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Inverse susceptibility expansions for the Ising and classical vector models

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Abstract. A new method of deriving high temperature series expansions for the susceptibility of the Ising and classical vector spin models is presented. The method involves generating the expansion for the inverse of the susceptibility, in which case only contributions from star graphs need to be considered. An additional term (the thirteenth) has been added to the Ising high temperature susceptibility series for the FCC lattice. Analysis of the extended series does not indicate that revision of previous critical estimates is required. In a test of the capabilities of the method for other systems, seven terms of the susceptibility series of the FCC Heisenberg and planar vector models have been reproduced. Techniques used in generating the graph data are discussed.

1. Introduction

The Ising model began its career as an idealized picture of a ferromagnet, but in recent years it has come to be regarded as a most useful device in its own right. Much of its significance lies in its application to the general question of identifying those features of the hamiltonian which determine the nature of the critical behaviour. Although the exactly known results for the Ising model are by no means abundant, use of series expansion techniques has led to what is generally regarded as a reasonable understanding of many of its properties, as well as those of other related systems. (Among the many reviews of the different aspects of the subject are Fisher (1967), Domb (1970a) and Stanley (1971).)

A number of schemes for generating series expansions have been proposed (eg Domb 1960, Wortis 1973); some of these techniques are more suited to a given problem than others. Our particular interest is the high temperature expansion for the Ising susceptibility, χ , for which two techniques have been used successfully in the past, one based on a 'counting theorem' (Sykes 1961, Sykes *et al* 1972a), the other on the renormalized linked cluster expansion (Wortis 1973, Moore *et al* 1969). The first method has been applied to a variety of two- and three-dimensional lattices. In the case of the face-centred cubic (FCC) lattice it has yielded the coefficients of the χ expansion to twelfth order; on lattices of lower coordination number many more terms have been generated. Use of this technique calls for an extensive list of graphs together with their weak lattice constants. The second method is of a more general nature; it too has been used to obtain twelve terms of the FCC lattice expansion, but with a difference of order 1 in 10^6 (itself a seven digit number) in the final term. Here use is made of free graphs of limited type ('free' in the sense that more than one graph edge may occupy a lattice bond, as opposed to the weak constants where graph edges must be located on distinct

bonds), and computing the required lattice constants is, therefore, a much simpler task. Compensation for this simplification comes in the form of a non-linear integral equation which requires solution. This method has not kept pace with the counting theorem approach on the other lattices, but it has proved to be ideal for computing correlation functions, and immediately generalizes to handle the classical vector models.

A third technique which has also proved useful in limited circumstances is the finite-cluster method. Its sole advantage is that it can be used in studies of Ising systems with random non-magnetic impurities (Rapaport 1972a, b), whereas the two methods mentioned above are inapplicable. Ten terms of the FCC series were derived by this method. The three different methods have one very noticeable feature in common—they all require substantial amounts of computer time.

The purpose of this article is to describe an entirely different technique which has been used successfully to add yet another term to the FCC Ising susceptibility series. We have called it the 'inverse susceptibility' expansion method because the computations yield an expansion for χ^{-1} rather than χ . Only multiply connected graphs (stars) are required in the calculation, and the necessary graphical data are more readily obtained than for the calculation based on the counting theorem; the latter involving both articulated and multi-component graphs of certain types, in addition to a large fraction of the star graphs. The method originated out of the work of Domb and Hiley (1962, to be referred to as DH) who computed a sequence of closed-form approximations to χ^{-1} in terms of star graphs alone; it is only a small jump from these approximations to the coefficients of an exact power series expansion for χ^{-1} , and progress to much higher order is possible.

In § 2 we discuss the derivation of the χ^{-1} series, starting from the DH analysis. The results serve as the motivation for a direct derivation, whose aim is to by-pass the need to rely on the results of the multi-component Mayer theory at the start of the analysis. This direct derivation is also discussed. Section 3 outlines the technicalities of the calculation—mainly the problems involved in deriving the graph data. The analysis of the extended series is discussed in § 4. In § 5 we show how the same technique can be applied to classical isotropic vector spin systems such as the Heisenberg and planar models.

2. The star expansion

2.1. Derivation from the Mayer theory

The Mayer cluster formalism, originally developed for the study of an interacting gas, was applied to the Ising lattice problem by Fuchs (1942a). Rushbrooke and Scoins (1955) showed that after suitable re-arrangement, the free energy could be expressed in terms of the contributions of finite star clusters of spins (for a review of graph terminology see Essam and Fisher 1970). DH extended the treatment by employing the Mayer theory for multi-component systems (Fuchs 1942b) and were able to obtain a sequence of closed-form approximations for the reciprocal of the susceptibility in terms of stars alone. This work is discussed briefly in what follows. More significant, however, is the fact that the same basic analysis is capable of yielding a power series expansion for χ^{-1} whose coefficients are determined by studying the form of χ^{-1} (or a generalization thereof) for the various finite star clusters of spins which can be embedded in the lattice. We start by describing the derivation of the series from the Mayer theory; an alternative method of derivation, which does not utilize the Mayer result, appears in § 2.2.

Consider an inhomogeneous cluster G of v_G Ising spins with e_G nearest-neighbour bonds connecting them (in other words a graph with v_G vertices and e_G edges). The spins are to be divided into R classes according to the degree of inhomogeneity of the cluster (we will elaborate on this matter shortly) and, in order to distinguish between the different classes, the magnetic moments of the spins in the i th class are denoted by m_i . DH confined their attention to the particular case $R = 2$, but their analysis is readily extended to arbitrary R . The expansion for the configurational partition function Λ_G (ie the normal partition function Z_G without the contribution of the ground state) is

$$\ln \Lambda_G(\alpha, z) = v_G \sum_{i=1}^R \alpha_i - v_G \sum_t \left(\sum_{i=1}^R t_i - 1 \right) B_G(t, z) \prod_{i=1}^R \alpha_i^{t_i} \tag{2.1}$$

where $z = \exp(-2\beta J)$; J is the exchange interaction, $\beta = 1/k_B T$. t denotes the set $\{t_e | 1 \leq e \leq e_G\}$, and the sum over t is over all sets $\{t_e\}$. The B_G are the irreducible cluster sums for G (see DH). α denotes the set $\{\alpha_i | 1 \leq i \leq R\}$; α_i is the fraction of spins in the i th class overturned from the ground state and is defined as

$$\alpha_i = \frac{\mu_i}{v_G} \frac{\partial}{\partial \mu_i} \ln \Lambda_G(\mu, z) \tag{2.2}$$

where $\mu_i = \exp(-2\beta m_i H)$ (H is the applied magnetic field). For the homogeneous cluster ($R = 1$) we have the familiar relation $\alpha = \frac{1}{2}$ (magnetization + 1).

Equation (2.1) is essentially an expansion in terms of the magnetization with the temperature entering as a parameter, but it contains sufficient information to permit deduction of both high and low temperature expansions with either the magnetization or the magnetic field entering as parameters in the coefficients. The high temperature series which can be deduced from (2.1) has the form

$$\ln \Lambda_G(\alpha, w) = \sum_{s \subseteq G} (s; G) \theta_s(\alpha, w) \tag{2.3}$$

where w is the commonly used Ising high temperature variable $\tanh \beta J$. The sum is over all star subgraphs s of G , with $(s; G)$ denoting the number of weak embeddings of s in G . The isolated vertex and edge are regarded as stars for the purpose of this discussion, and their contributions are included in (2.3). θ_s is the weight of star s and is, by definition, independent of G . It can, therefore, be calculated by considering only s and its star subgraphs—this leads to an iterative scheme for calculating weights which treats the clusters in order of increasing e_G (Sykes *et al* 1966).

If stars with more than e_{\max} edges are ignored in the computation of (2.3) the result is an expansion for $\ln \Lambda_G$ in the variable w correct to order e_{\max} . This follows from the fact that the leading order term of the power series for θ_s in w is of order e_s or greater. For the special case $H = 0$, (2.3) also follows directly from the partition function definition (Domb 1970b).

If G is a homogeneous cluster, and this includes the infinite regular lattice, the zero field susceptibility per spin is defined (neglecting a factor of βm^2) as

$$\chi_G = \frac{4}{v_G} \left(\mu \frac{\partial}{\partial \mu} \right)^2 \ln \Lambda_G(\mu, z) \Big|_{\mu=1}$$

Its reciprocal is readily seen to have the form

$$\chi_G^{-1} = \frac{1}{2v_G} \frac{\partial}{\partial \alpha} \ln \Lambda_G(\alpha, z) \Big|_{\alpha=\frac{1}{2}} \tag{2.4}$$

Rushbrooke and Scoins (1962) derived the early terms of the expansion of χ^{-1} for the infinite lattice by applying (2.4) to the single component version of the Mayer expansion (2.1). The question of inhomogeneity did not arise in this study; it is only when one attempts to obtain χ_G^{-1} from the cluster expansion (2.3) that inhomogeneity becomes important.

DH (see also Hiley and Joyce 1965) generalized (2.4) to the inhomogeneous case by replacing $\partial/\partial\alpha$ by a sum over $\partial/\partial\alpha_i$ weighted according to the number v_i of vertices in the cluster containing spins of type i . The result is no longer χ_G^{-1} if G is inhomogeneous, but since we are interested in the contribution of G to the expansion for the infinite lattice, and not in χ_G^{-1} itself, this is irrelevant.

We define the generalization of (2.4)—actually of $v_G\chi_G^{-1}$ —to be

$$\psi_G = \sum_{i=1}^R \frac{v_i}{2} \frac{\partial}{\partial\alpha_i} \ln \Lambda_G(\boldsymbol{\alpha}, z) \Big|_{\alpha_i = v_i/2v_G} \quad (2.5)$$

A change of variable and use of (2.2) results in

$$\psi_G = \sum_{i=1}^R \sum_{j=1}^R \frac{v_i v_j}{4v_G} \frac{\partial \mu_j}{\partial\alpha_i} \Big|_{\mu_j = 1} \quad (2.6)$$

The $\partial\mu_j/\partial\alpha_i$ are determined by differentiating the functions

$$F_i(\boldsymbol{\alpha}, \boldsymbol{\mu}, z) = \alpha_i - \frac{\mu_i}{v_G} \frac{\partial}{\partial\mu_i} \ln \Lambda_G(\boldsymbol{\mu}, z) \equiv 0$$

(which are merely (2.2)) with respect to α_k . We obtain

$$\frac{\partial F_i}{\partial\alpha_k} + \sum_{j=1}^R \frac{\partial F_i}{\partial\mu_j} \frac{\partial \mu_j}{\partial\alpha_k} = 0.$$

Now let

$$E_{ij} = -\omega \frac{\partial F_i}{\partial\mu_j} \Big|_{\mu_j = 1} \quad 1 \leq i, j \leq R \quad (2.7)$$

with ω left undefined for the present. Since

$$\frac{\partial F_i}{\partial\alpha_k} = \delta_{ik}$$

we have

$$\sum_{j=1}^R E_{ij} \frac{\partial \mu_j}{\partial\alpha_k} = \omega \delta_{ik},$$

and if we define

$$x_j = \omega^{-1} \sum_{i=1}^R v_i \frac{\partial \mu_j}{\partial\alpha_i} \quad (2.8)$$

then

$$\mathbf{E}\mathbf{x} = \mathbf{v} \quad (2.9)$$

where \mathbf{x} and \mathbf{v} are R component vectors, and \mathbf{E} denotes the matrix (E_{ij}) . Also

$$\psi_G = \frac{\omega}{4v_G} \mathbf{v}^T \mathbf{x}. \quad (2.10)$$

The question of the degree of inhomogeneity of a cluster involves a study of the symmetry transformations of the graph, and, in fact, it is sufficient that the vertices in each of the R classes be equivalent under any one of these symmetry transformations. The assumption of DH that it is sufficient to group the vertices according to their degrees is incorrect. For practical purposes it suffices to assign each spin to a different class, ie $v_i = 1$ and $R = v_G$, thereby entirely avoiding the supplementary problem of determining sets of equivalent vertices. In this case (2.9) and (2.10) become

$$\mathbf{E}\mathbf{x} = \mathbf{1} \tag{2.11}$$

and

$$\psi_G = \frac{\omega}{4v_G} \mathbf{1}^T \mathbf{x} \tag{2.12}$$

with $\mathbf{1}$ denoting a vector of v_G ones.

Explicit forms for the E_{ij} are obtained from (2.7). Above the critical temperature

$$E_{ij} = \frac{\omega}{v_G} \left(\frac{1}{2} \delta_{ij} + \frac{\partial^2}{\partial \mu_i \partial \mu_j} \ln \Lambda_G(\boldsymbol{\mu}, z) \Big|_{\mu_i=1} \right) = \frac{\omega}{v_G} \frac{\partial^2}{\partial \mu_i \partial \mu_j} \ln Z_G(\boldsymbol{\mu}, w) \Big|_{\mu_i=1} \tag{2.13}$$

in terms of the full partition function Z_G . Z_G itself can be expanded in terms of w (DH):

$$Z_G = (\cosh \beta J)^{e_G} \prod_{i=1}^{v_G} (2 \cosh \beta m_i H) \left(1 + \sum_{l \geq 1} p^{(l)} w^l + \sum_{i>j} \tau_i \tau_j \sum_{l \geq 1} p_{ij}^{(l)} w^l + \dots \right)$$

where $\tau_i = \tanh \beta m_i H$. $p^{(l)}$ is the total number of l -edged subgraphs (connected and otherwise) of G with all vertices of even degree; $p_{ij}^{(l)}$ is the corresponding number with vertices i and j odd, and all the others even. It then follows from (2.13) that

$$\begin{aligned} E_{ii} &= P = 1 + \sum_{l \geq 1} p^{(l)} w^l & 1 \leq i \leq v_G \\ E_{ij} &= \sum_{l \geq 1} p_{ij}^{(l)} w^l, & i \neq j, \quad 1 \leq i, j \leq v_G \end{aligned} \tag{2.14}$$

where we have chosen $\omega = 4v_G P$. For this value of ω (2.12) reduces to

$$\psi_G = P \mathbf{1}^T \mathbf{x}. \tag{2.15}$$

The elements of matrix \mathbf{E} are calculated by computer enumeration of the relevant subgraphs of G . Then, in order to obtain ψ_G , equation (2.11) must be solved for \mathbf{x} . If, as in DH, the goal is an exact expression for ψ_G , the complete solution of (2.11) in terms of determinants must be evaluated. Our goal, however, is a series expansion, and for this only a limited number of terms in the expansions of the components of \mathbf{x} need be computed.

The matrix \mathbf{E} is written in polynomial form

$$\mathbf{E} = \mathbf{I} + \sum_{l=1}^{e_G} \mathbf{E}^{(l)} w^l$$

where \mathbf{I} is the identity matrix and

$$E_{ii}^{(l)} = p^{(l)}; \quad E_{ij}^{(l)} = E_{ji}^{(l)} = p_{ij}^{(l)}, \quad i \neq j.$$

The solution to (2.11) is the infinite series

$$\mathbf{x} = \mathbf{x}^{(0)} + \mathbf{x}^{(1)} w + \mathbf{x}^{(2)} w^2 + \dots$$

with $\mathbf{x}^{(0)} = \mathbf{1}$, $\mathbf{x}^{(1)} = -\mathbf{E}^{(1)}\mathbf{1}$, etc. The general term follows by iteration and is

$$\mathbf{x}^{(k)} = - \sum_{n=0}^{k-1} \mathbf{E}^{(k-n)} \mathbf{x}^{(n)} = \left(\sum_{n=1}^k (-1)^n \sum_t' \prod_{m=1}^n \mathbf{E}^{(t_m)} \right) \mathbf{1} \tag{2.16}$$

where the primed sum is over all sets $\{t_m | 1 \leq m \leq n\}$ satisfying $t_1 + \dots + t_n = k$. (2.15) then yields the result

$$\psi_G = \left(1 + \sum_{l \geq 1} p^{(l)} w^l \right) \left(v_G + \sum_{k \geq 1} y^{(k)} w^k \right) \tag{2.17}$$

where $y^{(k)} = \mathbf{1}^T \mathbf{x}^{(k)}$.

Application of (2.5) to (2.3) yields the cluster expansion

$$\psi_G(w) = \sum_{s \in G} (s; G) \Phi_s(w), \tag{2.18}$$

with Φ_s being the weight of star s in the expansion of χ^{-1} for the infinite lattice. The discussion following (2.3) is applicable to (2.18); the Φ_s are obtained iteratively in order of increasing e_s , and the first non-zero term in the expansion of each Φ_s will be of order e_s or higher. The final expansion is

$$\chi^{-1}(w) = \sum_s (s; \mathcal{L}) \Phi_s(w) \tag{2.19}$$

with $(s; \mathcal{L})$ denoting the number of weak embeddings of s in the infinite lattice, evaluated per lattice site, ie the lattice constant of s . If only those stars with up to e_{\max} edges are used in computing (2.19) the expansion will be correct to order e_{\max} in w .

An outline of the techniques used to generate the graph data required for the expansion appears in § 3.

2.2. A direct derivation

The existence of the star cluster expansion for χ^{-1} can be established directly without having to rely on the results of the Mayer development. The relation

$$\chi_G = 1 + \frac{2}{v_G} \sum_{i > j} s_{ij}$$

between the susceptibility of a cluster of Ising spins G and the spin correlation functions s_{ij} can be written as

$$v_G \chi_G = \mathbf{1}^T \mathbf{S} \mathbf{1}, \tag{2.20}$$

where $\mathbf{S} = (s_{ij})$. In terms of quantities defined earlier we have

$$s_{ij} = P^{-1} \sum_{l \geq 1} p_{ij}^{(l)} w^l,$$

and since $s_{ii} = 1$ it follows from (2.14) that $\mathbf{S} = P^{-1} \mathbf{E}$.

The inverse of (2.20) for a homogeneous cluster is simply

$$v_G \chi_G^{-1} = \mathbf{1}^T \mathbf{S}^{-1} \mathbf{1}. \tag{2.21}$$

Since all the sites of G are equivalent, the sum of the elements in each row (or column) of \mathbf{S} is equal to a constant $\Sigma_G(\mathbf{S})$. Now $\mathbf{S} \mathbf{1} = \Sigma_G(\mathbf{S}) \mathbf{1}$, so that if \mathbf{S}^{-1} exists $\Sigma_G(\mathbf{S}^{-1}) = \Sigma_G(\mathbf{S})^{-1}$, and the result (2.21) follows immediately.

From (2.11) and (2.15)

$$\psi_G = P\mathbf{1}^T \mathbf{E}^{-1} \mathbf{1} = \mathbf{1}^T \mathbf{S}^{-1} \mathbf{1}. \tag{2.22}$$

If G is homogeneous ψ_G reduces to $v_G \chi_G^{-1}$. In the inhomogeneous case we assume (2.22) to be the appropriate generalization and demonstrate that it leads to the star cluster expansion for χ^{-1} .

The vector $\mathbf{S}^{-1} \mathbf{1}$ in (2.22) is the solution to the equation $\mathbf{S} \mathbf{f} = \mathbf{1}$. Application of Cramers' rule yields

$$f_n = \frac{\det |\mathbf{S}^{(n)}|}{\det |\mathbf{S}|},$$

where $\mathbf{S}^{(n)}$ is obtained from \mathbf{S} by replacing the n th column with the vector $\mathbf{1}$.

Consider the behaviour of $\psi_{G'}$ for a cluster G' which is not a star, but which has an articulation point at vertex t . Choose the vertex labels so that if G' is separated into its two star components at t , vertices numbered 1 to t will lie in component 1, and vertices t to $v_{G'}$ in component 2. Above the critical point ($H = 0$) the correlation between two spins located at vertices i and j in different star components of G' (ie $i < t < j$) factorizes: $s_{ij} = s_{it} s_{tj}$. This follows directly from the definition of the correlation function. Because of this factorization, \mathbf{S} can be written in the form of a partitioned matrix and we have

$$\det |\mathbf{S}| = \det \begin{vmatrix} \mathbf{S}'_{(1)} & \mathbf{S}_{(1t)} & \mathbf{S}_{(1t)} \mathbf{S}_{(2t)}^T \\ \mathbf{S}_{(1t)}^T & 1 & \mathbf{S}_{(2t)}^T \\ \mathbf{S}_{(2t)} \mathbf{S}_{(1t)}^T & \mathbf{S}_{(2t)} & \mathbf{S}'_{(2)} \end{vmatrix} \tag{2.23}$$

Here $\mathbf{S}'_{(d)}$ ($d = 1, 2$) is the matrix of correlation functions between the spins of star component d excluding the spin at t , and vector $\mathbf{S}_{(dt)}$ contains the correlations between the spin at t and the remaining spins of d .

The result of subtracting appropriate multiples of the middle row of (2.23) from both top and bottom rows is

$$\det |\mathbf{S}| = \prod_{d=1}^2 \det |\mathbf{S}'_{(d)} - \mathbf{S}_{(dt)} \mathbf{S}_{(dt)}^T| = \det |\mathbf{S}'_{(1)}| \times \det |\mathbf{S}'_{(2)}|,$$

with $\mathbf{S}'_{(d)}$ the correlation matrix involving all the spins of d , including the spin at t . A similar analysis for $\mathbf{S}^{(n)}$ with $n < t$ yields

$$\det |\mathbf{S}^{(n)}| = \det |\mathbf{S}'_{(1)}^{(n)}| \times \det |\mathbf{S}'_{(2)}|,$$

with an analogous result holding for $n > t$. Thus for $n \neq t$

$$f_n = \frac{\det |\mathbf{S}'_{(d)}^{(n)}|}{\det |\mathbf{S}'_{(d)}|} \tag{2.24}$$

with $d = 1$ or 2 depending on which component contains vertex n . For $n = t$ we obtain

$$f_t = \sum_{d=1}^2 \frac{\det |\mathbf{S}'_{(d)}^{(t)}|}{\det |\mathbf{S}'_{(d)}|} - 1. \tag{2.25}$$

These results immediately generalize to clusters with more than one articulation point.

The subtraction of the star subgraph weights in (2.18) during the calculation of $\psi_{G'}$ includes the subtraction of the vertex contributions, namely a constant $v_{G'}$ is to be

subtracted from $\psi_{G'}$. If we define $\bar{\psi}_{G'} = \psi_{G'} - v_{G'}$, then from (2.22) and (2.24–5) we find that for a general articulated cluster G' (which may now have any number of articulation points)

$$\bar{\psi}_{G'} = \sum_{s_d} \bar{\psi}_{s_d}$$

the sum being over the star components of G' . It follows from (2.18) that $\Phi_{G'} = 0$, because every star subgraph of G' is a subgraph of one of the star components of G' . Hence only the star subgraphs of G contribute to χ_G^{-1} , and if G is now taken to be the infinite lattice the expansion of χ^{-1} is in terms of star graphs alone.

2.3. *Weights by the labelled edge method*

The great proliferation of stars entering into the computation of the higher order terms of the expansion can turn the counting of the star subgraph embeddings ($s; G$) into a relatively time consuming operation. A scheme for by-passing this calculation entirely was described in a different context by Domb (1970b), and used in computing the Ising partition function (Hunter 1968) and the susceptibility of Ising systems with impurities (Rapaport 1972a).

The essence of the idea as applied to our problem is to compute ψ_G by inverting the polynomial expansion of \mathbf{E} (§ 2.1), but only after assigning a different variable w_e (ie a label) to each edge of G . The distinction between the different w_e is retained throughout the calculation and, at its conclusion, the weight Φ_G is deduced simply by discarding all terms of the multi-variable expansion of ψ_G which do not contain contributions from all the edges of G .

This approach is not particularly effective in dealing with large graphs because of the multi-variable expansions involved. It can however be modified to yield, for example, only the term of order e_G in the expansion of Φ_G , ie the earliest possible contribution of G to the expansion, even for the largest graphs considered.

2.4. *General properties of the weights*

Certain general features of the weights are apparent from the calculations and merit some discussion. First, if a star G has four or more odd vertices, the leading order term in the expansion of Φ_G is of order $e_G + 1$ or greater. That this is to be expected follows from (2.16–7) where it is seen that each contribution to ψ_G arises from the product of a subgraph of G with all vertices of even degree and zero, one, or more subgraphs which have just two odd vertices and which are embedded in G in such a manner that their product is a graph (possibly multi-edged) with at most two vertices of odd degree. Since all the edges of G must contribute to the terms of Φ_G , and the subgraph products arising from (2.17) can have at most two odd vertices, it is obvious that there can be no term of order e_G which utilizes all the edges of G , and hence the first non-zero term in Φ_G will be at least of order $e_G + 1$.

The second observation is that if G has exactly two odd vertices the coefficient of the order e_G term in Φ_G depends only on the topology of G and not on e_G ; if all the vertices are even the coefficient depends on e_G as well. These observations are related to the rules for determining graph weights when the χ expansion is computed directly using the counting theorem (Sykes 1961, Nagle and Temperley 1968). The precise relationship between the structures of the series for χ and χ^{-1} may be explored by

following the fate of each of the graphs contributing to the χ expansion when it is inverted; we do not intend to pursue such a study here.

The proof that the term of order e_G in the weight of a star G with two odd vertices depends on topology alone is straightforward. We see from (2.16–7) that the coefficients in the expansion of ψ_G are sums of terms of general form

$$(-1)^n p^{(l)} p_{i_0, i_1}^{(t_1)} p_{i_1, i_2}^{(t_2)} \dots p_{i_{n-1}, i_n}^{(t_n)} \tag{2.26}$$

The subscripts in (2.26) correspond to vertices of G and need not all be distinct. Some of these terms will have the property that one or more of their subscripts correspond to a particular vertex m . These can be written as

$$(-1)^n p^{(l)} F_1 p_{i', m}^{(t')} p_{m, i''}^{(t'')} F_2 \tag{2.27}$$

with F_1 and F_2 denoting the remaining $p_{ij}^{(t)}$, and perhaps themselves involving further appearances of subscript m . We now construct a new star G' with the same topology as G by inserting an additional vertex m' into the edge $m-i''$. If we assert that (2.27) is one of the terms which contribute to the expansion of Φ_G at order e_G the corresponding contribution to $\Phi_{G'}$ at order $e_{G'} = e_G + 1$ is

$$(-1)^n p^{(l)} F_1 (p_{i', m}^{(t')} p_{m, i''}^{(t''+1)} + p_{i', m'}^{(t'+1)} p_{m', i''}^{(t'')} - p_{i', m}^{(t')} p_{m, m'}^{(1)} p_{m', i''}^{(t'')}) F_2. \tag{2.28}$$

Since by definition $p_{m, m'}^{(1)} = 1$, $p_{i', m'}^{(t'+1)} = p_{i', m}^{(t')}$, etc, (2.28) is identical to (2.27). There are also terms of form (2.26) which contribute to Φ_G at order e_G and do not involve vertex m explicitly; these terms are unaffected by the additional vertex and make identical contributions to $\Phi_{G'}$ at order $e_{G'}$. It follows that the order e_G term of Φ_G is a function of the topology of G only.

3. Series generation techniques

The first stage in generating the series expansion is to obtain a complete list of those star graphs which are possible contributors to the series. The largest stars which have to be considered are those with as many edges (e_{\max}) as the order of the last term required in the expansion; in this case $e_{\max} = 13$. Furthermore, only those e_{\max} edge stars with not more than two odd vertices need be studied; for other stars there is no need to go beyond $e_{\max} - 1$ edges (a more careful analysis would show that there are small classes of stars—among them, for example, those having six odd vertices—where even this is unnecessary).

In a previous susceptibility calculation (Rapaport 1972a) the approach called for a list of connected graphs (ie both stars and articulated graphs). In that case we were able to build up a suitable graph list by generating the e edge graphs from those with $e - 1$ edges simply by adding single edges. This technique is not ideal for star generation because the majority of graphs generated are not stars.

A more suitable method for generating stars only begins with the generation of a list of homeomorphically irreducible stars, ie stars with all vertices of degree two suppressed. Stars of this type are called topologies; all their vertices are of degree three or greater (nodes) and, for clarity, the edges of the topologies will be referred to as bridges. When the topology generation is complete the stars required for the series expansion are obtained by replacing the bridges with chains of edges (see later).

The topologies are generated by an iterative scheme (Heap 1966). All topologies (b, n) having b bridges and n nodes can be obtained from a complete list of $(b - 1, n)$,

$(b-2, n-1)$ and $(b-3, n-2)$ topologies. The (b, n) are obtained: (i) from $(b-1, n)$ by joining any pair of existing nodes with a single bridge; (ii) from $(b-2, n-1)$ by inserting a new node on an existing bridge and connecting it to an existing node; (iii) from $(b-3, n-2)$ by inserting two nodes on either the same bridge or on different bridges and joining them. In each process the cyclomatic index $c = b - n + 1$ is increased by unity. This scheme permits the generation of topologies in order of increasing c , starting with the $c = 1$ topology—the simple polygon.

The possibility of generating any given topology in more than one way cannot be neglected; in fact the technique just described generates most of the topologies more than once, and some means of eliminating duplicates must be devised. This is most readily achieved by prescribing a canonical scheme for labelling the nodes. Each topology will then possess a unique description, and if the topologies are sorted into a suitable dictionary order the problem of identifying duplicates is reduced to triviality.

The labelling method used here is a generalization of one proposed by Nagle (1966), and is as follows. Initially the nodes are labelled $1, 2, \dots$ in order of decreasing degree. If, as is usually the case, there is more than one node with a given degree, the labels are assigned in such a manner that when the elements of the adjacency matrix \mathbf{A} (A_{ij} = number of bridges between nodes i and j) are written in the form of a string

$$\mathcal{A} = A_{11}A_{12}A_{13} \dots A_{21}A_{22} \dots$$

the numerical value of \mathcal{A} is maximized. Maximization of \mathcal{A} requires the examining of all node label permutations consistent with the ordering by degree. \mathcal{A} is unambiguously defined and has a different value for each distinct topology, although the prescription for arriving at its value is highly arbitrary.

If too many nodes of the topology have the same degree, the number of label permutations required to maximize \mathcal{A} becomes inconveniently large. In this case the labelling process is accelerated by grouping the nodes according to the numbers of two-, three-, ... step returns to each node, in addition to the degree grouping. The number of N -step returns to node i is just $(\mathbf{A}^N)_{ii}$.

Taking into account the symmetries of the topologies reduces the amount of over-generation, eg if in process (ii) the $(b-2, n-1)$ topology under consideration has two bridges b_1 and b_2 equivalent under a symmetry transformation, there is no need to insert a new node into b_2 . Additional economies arise from the manner in which the graph descriptions are handled by the computer, the sorting techniques used, and so on.

Application of the techniques just outlined yields a list of all the topologies required for the series generation. The enumeration of the star graphs themselves is then merely a matter of assigning lengths (in terms of chains of edges) to the bridges. By running through the possible combinations of bridge lengths (excluding those which lead to multi-edges) subject to a fixed total number of edges, all realizations of a given topology with given e are produced. Care is required to avoid repeated generation of realizations equivalent under a symmetry transformation. In this manner the list of nearly 3000 distinct star graphs needed for the χ^{-1} series was constructed from the topology list.

The most time consuming part of the calculation is the evaluation of the lattice constants ($s; \mathcal{L}$). The computer program used for this task is a refinement of one used in an earlier calculation (Rapaport 1972a), the principal difference being that rather than constructing the possible embeddings by laying the graph edges on the lattice bonds one at a time, the graph is constructed from short self-avoiding walks (eg up to three edges at a time). This idea was first incorporated in a much used program developed by J L Martin (unpublished); use of walks instead of edges means a significant

reduction in the number of partially completed embeddings which have to be rejected because of their failure to meet the self-avoiding condition. A further marked reduction in computer time is achieved by coding the program in assembler language, and rates of up to a quarter of a million successful embeddings per minute have been achieved on an IBM 360/50 computer.

All the necessary stars were counted with this program, except the very largest polygons whose counts appear in the literature (Sykes *et al* 1972c) and which are best obtained by an indirect method. The star subgraph embeddings required for the weight calculation were handled by similar means; an iterative scheme (Sykes *et al* 1966) which proved useful when embeddings of all subgraphs—including multi-component—were required (Rapaport 1972b), and which avoided the explicit counting of embeddings, is not suited to the star problem.

The final stage is the computation of the star weights Φ_G , either by determining ψ_G and subtracting the subgraph contributions (§ 2.1), or, in the case of the $e = 13$ stars, by using the labelled edge method of § 2.3. The weights, together with the lattice constants, yield the following expansion for the Ising model on the FCC lattice:

$$\begin{aligned} \chi^{-1} = & 1 - 12w + 12w^2 + 36w^3 + 180w^4 + 948w^5 + 5556w^6 + 36\,132w^7 + 256\,452w^8 \\ & + 1\,899\,332w^9 + 14\,470\,572w^{10} + 112\,925\,988w^{11} + 899\,987\,260w^{12} \\ & + 7\,303\,456\,548w^{13} \end{aligned}$$

the inverse of which (χ) appears in the appendix. The terms to twelfth order are identical to those of Sykes *et al* (1972a). The thirteenth is of course new.

A partial check on the accuracy of the star data is to use them in the generation of the partition function ($\ln Z$) expansion. Included among the stars generated for the χ^{-1} study are the majority of those needed to compute $\ln Z$ to fourteenth order. What is missing is the set of fourteen edge stars with all vertices of even degree, but these can be obtained using the techniques described earlier. The resulting $\ln Z$ expansion agrees with the published one (Sykes *et al* 1972b). This by no means constitutes a complete check, because there are a number of stars which contribute to χ^{-1} but not to $\ln Z$ to the orders considered.

4. Analysis of the series

In their analysis of the first eight terms of the FCC susceptibility series Domb and Sykes (1957) were able to obtain estimates of the critical temperature corresponding to $w_c = 0.10174$ and exponent $\gamma = 1.25$. The same values were obtained after the addition of a further four terms (Sykes *et al* 1972a), together with the critical amplitude and tentative estimates of the corrections to critical behaviour. More generally, all available numerical evidence for two- and three-dimensional Ising systems points to critical behaviour of the form

$$\chi \sim f(w) + C_0(1 - w/w_c)^{-\gamma} + C_1(1 - w/w_c)^{-\gamma+1} + \dots \quad w \leq w_c \quad (4.1)$$

with $f(w)$ regular in the neighbourhood of w_c . (4.1) applies to close-packed lattices; in the loose-packed case it must be supplemented by the antiferromagnetic singularity at $-w_c$ (Sykes *et al* 1972a). In three dimensions (4.1) has no rigorous basis, and it is only recently that exact results for C_0 and C_1 have been obtained for the two-dimensional square lattice (Barouch *et al* 1973).

Expansion of (4.1) in terms of w suggests that for $n \gg 1$ the coefficients of the χ series should become

$$a_n \sim w_c^{-n}(G_0 n^{\gamma-1} + G_1 n^{\gamma-2} + \dots) \tag{4.2}$$

The ratios of successive coefficients are then

$$r_n = a_n/a_{n-1} \sim w_c^{-1}(1 + b_1/n + \dots + b_k/n^k \dots) \tag{4.3}$$

with $b_1 = \gamma - 1$. Truncation of (4.3) at order k corresponds to the k th order Neville extrapolant (Hunter and Baker 1973). In a preliminary report (Rapaport 1973) the Neville method was used to compute estimates for w_c and biased estimates for γ . Unbiased estimates of γ are obtained by truncating (4.3) at k th order and solving the resulting sets of equations using the known r_{n-k+1}, \dots, r_n , for various n . The results appear in table 1. The calculation also yields w_c (identical to the Neville results—see figure 1) and the higher order coefficients b_2, \dots . The latter were not observed to settle into any regular pattern.

Table 1. Unbiased estimates of γ (ie $b_1 + 1$) obtained from equation (4.3) using a k th degree polynomial in $1/n$.

$n \backslash k$	1	2	3
9	1.24594	1.24952	1.25839
10	1.24619	1.24833	1.24394
11	1.24626	1.24684	1.24059
12	1.24622	1.24590	1.24152
13	1.24616	1.24544	1.24305

If γ is (believed) known one can compute w_c from

$$r'_n = \frac{n}{n + \gamma - 1} r_n \sim w_c^{-1}(1 + b'_2/n^2 + \dots + b'_k/n^k \dots) \tag{4.4}$$

Since the term linear in $1/n$ is absent the convergence of the w_c estimates ought to be more rapid than with (4.3). The results appear in figure 1. They lie slightly above the estimates from (4.3), but there is no significant improvement in convergence.

The amplitudes C_m are computed by fitting (4.1) to the χ expansion. Using the values $w_c = 0.10174$, $\gamma = 1.25$ we obtain $C_0 = 0.963$ —as in Sykes *et al* (1972a), but the result is sensitive to the choice of w_c . The higher order amplitudes are more difficult to determine; the analysis indicates that $C_1 \approx 0.21$, but is unable to provide a satisfactory estimate for C_2 .

Analysis by the Padé method has also been tried. The diagonal and immediate off-diagonal approximants of $d/dw \ln \chi$ yield results which indicate $w_c = 0.10174$, $\gamma = 1.248$. A number of the approximants contain defects and therefore present a possibly over-optimistic picture of the degree of convergence (Hunter and Baker 1973).

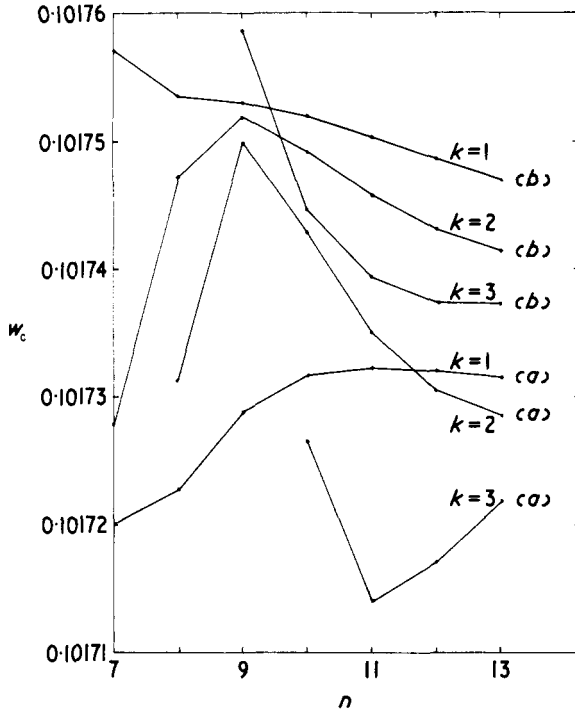


Figure 1. Plots of the w_c estimates obtained from a fit to a k th degree polynomial in $1/n$ of form: (a) equation (4.3); (b) equation (4.4). The latter involves the assumption $\gamma = \frac{1}{4}$. Note the ordinate scale—it is only the 5th and 6th significant digits which are at issue.

Padé analysis of $\chi^{1/\gamma}$ yields essentially the same w_c , and from the [7, 6] and [6, 7] approximants we deduce $C_0 = 0.962$.

A different approach to the analysis is motivated by the fact that the series originally derived was that of χ^{-1} . The critical point singularity at w_c corresponds to the appropriate zero of $\chi(w)^{-1}$. The w_c estimates obtained from the first n terms of χ^{-1} together with their Neville extrapolants appear in table 2, and are in complete agreement with those obtained previously.

Table 2. Zeros of the first n terms of χ^{-1} ($k = 0$ column) and w_c estimates obtained by Neville extrapolation.

$n \backslash k$	0	1	2	3
9	0.099549	0.101755	0.101785	0.101814
10	0.099769	0.101753	0.101747	0.101660
11	0.099949	0.101748	0.101725	0.101665
12	0.100099	0.101743	0.101719	0.101700
13	0.100225	0.101740	0.101719	0.101722

5. Application to the classical vector models

The derivation of the expansion for χ^{-1} (§ 2.2) is readily extended to include the isotropically interacting classical vector models—namely the planar model (Bowers and Joyce 1967), the Heisenberg model (Wood and Rushbrooke 1966), and the range of systems with higher-dimensional spin vectors (Stanley 1971).

In the Ising case the crucial element in establishing the zero weight of an articulated graph G' is that the correlation between spins σ_i and σ_j on different star components of G' can be factorized as $\langle \sigma_i \sigma_j \rangle = \langle \sigma_i \sigma_i \rangle \langle \sigma_i \sigma_j \rangle$ with σ_i the spin at the articulation point. In the isotropic Heisenberg model symmetry considerations lead to the result (Joyce 1967) $\langle \sigma_i \cdot \sigma_j \rangle = \langle \sigma_i \cdot \sigma_i \rangle \langle \sigma_i \cdot \sigma_j \rangle$ so that the correlation between the z components of the spins is

$$s_{ij} = \langle \sigma_{iz} \sigma_{jz} \rangle = 3 \langle \sigma_{iz} \sigma_{iz} \rangle \langle \sigma_{iz} \sigma_{jz} \rangle = 3s_{ii} s_{ij}.$$

We construct the correlation matrix $\mathbf{S} = (s_{ij})$ —the diagonal elements are simply $s_{ii} = \langle \sigma_{iz} \rangle^2 = \frac{1}{3}$. The subsequent analysis parallels the Ising case, and the result is again that only the star subgraphs of G contribute to ψ_G .

The star expansion for χ^{-1} may be shown to exist for isotropic systems having any spin dimensionality d , the only difference in the analysis is that the number 3 which appears when s_{ij} is factorized must be replaced by d . The analysis does not apply when the interaction is anisotropic, as in a mixed Heisenberg–Ising system, because s_{ij} no longer factorizes.

Actual development of the expansions for the vector models requires the computation of the elements of a matrix analogous to \mathbf{E} in (2.14). The partition function of a spin cluster G is ($K = \beta J, L = \beta m H$)

$$Z_G = \text{Tr} \left[\exp \left(K \sum_e \sigma_i \cdot \sigma_j + L \sum_i \sigma_{iz} \right) \right]$$

where the trace is just the normalized integral over the surface of a d -dimensional hypersphere for each spin of G and e denotes the edge $i-j$. Expanding the exponential and setting $L = 0$ leads to

$$Z_G = \sum_{\{M_{e\tau}\}} \frac{K^{\sum_{e,\tau} M_{e\tau}}}{\prod_{e,\tau} M_{e\tau}!} \text{Tr} \left(\prod_{e,\tau} (\sigma_{i\tau} \sigma_{j\tau})^{M_{e\tau}} \right) \tag{5.1}$$

Each set $\{M_{e\tau}\}$ corresponds to choosing a subgraph of G and replacing each edge e by $M_{e\tau}$ edges of type τ , with τ running through the values x, y , and z for Heisenberg spins, and correspondingly for the other kinds of system. The sum is over all such sets; an upper limit on the values of the $M_{e\tau}$ is set by the greatest power of K sought. For convenience we now specialize to the Heisenberg case.

If $D_{v\tau}$ is the degree of vertex v with respect to edges of type τ in the graph corresponding to the particular set $\{M_{e\tau}\}$, then the trace in (5.1) can be written as

$$\prod_v F(D_{vx}, D_{vy}, D_{vz})$$

where

$$F(D_{vx}, \dots) = \frac{1}{2\pi} \prod_{\tau} \Gamma\left(\frac{D_{v\tau} + 1}{2}\right) \left[\Gamma\left(\frac{\sum_{\tau} D_{v\tau} + 3}{2}\right) \right]^{-1} \tag{5.2}$$

if all the $D_{v\tau}$ are even, and zero otherwise. This is a consequence of

$$\prod_e (\sigma_{i\tau} \sigma_{j\tau})^{M_{e\tau}} = \prod_v (\sigma_{v\tau})^{D_{v\tau}}$$

and the evaluation of the spin integrals arising from the trace.

We define $\psi_G = 3Z_G \mathbf{1}^T \mathbf{x}$. It is then readily established that the elements of \mathbf{E} are

$$\begin{aligned} E_{ij} &= 3 \text{Tr} \left[\sigma_{iz} \sigma_{jz} \exp \left(K \sum_e \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \right) \right] \\ &= 3 \sum'_{\{M_{e\tau}\}} \frac{K^{\sum_{e,\tau} M_{e\tau}}}{\prod_{e,\tau} M_{e\tau}!} \prod_{v \neq i,j} F(D_{vx}, D_{vy}, D_{vz}) \prod_{v=i,j} F(D_{vx}, D_{vy}, D_{vz} + 1) \end{aligned}$$

with the prime denoting a sum over $\{M_{e\tau}\}$ such that all the $D_{v\tau}$ are even, except D_{iz} and D_{jz} . The diagonal elements are $E_{ii} = Z_G$. In the planar model case we define $\psi_G = 2Z_G \mathbf{1}^T \mathbf{x}$, and obtain similar results, but with a modified form of (5.2). The analysis is readily extended to handle the other spin systems.

These results, together with the star graph data generated for the Ising study were used to compute the terms of χ^{-1} to seventh order for both Heisenberg and planar models on the FCC lattice. The results agreed with the published expansions. Ten terms are currently available for both Heisenberg and planar model series (Ferer *et al* 1971, 1973). The method is capable of yielding longer series, but the computation time required in forming the matrix \mathbf{E} increases rapidly with star size.

6. Summary

A new approach to the derivation of exact high temperature series expansions for the susceptibility of the Ising and classical vector models has been presented. The idea behind the method is that one computes the expansion of the inverse susceptibility, for which only data on star graphs are required. The method has been used to extend the FCC Ising susceptibility series to thirteenth order, and has also reproduced parts of the expansions for the classical Heisenberg and planar spin models. The behaviour of the Ising series is already so smooth at twelfth order that the addition of the extra term has no significant effect on the estimated critical behaviour of the susceptibility, and merely reinforces earlier conclusions. It appears probable that, should the need arise, the method could be used to extend the series even further with the extremely powerful computers currently available.

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Appendix. Coefficients of the susceptibility expansion in terms of $w = \tanh \beta J$

n	χ
0	1
1	12
2	132
3	1404
4	14652
5	151116
6	1546332
7	15734460
8	159425580
9	1609987708
10	16215457188
11	162961837500
12	1634743178420
13	16373484437340

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