1, 0, 6, 9, 1, 0, 0, 0, 3, 0, 0, 0,
6, 0, 2, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 3, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 1.

g_{102}  : 7, 11, 1, 10, 5, 2, 0, 4, 11, 1, 0, 0, 1, 2, 0, 0, 0,
2, 4, 2, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 2, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 1.

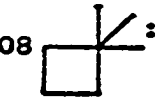
g_{103}  : 7, 13, 1, 10, 10, 3, 0, 2, 12, 5, 0, 0, 3, 1, 0, 0, 0,
0, 4, 6, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 1,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 1.

g_{104}  : 7, 17, 1, 8, 20, 4, 0, 0, 12, 15, 0, 0, 6, 0, 0, 0, 0,
0, 0, 8, 0, 6, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 4,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 1.

g_{105}  : 7, 10, 0, 12, 3, 0, 1, 8, 10, 0, 0, 0, 0, 0, 3, 0, 2,
4, 5, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 2, 1, 0, 0, 0, 0, 2, 0, 0, 2.

g_{106}  : 7, 11, 0, 10, 5, 0, 1, 10, 8, 1, 0, 0, 0, 0, 3, 0, 0,
12, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 1, 0, 2, 0, 0, 0, 0, 0, 0, 2, 0, 2.

g_{107}  : 7, 11, 0, 12, 5, 0, 1, 6, 13, 1, 0, 0, 0, 0, 3, 0, 2,
2, 4, 3, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 1, 2, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 1, 1.

g_{108}  : 7, 13, 0, 10, 10, 0, 1, 6, 12, 5, 0, 0, 0, 0, 3, 0, 0,
6, 0, 8, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 2.

Appendix B. Tables of Characters of the Symmetric Groups and the Values of tr P_k and tr P_kQ^2

Note: The values of tr P_kQ^2 should be multiplied by the factor $\frac{X}{3}$ tr P_k which is dropped out in these tables for convenience.

Degree 2

Class k	1^2	2
Order h_k	1	1
$\chi_k^{(\nu)}$ (2)	1	1
$\chi_k^{(\nu)}$ (1^2)	1	-1
tr P_k	Y^2	Y
tr P_kQ^2	2	4

Degree 3

Class k	1^3	12	3
Order h_k	1	3	2
$\chi_k^{(\nu)}$ (3)	1	1	1
$\chi_k^{(\nu)}$ (21)	2	0	-1
$\chi_k^{(\nu)}$ (1^3)	1	-1	1
tr P_k	Y^3	Y^2	Y
tr P_kQ^2	3	5	9

Degree 4

Class k	1^4	$1^2 2$	13	4	2^2
Order h_k	1	6	8	6	3
$\chi_k^{(\nu)}$ (4)	1	1	1	1	1
(31)	3	1	0	-1	-1
(2^2)	2	0	-1	0	2
(21^2)	3	-1	0	1	-1
(1^4)	1	-1	1	-1	1
tr P_k	Y^4	Y^3	Y^2	Y	Y^2
tr $P_k Q^2$	4	6	10	16	8

Degree 5

Class k	1^5	$1^3 2$	$1^2 3$	14	12^2	23	5
Order h_k	1	10	20	30	15	20	24
$\chi_k^{(\nu)}$ (5)	1	1	1	1	1	1	1
(41)	4	2	1	0	0	-1	-1
(32)	5	1	-1	-1	1	1	0
(31^2)	6	0	0	0	-2	0	1
$(2^2 1)$	5	-1	-1	1	1	-1	0
(21^3)	4	-2	1	0	0	1	-1
(1^5)	1	-1	1	-1	1	-1	1
tr P_k	Y^5	Y^4	Y^3	Y^2	Y^3	Y^2	Y
tr $P_k Q^2$	5	7	11	17	9	13	25

Degree 6

Class k	1^6	$1^4 2$	$1^3 3$	$1^2 4$	$1^2 2^2$	123	15	6	24	2^3	3^2
Order h_k	1	15	40	90	45	120	144	120	90	15	40
$\chi_k^{(\nu)}$ (6)	1	1	1	1	1	1	1	1	1	1	1
(51)	5	3	2	1	1	0	0	-1	-1	-1	-1
(42)	9	3	0	-1	1	0	-1	0	1	3	0
(41^2)	10	2	1	0	-2	-1	0	1	0	-2	1
(3^2)	5	1	-1	-1	1	1	0	0	-1	-3	2
(321)	16	0	-2	0	0	0	1	0	0	0	-2
(2^3)	5	-1	-1	1	1	-1	0	0	-1	3	2
(31^3)	10	-2	1	0	-2	1	0	-1	0	2	1
$(2^2 1^2)$	9	-3	0	1	1	0	-1	0	1	-3	0
(21^4)	5	-3	2	-1	1	0	0	1	-1	1	-1
(1^6)	1	-1	1	-1	1	-1	1	-1	1	-1	1
tr P_k	Y^6	Y^5	Y^4	Y^3	Y^4	Y^3	Y^2	Y	Y^2	Y^3	Y^2
tr $P_k Q^2$	6	8	12	18	10	14	26	36	20	12	18

Degree 7

Class k	1^7	$1^5 2$	$1^4 3$	$1^3 4$	$1^3 2^2$	$1^2 23$	$1^2 5$	16	124	12^3	13^2	25	$2^2 3$	34	7
Order h_k	1	21	70	210	105	420	504	840	630	105	280	504	210	420	720
$\chi_k^{(\nu)}$ (7)	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
(61)	6	4	3	2	2	1	1	0	0	0	0	-1	-1	-1	-1
(52)	14	6	2	0	2	0	-1	-1	0	2	-1	1	2	0	0
(51^2)	15	5	3	1	-1	-1	0	0	-1	-3	0	0	-1	1	1
(43)	14	4	-1	-2	2	1	-1	0	0	0	2	-1	-1	1	0
(421)	35	5	-1	-1	-1	-1	0	1	1	1	-1	0	-1	-1	0
$(3^2 1)$	21	1	-3	-1	1	1	1	0	-1	-3	0	1	1	-1	0
(41^3)	20	0	2	0	-4	0	0	0	0	0	2	0	2	0	-1
(32^2)	21	-1	-3	1	1	-1	1	0	-1	3	0	-1	1	1	0
(321^2)	35	-5	-1	1	-1	1	0	-1	1	-1	-1	0	-1	1	0
$(2^3 1)$	14	-4	-1	2	2	-1	-1	0	0	0	2	1	-1	-1	0
(31^4)	15	-5	3	-1	-1	1	0	0	-1	3	0	0	-1	-1	1
$(2^2 1^3)$	14	-6	2	0	2	0	-1	1	0	-2	-1	-1	2	0	0
(21^5)	6	-4	3	-2	2	-1	1	0	0	0	0	1	-1	1	-1
(1^7)	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1
tr P_k	Y^7	Y^6	Y^5	Y^4	Y^5	Y^4	Y^3	Y^2	Y^3	Y^4	Y^3	Y^2	Y^3	Y^2	Y
tr $P_k Q^2$	7	9	13	19	11	15	27	37	21	13	19	29	17	25	49

Appendix C. Irreducible Representations of the Symmetric Groups

Note: 1. As described in Chapter VI for two conjugate representations we need only one of them for trace calculations. Therefore, only one of each pair of conjugate representations is given here.

2. For each representations only the interchanges P_{12}, P_{23}, ... , and $P_{N-1\ N}$ are shown. Other elements are multiplications of these interchanges.

3. Since the matrices are symmetric, only the diagonal elements and the non-zero upper triangular elements are shown.

4. We use the notations $Rn = \frac{1}{n}$, $Sn = (n^2-1)^{1/2}/n$.

Degree 2

Representation 2

$$P_{12} = [1]$$

Degree 3

Representation 3

$$P_{12} = P_{23} = [1]$$

Representation 21

$$P_{12} = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix}, \quad P_{23} = \begin{bmatrix} -R2 & S2 \\ & R2 \end{bmatrix}$$

Degree 4

Representation 4

$$P_{12} = P_{23} = P_{34} = \begin{bmatrix} 1 \end{bmatrix}$$

Representation 31

$$P_{12} = \begin{bmatrix} 1 & & \\ & 1 & \\ & & -1 \end{bmatrix} \quad P_{23} = \begin{bmatrix} 1 & & \\ & -R2 & S2 \\ & & R2 \end{bmatrix} \quad P_{34} = \begin{bmatrix} -R3 & S3 & \\ & R3 & \\ & & 1 \end{bmatrix}$$

Representation 2^2

$$P_{12} = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix} \quad P_{23} = \begin{bmatrix} -R2 & S2 \\ & R2 \end{bmatrix} \quad P_{34} = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix}$$

Degree 5

Representation 5

$$P_{12} = P_{23} = P_{34} = P_{45} = \begin{bmatrix} 1 \end{bmatrix}$$

Representation 41

$$P_{12} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{bmatrix} \quad P_{23} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & -R2 & S2 \\ & & & R2 \end{bmatrix} \quad P_{34} = \begin{bmatrix} 1 & & & \\ & -R3 & S3 & \\ & & R3 & \\ & & & 1 \end{bmatrix}$$

$$P_{45} = \begin{bmatrix} -R4 & S4 & & \\ & R4 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

Repersentation 32

$$P_{12} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & 1 \\ & & & & -1 \end{bmatrix} \quad P_{23} = \begin{bmatrix} 1 & & & \\ & -R2 & S2 & \\ & & R2 & \\ & & & -R2 & S2 \\ & & & & R2 \end{bmatrix}$$

$$P_{34} = \begin{bmatrix} -R3 & S3 & & & \\ & R3 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & -1 \end{bmatrix} \quad P_{45} = \begin{bmatrix} 1 & & & & \\ & -R2 & & S2 & \\ & & -R2 & & S2 \\ & & & R2 & \\ & & & & R2 \end{bmatrix}$$

Representation 31^2

$$P_{12} = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & -1 & & \\ & & & 1 & \\ & & & & -1 \end{bmatrix} \quad P_{23} = \begin{bmatrix} 1 & & & & \\ & -R2 & S2 & & \\ & & R2 & & \\ & & & -R2 & S2 \\ & & & & R2 \end{bmatrix}$$

$$P_{34} = \begin{bmatrix} -R3 & S3 & & & \\ & R3 & & & \\ & & 1 & & \\ & & & -1 & \\ & & & & -1 \end{bmatrix} \quad P_{45} = \begin{bmatrix} -1 & & & & \\ & -R4 & & S4 & \\ & & -R4 & & S4 \\ & & & R4 & \\ & & & & R4 \end{bmatrix}$$

Degree 6

Representation 6

$$P_{12} = P_{23} = P_{34} = P_{45} = P_{56} = [1]$$

Representation 51

$$P_{12} = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & -1 \end{bmatrix} \quad P_{23} = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & -R2 & S2 \\ & & & & R2 \end{bmatrix} \quad P_{34} = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & -R3 & S3 & \\ & & & R3 & \\ & & & & 1 \end{bmatrix}$$

$$P_{45} = \begin{bmatrix} 1 & & & & \\ & -R4 & S4 & & \\ & & R4 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix} \quad P_{56} = \begin{bmatrix} -R5 & S5 & & & \\ & R5 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}$$

Note: For the following matrices we first write the diagonal elements $P_{ij}(1,1)$, $P_{ij}(2,2)$, $P_{ij}(3,3)$, etc., then, the non-zero upper triangular elements.

Representation 42

P_{12} diag(1, 1, 1, -1, 1, 1, -1, 1, -1)

P_{23} diag(1, 1, -R2, R2, 1, -R2, R2 -R2, R2)

$P_{23}(3,4) = P_{23}(6,7) = P_{23}(8,9) = S2$

P_{34} diag(1, -R3, R3, 1, -R3, R3, 1, 1, -1)

$P_{34}(2,3) = P_{34}(5,6) = S3$

P_{45} diag(-R4, R4, 1, 1, 1, -R2, -R2, R2, R2)

$P_{45}(1,2) = S4$, $P_{45}(6,8) = P_{45}(7,9) = S2$

P_{56} diag(1, -R3, -R3, -R3, R3, R3, R3, 1, 1)

$P_{56}(2,5) = P_{56}(3,6) = P_{56}(4,7) = S3$

Representation 41^2

P_{12} diag(1, 1, 1, -1, 1, 1, -1, 1, -1, -1)

P_{23} diag(1, 1, -R2, R2, 1, -R2, R2, -R2, R2, -1)

$P_{23}(3,4) = P_{23}(6,7) = P_{23}(8,9) = S2$

P_{34} diag(1, -R3, R3, 1, -R3, R3, 1, -1, -R3, R3)

$P_{34}(2,3) = P_{34}(5,6) = P_{34}(9,10) = S3$

P_{45} diag(-R4, R4, 1, 1, -1, -R4, -R4, R4, R4, 1)

$P_{45}(1,2) = P_{45}(6,8) = P_{45}(7,9) = S4$

P_{56} diag(-1, -R5, -R5, -R5, R5, R5, R5, 1, 1, 1)

$P_{56}(2,5) = P_{56}(3,6) = P_{56}(4,7) = S5$

Representation 3^2

P_{12} diag(1, 1, -1, 1, -1)

P_{23} diag(1, -R2, R2, -R2, R2)

$P_{23}(2,3) = P_{23}(4,5) = S2$

P_{34} diag(-R3, R3, 1, 1, -1)

$P_{34}(1,2) = S3$

P_{45} diag(1, -R2, -R2, R2, R2)

$P_{45}(2,4) = P_{45}(3,5) = S2$

P_{56} diag(1, 1, 1, -1, -1)

Representation 321

P_{12} diag(1, 1, -1, 1, -1, 1, 1, -1, 1, -1, -1, 1, -1, 1, -1, -1)

P_{23} diag(1, -R2, R2, -R2, R2, 1, -R2, R2, -R2, R2, -1, -R2, R2,
-R2, R2, -1)

$P_{23}(2,3) = P_{23}(4,5) = P_{23}(7,8) = P_{23}(9,10) = P_{23}(12,13)$
$= P_{23}(14,15) = S2$

P_{34} diag(-R3, R3, 1, 1, -1, -R3, R3, 1, -1, -R3, R3, 1, -1, -1,
-R3, R3)

$P_{34}(1,2) = P_{34}(6,7) = P_{34}(10,11) = P_{34}(15,16) = S3$

P_{45} diag(1, -R2, -R2, R2, R2, -1, -R4, -R4, R4, R4, 1, -R2, -R2,
R2, R2, -1)

$P_{45}(2,4) = P_{45}(3,5) = P_{45}(12,14) = P_{45}(13,15) = S2$

$P_{45}(7,9) = P_{45}(8,10) = S4$

P_{56} diag(-R2, -R2, -R2, -R4, -R4, R2, R2, R2, -R2, -R2, -R2,

R4, R4, R2, R2, R2)

$P_{56}(1,6) = P_{56}(2,7) = P_{56}(3,8) = S2$

$P_{56}(4,12) = P_{56}(5,13) = S4$

$P_{56}(9,14) = P_{56}(10,15) = P_{56}(11,16) = S2$

Degree 7

Representation 7

$P_{12} = P_{23} = P_{34} = P_{45} = P_{56} = P_{67} = [1]$

Representation 61

P_{12} diag(1, 1, 1, 1, 1, -1)

P_{23} diag(1, 1, 1, 1, -R2, R2)

$P_{23}(5,6) = S2$

P_{34} diag(1, 1, 1, -R3, R3, 1)

$P_{34}(4,5) = S3$

P_{45} diag(1, 1, -R4, R4, 1, 1)

$P_{45}(3,4) = S4$

P_{56} diag(1, -R5, R5, 1, 1, 1)

$P_{56}(2,3) = S5$

P_{67} diag(-R6, R6, 1, 1, 1, 1)

$P_{67}(1,2) = S6$

Representation 52

P_{12} diag(1, 1, 1, 1, -1, 1, 1, 1, -1, 1, 1, -1, 1, -1)

P_{23} diag(1, 1, 1, -R2, R2, 1, 1, -R2, R2, 1, -R2, R2, -R2, R2)

$P_{23}(4,5) = P_{23}(8,9) = P_{23}(11,12) = P_{23}(13,14) = S2$

P_{34} diag(1, 1, -R3,R3, 1, 1, -R3, R3,1, -R3, R3, 1, 1, -1)

$P_{34}(3,4) = P_{34}(7,8) = P_{34}(10,11) = S3$

P_{45} diag(1, -R4, R4, 1, 1, -R4, R4, 1, 1, 1, -R2, -R2, R2, R2)

$P_{45}(2,3) = P_{45}(6,7) = S4$, $P_{45}(11,13) = P_{45}(12,14) = S2$

P_{56} diag(-R5, R5, 1, 1, 1, 1, -R3, -R3, -R3, R3, R3, R3, 1, 1)

$P_{56}(1,2) = S5$, $P_{56}(7,10) = P_{56}(8,11) = P_{56}(9, 12) = S3$

P_{67} diag(1, -R4, -R4, -R4, -R4, R4, R4, R4, R4, 1, 1, 1, 1, 1)

$P_{67}(2,6) = P_{67}(3,7) = P_{67}(4,8) = P_{67}(5,9) = S4$

Representation 51^2

P_{12} diag(1, 1, 1, 1, -1, 1, 1, 1, -1, 1, 1, -1, 1, -1, -1)

P_{23} diag(1, 1, 1, -R2, R2, 1, 1, -R2, R2, 1, -R2, R2, -R2, R2, -1)

$P_{23}(4,5) = P_{23}(8,9) = P_{23}(11,12) = P_{23}(13,14) = S2$

P_{34} diag(1, 1, -R3, R3, 1, 1, -R3, R3,1,-R3, R3, 1, -1, -R3, R3)

$P_{34}(3,4) = P_{34}(7,8) = P_{34}(10,11) = P_{34}(14,15) = S3$

P_{45} diag(1, -R4, R4, 1, 1, -R4, R4, 1, 1, -1, -R4, -R4, R4, R4, 1)

$P_{45}(2,3) = P_{45}(6,7) = P_{45}(11,13) = P_{45}(12,14) = S4$

P_{56} diag(-R5, R5, 1, 1, 1, -1 , -R5, -R5,-R5, R5, R5, R5, 1, 1, 1)

$P_{56}(1,2) = P_{56}(7,10) = P_{56}(8,11) = P_{56}(9,12) = S5$

P_{67} diag(-1,-R5, -R6, -R6, -R6, R6, R6, R6, R6, 1, 1, 1, 1, 1, 1)

$P_{67}(2,6) = P_{67}(3,7) = P_{67}(4,8) = P_{67}(5,9) = S6$

Representation 43

P_{12} diag(1, 1, 1, -1, 1, 1, -1, 1, -1, 1, 1, -1, 1, -1)

P_{23} diag(1, 1, -R2, R2, 1, -R2, R2, -R2, R2, 1, -R2, R2, -R2, R2)

$P_{23}(3,4) = P_{23}(6,7) = P_{23}(8,9) = P_{23}(11,12) = P_{23}(13,14) = S2$

P_{34} diag(1, -R3, R3, 1, -R3, R3, 1, 1, -1, -R3, R3, 1, 1, -1)

$P_{34}(2,3) = P_{34}(5,6) = P_{34}(10,11) = S3$

P_{45} diag(-R4, R4, 1, 1, 1, -R2, -R2, R2, R2, 1, -R2,-R2, R2, R2)

$P_{45}(1,2) = S4$

$P_{45}(6,8) = P_{45}(7,9) = P_{45}(11,13) = P_{45}(12,14) = S2$

P_{56} diag(1, -R3, -R3, -R3, R3, R3, R3, 1, 1, 1, 1, 1, -1,-1)

$P_{56}(2,5) = P_{56}(3,6) = P_{56}(4,7) = S3$

P_{67} diag(1, 1, 1, 1, -R2, -R2, -R2, -R2, -R2, R2, R2, R2, R2, R2)

$P_{67}(5,10) = P_{67}(6,11) = P_{67}(7,12) = P_{67}(8,13) = P_{67}(9,14) = S2$

Representation 421

P_{12} diag(1, 1, 1, -1, 1, 1, -1, 1, -1, 1, 1, 1, -1, 1, 1, -1, 1,
-1, -1, 1, 1, -1, 1, -1, 1, 1, -1, 1, -1, -1, 1, -1, 1,
-1, -1)

P_{23} diag(1, 1, -R2, R2, 1, -R2, R2, -R2, R2, 1, 1, -R2, R2, 1,
-R2, R2, -R2, R2, -1, 1, -R2, R2, -R2, R2, 1, -R2, R2,
-R2, R2, -1, -R2, R2, -R2, R2, -1)

$P_{23}(3,4) = P_{23}(6,7) = P_{23}(8,9) = P_{23}(12,13) = P_{23}(15,16)$
$= P_{23}(17,18) = P_{23}(21,22) = P_{23}(23,24) = P_{23}(26,27)$
$= P_{23}(28,29) = P_{23}(31,32) = P_{23}(33,34) = S2$

P_{34} diag(1, -R3, R3, 1, -R3, R3, 1, 1, -1, 1, -R3, R3, 1, -R3, R3, 1, -1, -R3, R3, -R3, R3, 1, 1, -1, -R3, R3, 1, -1, -R3, R3, 1, -1, -1, -R3, R3)

$P_{34}(2,3) = P_{34}(5,6) = P_{34}(11,12) = P_{34}(14,15) = P_{34}(18,19) = P_{34}(20,21) = P_{34}(25,26) = P_{34}(29,30) = P_{34}(34,35) = S3$

P_{45} diag(-R4, R4, 1, 1, 1, -R2, -R2, R2, R2, -R4, R4, 1, 1, -1, -R4, -R4, R4, R4, 1, 1, -R2, -R2, R2, R2, -1, -R4, -R4 R4, R4, 1, -R2, -R2, R2, R2, -1)

$P_{45}(1,2) = P_{45}(10,11) = P_{45}(15,17) = P_{45}(16,18) = P_{45}(26,28) = P_{45}(27,29) = S4$

$P_{45}(6,8) = P_{45}(7,9) = P_{45}(21,23) = P_{45}(22,24) = P_{45}(31,33) = P_{45}(32,34) = S2$

P_{56} diag(1, -R3, -R3, -R3, R3, R3, R3, 1, 1, -1, -R5, -R5, -R5, R5, R5, R5, 1, 1, 1, -R2, -R2, -R2, -R4, -R4, R2, R2, R2, -R2, -R2, -R2, R4, R4, R2, R2, R2)

$P_{56}(2,5) = P_{56}(3,6) = P_{56}(4,7) = S3$

$P_{56}(11,14) = P_{56}(12,15) = P_{56}(13, 16) = S5$

$P_{56}(20,25) = P_{56}(21,26) = P_{56}(22, 27) = S2$

$P_{56}(23,31) = P_{56}(24,32) = S4$

$P_{56}(28,33) = P_{56}(29,34) = P_{56}(30,35) = S2$

P_{67} diag(-R2, -R2, -R2, -R2, -R5, -R5, -R5, -R5, -R5, R2, R2, R2, R2, -R3, -R3, -R3, -R3, -R3, -R3, R5, R5, R5, R5, R5, R3, R3, R3, R3, R3, R3, 1, 1, 1, 1, 1)

$P_{67}(1,10) = P_{67}(2,11) = P_{67}(3,12) = P_{67}(4,13) = S2$

$P_{67}(5,20) = P_{67}(6,21) = P_{67}(7,22) = P_{67}(8,23) = P_{67}(9,24) = S5$

$P_{67}(14,25) = P_{67}(15,26) = P_{67}(16,27) = P_{67}(17,28)$

$= P_{67}(18,29) = P_{67}(19,30) = S3$

Representation $3^2 1$

P_{12} diag(1, 1, -1, 1, -1, 1, 1, -1, 1, -1, 1, 1, -1, 1, -1,
-1, 1, -1, 1, -1, -1)

P_{23} diag(1, -R2, R2, -R2, R2, 1, -R2, R2, -R2, R2, 1, -R2, R2,
-R2, R2, -1, -R2, R2, -R2, R2, -1)

$P_{23}(2,3) = P_{23}(4,5) = P_{23}(7,8) = P_{23}(9,10) = P_{23}(12,13)$

$P_{23}(14,15) = P_{23}(17,18) = P_{23}(19,20) = S2$

P_{34} diag(-R3, R3, 1, 1, -1, -R3, R3, 1, 1, -1, -R3, R3, 1, -1,
-R3, R3, 1, -1, -1, -R3, R3)

$P_{34}(1,2) = P_{34}(6,7) = P_{34}(11,12) = P_{34}(15,16)$

$= P_{34}(20,21) = S3$

P_{45} diag(1, -R2, -R2, R2, R2,1, -R2, -R2, R2, R2, -1, -R4, -R4,
R4, R4, 1, -R2, -R2, R2, R2, -1)

$P_{45}(2,4) = P_{45}(3,5) = P_{45}(7,9) = P_{45}(8,10) = P_{45}(17,19)$

$= P_{45}(18,20) = S2$

$P_{45}(12,14) = P_{45}(13,15) = S4$

P_{56} diag(1, 1, 1, -1, -1, -R2, -R2, -R2, -R4, -R4, R2, R2, R2,
-R2, -R2, -R2, R4, R4, R2, R2, R2)

$P_{56}(6,11) = P_{56}(7,12) = P_{56}(8,13) = S2$

$P_{56}(9,17) = P_{56}(10,18) = S4$

$P_{56}(14,19) = P_{56}(15,20) = P_{56}(16,21) = S2$

P_{67} diag(-R3, -R3, -R3, -R3, -R3, R3, R3, R3, R3, R3, 1, 1, 1, 1, 1, 1, -1, -1, -1, -1, -1)

$P_{67}(1,6) = P_{67}(2,7) = P_{67}(3,8) = P_{67}(4,9) = P_{67}(5,10) = S3$

Representation 41^3

P_{12} diag(1, 1, 1, -1, 1, 1, -1, 1, -1, -1, 1, 1, -1, 1, -1, -1, 1, -1, -1, -1)

P_{23} diag(1, 1, -R2, R2, 1, -R2, R2, -R2, R2,-1, 1, -R2, R2, -R2, R2,-1, -R2, R2, -1, -1)

$P_{23}(3,4) = P_{23}(6,7) = P_{23}(8,9) = P_{23}(12,13) = P_{23}(14,15)$
$= P_{23}(17,18) = S2$

P_{34} diag(1, -R3, R3, 1, -R3, R3,1, -1, -R3, R3, -R3, R3,1, -1, -R3, R3,-1, -R3, R3, -1)

$P_{34}(2,3) = P_{34}(5,6) = P_{34}(9,10) = P_{34}(11,12) = P_{34}(15,16)$
$= P_{34}(18,19) = S3$

P_{45} diag(-R4, R4, 1, 1, -1, -R4, -R4, R4, R4, 1, -1, -R4, -R4, R4, R4, 1, -1, -1, -R4, R4)

$P_{45}(1,2) = P_{45}(6,8) = P_{45}(7,9) = P_{45}(12,14) = P_{45}(13,15)$
$P_{45}(19,20) = S4$

P_{56} diag(-1, -R5, -R5, -R5, R5, R5, R5, 1, 1, 1, -1, -1, -1, -R5, -R5, -R5, R5, R5, R5, 1)

$P_{56}(2,5) = P_{56}(3,6) = P_{56}(4,7) = P_{56}(14,17) = P_{56}(15,18)$
$= P_{56}(16,19) = S5$

P_{67} diag(-1, -1, -1, -1, -R6, -R6, -R6, -R6, -R6, -R6, R6,
R6, R6, R6, R6, R6, 1, 1, 1, 1)

$P_{67}(5,11) = P_{67}(6,12) = P_{67}(7,13) = P_{67}(8,14) = P_{67}(9,15)$
$= P_{67}(10,16) = S6$

Appendix D. Series Coefficients $e_n^{(m)}(g_i)$ and $a_n^{(m)}(g_i)$

D-1. Coefficients $e_n^{(m)}(g_i)$. [see Eqs.(77) and (80)]

Following each graph are the numbers $e_1^{(1)}(g_i)$; $e_2^{(0)}(g_i)$, $e_2^{(2)}(g_i)$; $e_3^{(1)}(g_i)$, $e_3^{(3)}(g_i)$; $e_4^{(0)}(g_i)$, $e_4^{(2)}(g_i)$, $e_4^{(4)}(g_i)$; $e_5^{(1)}(g_i)$, $e_5^{(3)}(g_i)$, $e_5^{(5)}(g_i)$; $e_6^{(0)}(g_i)$, $e_6^{(2)}(g_i)$, $e_6^{(4)}(g_i)$, $e_6^{(6)}(g_i)$; $e_7^{(1)}(g_i)$, $e_7^{(3)}(g_i)$, $e_7^{(5)}(g_i)$, $e_7^{(7)}(g_i)$.

Graphs with all the numbers zero are not shown.

g_1  : 1; 1, -1; -2, 2; -2, 8, -6; 16, -40, 24; 16, -136, 240, -120; -272, 1232, -1680, 720.

g_2  : 0; 0, 0; 0, 0; -2, 2, 0; 20, -20, 0; 50, -230, 180, 0; -980, 2660, -1680, 0.

g_3  : 0; 0, 0; 6, -6; 12, -84, 72; -270, 990, -720; -360, 4500, -10980, 6840; 11046, -62706, 112140, -60480.

g_4  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 12, -12, 0, 0; -280, 280, 0, 0.

g_5  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 30, -30, 0, 0; -630, 630, 0, 0.

g_6  : 0; 0, 0; 0, 0; 0, 0, 0; -20, 20, 0; -84, 684, -600, 0; 4270, -16870, 12600, 0.

g_7  : 0; 0, 0; 0, 0; 0, 24, -24; 80, -560, 480; 72, -2712, 9840, -7200; -6160, 66640, -161280, 100800.

g_{11}  : 0; 0, 0; 0, 0; 0, 0, 0; 60, -300, 240; 132, -3372, 11160, -7920; -12600, 112560, -271320, 171360.

g_{12}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 140, -140, 0, 0.

g_{13}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 420. -420, 0, 0.

g_{14}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 168, -168, 0, 0.

g_{15}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, -120, 120, 0; -700, 5740, -5040, 0.

g_{16}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 120, -120; 0, 600, -4200, 3600; 910, -28210, 102900, -75600.

g_{23}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 96, -1536, 5760, -4320; -9240, 89880, -262080, 181440.

g_{24}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; -448, 2128, -1680, 0.

g_{25}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; -630, 3150, -2520, 0.

g_{26}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, -240, 240, 0; -2352, 15792, -13440, 0.

g_{27}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 360, -1800, 1440; 1260, -21420, 80640, -60480.

g_{28}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 360, -1800, 1440; 1456, -28336, 92400, -65520.

g_{40}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 0, -840, 840, 0.

g_{41}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 720, -720; 0, 5040, -35280, 30240.

g_{54}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 798, -9198, 28560, -20160.

g_{55}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 644, -10724, 40320, -30240.

g_{56}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 840, -21000, 50400, -30240.

g_{70}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 0, -1680, 1680, 0.

g_{71}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 0, 2520, -12600, 10080.

g_{72}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 0, 2520, -12600, 10080.

g_{73}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 0, 2520, -12600, 10080.

g_{93}  : 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 0, 0, 0; 0, 0, 5040, -5040.

D-2. Coefficients $a_n^{(m)}(g_i)$. [see Eqs.(78) and (81)]

Following each graph are the numbers $a_1^{(1)}(g_i)$; $a_2^{(2)}(g_2)$; $a_3^{(1)}(g_i)$, $a_3^{(3)}(g_i)$; $a_4^{(2)}(g_i)$, $a_4^{(4)}(g_i)$; $a_5^{(1)}(g_i)$, $a_5^{(3)}(g_i)$, $a_5^{(5)}(g_i)$; $a_6^{(2)}(g_i)$, $a_6^{(4)}(g_i)$, $a_6^{(6)}(g_i)$; $a_7^{(1)}(g_i)$, $a_7^{(3)}(g_i)$, $a_7^{(5)}(g_i)$, $a_7^{(7)}(g_i)$. Graphs with all the numbers zero are not shown.

g_1  : 2; -4; -4, 12; 32, -48; 32, -240, 240; -544, 1920, -1440; -544, 7392, -16800, 10080.

g_2  : 0; 4; 0, -24; -20, 144; 40, 320, -960; -356, -4080, 7200; -1960, -224, 50400, -60480.

g_3  : 0; 0; 12, -72; -360, 1008; -540, 6240, -10800; 17280, -81000, 99360; 22092, -307272, 715680, -665280.

g_4  : 0; 0; 0, 12; 8,-144; 0, -280, 1440; -120, 5520, -14400; -560, 8512, -92400, 151200.

g_5  : 0; 0; 0, 0; -24, 0; 0, 480, 0; 1320, -7200, 0; -1260, -42420, 100800, 0.

g_6  : 0; 0; 0, 0; 32, -192; -40, -1080, 4320; 600, 24960, -69120; 8540, 1260, -455280, 947520.

g_7  : 0; 0; 0, 0; 112, -576; 160, -4320, 12480; -11280, 105600, -195840; -12320, 430080, -2184000, 2822400.

g_8  : 0; 0; 0, 0; 0, 48; 0, 80, -960; 12, -3240, 14400; 0, -3472, 82320, -201600.

g_9  : 0; 0; 0, 0; 0, 0; 0, -80, 0; -72, 2400, 0; 0, 8372, -50400, 0.

g_{10}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 720, 0, 0; 0, -25200, 0, 0.

g_{11}  : 0; 0; 0, 0; 0, 0; 120, -2640, 6720; -14640, 120240, -221760; -25200, 706440, -3087840, 4475520.

g_{12}  : 0; 0; 0, 0; 0, 0; 0, 120, -480; -168, -4080, 15840; 280, 4788, 104160, -352800.

g_{13}  : 0; 0; 0, 0; 0, 0; 0, -80, 0; -816, 6240, 0; 840, 61376, -228480, 0.

g_{14}  : 0; 0; 0, 0; 0, 0; 0, 160, -960; 96, -9360, 31680; 336, -24752, 319200, -705600.

g_{15}  : 0; 0; 0, 0; 0, 0; 0, 280, -1440; -72, -11520, 46080; -1400, -1176, 344400, -1008000.

g_{16}  : 0; 0; 0, 0; 0, 0; 0, 1000, -4800; 2760, -52800, 151200; 1820, -203140, 1730400, -3276000.

g_{17}  : 0; 0; 0, 0; 0, 0; 0, 0, 240; 0, 720, -7200; 0, 448, -36960, 151200.

g_{18}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, -480, 0; 0, -1400, 20160, 0.

g_{19}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, -240, 0; 0, -168, 10080, 0.

g_{20}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 2520,
0, 0.

g_{21}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0; 0, 1120,
0, 0.

g_{23}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; -5280, 46080, -103680;
-18480, 327600, -1774080, 3870720.

g_{24}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 384, -6720, 20160;
-896, -23408, 342720, -887040.

g_{25}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 336, -9120, 20160;
-1260, -34608, 477120, -947520.

g_{26}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; -432, -1920, 23040;
-4704, 59136, 221760, -1128960.

g_{27}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 1512, -25920, 69120;
2520, -159264, 1310400, -2903040.

g_{28}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 1656, -25920, 66240;
2912, -209104, 1592640, -3003840.

g_{29}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, -2688, 10080, 0.

g_{30}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 720, -2880;
0, 420, -42000, 131040.

g_{31}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, -1960, 10080, 0.

g_{32}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 960, -5760;
0, 1792, -78960, 262080.

g_{33}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, -1568, 13440, 0.

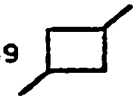
g_{34}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, -480, 0;
0, -4872, 36960, 0.

g_{35}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 5040, 0, 0.

g_{36}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 1680, -8640;
0, 4452, -117600, 383040.

g_{37}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, -480, 0;
0, -8680, 57120, 0.

g_{38}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 720, -2880;
0, -1680, -30240, 131040.

g_{39}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 720, -2880;
0, -2240, -16800, 120960.

g_{40}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 2400, -11520;
0, 784, -129360, 504000.

g_{41}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 9360, -43200;
0, 41664, -665280, 1874880.

g_{42}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 1440;
0, 0, 6720, -60480.

g_{43}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, -3360, 0.

g_{44}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, -1680, 0.

g_{53}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, -18480, 161280, -362880.

g_{54}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
1596, -76608, 510720, -987840.

g_{55}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
1288, -62888, 540960, -1249920.

g_{56}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
1680, -148008, 987840, -1330560.

g_{57}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 1288, -20160, 60480.

g_{58}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 1680, -40320, 60480.

g_{59}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 1596, -16800, 40320.

g_{60}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 2688, -47040, 141120.

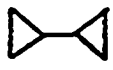
g_{61}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 2352, -63840, 141120.

g_{62}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, -2520, 10080, 0.

g_{63}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, -1792, 6720, 0.

g_{64}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, -6720, 40320, 0.

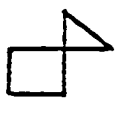
g_{65}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 168, -16800, 80640.

g_{66}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 4480, -53760, 161280.

g_{67}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 3920, -67200, 201600.

g_{68}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 4116, -80640, 181440.

g_{69}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 5516, -67200, 181440.

g_{70}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, -4872, -23520, 241920.

g_{71}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 19432, -272160, 705600.

g_{72}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 20356, -272160, 685440.

g_{73}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 18088, -272160, 725760.

g_{74}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 4200, -80640, 181440.

g_{75}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 4256, -67200, 201600.

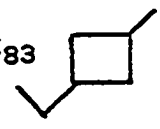
g_{76}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 5040, -20160.

g_{77}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 5040, -20160.

g_{78}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 6720, -40320.

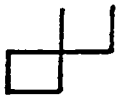
g_{81}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, -3360, 0.

g_{82}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, -3360, 0.

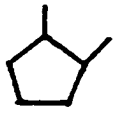
g_{83}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 5040, -20160.

g_{84}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 5040, -20160.

g_{85}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 11760, -60480.

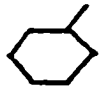
g_{87}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, -3360, 0.

g_{88}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 5040, -20160.

g_{89}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 5040, -20160.

g_{90}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 16800, -80640.

g_{91}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, -3360, 0.

g_{92}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 21840, -100800.

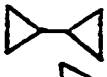
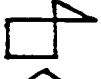
g_{93}  : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 94080, -423360.

- - - - - - - - - - - - - - - - - -

g_{109}(simple chain of 8 points)

 : 0; 0; 0, 0; 0, 0; 0, 0, 0; 0, 0, 0;
0, 0, 0, 10080.

Appendix E. Values of p_{nx} for Various Crystal Lattices

p_{nx}	Face-centered cubic	Body-centered cubic	Simple cubic	Plane triangle	Diamond	Plane square	Honey-comb	Linear
q	12	8	6	6	4	4	3	2
p_3 	8	0	0	2	0	0	0	0
p_4 	33	12	3	3	0	1	0	0
p_5 	168	0	0	6	0	0	0	0
p_{5a} 	36	0	0	3	0	0	0	0
p_6 	970	148	22	15	2	2	$\frac{1}{2}$	0
p_{6a} 	36	12	0	0	0	0	0	0
p_{6b} 	384	0	0	12	0	0	0	0
p_{6c} 	204	0	0	9	0	0	0	0
p_{6d} 	2	0	0	0	0	0	0	0
p_7 	6168	0	0	42	0	0	0	0
p_{7a} 	966	192	18	12	0	2	0	0
p_{7b} 	2400	0	0	30	0	0	0	0
p_{7c} 	192	0	0	6	0	0	0	0
p_{7d} 	2196	0	0	42	0	0	0	0
p_{7e} 	2040	0	0	30	0	0	0	0
p_{7f} 	600	0	0	0	0	0	0	0
p_{7g} 	24	0	0	0	0	0	0	0
p_{7h} 	48	0	0	0	0	0	0	0

Appendix F. Values of e_n and a_n for Several Lattices

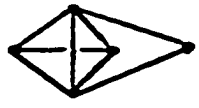
	$S = \frac{1}{2}$	$S = 1$	$S = \frac{3}{2}$	$S = 2$	$S = \frac{5}{2}$
Face-centered cubic lattice					
e_2	2.25	2.66667	2.8125	2.88	2.91667
e_3	2.25	1.77778	1.40625	1.152	0.97222
e_4	0.46875	-0.74074	-1.25976	-1.5168	-1.66088
e_5	-1.3125	-1.48148	-1.29492	-1.10745	-0.95602
e_6	3.51562	4.34842	4.25171	4.12301	4.02917
e_7	22.57812	13.33333	8.65661	6.28234	4.91030
Body-centered cubic lattice					
e_2	1.5	1.77778	1.875	1.92	1.94444
e_3	-0.5	-0.39506	-0.3125	-0.256	-0.21605
e_4	0.4375	-1.08642	-1.73828	-2.0608	-2.24152
e_5	0.375	2.30453	2.37891	2.15962	1.91924
e_6	0.53125	1.28578	3.68896	5.25901	6.24193
e_7	-0.46042	-6.28514	-9.53458	-9.96130	-9.48678
Simple cubic lattice					
e_2	1.125	1.33333	1.40625	1.44	1.45833
e_3	-0.375	-0.29629	-0.23437	-0.192	-0.16204
e_4	-0.42187	-0.96296	-1.18652	-1.296	-1.35706
e_5	0.65625	1.03704	0.96387	0.84403	0.73727
e_6	0.72031	1.38354	2.10339	2.53984	2.80617
e_7	-1.57969	-2.81536	-3.14886	-2.99927	-2.73934

	$S = \frac{1}{2}$	$S = 1$	$S = \frac{3}{2}$	$S = 2$	$S = \frac{5}{2}$
Face-centered cubic lattice					
a_1	6.0	4.0	3.0	2.4	2.0
a_2	30.0	13.33333	7.5	4.8	3.33333
a_3	138.0	43.11111	19.5	10.848	6.88889
a_4	611.25	140.55555	53.25	26.4336	15.47222
a_5	2658.55	456.03951	142.4	60.49024	30.75123
a_6	11432.5125	1461.63621	372.44062	134.67033	59.84501
a_7	48726.7262	4664.54243	988.93048	317.95349	132.51504
Body-centered cubic lattice					
a_1	4.0	2.66667	2.0	1.6	1.33333
a_2	12.0	5.33333	3.0	1.92	1.33333
a_3	34.66667	9.77778	3.83333	1.77066	0.88889
a_4	95.83333	21.85185	8.20833	4.04373	2.35185
a_5	262.7	45.19506	16.4125	8.99072	6.13456
a_6	708.04166	83.48148	16.80729	3.55153	0.06636
a_7	1893.28968	168.43935	24.68573	-3.13239	-10.69658
Simple cubic lattice					
a_1	3.0	2.0	1.5	1.2	1.0
a_2	6.0	2.66667	1.5	0.96	0.66667
a_3	11.0	2.88889	1.0	0.368	0.11111
a_4	20.6250	4.72222	1.78125	0.88080	0.51389
a_5	39.025	7.45185	3.34063	2.20864	1.71204
a_6	68.77708	7.19053	0.61809	-0.48737	-0.64719
a_7	119.42976	8.19700	-1.84097	-3.86818	-4.26662

	$S = \frac{1}{2}$	$S = 1$	$S = \frac{3}{2}$	$S = 2$	$S = \frac{5}{2}$
Plane triangular					
a_1	3.0	2.0	1.5	1.2	1.0
a_2	6.0	2.66666	1.5	0.96	0.66667
a_3	8.5	2.88889	1.4375	0.88	0.61111
a_4	9.375	2.5	1.07813	0.5928	0.375
a_5	11.025	1.62469	0.09844	-0.28224	-0.38673
a_6	16.96458	2.06914	0.20989	-0.13444	-0.19221
a_7	21.15268	4.76614	2.47238	1.77123	1.42805
Plane square					
a_1	2.0	1.33333	1.0	0.8	0.66667
a_2	2.0	0.88889	0.5	0.32	0.22222
a_3	1.33333	0.14815	-0.08333	-0.13867	-0.14815
a_4	1.08333	0.48148	0.27083	0.17333	0.12037
a_5	1.18333	0.73745	0.68542	0.61781	0.55082
a_6	0.50972	-0.67702	-0.67726	-0.05345	-0.41181
a_7	-4.82183	-0.96341	-1.12563	-1.21300	-1.19045

Appendix G. Clusters Used to Check the General Expressions for $e_n^{(m)}(g_i)$ and $a_n^{(m)}(g_i)$

Following each graph G are the lattice constants $(g_1;G)$, $(g_2;G)$, ... , $(g_{108};G)$, and then e_1, e_2, e_3, e_4, e_5, e_6, e_7 and a_1, a_2, a_3, a_4, a_5, a_6, a_7, respectively.[see Eqs.(14), (24)]



$(g_i;G)$: 8, 19, 5, 28, 10, 22, 5, 18, 20, 2, 8, 14, 8, 12, 12,
2, 0, 0, 0, 0, 0, 0, 1, 8, 10, 2, 1, 6, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 4, 1,
1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0.

$e_1 = 8\,Y^{-1}$,

$e_2 = 8 - 8Y^{-2}$,

$e_3 = 14Y^{-1} - 14Y^{-3}$,

$e_4 = 6 - 198Y^{-2} + 192Y^{-4}$,

$e_5 = -402Y^{-1} - 270Y^{-3} + 672Y^{-5}$,

$e_6 = -422 - 8818Y^{-2} + 62400Y^{-4} - 53160Y^{-6}$,

$e_7 = -25766Y^{-1} + 538706Y^{-3} - 1526700Y^{-5} + 1013760Y^{-7}$.

$a_1 = 16Y^{-1}$,

$a_2 = 44Y^{-2}$,

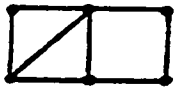
$a_3 = 28Y^{-1} - 384Y^{-3}$,

$a_4 = -676Y^{-2} - 2880Y^{-4}$,

$a_5 = -804Y^{-1} - 26000Y^{-3} + 118800Y^{-5}$,

$a_6 = -66316Y^{-2} + 996600Y^{-4} - 1566720Y^{-6}$,

$a_7 = -51532Y^{-1} + 4001816Y^{-3} - 10345440Y^{-5} - 8225280Y^{-7}$.



$(g_i;G)$: 8, 15, 2, 21, 6, 7, 2, 18, 16, 1, 1, 5, 2, 5, 5,
1, 11, 5, 10, 2, 1, 0, 0, 1, 1, 0, 0, 1, 1, 5, 1, 3, 0, 3, 0,
5, 1, 2, 0, 2, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 1, 1, 1, 0, 0, 0, 0, 0, 1, 1, 0, 1, 1, 1, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0.

$e_1 = 8Y^{-1}$,

$e_2 = 8 - 8Y^{-2}$,

$e_3 = -4Y^{-1} + 4Y^{-3}$,

$e_4 = -22 - 26Y^{-2} + 48Y^{-4}$,

$e_5 = -32Y^{-1} + 200Y^{-3} - 168Y^{-5}$,

$e_6 = 278 + 382Y^{-2} + 4620Y^{-4} - 5280Y^{-6}$,

$e_7 = 694Y^{-1} + 43526Y^{-3} - 211260Y^{-5} + 167040Y^{-7}$,

$a_1 = 16Y^{-1}$,

$a_2 = 28Y^{-2}$,

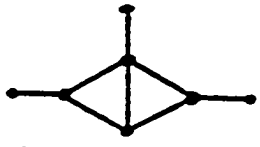
$a_3 = -8Y^{-1} - 156Y^{-3}$,

$a_4 = -292Y^{-2} - 864Y^{-4}$,

$a_5 = -64Y^{-1} - 2680Y^{-3} + 24240Y^{-5}$,

$a_6 = -164Y^{-2} + 175920Y^{-4} - 345600Y^{-6}$,

$a_7 = 1388Y^{-1} + 627592Y^{-3} - 4604880Y^{-5} + 6199200Y^{-7}$.



$(g_i;G)$: 8, 15, 2, 20, 7, 8, 1, 14, 19, 1, 1, 8, 2, 4, 3,
0, 4, 6, 11, 2, 2, 0, 0, 2, 1, 0, 0, 0, 2, 6, 2, 0, 0, 2, 0,
0, 0, 2, 1, 0, 0, 0, 0, 4, 1, 0, 2, 0, 1, 0, 0, 0, 0, 0, 0,
0, 1, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0,
0, 2, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0.

$e_1 = 8Y^{-1}$,

$e_2 = 8 - 8Y^{-2}$,

$e_3 = -4Y^{-1} + 4Y^{-3}$,

$e_4 = -22 - 50Y^{-2} + 72Y^{-4}$,

$e_5 = -132Y^{-1} + 660Y^{-3} - 528Y^{-5}$,

$e_6 = 140 + 3040Y^{-2} - 780Y^{-4} - 2400Y^{-6}$,

$e_7 = 9612Y^{-1} + 588Y^{-3} - 167160Y^{-5} + 156960Y^{-7}$,

$a_1 = 16Y^{-1}$,

$a_2 = 28Y^{-2}$,

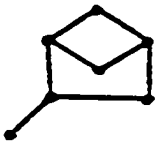
$a_3 = -8Y^{-1} - 168Y^{-3}$,

$a_4 = -404Y^{-2} - 528Y^{-4}$,

$a_5 = -264Y^{-1} - 600Y^{-3} + 24000Y^{-5}$,

$a_6 = 8404Y^{-2} + 166080Y^{-4} - 364320Y^{-6}$,

$a_7 = 19224Y^{-1} + 504672Y^{-3} - 4151280Y^{-5} + 3447360Y^{-7}$.



$(g_i;G)$: 8, 12, 0, 16, 3, 0, 1, 18, 10, 0, 0, 0, 0, 0, 2,
2, 12, 11, 8, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
3, 0, 0, 1, 6, 0, 2, 4, 6, 0, 1, 3, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0,
0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 1, 0, 2, 2, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0.

$e_1 = 8Y^{-1}$,

$e_2 = 8 - 8Y^{-2}$,

$e_3 = -16Y^{-1} + 16Y^{-3}$,

$e_4 = -40 + 112Y^{-2} - 72Y^{-4}$,

$e_5 = 448Y^{-1} - 880Y^{-3} + 432Y^{-5}$,

$e_6 = 1082 - 5882Y^{-2} + 5760Y^{-4} - 960Y^{-6}$,

$e_7 = -26046Y^{-1} + 67326Y^{-3} - 6720Y^{-5} - 34560Y^{-7}$,

$$a_1 = 16Y^{-1},$$

$$a_2 = 16Y^{-2},$$

$$a_3 = -32Y^{-1},$$

$$a_4 = 184Y^{-2} - 672Y^{-4},$$

$$a_5 = 896Y^{-1} - 2240Y^{-3} - 960Y^{-5},$$

$$a_6 = -12992Y^{-2} - 2640Y^{-4} + 120960Y^{-6},$$

$$a_7 = -52092Y^{-1} + 131712Y^{-3} + 705600Y^{-5} - 1048320Y^{-7}.$$

Appendix H. Proof of Theorems IX and X

Theorem A-1. Let i and j be any two sites in a finite cluster of N sites. Then

$$\langle S^n_{zi} S^n_{zj} \rangle_\beta - \langle S^n_{zi} \rangle_\beta \langle S^n_{zj} \rangle_\beta = (W_{2n} - W_n^2)\, X^{-1} \langle \underset{\sim}{S}_i \cdot \underset{\sim}{S}_j \rangle_\beta . \tag{A1}$$

Proof: From Eq.(61), it is straightforward to show that

$$\langle S^n_{zi} \rangle_\beta = W_n . \tag{A2}$$

Hence

$$\langle S^n_{zi} S^n_{zj} \rangle_\beta - \langle S^n_{zi} \rangle_\beta \langle S^n_{zj} \rangle_\beta = \frac{\sum_{r=0}^{\infty} \frac{K^r}{r!} \operatorname{tr} (S^n_{zi} S^n_{zj} \mathcal{P}^r - W_n^2 \mathcal{P}^r)}{\sum_{r=0}^{\infty} \frac{K^r}{r!} \operatorname{tr} \mathcal{P}^r} . \tag{A3}$$

If the finite cluster of N sites contains ℓ_c nearset-neighbor pairs, there are $r\ell_c$ terms in $\mathcal{P}^r$ and each term is also an element of S_N. Denote the sum of terms with i, j in the same cycle by $\mathcal{P}^{(1)}_r$ and the sum of terms with i, j in different independent cycles by $\mathcal{P}^{(2)}_r$:

$$\mathcal{P}^r = \mathcal{P}^{(1)}_r + \mathcal{P}^{(2)}_r . \tag{A4}$$

It then follows from Eq.(62) that for any r in Eq.(A3)

$$\operatorname{tr} S^n_{zi} S^n_{zj} \mathcal{P}^r - W_n^2 \operatorname{tr} \mathcal{P}^r = (W_{2n} - W_n^2) \operatorname{tr} \mathcal{P}^{(1)}_r . \tag{A5}$$

Hence

$$\langle S^n_{zi} S^n_{zj} \rangle_\beta - \langle S^n_{zi} \rangle_\beta \langle S^n_{zj} \rangle_\beta = (W_{2n} - W_n^2) \frac{\sum_{r=0}^{\infty} \frac{K^r}{r!} \operatorname{tr} \mathcal{P}^{(1)}_r}{\sum_{r=0}^{\infty} \frac{K^r}{r!} \operatorname{tr} \mathcal{P}^r} . \qquad \text{(A6)}$$

For n=1, $\langle S_{zi} \rangle_\beta = W_1 = 0$, $W_2 = \frac{X}{3}$, and

$$\langle \underset{\sim}{S}_i \cdot \underset{\sim}{S}_j \rangle_\beta = 3 \langle S_{zi} S_{zj} \rangle_\beta = \frac{X\left(\sum_{r=0}^{\infty} \frac{K^r}{r!} \operatorname{tr} \mathcal{P}^{(1)}_r \right)}{\sum_{r=0}^{\infty} \frac{K^r}{r!} \operatorname{tr} \mathcal{P}^r} . \qquad \text{(A7)}$$

Comparison of Eqs.(A6),and (A7) immediately yields the statement of Theorem A-1, Eq.(A1).

Theorem A-2. Let i and j be two different sites in a finite cluster of N sites, Then

$$\langle P_{ij} - \frac{1}{Y} \underset{\sim}{I} \rangle_\beta = \frac{4}{Y} \langle \underset{\sim}{S}_i \cdot \underset{\sim}{S}_j \rangle_\beta . \qquad \text{(A8)}$$

Proof: From a consideration of Eqs.(23) and (A7), we need only prove for each r that

$$\operatorname{tr} (P_{ij} - \frac{1}{Y} \underset{\sim}{I}) \mathcal{P}^r = \frac{12}{Y} \operatorname{tr} S_{zi} S_{zj} \mathcal{P}^r . \qquad \text{(A9)}$$

From Eqs.(A4) and (65)

$$\operatorname{tr} (P_{ij} - \frac{1}{Y} \underset{\sim}{I}) \mathcal{P}^r = (Y - \frac{1}{Y}) \operatorname{tr} \mathcal{P}^{(1)}_r$$

$$= \frac{4X}{Y} \operatorname{tr} \mathcal{P}^{(1)}_r . \qquad \text{(A10)}$$

Now let n=1 in Eq.(A5)

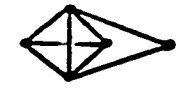
$$\mathrm{tr}\, S_{zi} S_{zj} \mathcal{P}^r = \frac{X}{3} \mathrm{tr}\, \mathcal{P}_r^{(1)} \tag{A11}$$

Eqs.(A9) and thence (A8) follows directly from Eqs.(A10) and (A11), so that Theorem A-2 is proved.

Performing the appropriate sums over lattice sites, Theorems IX and X follow directly from Theorems A-1 and A-2, respectively, for the case of finite clusters. Since both χ_n and $\sum_{i,j}{}' \langle P_{ij} - \frac{1}{Y}\underset{\sim}{I}\rangle_\beta$ are extensive quantities it follows from the cluster expansion method that Theorems IX and X hold for the infinite lattice.

Note that Theorems A-1 and A-2 contain considerably more information in them than Theorems IX and X. For example, since for $T>T_c$ the spontaneous magnetization per spin is zero, $\langle \underset{\sim}{S}_0 \cdot \underset{\sim}{S}_\infty \rangle_\beta = 0$, it follows from Theorem A-2 that $\langle P_{0\infty} - \frac{1}{Y}\underset{\sim}{I}\rangle = 0$. Here the subscripts indicate the limit of infinite separation of two spins. It also follows from Theorems A-1 and A-2 that for S=1, $\langle S_{xi} S_{xj} S_{zi} S_{zj} \rangle_\beta = 0$, for $i \neq j$, here S_{xi} is the x-component of $\underset{\sim}{S}_i$.

Appendix I. Computer Programs

(a) Calculations of $tr(\rho^{(\nu)})^n$ for all irreducible representations and $n \leq 7$, for the finite cluster  .

(b) Calculations of $tr\rho^n$ and $tr\rho^n Q^2$.

(c) Calculation of ln Z series.

(d) Calculation of χ series.

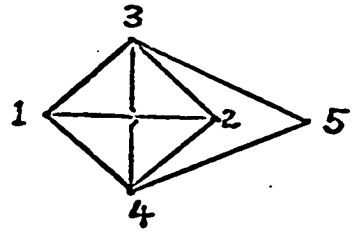
(a) Calculations of tr $(\mathcal{P}^{(y)})^n$ for all representations and for $n \leq 7$.

```
C  ALL MATRICES ARE SYMMETRIC
      DIMENSION P12(6, 6), P13(6, 6), P14(6, 6), P23(6, 6), P24(6, 6)
     1  P34(6, 6), P35(6, 6), P45(6, 6), P00(6, 6),
     1  SM1(6, 6), SM2(6, 6), SM3(6, 6), SM4(6, 6)
      R2 = 0.5
      R3 = 1.0 / 3.0
      R4 = 0.25
      R5 = 0.2
      R6 = 1.0 / 6.0
      S2 = SQRT(3.0) / 2.0
      S3 = SQRT(8.0) / 3.0
      S4 = SQRT(15.0) / 4.0
      S5 = SQRT(24.0) / 5.0
      S6 = SQRT(35.0) / 6.0
      NB = 0
  800 NB = NB + 1
      IF (NB .GE. 4) STOP
C  CLEAR MATRICES
      DO 80 I = 1, 6
      DO 80 J = 1, 6
      P12(I, J) = 0.0
      P23(I, J) = 0.0
      P34(I, J) = 0.0
      P45(I, J) = 0.0
   80 P00(I, J) = 0.0
      IF (NB .EQ. 2) GO TO 902
      IF (NB .EQ. 3) GO TO 903
C
  901 KAI = 41
      P12(1, 1) = 1.0
      P12(2, 2) = 1.0
      P12(3, 3) = 1.0
      P12(4, 4) = -1.0
      P23(1, 1) = 1.0
      P23(2, 2) = 1.0
      P23(3, 3) = -R2
      P23(4, 4) = R2
      P23(4, 3) = S2
      P34(1, 1) = 1.0
      P34(2, 2) = - R3
      P34(3, 3) = R3
      P34(4, 4) = 1.0
      P34(3, 2) = S3
      P45(1, 1) = -R4
      P45(2, 2) = R4
      P45(3, 3) = 1.0
      P45(4, 4) = 1.0
      P45(2, 1) = S4
      GO TO 900
  902 KAI = 32
      P12(1, 1) = 1.0
      P12(2, 2) = 1.0
      P12(3, 3) = -1.0
      P12(4, 4) = 1.0
```

```
      P12(5, 5) = -1.0
      P23(1, 1) = 1.0
      P23(2, 2) = -R2
      P23(3, 3) = R2
      P23(4, 4) = -R2
      P23(5, 5) = R2
      P23(3, 2) = S2
      P23(5, 4) = S2
      P34(1, 1) = -R3
      P34(2, 2) = R3
      P34(3, 3) = 1.0
      P34(4, 4) = 1.0
      P34(5, 5) = -1.0
      P34(2, 1) = S3
      P45(1, 1) = 1.0
      P45(2, 2) = -R2
      P45(3, 3) = -R2
      P45(4, 4) = R2
      P45(5, 5) = R2
      P45(4, 2) = S2
      P45(5, 3) = S2
      GO TO 900
  903 KAI = 311
      P12(1, 1) = 1.0
      P12(2, 2) = 1.0
      P12(3, 3) = -1.0
      P12(4, 4) = 1.0
      P12(5, 5) = -1.0
      P12(6, 6) = -1.0
      P23(1, 1) = 1.0
      P23(2, 2) = -R2
      P23(3, 3) = R2
      P23(4, 4) = -R2
      P23(5, 5) = R2
      P23(6, 6) = -1.0
      P23(3, 2) = S2
      P23(5, 4) = S2
      P34(1, 1) = -R3
      P34(2, 2) = R3
      P34(3, 3) = 1.0
      P34(4, 4) = -1.0
      P34(5, 5) = -R3
      P34(6, 6) = R3
      P34(2, 1) = S3
      P34(6, 5) = S3
      P45(1, 1) = -1.0
      P45(2, 2) = -R4
      P45(3, 3) = -R4
      P45(4, 4) = R4
      P45(5, 5) = R4
      P45(6, 6) = 1.0
      P45(4, 2) = S4
      P45(5, 3) = S4
      GO TO 900

  900 DO 98 L = 1, 6
```

```
      DO 98 K = 1, L
      P12(K, L) = P12(L, K)
      P23(K, L) = P23(L, K)
      P34(K, L) = P34(L, K)
      P45(K, L) = P45(L, K)
   98 P00(K, L) = P00(L, K)
      CALL MATMP (P12, P23, P13, 6)
      CALL MATMP (P13, P34, P14, 6)
      CALL MATMP (P23, P34, P24, 6)
      CALL MATMP (P34, P45, P35, 6)
      WRITE (6, 111) KAI
  111 FORMAT (12HOPARTITION = , I6)
      CALL TRACES (P12, P13, P14, P23, P24, P34, P35, P45,
     1  SM1, SM2, SM3, SM4, 801, 6)
      GO TO 800
      END
```




```
C  THIS IS THE SUBROUTINE FOR MATRIX MULTIPLICATION Q3 = Q1 * Q2 * Q1
      SUBROUTINE MATMP (Q1, Q2, Q3, N)
      DIMENSION Q1(N, N), Q2(N, N), Q3(N, N)
      DO 16 I = 1, N
      DO 16 J = 1, I
      Q3(I, J) = 0.0
      DO 16 K = 1, N
      DO 16 L = 1, N
      Q3(I, J) = Q3(I, J) + Q1(I, L) * Q2(L, K) * Q1(K, J)
   16 Q3(J, I) = Q3(I, J)
      RETURN
      END
```

```
C  THIS IS THE SUBROUTINE FOR TRACES CALCULATIONS
      SUBROUTINE TRACES (A, B, C, D, E, F, G, H, SUM1, SUM2, SUM3, SUM4,
     1  M, N)
      DIMENSION A(N, N), B(N, N), C(N, N), D(N, N), E(N, N), F(N, N),
     1  G(N, N), H(N, N), SUM1(N, N), SUM2(N, N), SUM3(N, N), SUM4(N, N)
C  SUM1 = A + B + C + D + E + F + G + H
      DO 15 I = 1, N
      DO 15 J = 1, I
      SUM1(I, J) = A(I, J) + B(I, J) + C(I, J) + D(I, J) + E(I, J)
     1  + F(I, J) + G(I, J) + H(I, J)
   15 SUM1(J, I) = SUM1(I, J)
      TRACE1 = 0.0
      DO 115 I = 1, N
  115 TRACE1 = TRACE1 + SUM1(I, I)
C  SUM2 = SUM1 * SUM1
      DO 25 I = 1, N
      DO 25 J = 1, I
      SUM2(I, J) = 0.0
      DO 25 L = 1, N
      SUM2(I, J) = SUM2(I, J) + SUM1(I, L) * SUM1(L, J)
   25 SUM2(J, I) = SUM2(I, J)
      TRACE2 = 0.0
      DO 125 I = 1, N
  125 TRACE2 = TRACE2 + SUM2(I, I)
C  SUM3 = SUM1 * SUM2
      DO 35 I = 1, N
      DO 35 J = 1, I
      SUM3(I, J) = 0.0
      DO 35 L = 1, N
      SUM3(I, J) = SUM3(I, J) + SUM1(I, L) * SUM2(L, J)
   35 SUM3(J, I) = SUM3(I, J)
      TRACE3 = 0.0
      DO 135 I = 1, N
  135 TRACE3 = TRACE3 + SUM3(I, I)
C  SUM4 = SUM2 * SUM2
      DO 45 I = 1, N
      DO 45 J = 1, I
      SUM4(I, J) = 0.0
      DO 45 L = 1, N
      SUM4(I, J) = SUM4(I, J) + SUM2(I, L) * SUM2(L, J)
   45 SUM4(J, I) = SUM4(I, J)
      TRACE4 = 0.0
      DO 145 I = 1, N
  145 TRACE4 = TRACE4 + SUM4(I, I)
C  SUM1 = DIAGONAL ELEMENTALS OF SUM2 * SUM3      (SUM5)
      DO 55 I = 1, N
      SUM1(I, I) = 0.0
      DO 55 L = 1, N
   55 SUM1(I, I) = SUM1(I, I) + SUM2(I, L) * SUM3(L, I)
      TRACE5 = 0.0
      DO 155 I = 1, N
  155 TRACE5 = TRACE5 + SUM1(I, I)
C  SUM1 = DIAGONAL ELEMENTALS OF SUM3 * SUM3      (SUM6)
      DO 65 I = 1, N
      SUM1(I, I) = 0.0
```

```
      DO 65 L = 1, N
   65 SUM1(I, I) = SUM1(I, I) + SUM3(I, L) * SUM3(L, I)
      TRACE6 = 0.0
      DO 165 I = 1, N
  165 TRACE6 = TRACE6 + SUM1(I, I)
C  SUM1 = DIAGONAL ELEMENTALS OF SUM3 * SUM4      (SUM7)
      DO 75 I = 1, N
      SUM1(I, I) = 0.0
      DO 75 L = 1, N
   75 SUM1(I, I) = SUM1(I, I) + SUM3(I, L) * SUM4(L, I)
      TRACE7 = 0.0
      DO 175 I = 1, N
  175 TRACE7 = TRACE7 + SUM1(I, I)
C  PRINT THE RESULTS
      WRITE ( 6, 101) M, TRACE1, TRACE2, TRACE3, TRACE4, TRACE5,
     1  TRACE6, TRACE7
  101 FORMAT ( I8, 2F9.2, 2F10.2, 2F11.2, F12.2 )
      RETURN
      END
```

```
PARTITION =     41
   801     16.00     70.00    334.00    1714.00    9286.00   52209.99   300693.97

PARTITION =     32
   801      8.00     20.00     56.00     164.00     488.00    1460.00     4375.00

PARTITION =    311

UNDRFLOW AT 05723 IN MQ

UNDRFLOW AT 05723 IN MQ

UNDRFLOW AT 05723 IN MQ

UNDRFLOW AT 05723 IN MQ
   801     -0.00     12.00     -0.00      36.00     -0.00     132.00       -0.00
```

(b) Calculations of $tr\rho^n$ and $tr\,\rho^n Q^2$ for $n \leq 7$.

```
C  PI(N) MEANS THE 1.0/Y**I PART OF (P**N)
C  QI(N) MEANS THE 1.0/Y**I PART OF (P**N*Q**2)*3.0/X
      DIMENSION  A(8), B(8), C(8), D(8),
     1      P1(7), P2(7), P3(7), P4(7), P5(7), P6(7), P0(7),
     1      Q1(7), Q2(7), Q3(7), Q4(7), Q5(7), Q6(7)
      K = 5
      NB = 801
      WRITE (6, 108) NB
  108 FORMAT (6HOGRAPH , I4)
      A(1) = 8.0
      A(2) = 64.0
      A(3) = 512.0
      A(4) = 4096.0
      A(5) = 32768.0
      A(6) = 262144.0
      A(7) = 2097152.0
      B(1) = 16.0
      B(2) = 70.0
      B(3) = 334.0
      B(4) = 1714.0
      B(5) = 9286.0
      B(6) = 52210.0
      B(7) = 300694.0
      C(1) = 8.0
      C(2) = 20.0
      C(3) = 56.0
      C(4) = 164.0
      C(5) = 488.0
      C(6) = 1460.0
      C(7) = 4376.0
      D(1) = 0.0
      D(2) = 12.0
      D(3) = 0.0
      D(4) = 36.0
      D(5) = 0.0
      D(6) = 132.0
      D(7) = 0.0
      DO 840 I = 1, 7, 2
      P1(I) = ( A(I) + 2.0 * B(I) + C(I) ) / 6.0
      Q1(I) = ( A(I) + 2.0 * B(I) + C(I) ) / 6.0 *7.0
      P3(I) = ( A(I) - C(I) ) / 2.0
     1   + ( A(I) - B(I) + C(I) )/ 3.0
      Q3(I) = ( A(I) - C(I) ) / 2.0 *17.0
     1   + ( A(I) - B(I) + C(I) )/ 3.0 * 13.0
      P5(I) = 0.0
  840 Q5(I) = 0.0
      DO 880 I = 2, 6, 2
      P0(I) = ( A(I) + 4.0*B(I) + 5.0*C(I) + 3.0*D(I)) / 60.0
      P2(I) = ( A(I) + B(I) - C(I) ) / 3.0
     1   + ( A(I) + C(I) - D(I) ) / 4.0
      Q2(I) = ( A(I) + B(I) - C(I) ) / 3.0 * 11.0
     1   + ( A(I) + C(I) - D(I) ) / 4.0 * 9.0
      P4(I) = ( 2.0 * A(I) - 2.0 * B(I) + D(I) ) / 5.0
      Q4(I) = ( 2.0 * A(I) - 2.0 * B(I) + D(I) ) * 5.0
```

```
      P6(I) = 0.0
  880 QS(I) = 0.0
      WRITE (6, 120) K, PO(2), PO(4), PO(6)
  120 FORMAT (I8, 3F16.2)
      WRITE (6,102) P1(1), P2(2), P1(3), P3(3), P2(4), P4(4), P1(5),
     1 P3(5), P5(5), P2(6), P4(6), P6(6), P1(7), P3(7), P5(7),
     1 Q1(1), Q2(2), Q1(3), Q3(3), Q2(4), Q4(4), Q1(5), Q3(5), Q5(5),
     1 Q2(6), Q4(6), Q6(6), Q1(7), Q3(7), Q5(7).

  102 FORMAT (5F16.2)
      STOP
      END
```

```
RAPH 801
   5          8.00          198.00          7978.00
        8.00          56.00          206.00          306.00          2938.00
      960.00        8638.00        24130.00            0.00        170155.00
    84000.00           0.00       450486.00      1646666.00             0.00
       56.00         580.00         1442.00         4890.00         30206.00
    24000.00       60466.00       378250.00            0.00       1740090.00
  2100000.00           0.00      3153402.00      25592210.00             0.00
```

(c) Calculation of ln Z series,

```
C  LOG(Z) SERIES FOR EXCHANGE INTERACTION MODEL OF FERROMAGNETISM
      DOUBLE PRECISION Z
      DIMENSION P(122,60), Z(122,19), IZ(122,19)
      READ (5,100) ((P(I,J), J = 1,30), I = 1,122)
  100 FORMAT (5F16.0)
      READ (5,120) ((P(I,J), J = 31,34), I = 1,122)
  120 FORMAT (4F20.0)
      DO 800 I = 1,122
      Z(I,1) = P(I,1)
      Z(I,2) = P(I,32)
      Z(I,3) = P(I,2) - P(I,1)**2
      Z(I,4) = P(I,3) - 3.0*P(I,32)*P(I,1)
      Z(I,5) = P(I,4) - 3.0*P(I,2)*P(I,1) + 2.0*P(I,1)**3
      Z(I,6) = P(I,33) - 3.0*P(I,32)**2
      Z(I,7) = P(I,5) - 4.0*P(I,3)*P(I,1) - 6.0*P(I,2)*P(I,32)
     1  + 12.0*P(I,32)*P(I,1)**2
      Z(I,8) = P(I,6) - 4.0*P(I,4)*P(I,1) - 3.0*P(I,2)**2
     1  + 12.0*P(I,2)*P(I,1)**2 - 6.0*P(I,1)**4
      Z(I,9) = P(I,7) - 5.0*P(I,33)*P(I,1) - 10.0*P(I,3)*P(I,32)
     1  + 30.0*P(I,32)**2*P(I,1)
      Z(I,10) = P(I,8) - 5.0*P(I,5)*P(I,1) - 10.0*P(I,3)*P(I,2)
     1  - 10.0*P(I,4)*P(I,32) + 20.0*P(I,3)*P(I,1)**2
     1  + 60.0*P(I,2)*P(I,32)*P(I,1) - 60.0*P(I,32)*P(I,1)**3
      Z(I,11) = P(I,9) - 5.0*P(I,6)*P(I,1) - 10.0*P(I,4)*P(I,2)
     1  + 20.0*P(I,4)*P(I,1)**2 + 30.0*P(I,2)**2*P(I,1)
     1  - 60.0*P(I,2)*P(I,1)**3 + 24.0*P(I,1)**5
      Z(I,12) = P(I,34) - 15.0*P(I,33)*P(I,32) + 30.0*P(I,32)**3
      Z(I,13) = P(I,10) - 6.0*P(I,7)*P(I,1) - 15.0*P(I,5)*P(I,32)
     1  - 15.0*P(I,33)*P(I,2) + 30.0*P(I,33)*P(I,1)**2
     1  - 10.0*P(I,3)**2 + 120.0*P(I,3)*P(I,32)*P(I,1)
     1  + 90.0*P(I,2)*P(I,32)**2 - 270.0*P(I,32)**2*P(I,1)**2
      Z(I,14) = P(I,11) - 6.0*P(I,8)*P(I,1) - 15.0*P(I,5)*P(I,2)
     1  - 15.0*P(I,6)*P(I,32) + 30.0*P(I,5)*P(I,1)**2
     1  - 20.0*P(I,4)*P(I,3) + 120.0*P(I,3)*P(I,2)*P(I,1)
     1  + 120.0*P(I,4)*P(I,32)*P(I,1) - 120.0*P(I,3)*P(I,1)**3
     1  + 90.0*P(I,2)**2*P(I,32) - 540.0*P(I,2)*P(I,32)*P(I,1)**2
     1  + 360.0*P(I,32)*P(I,1)**4
      Z(I,15) = P(I,12) - 6.0*P(I,9)*P(I,1) - 15.0*P(I,6)*P(I,2)
     1  + 30.0*P(I,6)*P(I,1)**2 - 10.0*P(I,4)**2
     1  + 120.0*P(I,4)*P(I,2)*P(I,1) - 120.0*P(I,4)*P(I,1)**3
     1  + 30.0*P(I,2)**3 - 270.0*P(I,2)**2*P(I,1)**2
     1  + 360.0*P(I,2)*P(I,1)**4 - 120.0*P(I,1)**6
      Z(I,16) = P(I,13) - 7.0*P(I,34)*P(I,1) - 21.0*P(I,7)*P(I,32)
     1  - 35.0*P(I,33)*P(I,3) + 210.0*P(I,33)*P(I,32)*P(I,1)
     1  + 210.0*P(I,3)*P(I,32)**2 - 630.0*P(I,32)**3*P(I,1)
      Z(I,17) = P(I,14) - 7.0*P(I,10)*P(I,1) - 21.0*P(I,8)*P(I,32)
     1  - 21.0*P(I,7)*P(I,2) + 42.0*P(I,7)*P(I,1)**2
     1  - 35.0*P(I,33)*P(I,4) - 35.0*P(I,5)*P(I,3)
     1  + 210.0*P(I,33)*P(I,2)*P(I,1) + 210.0*P(I,5)*P(I,32)*P(I,1)
     1  - 210.0*P(I,33)*P(I,1)**3 + 140.0*P(I,3)**2*P(I,1)
     1  + 420.0*P(I,3)*P(I,2)*P(I,32) + 210.0*P(I,4)*P(I,32)**2
     1  - 1260.0*P(I,3)*P(I,32)*P(I,1)**2
     1  - 1890.0*P(I,2)*P(I,32)**2*P(I,1) + 2520.0*P(I,32)**2*P(I,1)**3
      Z(I,18) = P(I,15) - 7.0*P(I,11)*P(I,1) - 21.0*P(I,9)*P(I,32)
     1  - 21.0*P(I,8)*P(I,2) + 42.0*P(I,8)*P(I,1)**2
```

```
     1  - 35.0*P(I,5)*P(I,4) - 35.0*P(I,6)*P(I,3)
     1  + 210.0*P(I,6)*P(I,32)*P(I,1) + 210.0*P(I,5)*P(I,2)*P(I,1)
     1  - 210.0*P(I,5)*P(I,1)**3 + 280.0*P(I,4)*P(I,3)*P(I,1)
     1  + 210.0*P(I,3)*P(I,2)**2 + 420.0*P(I,2)*P(I,4)*P(I,32)
     1  - 1260.0*P(I,4)*P(I,32)*P(I,1)**2
     1  - 1260.0*P(I,3)*P(I,2)*P(I,1)**2
     1  + 840.0*P(I,3)*P(I,1)**4 - 1890.0*P(I,2)**2*P(I,32)*P(I,1)
     1  + 5040.0*P(I,2)*P(I,32)*P(I,1)**3 - 2520.0*P(I,32)*P(I,1)**5
800  Z(I,19) = - 7.0*P(I,12)*P(I,1) - 21.0*P(I,9)*P(I,2)
     1  + 42.0*P(I,9)*P(I,1)**2 - 35.0*P(I,6)*P(I,4)
     1  + 210.0*P(I,6)*P(I,2)*P(I,1) - 210.0*P(I,6)*P(I,1)**3
     1  + 140.0*P(I,4)**2*P(I,1) + 210.0*P(I,4)*P(I,2)**2
     1  - 1260.0*P(I,4)*P(I,2)*P(I,1)**2 + 840.0*P(I,4)*P(I,1)**4
     1  - 630.0*P(I,2)**3*P(I,1) + 2520.0*P(I,2)**2*P(I,1)**3
     1  - 2520.0*P(I,2)*P(I,1)**5 + 720.0*P(I,1)**7
      DO 820 I = 1, 122
      DO 820 J = 1, 19
820  IZ(I,J) = Z(I,J)
      M = 1
      WRITE (6,101) M
101  FORMAT (16H1FINITE CLUSTERS , I8)
      DO 174 I = 1, 122
      WRITE (6, 158) I
158  FORMAT (6HOGRAPH , I4)
      WRITE (6, 160) IZ(I,1)
160  FORMAT (I48)
      WRITE (6, 162) IZ(I,2), IZ(I,3)
162  FORMAT (I36, I12)
      WRITE (6, 164) IZ(I,4), IZ(I,5)
164  FORMAT (I36, I12)
      WRITE (6, 166) IZ(I,6), IZ(I,7), IZ(I,8)
166  FORMAT (I24, 2I12)
      WRITE (6, 168) IZ(I,9), IZ(I,10), IZ(I,11)
168  FORMAT (I24, 2I12)
      WRITE (6, 170) IZ(I,12), IZ(I,13), IZ(I,14), IZ(I,15)
170  FORMAT (4I12)
174  WRITE (6, 172) IZ(I,16), IZ(I,17), IZ(I,18), IZ(I,19)
172  FORMAT (4I12)
      READ (5, 140) ((P(I,J), J=1,60), I=1,122)
140  FORMAT (20F4.0)
      DO 840 I = 2, 122
      DO 840 J = 1, 19
      DO 840 N = 1, 60
840  Z(I,J) = Z(I,J) - P(I,N)*Z(N,J)
      READ (5, 142) ((P(I,J), J=1,60), I=1,14)
142  FORMAT (20F4.0)
      DO 842 I = 109, 122
      IM108 = I - 108
      DO 842 J = 1, 19
      DO 842 N = 1, 48
      NP60 = N + 60
842  Z(I,J) = Z(I,J) - P(IM108,N)*Z(NP60,J)
      DO 860 I = 1,122
      DO 860 J = 1,19
860  IZ(I,J) = Z(I,J)
      M = 2
```

```
      WRITE (6, 102) M
  102 FORMAT (16H1INFINITE LATTICES , I8)
      DO 194 I = 1, 122
      WRITE (6,178) I
  178 FORMAT (6HOGRAPH , I4)
      WRITE (6, 180) IZ(I,1)
  180 FORMAT (I48)
      WRITE (6, 182) IZ(I,2), IZ(I,3)
  182 FORMAT (I36, I12)
      WRITE (6, 184) IZ(I,4), IZ(I,5)
  184 FORMAT (I36, I12)
      WRITE (6, 186) IZ(I,6), IZ(I,7), IZ(I,8)
  186 FORMAT (I24, 2I12)
      WRITE (6, 188) IZ(I,9), IZ(I,10), IZ(I,11)
  188 FORMAT (I24, 2I12)
      WRITE (6, 190) IZ(I,12), IZ(I,13), IZ(I,14), IZ(I,15)
  190 FORMAT (4I12)
  194 WRITE (6, 192) IZ(I,16), IZ(I,17), IZ(I,18), IZ(I,19)
  192 FORMAT (4I12)
      STOP
      END
```

(d) Calculation of χ series.

```
C  SUSCEPTIBILITY SERIES OF FINITE CLUSTERS AND INFINITE LATTICES
      DOUBLE PRECISION KA
      REAL NB, LC
      DIMENSION  NB(122,60), KA(122,16), LC(14,60)  IKA(122,16)
      READ (5, 100)  ((NB(I, J), J=1, 30), I=1, 122)
  100 FORMAT (5F16.0)
      READ (5, 120)  ((NB(I, J), J=31, 34), I=1, 122)
  120 FORMAT (4F20.0)
      DO 800 I = 1, 122
      KA(I,1) = NB(I,16) - NB(I,31)*NB(I,1)
      KA(I,2) = NB(I,17) - NB(I,31)*NB(I,2) -2.*KA(I,1)*NB(I,1)
      KA(I,3) = NB(I,18) - NB(I,31)*NB(I,3) -3.*KA(I,1)*NB(I,32)
      KA(I,4) = NB(I,19) - NB(I,31)*NB(I,4) -3.*KA(I,1)*NB(I, 2)
     1  -3.*KA(I,2)*NB(I,1)
      KA(I,5) = NB(I,20) - NB(I,31)*NB(I,5) -4.*KA(I,1)*NB(I, 3)
     1  -6.*KA(I,2)*NB(I,32) -4.*KA(I,3)*NB(I,1)
      KA(I,6) = NB(I,21) - NB(I,31)*NB(I,6) -4.*KA(I,1)*NB(I, 4)
     1  -6.*KA(I,2)*NB(I,2) -4.*KA(I,4)*NB(I,1)
      KA(I,7) = NB(I,22) - NB(I,31)*NB(I,7) -5.*KA(I,1)*NB(I,33)
     1  -10.*KA(I,3)*NB(I,32)
      KA(I,8) = NB(I,23) - NB(I,31)*NB(I,8) -5.*KA(I,1)*NB(I, 5)
     1  -10.*KA(I,2)*NB(I,3) -10.*KA(I,3)*NB(I,2) -10.*KA(I,4)*NB(I,32)
     1  -5.*KA(I,5)*NB(I,1)
      KA(I,9) = NB(I,24) - NB(I,31)*NB(I,9) -5.*KA(I,1)*NB(I, 6)
     1  -10.*KA(I,2)*NB(I,4) -10.*KA(I,4)*NB(I,2) -5.*KA(I,6)*NB(I,1)
      KA(I,10)= NB(I,25) - NB(I,31)*NB(I,10)-6.*KA(I,1)*NB(I, 7)
     1  -15.*KA(I,2)*NB(I,33) -20.*KA(I,3)*NB(I,3)
     1  -15.*KA(I,5)*NB(I,32) -6.*KA(I,7)*NB(I,1)
      KA(I,11)= NB(I,26) - NB(I,31)*NB(I,11)-6.*KA(I,1)*NB(I, 8)
     1 -15.*KA(I,2)*NB(I,5) -20.*KA(I,3)*NB(I,4) -20.*KA(I,4)*NB(I,3)
     1  -15.*KA(I,5)*NB(I,2) -15.*KA(I,6)*NB(I,32) -6.*KA(I,8)*NB(I,1)
      KA(I,12)= NB(I,27) - NB(I,31)*NB(I,12)-6.*KA(I,1)*NB(I, 9)
     1  -15.*KA(I,2)*NB(I,6) -20.*KA(I,4)*NB(I,4)
     1  -15.*KA(I,6)*NB(I,2) -6.*KA(I,9)*NB(I,1)
      KA(I,13)= NB(I,28) - NB(I,31)*NB(I,13)-7.*KA(I,1)*NB(I,34)
     1  -35.*KA(I,3)*NB(I,33) -21.*KA(I,7)*NB(I,32)
      KA(I,14)= NB(I,29) - NB(I,31)*NB(I,14)-7.*KA(I,1)*NB(I,10)
     1  -21.*KA(I,2)*NB(I,7) -35.*KA(I,3)*NB(I,5) -35.*KA(I,4)*NB(I,33)
     1  -35.*KA(I,5)*NB(I,3) -21.*KA(I,7)*NB(I,2)
     1  -21.*KA(I,8)*NB(I,32) -7.*KA(I,10)*NB(I,1)
      KA(I,15)= NB(I,30) - NB(I,31)*NB(I,15)-7.*KA(I,1)*NB(I,11)
     1  -21.*KA(I,2)*NB(I,8) -35.*KA(I,3)*NB(I,6) -35.*KA(I,4)*NB(I,5)
     1  -35.*KA(I,5)*NB(I,4) -35.*KA(I,6)*NB(I,3) -21.*KA(I,8)*NB(I,2)
     1  -21.*KA(I,9)*NB(I,32) -7.*KA(I,11)*NB(I,1)
  800 KA(I,16) = -7.*KA(I,1)*NB(I,12) -21.*KA(I,2)*NB(I,9)
     1  -35.*KA(I,4)*NB(I,6) -35.*KA(I,6)*NB(I,4)
     1  -21.*KA(I,9)*NB(I,2) -7.*KA(I,12)*NB(I,1)
      DO 820 I = 1, 122
      DO 820 J = 1, 16
  820 IKA(I, J) = KA(I, J)
      M = 1
      WRITE (6,101) M
  101 FORMAT (16H1FINITE CLUSTERS , I8)
      DO 174 I = 1,122
      WRITE (6, 158) I
```

```
158 FORMAT (6HOGRAPH , I4)
    WRITE (6, 160) IKA(I, 1)
160 FORMAT (I48)
    WRITE (6, 162) IKA(I, 2)
162 FORMAT (I48)
    WRITE (6, 164) IKA(I, 3), IKA(I, 4)
164 FORMAT (I36, I12)
    WRITE (6, 166) IKA(I, 5), IKA(I, 6)
166 FORMAT (I36, I12)
    WRITE (6, 168) IKA(I, 7), IKA(I, 8), IKA(I, 9)
168 FORMAT (I24, 2I12)
    WRITE (6, 170) IKA(I,10), IKA(I,11), IKA(I,12)
170 FORMAT (I24, 2I12)
174 WRITE (6, 172) IKA(I,13), IKA(I,14), IKA(I,15), IKA(I,16)
172 FORMAT (4I12)
    READ (5, 140) ((NB(I, J), J=I,60), I=1,122)
140 FORMAT (20F4.0)
    DO 840 I = 2, 122
    DO 840 J = 1, 16
    DO 840 N = 1, 60
840 KA(I, J) = KA(I, J) - NB(I, N) * KA(N, J)
    READ (5, 142) ((LC(I, J), J=1,60), I=1,14)
142 FORMAT (20F4.0)
    DO 842 I = 109, 122
    IM108 = I-108
    DO 842 J = 1, 16
    DO 842 N = 1, 48
    NP60 = N+60
842 KA(I, J) = KA(I, J) - LC(IM108, N) * KA(NP60, J)
    DO 860 I = 1, 122
    DO 860 J = 1, 16
860 IKA(I, J) = KA(I, J)
    M = 2
    WRITE (6,102) M
102 FORMAT (18H1INFINITE LATTICES , I8)
    DO 194 I = 1,122
    WRITE (6, 178) I
178 FORMAT (6HOGRAPH , I4)
    WRITE (6, 180) IKA(I, 1)
180 FORMAT (I48)
    WRITE (6, 182) IKA(I, 2)
182 FORMAT (I48)
    WRITE (6, 184) IKA(I, 3), IKA(I, 4)
184 FORMAT (I36, I12)
    WRITE (6, 186) IKA(I, 5), IKA(I, 6)
186 FORMAT (I36, I12)
    WRITE (6, 188) IKA(I, 7), IKA(I, 8), IKA(I, 9)
188 FORMAT (I24, 2I12)
    WRITE (6, 190) IKA(I,10), IKA(I,11), IKA(I,12)
190 FORMAT (I24, 2I12)
194 WRITE (6, 192) IKA(I,13), IKA(I,14), IKA(I,15), IKA(I,16)
192 FORMAT (4I12)
    STOP
    END
```

SPIN S EXCHANGE INTERACTION MODEL OF FERROMAGNETISM

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The first 8 terms of the low field-high temperature susceptibility series are obtained for an exchange interaction model of ferromagnetism for general spin and crystal lattice. For the f.c.c. lattice $k_B T_C/J = 1.20 + 5.72/(2S+1)$.

Consider a system consisting of a lattice of N sites containing atoms of spin S and gyromagnetic ratio g, each atom having q nearest neighbors. The Hamiltonian of the system is taken to be

$$H = -J \sum_{\langle i,j \rangle} P_{ij} - g\mu H \sum_k S_{kz} .$$

Here H is the z directed external magnetic field, J the magnitude of a near neighbor exchange interaction and μ the Bohr magneton. P_{ij} is the Schrödinger exchange interaction operator which exchanges or permutes the spin coordinates of two electrons, labelled i and j. In general P_{ij} is a polynomial of degree $2S$ in $S_i \cdot S_j$ [1]. For $S = \frac{1}{2}$ this Hamiltonian is identical to that of the Heisenberg model. The high temperature series for the low field susceptibility is of the form

$$\chi = (C/T)\left[1 + \sum_{n=1}^{\infty} a_n (J/k_B T)^n\right] ,$$

where $C = Ng^2\mu^2 S(S+1)/3k_B$, k_B is the Boltzman constant and T the thermodynamic temperature. When $S = \frac{1}{2}$, coefficients through a_7 for close-packed lattices and a_9 for loose-packed lattices have been obtained by Domb and Wood [2]. Baker et al. [3] have added the quantities a_8 and a_9 for the f.c.c. lattice and a_{10} for the b.c.c. and s.c. lattices. For $S = 1$ Allan and Betts [4] obtained terms through a_7 for the f.c.c. lattice. Such a large number of terms was obtained through the use of the cluster expansion method [5] in conjunction with powerful group theoretic techniques [6]. In the present letter we report the results of a generalization of these group theoretic techniques to arbitrary spin to obtain the coefficients $a_1 - a_7$ for general lattices.

The most convenient way to represent the coefficients a_n is in the form

$$a_n = a_n^{(n)} Y^{-n} + a_n^{(n-2)} Y^{-n+2} + \ldots + a_n^{(2)} Y^{-2} \ (\text{or } a_n^{(1)} Y^{-1})$$

where $Y = 2S + 1$. Results for $a_n^{(m)}$ have been obtained in terms of Dombs "general lattice constants" $p_{n\gamma}$ [5]. For simplicity, however, we present the actual numerical values of $a_n^{(m)}$ for various crystal lattices in the accompanying table. The labor of evaluating the coefficients was greatly reduced by the use of a number of new theorems. Even then, however, we had to resort to the use of a high speed computer to evaluate the traces. The numbers of non-trivial diagrams required to evaluate the coefficients $a_1 - a_7$ are 1, 2, 4, 8, 16, 35, 82, respectively. For $S = \frac{1}{2}$ and 1 the present results reduce exactly to those contained in refs. 2 and 4 *.

A preliminary analysis of these series by

* For $S = 1$ and the f.c.c. lattice we get $a_7 = 4\,664.542\,426$ while the results of ref. 4 gives $a_7 = 4\,658.473\,838$. In private communication with Dr. Allan the mistake leading to the latter erroneous value has been discovered.

Table 1
Coefficients $a_n^{(m)}$ for various crystal lattices.

	Face-centered cubic	Body-centered cubic	Simple cubic	Plane triangle	Diamond	Plane square	Honeycomb	Linear
$a_1^{(1)}$	12	8	6	6	4	4	3	2
$a_2^{(2)}$	120	48	24	24	8	8	3	0
$a_3^{(1)}$	12	− 8/3	− 2	2	− 4/3	− 4/3	− 1	− 2/3
$a_3^{(3)}$	1056	288	96	60	16	16	3	0
$a_4^{(2)}$	321	142/3	21/2	21/2	− 1/3	13/3	1/2	5/6
$a_4^{(4)}$	8496	1344	288	108	32	0	3	0
$a_5^{(1)}$	− 62/5	132/5	49/5	− 21/5	38/15	58/15	7/5	3/5
$a_5^{(3)}$	5310	172	− 15	63	− 2	− 22	− 1	− 1
$a_5^{(5)}$	64032	7296	1152	168	64	64	3	0
$a_6^{(2)}$	− 441/5	− 164	− 694/15	− 443/30	− 83/45	− 827/45	− 131/60	− 7/5
$a_6^{(4)}$	67917	15722/3	1539/2	553/2	79/3	401/3	15/2	7/6
$a_6^{(6)}$	461424	26976	2064	216	− 16	− 208	− 33	0
$a_7^{(1)}$	1028/21	− 47386/315	− 2811/70	121/14	− 1748/315	− 3218/315	− 943/420	− 383/630
$a_7^{(3)}$	3952	121112/45	8221/15	− 211/10	73/3	5698/45	167/20	113/45
$a_7^{(5)}$	734980	30680/3	− 1256	668	− 524/3	− 1756/3	− 58	− 4/3
$a_7^{(7)}$	3230736	168000	14112	− 180	544	928	147	0

means of various ratio tests shows that the Curie temperature T_C is of the form $k_B T_C/J = A + B/Y$, where for the f.c.c. lattice $A = 1.20$ and $B = 5.72$ while for the b.c.c. lattice $A \approx 1.0$ and $B \approx 3.1$. In general T_C for the present model is less than that of the Heisenberg model, as can be anticipated from the higher degeneracy of the ground state of a pair of spins interacting with exchange Hamiltonian compared to the Heisenberg Hamiltonian.

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CRITICAL PROPERTIES OF THE EXCHANGE INTERACTION MODEL OF FERROMAGNETISM

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For the f.c.c. lattice $k_B T_c / J = 1.19 + 5.70 Y^{-1}$ for all S and $\gamma = 0.48 + 2.16\ Y^{-1}$ for $S > \frac{1}{2}$ where $Y = 2S+1$. The value of $\gamma(=1.41)$ for $S = \frac{1}{2}$ is anomalous with respect to extrapolation of the observed linear behaviour in Y^{-1} for other spins.

RECENTLY we reported[1] the results of a calculation of the first eight terms in the low field-high temperature susceptibility series of the Exchange Interaction Model of Ferromagnetism[2] for arbitrary spin and general lattice. We present here the results of a detailed Pade analysis[3] of these series to obtain the Curie temperature T_c and critical index γ, $\chi^{-1} \sim (T - T_c)^{\gamma}$, for $T \to T_c^+$.

Our findings are the following:

(1) For the f.c.c. lattice the Curie temperature is given by

$$k_B T_c / J = 1.19 + 5.70\ Y^{-1}$$

where $Y = 2S + 1$. This expression is valid for all S.

(2) The critical index γ is a strong function of spin. For the f.c.c. lattice and for $S > \frac{1}{2}$ it is

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

(3) The value of γ for $S = \frac{1}{2}$ is anomalous in the sense that our estimated value, $\gamma = 1.41 \pm 0.02$, differs markedly from what an extrapolation of the observed linear behaviour in γ^{-1} for other spins would yield, namely $\gamma = 1.56$.

(4) For the b.c.c. and s.c. lattices the coefficients are in general too irregular to estimate both T_c and γ. However, within our precision, γ for both seems to be the same as that of the f.c.c. lattice for each S. If the values of γ for the b.c.c. and s.c. lattices are chosen to be the same as those of the f.c.c. lattice, then an estimate of T_c from Padé approximants to $\chi^{1/\gamma}$ shows that for all the cubic lattices and for all S, T_c can be described to within a few percent by

$$k_B T_c / J = 0.547\,(q - 1.6)\,(Y^{-1} + 0.21)$$

where q is the coordination number of the lattice. This equation indirectly suggests that all the cubic lattices have the same critical index.

The values of γ for the present 3-dimensional quantum mechanical model differ considerably from the results of the Heisenberg model (for $S > \frac{1}{2}$). In fact, γ becomes less than unity for large enough spin. The existence of values of γ less than those appropriate to the Heisenbert model[4] ($1.33 \gamma \leqslant 1.43$) suggests, when compared to the results of a recent reanalysis of a large body of experimental data in magnets and fluids,[5] that the present model may have more physical significance than originally thought.[4] Hence we see that the inclusion of nonlinear terms in $S_i \cdot S_j$ in the Hamiltonian[2] can significantly affect theoretical estimates of γ.

The methods we have used to estimate T_c and γ are as follows:

(a) Choosing γ, $K_c = J/k_B T_c$ was represented by appropriate poles of the Padé approximants to $\chi^{1/\gamma}$. Instead of tabulating the various approximants in Padé tables for several values of γ, we have plotted the various approximants of K_c as functions of γ in the K_c-γ plane. The proper values of γ and K_c are easily obtained from these curves in the region in which the various order approximants coalesce.

(b) Choosing K_c, γ was obtained by evaluating Padé approximants to $(K - K_c)\,(d\ln\chi/dK)$ at $K = K_c$. If the approximants of γ as functions of K_c are plotted in the $K_c - \gamma$ plane, these curves are roughly parallel to and close to the curves obtained from method (a) in the region of interest. We have also explored the Padé approximants to χ'/χ and $\chi\chi''/(\chi')^2$. These results are more irregular but not inconsistent with what methods (a) and (b) yield. The present values of T_c are also in agreement with estimates based on various ratio tests.

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Dans le réseau cubique à faces centrées $k_B T_c/J = 1.19 + 5.70\,Y^{-1}$ pour tout S et d'autre part $\gamma = 0.48 + 2.16\,Y^{-1}$ pour $S > 1/2$, avec $Y = 2S + 1$. La valeur de $\gamma (= 1.41)$ pour le cas $S = 1/2$ est anormale par rapport, a l'extrapolation de la variation linéaire de Y^{-1} observée pour les autres spins.

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THERMODYNAMIC PROPERTIES OF THE EXCHANGE INTERACTION MODEL OF FERROMAGNETISM

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Terms through T^{-7} are obtained for the zero field–high temperature partition function series for general spin S and arbitrary lattice. For the f.c.c. lattice the fraction of the entropy change occurring above T_c is found to be $(S_\infty - S_c)/S_\infty = 0.494 - 0.353/(2S+1)$.

In zero external magnetic field the Hamiltonian for the exchange interaction model of ferromagnetism is

$$H = -J \sum_{\langle i,j \rangle} P_{ij} . \tag{1}$$

Here J is the magnitude of a near neighbor exchange interaction and P_{ij} is the Schrödinger exchange interaction operator which exchanges or permutes the spin coordinates of two electrons labelled i and j. In the present letter we report the results of a calculation of the high temperature expansion coefficients for the partition function Z which we write in the form *

$$(\ln Z)/N = \ln Y + \sum_{n=2}^{\infty} e_n (J/k_B T)^n , \tag{2}$$

where $Y = 2S + 1$.

By means of the cluster expansion method in conjunction with group theoretic techniques we have obtained terms through T^{-7} for arbitrary spin and general lattice. The numbers of diagrams which contribute to the coefficients $e_2 - e_7$ are 1, 2, 4, 7, 15, and 29, respectively. It is convenient to express e_n as

$$e_n = e_n^{(n)} Y^{-n} + e_n^{(n-2)} Y^{-n+2} + \ldots + e_n^{(1)} Y^{-1} \text{ (or } e_n^{(0)}). \tag{3}$$

Results for the $e_n^{(m)}$ in terms of the general lattice constants p_{nx} are too lengthy to present here: the actual numerical values for various crystal lattices are given in table 1. ** For $S = \frac{1}{2}$ our results and those of Rushbrooke and Wood [1] agree exactly. For $S = 1$ and the f.c.c. lattice our results reduce to those of Allan and Betts [2].

The thermodynamic functions can now be directly obtained:

internal energy: $-E/J = (\partial/\partial K)(\ln Z)$, (4)

entropy : $-S/k_B = K^2 (\partial/\partial K)[(\ln Z)/K]$, (5)

specific heat : $C_v/k_B = K^2 (\partial^2/\partial K^2)(\ln Z)$, (6)

with $K = J/k_B T$. Making use of the values of the Curie temperature T_c determined by analysis of the susceptibility series [3, 4]

$$k_B T_c/J = 0.547 (q - 1.6)(Y^{-1} + 0.21), \tag{7}$$

we have made a Padé analysis of the resultant series for these quantities. For the f.c.c. lattice we find that

$$(S_\infty - S_c)/S_\infty = 0.494 - 0.353/Y, \tag{8}$$

* e_1 is set equal to zero by adjusting the zero of energy such that $E_\infty = 0$, that is, the constant $1/(2S+1)$ is subtracted from P_{ij} to make H traceless.

** Note that every coefficient e_n has the common factor $(1 - Y^{-2})$.

Table 1
Coefficients $c_n^{(m)}$ for various crystal lattices [see eq. (3)]

	Face-centered cubic	Body-centered cubic	Simple cubic	Plane triangle	Diamond	Plane square	Honeycomb	Linear
$c_2^{(0)}$	3	2	3/2	3/2	1	1	3/4	1/2
$c_2^{(2)}$	-3	-2	-3/2	-3/2	-1	-1	-3/4	-1/2
$c_3^{(1)}$	6	-4/3	-1	1	-2/3	-2/3	-1/2	-1/3
$c_3^{(3)}$	-6	4/3	1	-1	2/3	2/3	1/2	1/3
$c_4^{(0)}$	-2	-8/3	-3/2	-1/2	-2/3	-2/3	-3/8	-1/6
$c_4^{(2)}$	25/2	47/3	21/4	-7/4	7/6	13/6	3/4	5/12
$c_4^{(4)}$	-21/2	-39/3	-15/4	9/4	-1/2	-3/2	-3/8	-1/4
$c_5^{(1)}$	-31/5	66/5	49/10	-21/10	19/15	29/15	7/10	3/10
$c_5^{(3)}$	17	-62	-35/2	3/2	-5/3	-19/3	-1	-1/2
$c_5^{(5)}$	-54/4	244/5	63/5	3/5	2/5	22/5	3/10	1/5
$c_6^{(0)}$	15/4	53/6	419/120	17/120	167/180	37/36	23/60	13/120
$c_6^{(2)}$	47/4	-615/6	-3209/120	433/120	-497/180	-283/36	-83/60	-21/40
$c_6^{(4)}$	-125/2	1015/3	303/4	7/4	25/6	115/6	7/4	7/12
$c_6^{(6)}$	47	-734/3	-105/2	-11/2	-7/3	-37/3	-3/4	-1/6
$c_7^{(1)}$	514/21	-23693/315	-2811/140	121/28	-874/315	-1609/315	-943/840	-383/1260
$c_7^{(3)}$	4067/21	32099/45	2813/20	11/4	322/45	9604/315	349/120	149/180
$c_7^{(5)}$	-519	-6020/3	-349	-15/2	-50/3	-185/3	-5	-2/3
$c_7^{(7)}$	2106/7	9580/7	1599/7	3/7	86/7	254/7	135/42	1/7

and $$(E_\infty - E_C)/JN = 3.98 - 5.04/Y, \qquad (9)$$

for all S with the exception that for $S = 1/2$, $(E_\infty - E_C)/JN = 1.60$. Here $S_\infty = Nk_B \ln Y$ and $E_\infty = 0$ *. The scatter in the various Padé approximants was too large to draw any conclusions concerning the nature of the divergence of the specific heat at T_C.

For the b.c.c. and s.c. lattices, within the reduced accuracy of our results, we find that $(S_\infty - S_C)/S_\infty$ again varies linearly in Y^{-1} and that for each spin value it is higher than that for the f.c.c. lattice by an amount 0.025 and 0.055, respectively. For each spin value and crystal lattice, $(S_\infty - S_C)/S_\infty$ for the present model is considerably higher than that of the Heisenberg model (0.23, 0.17, 0.145 for $S = 1$, 2, 3, respectively, for the f.c.c. lattice). It would be interesting to see how these numbers compare with an accurate experimental determination of this quantity.

* Footnote see preceeding page.

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