Specific heat of a three-dimensional Ising ferromagnet above the Curie temperature. III. The star cluster expansion

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Specific heat of a three-dimensional Ising ferromagnet above the Curie temperature III. The star cluster expansion

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Abstract. The star cluster expansion for the specific heat of a three-dimensional Ising ferromagnet is described. The classification of stars by ascending number of edges is studied and a canonical description developed. The construction of a general star-graph list for high temperature expansions is described.

1. Introduction

In this paper we describe a general cluster expansion for the high temperature specific heat of the Ising model of a ferromagnet. We have two main objectives in studying this expansion; first to derive as many terms as possible and use them to elucidate the critical behaviour of the specific heat and to evaluate it numerically for direct comparison with experiment; second to provide detailed configurational data for studies of the structure of the expansion.

The expansion coefficients we have derived are given in previous papers (Sykes *et al* 1967, 1972a, to be referred to as I and II) together with a numerical study; although convergence is slow it seems that reasonable estimates of the critical index (α) can be made and this is relevant to the theory of scaling (Fisher 1967, Kadanoff *et al* 1967, Stanley 1971). Numerical representations have found application to experimental work (Wielinga 1968a, b, Blöte 1972); certain compounds, notably Rb_3CoCl_5, fit the specific heat of the simple cubic Ising model very well. The structure of the expansion has been studied extensively by Domb (1970, 1972a, b).

We follow I and II and write the configurational free energy of a lattice of N sites and $\mathcal{N}$ edges in the form

$$N \ln \Lambda(v) = N \ln 2 - \mathcal{N} \ln(1+v) + NL(v) \tag{1.1}$$

where $v = \tanh K$ (the standard high temperature counting variable). The starting point of our treatment is the well known result that $L(v)$ may be written as a cluster expansion. (For a general introduction see Domb 1960, in particular § 5.2.10, Domb and Hiley 1962, in particular equation (31), Uhlenbeck and Ford 1962, Kubo 1962, Strieb *et al* 1963, Sykes *et al* 1966, in particular § 5, Sykes and Hunter 1973, Domb and

Green 1973). We use the notation of Sykes *et al* (1966). Explicitly if we expand in powers of v:

$$L(v) = \sum_r a_r v^r \tag{1.2}$$

then

$$a_r = \sum_G w_r(G)(G; \mathscr{L}) \tag{1.3}$$

where the last sum is taken over all star graphs G with r edges, or less, (other than the single edge) that occur as sub-graphs of the lattice $\mathscr{L}$ and $(G; \mathscr{L})$ denotes the number of weak embeddings per site of G in $\mathscr{L}$ (that is the weak lattice constant of G in $\mathscr{L}$). The $w_r(G)$ are numbers, independent of $\mathscr{L}$, which we call the L weights of G. Since the summation is restricted to stars of r edges or less, $w_r(G) = 0$ for $r < e$, the number of edges in G. We call $w_e(G)$, $w_{e+1}(G)$, $w_{e+2}(G)$ the primary, secondary and tertiary weights of G respectively.

The prescription for determining a_r for a lattice L is thus conceptually simple: from a complete list of stars with r or fewer edges select those with non-zero weights and form the sum (1.3). However, the number of stars with r edges increases rapidly with r; the scale of the problem may be judged from table 1.

Table 1.

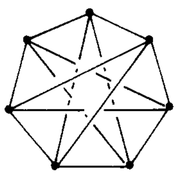
r	Number of stars with $e = r$	Number of stars with $e \leqslant r$	Number of stars contributing to a_r
3	1	1	1
4	1	2	1
5	2	4	1
6	4	8	3
7	7	15	4
8	16	31	10
9	42	73	19
10	111	184	42
11	331	515	86
12	1094	1609	237

To extend the expansion beyond $r = 12$ it is desirable to list and classify stars in some systematic way; to do this we have modified and extended an earlier topological classification (Sykes *et al* 1966). The restriction of the problem to a particular lattice results in some reduction in the number of stars that need be considered; for example of the 1609 stars with $e \leqslant 12$ only 1548 are embeddable in the face-centred cubic lattice. A much greater economy will be achieved as r increases; it is trivially clear that for a loose-packed lattice only loose-packed stars need be listed. The problems of classification and listing are considered in §§ 3 and 4.

In practice it is uneconomic to list all stars because of the large number of zero weights. We summarize in § 2 the salient properties of the L weights. Since we are describing a large project we do not give an immense amount of detail; we make a large number of statements without proof and these will be readily understood by anyone familiar with the cluster technique. Justification may be found in the literature cited.

In § 4 we describe the construction of complete lists of stars, in the appropriate format, for the more common crystal lattices. In considering the general problem of listing lattice constants we have not restricted the investigation to the free energy of the Ising model in zero field; we have made provision for studies of closely related problems which require data differing only in detail: for example the zero-field expansion for the free energy of the spin ∞ Heisenberg model, the classical vector model, and the susceptibility of the Ising model.

Once a list of stars has been compiled there remain the two problems of determining the lattice constants and the weights. In general the higher the connectivity of a graph the easier it is to determine the number of embeddings; at the same time problems of symmetry and weight are usually more complex. For example at $r = 14$ the star with the lowest connectivity is the polygon of 14 sides with a lattice constant of 8 798 329 080 on the face-centred cubic lattice; special methods are required to determine lattice constants of this size (Sykes *et al* 1972b). At the other extreme there are some graphs of cyclomatic number 8:



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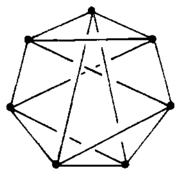


whose weights are not easily obtained by elementary methods.

The determination of the weights has been developed by Hunter (1967) and more recently by Domb (1972b); a summary, and a lead into the literature is given by Sykes and Hunter (1973). With the use of fast electronic computers the weights no longer present a serious problem. To count embeddings we have again largely relied on computers. Since the pioneer work of Rushbrooke and Eve (1959) and Martin (1962) many specialized techniques have been developed for this purpose.

2. Properties of the L weights

We begin by defining certain concepts (for a general introduction to the definitions of this section see Sykes *et al* 1966). A terminology which distinguishes each separate concept precisely is cumbersome; we are concerned both with linear graphs and graph topologies. These two concepts have many features in common and a certain overlapping of terms is inevitable. It is convenient to distinguish a graph topology (or more simply a *topology*) and a linear graph (or more simply a *graph*). A graph topology is a set of nodes connected by bridges; the number of bridges incident upon any node is the *valence* of that node and, for a star, is always greater than 2. (The polygon corresponds to the exceptional topology with no nodes.) If we introduce a *metric* by inserting on the bridges of a topology antinodes of valence 2 we obtain a (linear) graph which is a *realization* of the topology. To avoid confusion it is convenient to refer to the nodes and antinodes of the realization as vertices (or points or sites) and to each connection between two vertices as edges (or lines or bonds). The concept of *valence* is still applicable to a vertex; each vertex of valence 2 corresponding to an antinode, of valence more than two to a node; nodes are sometimes called the principal points of a graph. The bridges of a graph are the chains of edges which connect the vertices of valence more than 2 (without passing through vertices of valence more than 2) and the length of the bridge is the number of edges in it.

Nodes of odd valence (odd nodes) must occur an even number of times; nodes of even valence (even nodes) are unrestricted. Topologies all of whose vertices are even are of fundamental importance in series expansions for the Ising model in zero magnetic field (Wakefield 1951, Rushbrooke and Eve 1962, Domb and Sykes 1957, Domb 1960); we call such topologies *no-field topologies* and their realizations *no-field graphs* and use the abbreviation NF.

Topologies with two, and only two, nodes of odd valence are of fundamental importance in series expansions for the zero-field susceptibility of the Ising model (Oguchi 1951, Sykes 1961); we call such topologies *magnetic topologies* and their realizations *magnetic graphs* and use the abbreviation MG.

A topology with more than two odd nodes we call *hypermagnetic* and for n odd nodes we abbreviate this to HMn. Trivially HM0 is equivalent to NF and HM2 to MG but it is usually convenient to assume (consistent with the definition above) that $n > 2$.

A further sub-classification can be made into categories dependent upon structural details of special relevance to the theory of L weights; if for a topology with $2m$ odd nodes $(m+s-1)$ is the least number of bridges that can be selected to connect the odd nodes in pairs we call s the *category* of the topology. A *graph* is of category s if its topology is of category s. For example a magnetic topology has $m = 1$ and for it to be first category the two odd nodes must be directly connected by a bridge. We illustrate in figure 1 particular examples of category 1 and 2. The fourth graph in figure 1 has category 2 because this gives $(m+s-1) = 3$ and 3 is the least number of bridges that can be selected to connect the odd nodes in pairs. It is evident that 3 is sufficient and that 2 would not suffice.

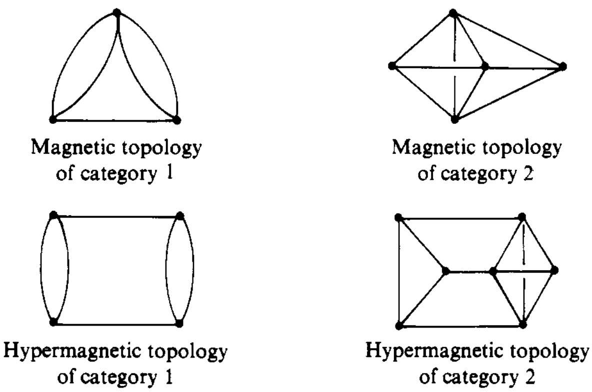
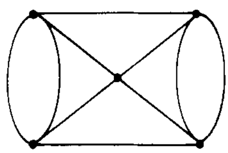


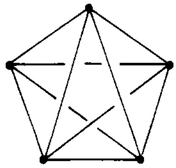
Figure 1. Examples of the sub-classification of graph topologies into categories.

2.1. *Primary weights*

We have defined the primary L weight of a graph of e edges to be its contribution to a_r for $r = e$ in (1.3). (Some authors have used the term entry parameter; a graph with non-zero primary weight has entry parameter zero.) *The only graphs with primary weights are no-field graphs*; further two graphs which are homeomorphic have the same primary weight which is therefore a property of their topology. In other words, the primary weight is not a *metric* property; it is independent of the lengths of the bridges. Primary weights are *metric invariants* or simply *invariants* (some authors have used the term topological invariant, but this is misleading). A few NF topologies have zero primary weight: for example



and

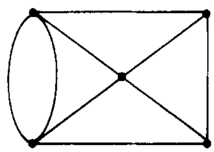


and we call these *cancellation zeros.* They arise as a result of cancellation from different contributions to the coefficient; we know of no theory that would make it clear in advance that certain topologies are cancellation zeros.

In general to develop (1.2) through v^r we should consider all no-field graphs with $e \leqslant r$; cancellation zeros may of course be ignored but for reasons stated in the introduction we have included them in our investigation. We illustrate in the appendix all the 53 no-field (NF) topologies of cyclomatic number 7 or less, together with their primary weights. There are 199 NF topologies of cyclomatic number 8 and we have enumerated all of these.

2.2. *Secondary weights*

The secondary L weight of a graph of e edges is its contribution to a_r in (1.3) for $r = e+1$. *The only graphs with non-zero secondary weight are first category magnetic graphs.* There is a further *metrical* condition that the bridge connecting the two odd vertices must be of unit length; this restriction is not very important in effecting economies since the first realization of any first category magnetic topology must always satisfy the metrical condition. Thus to develop (1.2) through v^r we should examine all first category magnetic graphs with $e \leqslant r-1$. There are a few first category magnetic topologies *all* of whose realizations have zero secondary weight (cancellation zeros). For example



is a first category magnetic cancellation zero. Again for reasons stated in the introduction we have chosen to extend our investigation to include all magnetic graphs with $e \leqslant r-1$. There are 112 magnetic topologies of cyclomatic number 6 and 601 of cyclomatic number 7, and we have enumerated all of these.

2.3. *Tertiary weights*

The tertiary L weight of a graph is its contribution to a_r in (1.2) for $r = e+2$. Contributions come from: (i) NF graphs (whose tertiary weight is a metric property); (ii) MG graphs of categories 1 and 2; (iii) HM4 graphs of category 1. The first two groups have already occurred above; to develop the expansion (1.2) through v^r we should examine all first category HM4 graphs with $e \leqslant r-2$. The extension of these general rules to higher weights is straightforward but increasingly complex.

2.4. General scheme

It is possible to exploit the occurrence of cancellation zeros and metrical conditions to reduce to a minimum the number of graphs that need be considered; a very detailed treatment is required. However, the economy effected by most of these constraints is a very small part of the whole; further, some of the constraints are specific to the Ising model (cancellation zeros); the metrical constraints are not so confined but only make a small economy. We have sought to achieve a list applicable to other problems and to effect worthwhile economies. From the above properties and considerations it should be clear that while extending (1.2) through v^r we should investigate:

(i) NF topologies and their realizations for $e \leqslant r$;

(ii) MG topologies and their realizations for $e \leqslant r-1$;

(iii) HM$2m$ topologies and their realizations for $e \leqslant r-m$.

Strictly we may exclude from (ii) magnetic topologies of category (s) greater than 1; these are only required for $e \leqslant r-s$. However by including them we form a list which can be used to derive the susceptibility through v^{r-1} (Oguchi 1951, Sykes 1961, Domb and Hiley 1962, Sykes *et al* 1972a, b).

3. Classification and listing of stars with a given number of edges (edge grouping)

To classify and list star graphs with a given number of edges we follow Sykes *et al* (1966) and group homeomorphic stars together; the idea is derived from the literature (Ford and Uhlenbeck 1957). For cyclomatic number 1 there is one topology (polygon) which has a unique realization for a given number of edges. For cyclomatic number 2 there is one topology, the *theta topology* which we illustrate in figure 2 (a). Any linear graph with this topology (a theta graph), that is a graph with two principal points connected by three distinct chains of edges (the bridges), is a *realization* of the topology. For example the two graphs illustrated in figure 2 (b) and (c) are realizations of the theta topology. In fact, if we exclude multigraphs, they are the only possible realizations with six edges of this topology. In general we shall simply say that *there are two theta graphs with six edges.*

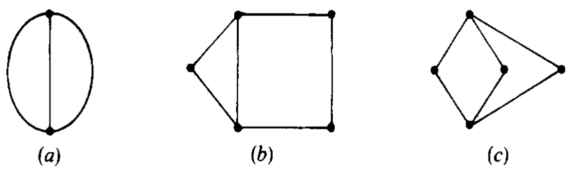


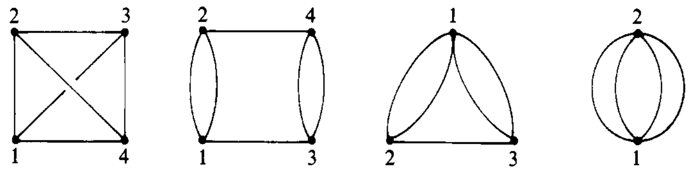
Figure 2. (a) Theta topology; (b) and (c) theta graphs with six edges.

It is possible to specify the realizations of a star S by labelling the bridges $a, b, c, \ldots$ and giving their lengths in some conventional order $S(a, b, c, \ldots)$. Such a notation always specifies the graph but it is possible for two specifications whose arguments are permutations of one another to specify the same (that is an isomorphic) graph. A trivial example is provided by the theta topology: if the bridges are labelled in any order the realizations $S(1, 2, 3)$ and $S(1, 3, 2)$ are clearly identical. For simple cases such ambiguities are readily removed; for the theta topology it suffices to write $S(a, b, c)$ with $a \leqslant b \leqslant c$ for isomorphic theta graphs to have identical descriptions.

For cyclomatic number 3 there are 4 star topologies and a convention for specifying their realizations has been devised (Sykes *et al* 1966). We now describe a general convention, applicable to any star topology or graph, which provides a unique specification which we have adopted as a *canonical specification.* A full mathematical treatment is given by McKenzie (1974a).

The 4 star topologies of cyclomatic number 3 are illustrated in figure 3. If we label the N nodes $1, 2, \ldots, N$ the topologies may be specified by listing the B bridges that connect the nodes in ordered number pairs:

Alpha	1 2	1 3	1 4	2 3	2 4	3 4	
Beta	1 2	1 2	1 3	2 4	3 4	3 4	(3.1)
Gamma	1 2	1 2	1 3	1 3	2 3		
Delta	1 2	1 2	1 2	1 2			

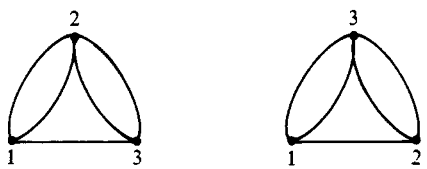


(*a*) Alpha $N = 4, B = 6$ (*b*) Beta $N = 4, B = 6$ (*c*) Gamma $N = 3, B = 5$ (*d*) Delta $N = 2, B = 4$

Figure 3. The four-star topologies of cyclomatic number 3.

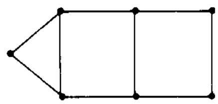
The bridge specifications (3.1) can be regarded as forming $(2B)$-tuples. We take as a *canonical description* of each topology the *minimum* $(2B)$-tuple that describes it. We assume the general conventions for the ordering of n-tuples as self-evident; a detailed treatment is given by Heap (1969, 1972). (The system of canonical descriptions we define is not the same as that used in these references.)

The descriptions (3.1) are all canonical. Any other description results in a larger $(2B)$-tuple. For example it is evident that any other ordering of the bridges in (3.1) for the gamma topology will result in a larger (10)-tuple; however the topology may be re-labelled in two other distinct ways:



which have minimum descriptions 1 2 1 2 1 3 2 3 2 3 and 1 2 1 3 1 3 2 3 2 3 respectively, both of which exceed that of (3.1). *Thus the canonical description of the topology also defines a canonical labelling.*

To describe the realization of a topology we specify the lengths of the bridges in their canonical order. When more than one specification is possible we choose the minimum. For example, the β graph:



can be specified in accordance with (3.1) in eight ways:

12	12	13	24	34	34	1 2 1 1 1 3
						1 2 1 1 3 1
						2 1 1 1 1 3
						2 1 1 1 3 1
						1 3 1 1 1 2
						1 3 1 1 2 1
						3 1 1 1 1 2
						3 1 1 1 2 1

of these the first yields the least 18-tuple and is the canonical description.

To summarize: we adopt as the canonical specification of a graph with B bridges the least $(3B)$-tuple that specifies the bridges and then their respective lengths in the same order. Under this regime isomorphic graphs have identical descriptions.

The canonical specification has the merit that it is not necessary to introduce arbitrary conventions from time to time; all that is arbitrary is introduced once for all in the definition. It is convenient for the handling of large numbers of topologies and realizations by electronic computers; it is somewhat inconvenient for hand calculations. It is useful to have simple names for the topologies with small cyclomatic number. We give the canonical description of the 17 topologies with cyclomatic number 4 in table 2.

Table 2. The star topologies of cyclomatic number 4 and their canonical descriptions

Topology	N	B	Canonical description								
A	6	9	12	13	14	25	26	35	36	45	46
B	6	9	12	13	14	23	25	36	45	46	56
C	6	9	12	12	13	24	35	36	45	46	56
D	6	9	12	12	13	24	34	35	46	56	56
E	6	9	12	12	13	24	35	35	46	46	56
F	5	8	12	13	14	15	23	24	35	45	
G	5	8	12	12	13	14	25	34	35	45	
H	5	8	12	12	13	14	23	35	45	45	
I	5	8	12	12	13	13	24	35	45	45	
J	4	7	12	12	13	14	23	24	34		
K	4	7	12	12	13	14	23	34	34		
L	4	7	12	12	13	13	24	24	34		
M	4	7	12	12	12	13	24	34	34		
N	4	7	12	12	13	13	14	24	34		
O	3	6	12	12	13	13	23	23			
P	3	6	12	12	12	13	13	23			
Q	2	5	12	12	12	12	12				

The number of topologies increases rapidly with cyclomatic number. The 118 topologies of cyclomatic number 5 have been described by Heap (1966, 1967), and the 1198 topologies of cyclomatic number 6 by Heap (1969). The number of topologies of cyclomatic number 7 is not available; we have derived all 1201 topologies with six nodes or less.

4. Construction of a star-graph list

4.1. Format

From the preceding sections the type of star-graph list required for the development of the specific heat expansion is clear; there remain some problems of format and listing and finally that of closing the list by supplying the few remaining stars of high cyclomatic number. The more common lattices that have been studied in critical phenomena fall into three groups:

(i) Close-packed lattices: triangular, face-centred cubic, close-packed hexagonal.

(ii) Loose-packed lattices: square, simple cubic, body-centred cubic.

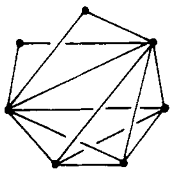
(iii) Very loose-packed lattices: honeycomb, diamond, white tin (ice) and the even more loosely-packed hydrogen peroxide and related structures.

For lattices in the first group it is a practical proposition to list and count all realizations of all topologies through r edges. For lattices in the second group only loose-packed realizations need be listed; if this is not done the number of zero lattice constants rapidly becomes prohibitively large. A loose-packed listing is still very inefficient for lattices like the simple cubic and even more so for lattices in the third group. To obtain efficient listings it is necessary to eliminate realizations whose counts must be zero because of the lattice structure. Special techniques have been developed for this purpose (McKenzie 1974b).

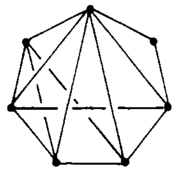
4.2.

4.2.1. Closure of the list. In compiling a list of all stars with a given number of edges (and supplemented as specified in § 3) we begin by an exhaustive enumeration of all the realizations of the possible topologies in order of ascending cyclomatic number. The procedure is limited by the fact that complete enumeration of topologies are not available beyond a certain cyclomatic number (currently 6 for all topologies, 7 for magnetic topologies and 8 for no-field topologies). Also for any fixed r the number of topologies becomes very large at the point where the number of realizations is small and the whole process becomes inefficient. For example to complete the listing of no-field graphs with $e \leqslant 14$ we need four graphs of cyclomatic number 8. These can be found by searching through the 119 topologies; it is more convenient to exploit the fact that such graphs have only seven points and must occur in lists of stars grouped by vertices. We describe the technique in the next sub-sections.

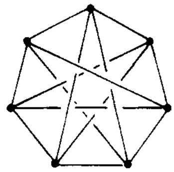
4.2.2. No-field graphs $e \leqslant 14$. We have illustrated in the appendix all the no-field topologies through cyclomatic number 7. To find all the remaining graphs we have used the seven-point stars in the seven-point graph list of F Harary and D W Crowe (1953, distributed privately), as corrected by Heap. Drawings of all the stars in the list have been published by Hoover and de Rocco (1962). A graph of 14 edges and cyclomatic number 8 must have seven points; there are 59 possible stars in the list. Inspection reveals that only 4 are no-field and they correspond to four distinct topologies:



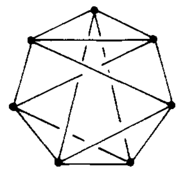
$w_{14} = 96$



$w_{14} = 80$



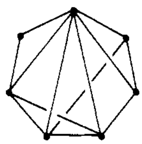
$w_{14} = 56$



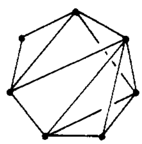
$w_{14} = 48$

None of these can be embedded in the face-centred cubic lattice. Finally there is only one star with 14 edges and cyclomatic number 9; it is hypermagnetic: the no-field list is closed.

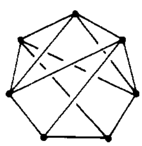
4.2.3. Magnetic graphs $e \leqslant 13$. The magnetic graphs are required up to $e \leqslant 13$; we have a complete listing of topologies of cyclomatic number 6 and we must supplement this. There are 81 possible stars with 7 vertices and 13 edges; 17 of these are first category magnetic. Only 4 of these 17 are embeddable in the face-centred cubic lattice:



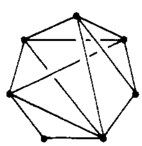
$w_{14} = 24$



$w_{14} = 24$

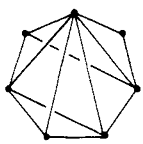


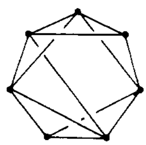
$w_{14} = 20$

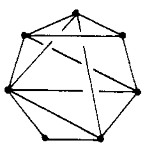


$w_{14} = 40$

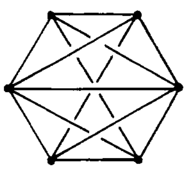
There are only 3 other magnetic graphs with 13 edges embeddable in the face-centred cubic lattice, all second category:







There are only two graphs of cyclomatic number 8 with 13 edges; only one is (first category) magnetic:



$w_{14} = 64$

It is not embeddable in the face-centred cubic lattice. The magnetic list is closed.

4.2.4. Hypermagnetic graphs $e \leqslant 12$. It remains to find any hypermagnetic graphs of cyclomatic number greater than or equal to 7 with $e \leqslant 12$. There are only five stars of 12 edges with cyclomatic number 7; two of these are hypermagnetic but they are not embeddable in the face-centred cubic lattice. There are no graphs of cyclomatic number 8 with 12 edges. The hypermagnetic list is closed and the star list should be complete.

4.2.5. Loose-packed listing. To close a list appropriate to a loose-packed lattice the same general principles apply; however larger values of r are accessible and no adequate list of loose-packed stars grouped by vertices is available. We have therefore used the general techniques proposed by Sykes *et al* (1966) and resorted to listing stars with strong embeddings to close the loose-packed list. In fact for the simple cubic lattice at $r = 18$ there are no stars of cyclomatic number greater than 6 required for a_r.

5. Summary and conclusions

We have studied the star-cluster expansion for the zero-field specific heat of the Ising model above the Curie temperature; explicitly we have examined the problem of determining the coefficients in the expansion for the configurational free energy in zero field (on which the specific heat depends).

We have developed a general method for the classification of stars together with a canonical description of their topologies and realizations. A study of the general properties of the weights has led to a format for a star list suitable for the derivation of successive coefficients a_r (no-field stars to $e \leqslant r$, magnetic stars to $e \leqslant r-1$, hypermagnetic stars to $e \leqslant r-2$). From such lists the series given in I and II were derived.

We have recently extended the expansion for the simple cubic lattice to $r = 20$ (unpublished) at which order more than 5000 stars contribute to the final coefficient. It should prove possible to add more coefficients to all the lattices studied previously, using the general approach we have described. There remains, for projects of this magnitude, the problem of verifying in some independent way that the lists are complete. We shall describe one such method in a subsequent paper.

Acknowledgments

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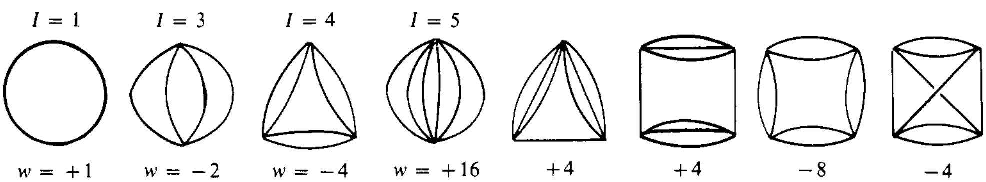
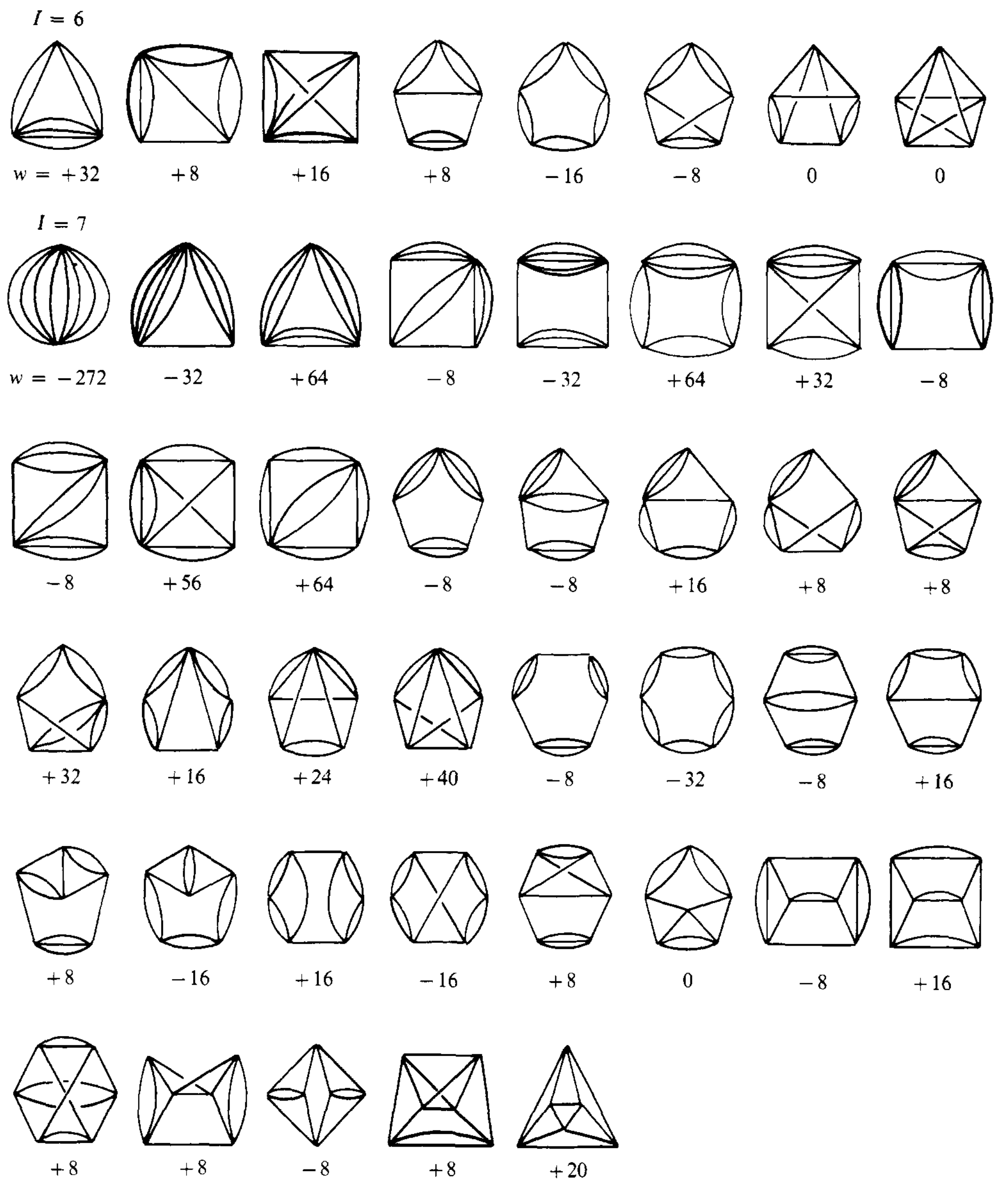
Appendix. The 53 no-field topologies of cyclomatic number (I) $\leqslant$ 7 and their primary weights (W)





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