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Extension of the high-temperature, free-energy series for the classical vector model of ferromagnetism in general spin dimensionality

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Abstract. In this paper we present the results of a study of the free energy and specific heat of the classical vector model of ferromagnetism. High-temperature series for the free energy are presented as far as the 12th term in general spin dimensionality (D) and the 13th term for the case $D = 3$. The techniques used to derive these series are discussed in some detail. The general series is shown to reduce to that for the Ising Model for $D = 1$, and to agree with the expansion of the exact result for the spherical model for the case $D = \infty$. The cases $D = 2$ and $D = 3$ correspond to the classical planar and classical Heisenberg models, respectively. We demonstrate that our general series reproduces previous results for both of these models, with the exception of a small disagreement with the calculated 11th terms of Ferer *et al* (1971, 1973). In addition, our general series extends the series for each of these models by one term, and our independent work for $D = 3$ provides one further term. We present the results of a ratio analysis of the series for $D = 2$ and $D = 3$, comparing previous work with our additional results. Although we are able to make predictions of both the critical point and the critical exponent, we conclude that further terms for the susceptibility series are required in order to refine the estimate of the critical point. We compare our estimate of the exponent α for $D = 2$ with the determination (Mueller *et al* 1976) of the exponent α for the λ transition in liquid helium II, finding striking agreement.

I. Introduction

The classical vector (n vector or D vector) model of ferromagnetism has been widely studied (Domb 1972, Stanley 1974). The model consists of D-dimensional spins arranged on a lattice, interacting according to the Hamiltonian

$$\mathcal{H} = -J \sum_{ij} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j - mH \sum_i \sigma_{z_i} \tag{1.1}$$

where J is the interaction energy, m the magnetic moment of a spin, H an external magnetic field, and the scalar product $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$ is taken in D dimensions.

It is noted that the dimensionality referred to in the present work is distinct from the dimensionality (commonly denoted in the literature by d) of the lattice on which the spins are situated. In the present work, we are considering general D, but restrict

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ourselves to the FCC lattice, which has $d = 3$, although the work could easily be further generalised. Extension to other lattices having $d = 2$ and $d = 3$ is currently being undertaken.

In this paper we present formulae for the free energy and specific heat in zero field of the general-D classical vector model, as a power series in $K \equiv J/k_B T$ on the FCC lattice. The coefficients in the series are functions of D. Our series extends as far as K^{12}, and we demonstrate that, as expected, the series reduces to that for the Ising model for $D = 1$, to that for the classical planar model for $D = 2$, to that for the classical Heisenberg model for $D = 3$ and to that for the spherical model (Joyce 1972) for $D \to \infty$. The series for $D = 2$ and 3 had previously been obtained as far as the 11th terms (Ferer *et al* 1971, 1973). We calculate the first 13 terms for $D = 3$ independently as a check on our general formula.

We also present here a preliminary analysis of our series for $D = 3$ and for $D = 2$. The simple ratio analysis of the specific heat now seems to be consistent with the analysis of the much shorter but smoother susceptibility series. In addition, we find that with the extra terms we are able to revise the estimates of the critical exponent α. In predicting α we employ biased procedures in which we use the values of the critical point estimated by the above authors from the short susceptibility series. Among other things we conclude that, before any further refinement of the estimates of the critical parameters is possible, it will be necessary to extend the susceptibility expansions. However, once this is done and a more precise value of K_c is available, the present specific heat series will probably produce more accurate values for α. Work on the susceptibility series is in progress and we shall report on it in the near future.

2. Graph terminology

Since the analysis uses graphical techniques, it is convenient to define at this point some of the terms used. The terminology is largely due to Sykes *et al* (1966).

A *graph* is a series of bonds (representing interaction variables) joining points (characterised as *nodes* or *antinodes* according to whether there are more than two or precisely two bonds leading from the point to other points in the graph, respectively). With each bond is associated a multiplicity. These different multiplicities of bonds correspond to different interaction variables between the spins in question. Multiplicity of a bond is represented in a graph diagram by multiple lines between the corresponding spins (i.e. lattice points).

It is convenient to classify and treat graphs according to *topology*. The topology to which a graph belongs may be determined by: (i) reducing the multiplicity of all bonds to unity and (ii) suppressing all antinodes.

Therefore, a topology consists only of nodes, and single lines representing the paths or *bridges* joining the nodes. A *realisation* of a topology is a graph with zero or more antinodes inserted along the bridges. Figure 1(a) illustrates a topology (the α) and figure 1(b) shows a specific realisation of this topology.

It is convenient to define a *bonding* of a topology which is obtained by assigning a specific multiplicity to each bridge. It may be represented by drawing the specified number of lines along each bridge of the topology. It is the property of all graphs with which we are concerned that both bonds meeting at an antinode must have the same multiplicity (see figure 1(c)). For most of our calculations it is convenient to assign a distinct interaction variable, say K_a, to each bridge. A bridge of multiplicity r cor-

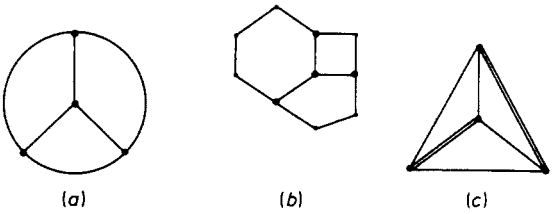


Figure 1. (*a*) The α topology; (*b*) realisation of the α topology; (*c*) bonding of the α topology.

responds to a variable $w_r(K_a)$ where

$$w_r(K_a) = \frac{I_{(D/2)+r-1}(K_a)}{I_{(D/2)-1}(K_a)} \tag{2.1}$$

and where the I's are modified spherical Bessel functions. The relations between the various w_r variables and the rules for determining which bondings of a given topology contribute to the series at a given order are explained by Domb (1976).

3. Computational techniques

We calculate the free energy as

$$F = -k_B T \ln Z \tag{3.1}$$

where Z is the partition function, defined as usual by

$$Z = \sum_{\text{spins}} \exp(-\mathcal{H}/k_B T). \tag{3.2}$$

Our expansion for Z is the star cluster expansion (see for example Domb 1974, Sykes and Hunter 1974) in which only multiply connected or star graphs need be considered. The expansion has the form (Domb 1972)

$$\ln Z = \sum_n a_n w^n \tag{3.3}$$

where

$$w \equiv w_1 = I_{D/2}(K)/I_{(D/2)-1}(K). \tag{3.4}$$

In the notation of Domb (1972) we write the coefficients a_n in the form

$$a_n = \sum_{\substack{l \leqslant n \\ x,y}} g_{ly} p_{lx} \tag{3.5}$$

where p_{lx} is the number of ways of embedding a particular star graph x, having l lines, in the lattice (i.e. the weak lattice constant of x) and g_{ly} is a *weight function* depending primarily on the bonding y of the topology to which x belongs. The g_{ly} have a simple dependence on the lengths of the bridges in x, but the non-trivial coefficients or *intrinsic weights* in g_{ly} depend only upon the bonding of the topology and the sub-topologies into which it can be decomposed and not upon the realisation x. Thus equation (3.3) contains an implied sum over all topologies. For each topology it is necessary to sum over all bondings (subject to the restrictions discussed below) and over all realisations of

each bonding. We shall henceforth refer to a particular realisation of a particular bonding of a topology simply as a graph.

The lattice constants, which are independent of D, are well known, having been calculated by Sykes *et al* (1967, 1972) in their work on the Ising model. It is, therefore, only necessary to calculate the weight functions g_{ly}.

A particular graph will contribute to the expansion (3.3) only at order n and above, where n is the total number of lines in the graph. Consider, for example, the three graphs shown in figure 2. Graphs (a) and (b) are different bondings of the same realisation of the θ topology. Graphs (a) and (c) are different realisations of the same bonding of the θ topology. These three graphs will begin to contribute to the series (3.3) at order 6, 9 and 10 respectively. Since free energy graphs must correspond to overlaps of polygons (Domb 1972) and since the smallest polygon is the triangle, a graph with a quintuply bonded bridge cannot occur until order 15. Therefore, in our calculations we need consider only bondings with multiplicities up to 4, since the present work extends only to order 13.

Although, in the final analysis, we naturally wish the reduced interaction strength K to be the same between all pairs of nearest neighbours, it is convenient, as a calculational artifice, to assume that the interaction along each *bridge* of a topology is unique. (Recall that a bridge is a path joining two nodes.) For example, in figure 2(c) the interactions along the three bridges a, b, c of the theta graph may be labelled K_a, K_b, K_c. Once this has been done, all the intrinsic weights for a given bonding can be expressed in the same form—for the bonding of figure 2(c) this has the form

$$(c_{121})_\theta w_1(K_a) w_2(K_b) w_1(K_c). \tag{3.6}$$

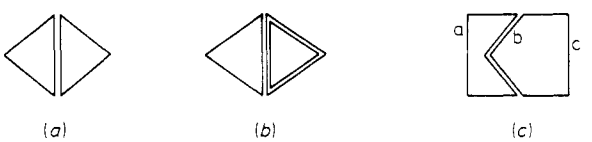


Figure 2. Examples of θ graphs.

By using the techniques described below, it was possible to obtain the weights for all bondings required in the free energy to order 13. The final step in the calculation was then the replacement of the $w_r(K_a)$ etc. with one w_r factor for every line in the bridge. Thus the graph of figure 2(c) contributes

$$(c_{121})_\theta w_1^6(K) w_2^2(K) \tag{3.7}$$

which is further simplified by substituting for $w_2(K)$ in terms of $w(K)$ defined in (2.1).

In the next section we shall consider methods of obtaining the intrinsic weights and hence the weight functions g_{ly}. For simplicity we will refer to the intrinsic weights as the *weights*.

4. Weight determination

The weights may be divided into three classes, according to the relative ease with which they may be obtained. The easiest of all are for the so-called ladder topologies, which may be obtained from simpler topologies by the replacement of a single interaction by a

pair of parallel interactions. An example is shown in figure 3. Domb (1972, 1976) has shown that the weight of such a ladder topology may be obtained simply by multiplying the weight of the root topology by a coefficient which is a simple function only of the spin dimensionality D. By starting from the known weights for the polygon (Bowers 1968), it is possible to generate, by successive ladderings, the vast majority of the weights which are required.

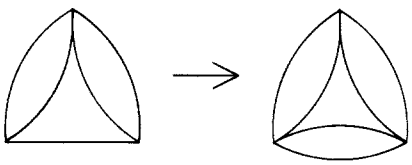


Figure 3. Example of ladder technique.

The problem of performing the ladder transformation lends itself easily to automation, provided only specific numerical results for a given value of D are required. A given bond in the topology to be laddered is chosen and the weight of each bonding of the new topology formed by laddering each bonding of the old topology is generated and stored in some suitable format. We note that a given bond can actually be laddered in three distinct ways, since in drawing a topology, vertices of degree two are suppressed. (See figure 4.)

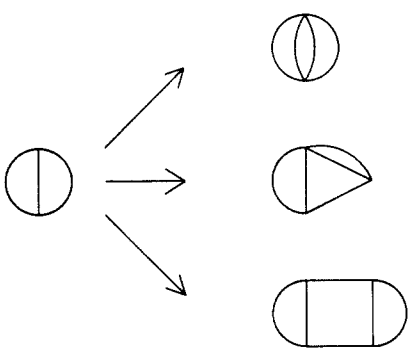


Figure 4. The three types of ladder.

To obtain the weights for general D, it is necessary to perform the explicit algebraic manipulations. We found that a preliminary computer laddering of each topology for $D = 3$ was invaluable in helping us to identify every one of the large number of bondings contributing to the free-energy series.

A calculation of the contribution of a specific graph using the ladder transformation is given in appendix 1. Clearly a necessary condition for a topology to be amenable to treatment by the laddering technique is the presence within it of a 'bubble' (two bridges having common nodes as endpoints).

Certain topologies do not contain such a bubble and to obtain the weights of such topologies it is necessary to devise other methods. Domb (1972, 1976) has shown that the weights for many such topologies can be obtained by considering the effect of

allowing the interaction along one bridge to become infinite. This will cause the two vertices at the end of this bridge to coalesce, forming a bonding of a different topology with the same cyclomatic index. Further, the weight of the new configuration so obtained must be equal to the sum of the weights of all bondings of the original topology in which the multiplicity of the bridge to be coalesced varies from zero to infinity, and the multiplicity of all the other bridges remains constant. However, as noted above, the free-energy weight of any graph which does not correspond to an overlap of polygons is zero, and this will eliminate most of the terms in the aforementioned sum.

Consider, for example, the bonding of the α topology shown in figure 5(a). To obtain its weight, we allow the interaction along the bridge labelled 'ab' to become infinite. This yields the γ bonding shown on the left-hand side of figure 5(b), whose weight can be obtained by laddering the θ graph (see figure 4). We equate this to the sum on the right-hand side in which term one is a θ graph (the broken line implying zero multiplicity), term three is the required weight, and term two and all terms higher than three have zero weight because of the 'polygon overlap' rule.

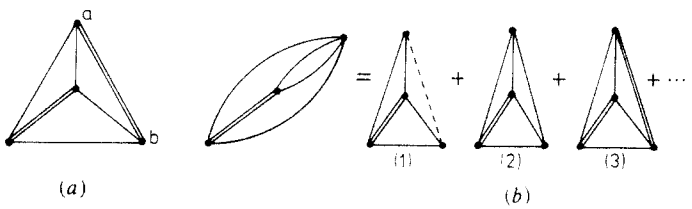


Figure 5. The infinite bond technique: (a) bonding whose weight is required; (b) symbolic equation produced by making bond ab infinite.

In most cases it was possible to obtain an equation involving only one unknown by using this 'infinite bond' technique. By this means the weights of the majority of bondings for non-ladder graphs were obtained. In addition, each non-ladder weight, once obtained, allowed several more weights to be calculated by using the ladder technique again. Figure 6 shows a J graph which can be obtained by laddering an α.

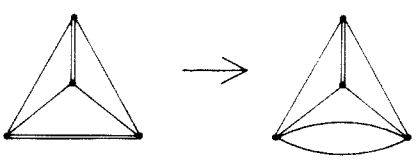


Figure 6. Derivation of J graph by laddering α.

Three bondings were found whose weights could be obtained neither by laddering nor by the 'infinite bond' method. These bondings, shown for reference in figure 7, possess such high symmetry that any attempt to use the 'infinite bond' technique leads to a situation in which the number of unknowns is greater than the number of equations. A third approach has been devised to determine these weights (Domb 1976). This method is demonstrated in appendix 2 using the highly symmetric 'octahedron' topology (figure 7(b)).

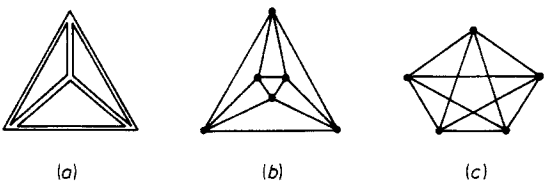


Figure 7. Bondings whose weights cannot be obtained by either the laddering or the infinite bond technique: (*a*) the (222222) α; (*b*) the (singly bonded) octahedron; (*c*) the (singly bonded) complete graph on five points.

5. Generation of the series

The combination of the weights and the lattice constants to obtain the series of equation (3.3) presents a non-trivial problem since each particular graph will contribute with a given weight (depending only on the bonding) but with a particular combination of the w variables (depending on the realisation), as discussed in § 2. In performing computer calculations for a specific value of D, these problems are easily overcome by storing the *weight* in a multidimensional array, and using the power of the various w variables at which it will contribute as the coordinates of the weight within the array. In performing calculations for general D, however, such an approach is not feasible since the weight to be stored is not a number, but an algebraic expression. For example, the contribution to the partition function from the particular θ graph shown in figure 2(*b*) is

$$(\text{lattice constant}) \times \tfrac{1}{2}D^2(D-1)w_1^2 w_2^2 w_3. \tag{5.1}$$

Using the expressions for w_2 and w_3 as functions of w_1 given by Domb (1972) the first contribution of this graph will be:

$$\text{l.c.} \times \tfrac{1}{2}D^2(D-1)[D^2/(D+2)^2][D^2/(D+2)(D+4)]w_1^9. \tag{5.2}$$

Since w_2 and w_3 are actually power series in w_1, there will also be contributions from this graph at higher powers of w_1. A further complication arises since the free energy is proportional to the *logarithm* of the partition function (Z) rather than Z itself. To obtain the contribution to ln Z from a given bonding, i.e. the weight function g, given its contribution to Z, it is necessary to allow for the contributions from all possible combinations of simpler graphs into which the bonding can be decomposed. A typical decomposition is shown in figure 8. Thus, returning to the graph of figure 2(*b*), its

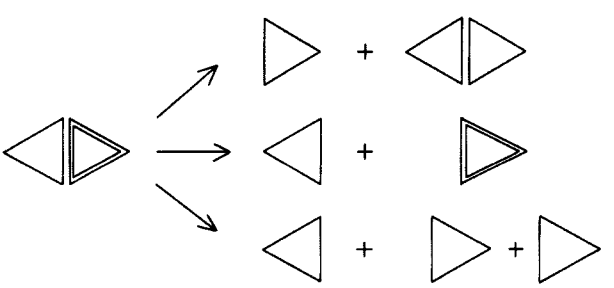


Figure 8. Example of decomposition of a bonding.

contribution to $\ln Z$ is:

$$(\text{l.c.})\left\{\frac{D^2(D-1)}{2}w_1^2w_2^2w_3+\tfrac{1}{3}(3)D^3w_1^9-\tfrac{1}{2}(2)D^2(D-1)w_1^7w_2\right.$$
$$\left.-\tfrac{1}{2}(2)\frac{D(D+2)(D-1)}{2}w_1^3w_2^3\right\}. \tag{5.3}$$

The four terms in expression (5.3) refer respectively to the θ bonding itself, the overlap of three triangles (note the presence of the $\frac{1}{3}$ factor from the logarithm expansion and the combinatoric factor of 3), the overlap of a triangle with the simpler (121) θ bonding, and the overlap of a singly bonded and a doubly bonded triangle.

As was the case in the previous calculations, for a specific value of D it is relatively easy to keep track of the contributions from the various graphs, on a computer, but for general D, unless one is in possession of a program which will allow manipulation of rational fractions of polynomials, it is necessary to perform the calculations manually. In the course of a manual calculation, it would be very easy to neglect one or more terms. For this reason, when performing the general D calculations, use was made of the computer results for $D = 3$ to obtain a list of all terms contributing to the series. The algebraic manipulations required to obtain the free-energy series were then performed manually on each term. It was originally felt that, due to the complexity of the mathematics, extension of the general D series beyond w_1^{12} would not be a feasible proposition. However, the authors have recently come into possession of computer programs (J L Martin, private communication; E W Grundke, private communication) which will enable the algebra to be performed automatically, and will be in a position to report the general form of the 13th term in the series shortly.

The free-energy series obtained by the methods described above is presented in table 1. Substitution of $D = 1$ yields the Ising model results (Sykes *et al* 1967) whilst $D = 2$ and $D = 3$ yield agreement with previous results for the classical planar model (Bowers and Joyce 1967, Ferer *et al* 1973) and the classical vector model (Ferer *et al* 1971, Gerber 1975) respectively.

We note that the denominator of the nth term in the series appears to take the general form

$$n\prod_{j=1}^{J}(D+2j-2)^{\mathrm{INT}(n-j)/j} \tag{5.4}$$

where $J \equiv \mathrm{INT}(n/2)$.

We present this form, which appeared as an empirical result of our calculations, as an hypothesis. It has been checked against the Sykes *et al* (1972) exact series for the Ising model, and was used to check our computer calculations for $D = 3$. It may be of use to future workers, if only to check the accuracy of their work.

6. Analysis and discussion for $D = 2$

Our calculation of the series in general D represents an extension of the general case by three terms (Stanley 1974). However, for the specific case $D = 1$ the series is already known to 14th order, while for the cases $D = 2$ and $D = 3$ our work provides one additional term.

Table 1. The first twelve terms in the high-temperature, free-energy series for the classical vector model on the FCC lattice.

	Coefficient of K^n—numerator.			
	Power of D			
n	0	1	2	3
2	6	—	—	—
3	24	—	—	—
4	264	126	—	—
5	1680	720	—	—
6	93120	104496	37368	4272
7	690816	735840	244944	26208
8	64617984	108435072	69058752	20823888
9	2083110912	3913860096	2925688320	1115272128
10	275425689600	676673310720	698049484800	394070319360
11	2321270341832	5597656289280	5648977010688	3107553960192
12	9541484795658240	32290078258888704	48532763592818688	42793815565025280
n	4	5	6	7
8	2996340	165294	—	—
9	230261856	24581568	1065120	—
10	133158505728	27647463264	3456505344	238638120
11	1019062454784	204634856448	24689231424	1643689872
12	24642176360239104	9764353972598784	2732299175361024	544738087572480
n	8	9	10	11
10	6980904	—	—	—
11	46392192	—	—	—
12	76918509345408	7514107489152	482781787392	18340982400
n	12			
12	311886144			

Denominator: $n \prod_{j=1}^{J} (D+2j-2)^{\mathrm{INT}(n-j)/j}$, where $J \equiv \mathrm{INT}(n/2)$.

In this paper we present only a preliminary analysis of our specific heat series for the two cases $D=2$ and $D=3$. Our general series, when evaluated for $D=1$, exactly reproduces the first 12 terms of the Ising model specific heat series of Sykes *et al* (1972), the analysis of which is quite complete. Our series also agrees exactly with the expansion of the exact solution of the spherical model (Berlin and Kac 1952, see Joyce 1972 for the expansion).

For $D=2$ the first nine terms of our series agree exactly with the specific heat series for the classical planar model calculated by Bowers and Joyce (1967) who also calculated eight terms of the susceptibility (χ) series. The 10th term of our series agrees exactly with the 10th term calculated by Ferer *et al* (1973). However, the 11th term of our series is in slight disagreement with theirs, the discrepancy occurring in the 11th significant figure. A discrepancy of this relative magnitude will not affect the conclusions one is able to draw from the standard methods of series analysis.

Bowers and Joyce estimated the critical temperature to be

$$K_c^{-1} = \frac{kT_c}{J} = 4{\cdot}823 \pm 0{\cdot}003$$

based on the analysis of their eight-term susceptibility series. Using that value of K_c they then estimated the specific heat exponent α to lie in the range

$$0 \leqslant \alpha < \tfrac{1}{32}.$$

Ferer *et al*, with two additional terms in both χ and C_H, estimated

$$K_c^{-1} = 4{\cdot}820 \pm 0{\cdot}003$$

$$\alpha = -0{\cdot}02 \pm 0{\cdot}03.$$

The reason for the rather significant shift in the ranges estimated for α is easily seen from the plot of the sequence α_n against $1/n$ in figure 11. The rapid change in slope around $n = 9$ suggests that the series was rather slow in settling down to its asymptotic behaviour. Indeed, one may well ask whether it has settled down by order 12!

In table 2, we present the series coefficients b_n for the free energy

$$F = -kT \ln Z = \sum_{n=2}^{\infty} b_n K^n \tag{6.1}$$

and a_n for the specific heat

$$C_H = kK^2 \frac{\partial^2}{\partial K^2} \ln Z = \sum_{n=2}^{\infty} a_n K^n. \tag{6.2}$$

We also tabulate the ratios

$$r_n = a_n / a_{n-1}, \tag{6.3}$$

the extrapolants

$$e_n = nr_n - (n-1)r_{n-1} \tag{6.4}$$

Table 2. Series coefficients and ratio analysis for $D = 2$ classical vector model free energy and specific heat.

n	b_n	a_n	r_n	e_n	α_n
2	1·5	3·0	—	—	—
3	2·0	12·0	4·0000	—	0·48963
4	4·03125	48·375	4·0313	4·1250	0·34544
5	9·75	195·0	4·0310	4·0300	0·18154
6	26·35416	790·625	4·0545	4·1719	0·04708
7	77·9375	3273·375	4·1402	4·6547	0·01279
8	247·1749269	13841·7958933	4·2286	4·8471	0·01843
9	825·9226707	59466·4322916	4·2962	4·8365	0·02186
10	2872·238384	258501·4546875	4·3470	4·8048	0·01870
11	10310·834928385	1134191·84212235	4·3876	4·7931	0·01312
12	37990·74045	5014777·739598253	4·4214	4·7942	0·00777

of successive pairs of ratios on a $1/n$ plot to the intercept $1/n = 0$, and the sequence of estimates

$$\alpha_n = nr_nK_c - n + 1 \tag{6.5}$$

for the critical exponent α of the specific heat. Using the well-known ratio method (Hunter and Baker 1973), if the series (6.2) represents a function which is singular at $K = K_c$ with an asymptotic form

$$C_H \approx A(1 - K/K_c)^{-\alpha}, \tag{6.6}$$

then the ratios of successive coefficients

$$r_n = a_n/a_{n-1} = [1 + (\alpha - 1)/n]K_c^{-1} \tag{6.7}$$

when plotted against $1/n$ should tend to the limit K_c^{-1} with a limiting slope $(\alpha - 1)/K_c$. The slopes of consecutive line segments of a $1/n$ plot could be used to find an 'unbiased' sequence of estimates for α, but if a reliable estimate of K_c is known, the sequence (6.5), which gives the slope of the line segments joining each successive point r_n to the predicted intercept K_c^{-1}, is a more rapidly converging sequence. It is 'biased' in the sense that this sequence, and hence predictions based upon it, depends upon the choice of K_c.

The sequences r_n and e_n for $D = 2$ are plotted in figure 10. The corresponding results for the Ising model ($D = 1$) are shown for comparison in figure 9. The new term for the specific heat shows the necessary change in sign of the slope in the e_n plot which indicates that the specific heat is beginning to settle down and show some compatibility with the Ferer *et al* prediction for the critical point based on the susceptibility expansion. The oscillation or bump in the extrapolant plot is probably caused by contributions from the next-strongest singularities. Padé analysis indicates that there is

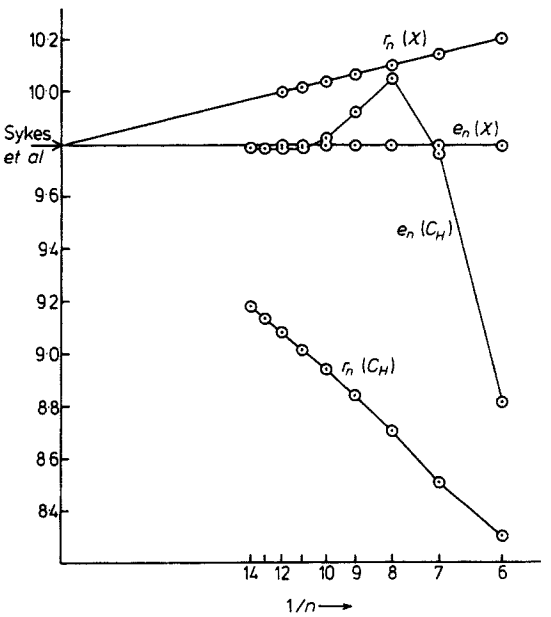


Figure 9. Ratio analysis: $D = 1$ classical vector model (Ising) specific heat.

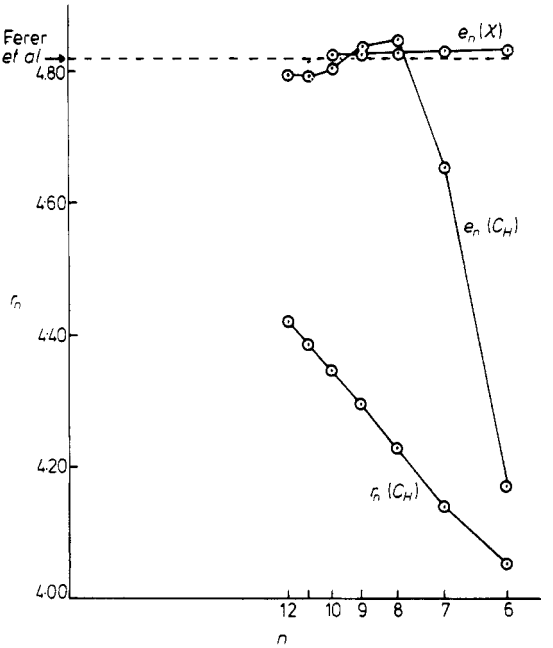


Figure 10. Ratio analysis: $D = 2$ classical vector model (classical planar) specific heat.

a pair of complex singularities near the imaginary axis at about $\pm 0{\cdot}3i$. Attempts to transform the series, so that the interfering singularities are even further from the origin, successfully remove the bump but leave sufficient curvature in the r_n and e_n plots that accurate extrapolation is difficult.

The sequence α_n is plotted in figure 11. It is quite significant that the new point indicates a straightening of the α_n plot. There would now seem to be even stronger evidence that α is small but negative—substantially in agreement with the Ferer *et al* prediction. However, using their value of $K_c^{-1} = 4{\cdot}820$ our conclusion would be that α is closer to $-0{\cdot}05$. We find it hard to believe that the data are any longer compatible

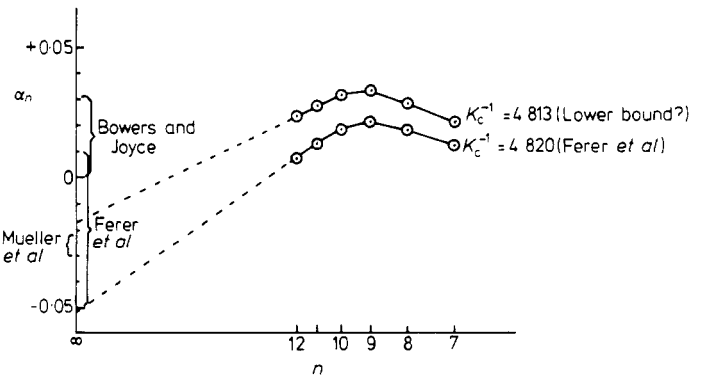


Figure 11. Sequence of biased estimates α_n for critical exponent: $D = 2$ (classical planar model).

with a logarithmic singularity and would suggest that

$$\alpha = -0{\cdot}05 \pm 0{\cdot}03$$

where the confidence limits might be over-optimistic. Further extension of the susceptibility series and refinement of K_c would be essential before a more definitive statement could be made. We find both the Ferer *et al* result and our own additional term in striking agreement with the Mueller *et al* (1976) determination of the exponent α at the λ point in liquid helium II, namely

$$\alpha = -0{\cdot}026 \pm 0{\cdot}004.$$

This agreement between an experiment on liquid helium and a classical model is an impressive piece of evidence in favour of universality. Betts and Lothian (1973) have shown that liquid helium and the XY models (both quantum and classical) fall into the same universality class—i.e. $D = 2$, $d = 3$.

Padé approximant analysis of the specific heat series is quite indeterminate, as indeed was the case for the Ising model (Hunter 1969). Once again we find evidence that the Padé approximants of the second derivative of the specific heat series are much better behaved than those for the undifferentiated series, again suggesting that the additive terms in the form of the specific heat function are much more important than in the case of the susceptibility (Hunter 1969). However, we regard the ratio analysis as far more significant for our specific heat series.

7. Analysis and discussion for $D = 3$

In table 3 we present the series coefficients for the free energy and specific heat, along with the specific heat ratios and extrapolants and the sequence of estimates α_n for the critical exponent, for the classical Heisenberg model ($D = 3$).

The first ten terms of our series again agree exactly with those of Ferer *et al* (1971), but we again find a discrepancy in the 11th significant digit of the 11th term. The 12th

Table 3. Series coefficients and ratio analysis for $D = 3$ classical vector model free energy and specific heat.

n	b_n	a_n	r_n	e_n	α_n†
2	1·0	2·0	—	—	—
3	0·88$\dot{8}$	5·3$\dot{3}$	2·666$\dot{6}$	—	0·51944
4	1·188$\dot{8}$	14·26$\dot{6}$	2·6750	2·7000	0·36975
5	1·8962$\dot{9}$6$\dot{2}$	37·925$\dot{9}$2$\dot{5}$	2·6584	2·5918	0·18599
6	3·363762490	100·91287478	2·6608	2·6729	0·02777
7	6·506478540	273·2720987	2·7080	2·9913	−0·03019
8	13·47476733	754·5869738	2·7613	3·1344	−0·04306
9	29·3907834	2116·136405	2·8044	3·1489	−0·05140
10	66·72564152	6005·307737	2·8379	3·1394	−0·06271
11	156·4127372402	17205·4090964	2·8650	3·1367	−0·07487
12	375·9299983	49689·48541	2·8880	3·1408	−0·08572
13	926·2679992	144497·8079	2·9080	3·1480	−0·09429

† Assuming $K_c^{-1} = 3{\cdot}1753$.

term, calculated from our general formula and independently by computer, is new, and the 13th term, at present obtained only by computer, is also new.

Bowers and Woolf (1969), on the basis of their eight-term susceptibility series, estimated

$$K_c^{-1} = 3{\cdot}18016 \pm 0{\cdot}00007$$

and then used this to estimate a specific heat exponent:

$$-\tfrac{1}{8} \leqslant \alpha \leqslant -\tfrac{1}{16}.$$

Ferer *et al* (1971), with their longer series, estimated

$$K_c^{-1} = 3{\cdot}1753 \pm 0{\cdot}0020,$$

from which they obtained a graphical estimate of

$$\alpha = -0{\cdot}14 \pm 0{\cdot}06$$

for the critical exponent.

Figure 12, which is analogous to figure 10, shows the sequences r_n and e_n for $D = 3$, along with the corresponding quantities from the ten-term susceptibility series of Ferer *et al.* Our two extra points again show a change in sign of the slope of the e_n plot, suggesting that, as in the case of $D = 2$, the series is beginning to settle down and show some compatibility with the Ferer *et al* susceptibility prediction.

The sequence α_n is plotted in figure 13. Using the Ferer *et al* prediction of $K_c^{-1} = 3{\cdot}1753$, we again observe a straightening of the α_n plot, and note that it is now pointing to a value of $\alpha = -0{\cdot}204$. If we use instead the value $K_c^{-1} = 3{\cdot}167$, suggested by χ extrapolants of figure 12, we obtain an estimate

$$\alpha \approx -0{\cdot}148,$$

closer to the Ferer *et al* prediction.

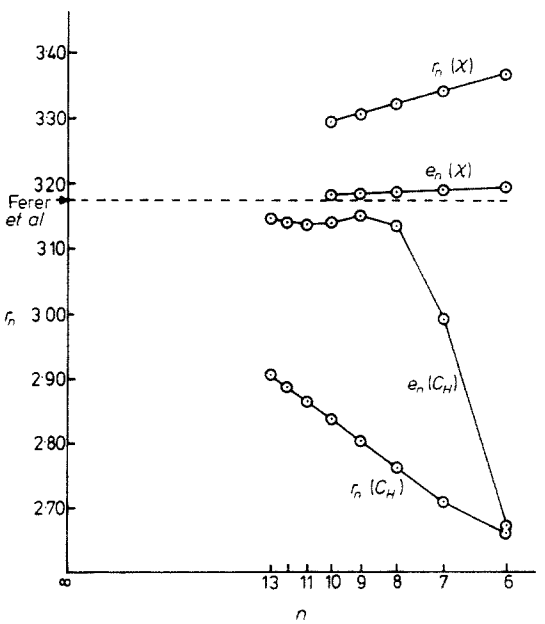


Figure 12. Ratio analysis: $D = 3$ classical vector model (classical Heisenberg) specific heat.

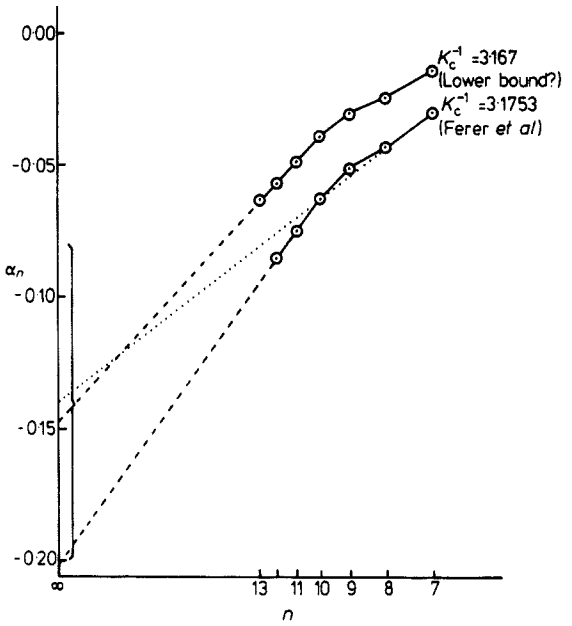


Figure 13. Sequence of biased estimates α_n for critical exponent: $D = 3$ (classical Heisenberg model).

This value of K_c^{-1} is probably a lower bound. It is drawn by a linear extrapolation of the χ extrapolant curve, and since this curve might reasonably approach the $(1/n = 0)$ axis with zero slope (Hunter and Baker 1973) we would expect the actual intercept to be a little higher.

It is clear that a more accurate estimate of the critical point is required. We again require further extension of the susceptibility series.

8. Conclusions

Our analysis for the classical planar and classical Heisenberg model series indicates that both of these series appear to be beginning to settle down by the 12th term. In both cases, the plots of the α_n sequences appear to be approaching straight lines. Work on the 13th term of our general series is almost complete, and this will enable us to add an extra point to the graphs for $D = 2$, as well as providing a useful check on our computer results for $D = 3$.

However, it has become evident that any further extension of the specific heat series will be of limited value until a better estimate of the critical point is available. This will be obtainable if the better behaved series for the susceptibility can be extended. Work is presently in progress on the susceptibility series. We hope to extend this series at least to order 12 for the cases $D = 2$ and $D = 3$.

Although the series presented in table 1 is general in D, its applicability is limited to a specific lattice—the FCC lattice. However, now that we have obtained the weights g_{iy} of equation (3.5) it is a simple matter to derive the corresponding series for any other lattice provided only that the lattice constants p_{ix} are known. We are currently in the

process of extending the present work to a number of other lattices, of lattice dimensionality $d = 2$ and 3, and will report the results shortly. The susceptibility series for these other lattices will also be presented.

Appendix 1. Calculation of the contribution of a specific graph

Consider the graph shown in figure A1(a). By removing the antinodes, we see that it is a realisation of the (121) bonding of the θ topology (figure A1(b)).

Figure A1. (a) The θ graph whose weight is calculated in the appendix; (b) the topology of which this is a realisation.

To determine the contribution of this graph, we require:

(1) the lattice constant of the θ realisation consisting of three bridges of lengths 1, 2 and 3. This is 384 (Sykes *et al* 1967, 1972);

(2) the weight of the (121) bonding of the θ topology.

We obtain the weight by noting that the given bonding can be obtained from the doubly bonded polygon by means of the ladder transformation. The polygon weight is $(D+2)(D-1)/2$ (Bowers 1968) and the relevant transformation coefficient is $d_{11}^{(2)}$, in the notation of Domb (1976), which has the value

$$d_{11}^{(2)} = 2D/D + 2.$$

The weight of the (121) theta bonding is thus

$$(c_{121})_\theta = (c_2)_{\text{polygon}} \times d_{11}^{(2)} = D(D-1).$$

The contribution to the partition function from any realisation of this θ bonding is thus, from equation (3.6),

$$\text{lattice constant} \times D(D-1) w_1(K_a) w_2(K_b) w_1(K_c).$$

For the specific realisation under consideration, bridge a contains three interactions, bridge b contains one, and bridge c, two. We therefore identify:

$$w_1(K_a) \rightarrow w_1^3(K)$$
$$w_2(K_b) \rightarrow w_2(K)$$
$$w_1(K_c) \rightarrow w_1^2(K)$$

so the contribution from this particular graph is

$$384\, D(D-1) w_1^5(K) w_2(K).$$

We now note from equation (3.4) (see, for example Abramowitz and Stegun 1964) that

$$w_1(K)=\frac{K}{D}-\frac{K^3}{D^2(D+2)}+\frac{2K^5}{D^3(D+2)(D+4)}-\cdots$$

and

$$w_2(K)=\frac{K^2}{D(D+2)}-\frac{2K^4}{D^2(D+2)(D+4)}+\cdots$$

so the contribution becomes:

$$384\,D(D-1)\left[\frac{K^5}{D^5}-\frac{5K^7}{D^6(D+2)}+\cdots\right]\left[\frac{K^2}{D(D+2)}-\frac{2K^4}{D^2(D+2)(D+4)}+\cdots\right]$$

$$=384\,D(D-1)\left[\frac{K^7}{D^6(D+2)}-\frac{(7D+24)K^9}{D^7(D+2)^2(D+4)}+\cdots\right].$$

We note that, as predicted, the graph shown, which has seven lines, contributes to the expansion first at K^7, and subsequently to every second term. These are general features of the expansion.

Appendix 2. Weights of highly symmetric bondings

The 'octahedron', a cyclomatic index seven topology (figure 7*b*), provides the most difficult weight determination problem we have yet encountered. If one attempts to apply the infinite bond technique to obtain the weight of the bonding having single multiplicity on every bridge, one discovers that the equation so obtained also contains the weight of the bonding containing one triple bridge. Because of the high symmetry (every bridge is equivalent) the procedure can be applied in only one way, leading to a single equation in two unknown weights.

Instead, from first principles we deduce the general *form* of the weight of the bonding we seek as it appears in the partition function for the octahedron. Stanley's (1968) result, that even for finite graphs there exists a finite limit (analogous to the spherical model limit for infinite clusters) for $\ln Z$ as $D\to\infty$, allows us to determine all but one unknown coefficient in the general form. Finally, using the value of the weight when $D=1$, obtained for the Ising model (Hunter 1967), we can completely determine the weight. These methods and their basis are described in more detail in Domb (1976).

From first principles the partition function for a graph G is

$$Z(G)=\left\langle\exp\sum_{i,j}\sum_{\alpha=1}^{D}K_{ij}\sigma_{\alpha i}\sigma_{\alpha j}\right\rangle=\left\langle\prod_{ij}\exp K_{ij}\sum_{\alpha=1}^{D}\sigma_{\alpha i}\sigma_{\alpha j}\right\rangle$$

$$=\left\langle\prod_{ij}\left[1+K_{ij}\sum_{\alpha=1}^{D}\sigma_{\alpha i}\sigma_{\alpha j}+\frac{K_{ij}^2}{2!}\left(\sum_{\alpha=1}^{D}\sigma_{\alpha i}\sigma_{\alpha j}\right)^2+\cdots+\frac{K_{ij}^r}{r!}\right.\right.$$

$$\left.\left.\times\left(\sum_{\alpha=1}^{D}\sigma_{\alpha i}\sigma_{\alpha j}\right)^r+\cdots\right]\right] \tag{A2.1}$$

where $\sigma_{\alpha i}$ is the αth component of a D-dimensional classical spin $\boldsymbol{\sigma}_i$. For a graph G, the index i runs over all the vertices of G while sums or products over the pair ij are assumed to run over all allowed interactions—or bonds—in G. The coefficient of

$K_{12}^{l}K_{23}^{m}K_{34}^{n}\ldots$ is clearly

$$\left\langle \frac{(\sum_{\alpha=1}^{D}\sigma_{\alpha 1}\sigma_{\alpha 2})^{l}}{l!}\frac{(\sum_{\alpha=1}^{D}\sigma_{\alpha 2}\sigma_{\alpha 3})^{m}}{m!}\frac{(\sum_{\alpha=1}^{D}\sigma_{\alpha 3}\sigma_{\alpha 4})^{n}}{n!}\ldots\right\rangle, \tag{A2.2}$$

there being one factor for each bond in the graph. For classical vectors the averages are obtained by integrating each spin over all possible orientations in D-space.

Following Domb, we represent each factor $\sigma_{\alpha i}\sigma_{\alpha j}$ in the expanded form of (A2.2) by a coloured bond on the graph, using a different colour for each of the D different values of α. One can then show that in the averaging process only those terms survive which correspond to configurations in which every vertex is of even order in *each* colour. Further, each vertex makes a contribution according to its total order: two-vertices make contributions proportional to $1/D$, four-vertices proportional to $1/D(D+2)$, six-vertices proportional to $1/D(D+2)(D+4)$, etc.

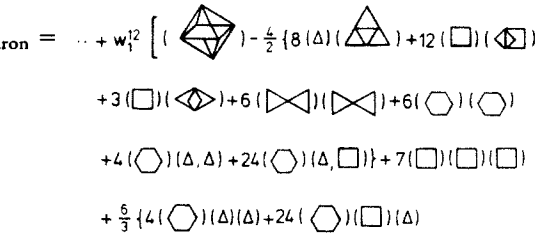
Hence to find the form of the D dependence of the weight corresponding to a particular bonding of G, we need to multiply together the form of the contributions from each vertex and a combinatorial factor accounting for the number of possible colourings subject to the constraints already described. The number of monochromatic colourings is proportional to $\binom{D}{1}$, dichromatic to $\binom{D}{2}$, n-chromatic to $\binom{D}{n}$.

Since every vertex must be of even order in each colour, every permissible colouring of a bonding must be decomposable into an overlap of monochromatic polygons and/or monochromatic double bonds. For example, the 'most colourful' colouring of the singly-bonded octahedron (figure 7*b*) contains four colours, corresponding to an overlap of four different triangles each of different colours, while for the entirely double-bonded α graph shown in Figure 7(*a*) it would contain six colours—the six different double bonds each being of a distinct colour.

Hence the general form of the weight W for the singly-bonded octahedron is

$$\begin{aligned} W &= [1/D(D+2)]^{6}[aD+bD(D-1)+cD(D-1)(D-2) \\ &\quad +dD(D-1)(D-2)(D-3)]K^{12} \\ &= [1/D^{5}(D+2)^{6}][\alpha+\beta D+\gamma D^{2}+\delta D^{3}]K^{12} \\ &= [D^{7}/(D+2)^{6}][\alpha+\beta D+\gamma D^{2}+\delta D^{3}]w_{1}^{12}. \end{aligned} \tag{A2.3}$$

The expansion of Z will contain terms corresponding, among others, to every singly-bonded subgraph of the octahedron which contains only even-order vertices. In taking the logarithm, all such terms are multiplied by each other in all possible ways. We find the coefficient of w_1^{12} corresponds to the sum of the products of weights of subgraphs (represented diagramatically) with the coefficients shown:

$\ln Z_{\text{octahedron}} =$ 

(A2.4)

Substituting the known weights of all the subgraphs and collecting terms we obtain

$$\ln Z_{\text{octahedron}} = +w_1^{12}\left[\frac{D^7}{(D+2)^6}(\alpha+\beta D+\gamma D^2+\delta D^3)-8\left(\frac{D^5(D+8)}{(D+2)^2}\right)\right.$$
$$\left.-15\left(\frac{3D^4}{D+2}\right)-6D^2+42D^3+6D^4\right]+\ldots. \tag{A2.5}$$

Stanley's proof that if the interaction J is replaced by λJ^*, where λ is of order D in the spin dimensionality, then $\ln Z/\lambda$ tends to a finite limit as D tends to ∞ implies that, when expressed in powers of w_1, no term in the $\ln Z$ expansion can have a coefficient of order greater than D. Expanding the coefficient in equation (A2.5) and separately equating the coefficients of D^4, D^3 and D^2 equal to zero gives

$$\delta = 2, \qquad \gamma = 59, \qquad \beta = 296 \tag{A2.6}$$

respectively. Finally using the Ising model results (Hunter 1967) that the coefficient of w_1^{12} in the $\ln Z$ expansion for the octahedron is 20, enables us to find $\alpha = 372$. Thus the difficult octahedron weight is found to be

$$W = (C_{111111111111})_{\text{octahedron}} = \frac{D^7}{(D+2)^6}(372+296D+59D^2+2D^3). \tag{A2.7}$$

When we substitute $D = 2$ into (A2.7) we obtain $W = 38$ which we have checked using other methods peculiar to the two-dimensional case (Domb 1976).

Acknowledgments

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