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# The Ising model on the tetrahedron lattice I. An extended susceptibility series

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**Abstract.** We have calculated the first 16 terms of the series expansion for the high-temperature susceptibility of the Ising model for a lattice made up of the B sites of the crystalalite or spinel structures (the 'tetrahedron' lattice). By means of a transformation technique which allows the enumeration of graphs to be carried out on the simpler diamond lattice we have added six new terms to previously published results. We estimate that the critical temperature is given by

$$v_c = 0.23300 \pm 0.00001$$

and that the exponent  $\gamma$  is

$$\gamma = 1.250 \pm 0.001,$$

a result which gives further confirmation of the universality hypothesis.

## 1. Introduction

It is generally believed that near the critical point the high-temperature zero-field susceptibility of the Ising model has the asymptotic form

$$\chi(T) \sim C(T - T_c)^{-\gamma}, \quad T \rightarrow T_c^+.$$

The high-temperature susceptibility can be expanded in the form

$$\chi = 1 + \sum_{r=1}^{\infty} a_r v^r$$

where  $v = \tanh(J/kT)$ ,  $J$  being the exchange constant. It is well known that the coefficients  $a_r$  can be related to a graph counting problem and can be evaluated exactly. If the coefficients up to and including  $r = N$  are known we will refer to this as an  $N$ -term series.

Evidence from such high-temperature series for the spin  $\frac{1}{2}$  nearest-neighbour Ising model on the face-centred cubic, body-centred cubic and simple cubic lattices suggests that  $\gamma = 1.25$  exactly for all three lattices. The latest results are due to Sykes *et al* (1972).

Early results of this type led the way to the 'universality' hypothesis (Kadanoff 1970, Griffiths 1970), according to which all critical exponents should be independent of the lattice structure for a given dimension.

High-temperature series have also been derived for a number of less common three-dimensional lattices. In table 1 we give a summary of such work. We only consider the

**Table 1.** Summary of published high-temperature susceptibility series for the spin  $\frac{1}{2}$  nearest-neighbour Ising model on three-dimensional lattices.

Lattice	Author(s)	Number of terms
Simple cubic	Sykes <i>et al</i> (1972)	17
Face-centred cubic	Rapaport (1974)	13
Body-centred cubic	Sykes <i>et al</i> (1972)	15
Diamond	Gaunt and Sykes (1973)	22
Crystobalite } B-site spinel }	Betts and Ditzian (1968)	10
	Lambeth <i>et al</i> (1974)	10
Hydrogen peroxide	Leu <i>et al</i> (1969)	27
Hyper-triangular	Leu <i>et al</i> (1969)	13
Octahedral	Oitmaa and Elliott (1970)	9

spin  $\frac{1}{2}$  nearest-neighbour case. Although these series are generally less regular in behaviour than the three common cubic lattices, the results are in all cases quite consistent with the hypothesis  $\gamma = 1.25$ . Of course the critical temperature  $T_c$  (or  $v_c$ ) depends on the lattice structure and the susceptibility series provide the best means of estimating  $v_c$  for a particular lattice structure.

Betts and Ditzian (1968) have derived high-temperature series for the specific heat and susceptibility for a spin  $\frac{1}{2}$  nearest-neighbour Ising model on a particular lattice which they called the crystobalite lattice. This lattice is illustrated in figure 1—it consists of regular tetrahedra joined corner to corner. The mineral crystobalite is a form of  $\text{SiO}_2$  in which the oxygen atoms occupy the sites of the lattice and the silicon atoms the centres of the tetrahedra. There are a number of alloys of the form  $\text{AB}_2$  which also have this structure. Jasnow and Moore (1968) and Lambeth *et al* (1974) have also derived high-temperature susceptibility series for this lattice, which they call the B-site spinel lattice, since it is the lattice occupied by the magnetic B ions in a number of spinel structure ferromagnetic insulators with the general formula  $\text{AB}_2\text{X}_4$ . Thus this lattice, which for simplicity we will call the 'tetrahedron lattice' is of interest not only from a purely theoretical point of view but also as the structure of a number of real ferromagnetic materials.

There is a great deal of similarity between the tetrahedron lattice and the diamond lattice—in fact the centres of the tetrahedra lie on the diamond lattice. Using this property Gibberd (1970) was able to extend the specific heat series derived initially by Betts and Ditzian from 11 terms to 19. This was done by using a transformation technique and the existing free energy series for the diamond lattice. Unfortunately specific heat series are invariably much more irregular than susceptibility series and Gibberd was unable to obtain consistent estimates of either the critical temperature  $v_c$  or exponent  $\alpha$ .

Gibberd's transformation method, in its original form, is applicable only to the zero-field free energy. We have been able to generalize the method to the calculation of the zero-field susceptibility. In this way we have been able to extend the 10-term susceptibility series of Betts and Ditzian (1968) and Lambeth *et al* (1974) to 16 terms. With the additional terms we are able to obtain much more accurate estimates for the critical temperature and the exponent  $\gamma$ . We estimate that  $\gamma = 1.250 \pm 0.001$ , a result in convincing agreement with the universality hypothesis. In the process we have obtained exact agreement with the terms given by Lambeth, Lee and Stanley and have confirmed a small error in the tenth coefficient of Betts and Ditzian.

In § 2 of the paper we will discuss the transformation technique and give the resulting series coefficients. In § 3 we present the results of the series analysis, based on standard ratio and Padé approximant techniques. In § 4 we present our conclusions and suggest areas for further work.

**2. Derivation of series**

We consider the spin  $\frac{1}{2}$  nearest-neighbour Ising model on the tetrahedron lattice shown in figure 1. The Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - mH \sum_i \sigma_i \tag{1}$$

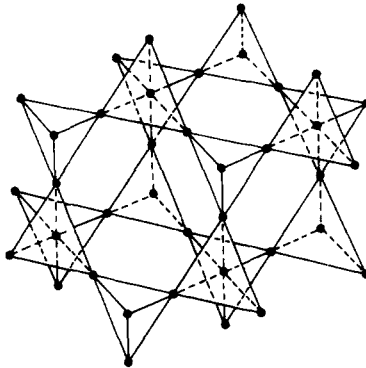
where the symbols have the usual meaning. The zero-field dimensionless susceptibility per spin is

$$\chi = \left( \frac{kT}{m} \right)^2 \lim_{H \rightarrow 0} \frac{\partial^2}{\partial H^2} \left( \frac{1}{N} \ln Z \right) \tag{2}$$

and the partition function is

$$Z = \sum_{\{\sigma\}} e^{-\beta \mathcal{H}} = (\cosh K)^{3N} \sum_{\{\sigma\}} \prod_{\langle ij \rangle} (1 + v \sigma_i \sigma_j) \prod_k \exp(h \sigma_k) \tag{3}$$

where  $\beta = 1/kT$ ,  $K = \beta J$ ,  $v = \tanh K$ , and  $h = \beta mH$ . The summation is over all spin configurations, the first product over all nearest-neighbour pairs of spins, and the second product over all spins.



**Figure 1.** The tetrahedron lattice. This is the lattice made up of the B sites in either the crystalite structure  $AB_2$  or the spinel structure  $AB_2X_4$ .

From the product  $\prod_{\langle ij \rangle}$  we explicitly multiply out the terms arising from a single tetrahedron, as described by Gibberd (1970). This yields for the partition function

$$Z = (\cosh K)^{3N} (1 + 4v^3 + 3v^4)^{N/2} \sum_{\{\sigma\}} \prod_k \exp(h \sigma_k) \prod_{\text{tetrahedra}} \times [1 + A(\sigma_1 \sigma_2 + \sigma_1 \sigma_3 + \sigma_1 \sigma_4 + \sigma_2 \sigma_3 + \sigma_2 \sigma_4 + \sigma_3 \sigma_4) + B \sigma_1 \sigma_2 \sigma_3 \sigma_4] \tag{4}$$

where

$$A = (v + 2v^2 + 2v^3 + 2v^4 + v^5)(1 + 4v^3 + 3v^4)^{-1}$$

$$B = (3v^2 + 4v^3 + v^6)(1 + 4v^3 + 3v^4)^{-1} \tag{5}$$

and the second product runs over the  $N/2$  tetrahedra which make up the lattice of  $N$  sites.

The product over the set of  $N/2$  tetrahedra can be expanded and the various terms associated with graphs on the lattice in the usual way (see Domb 1974 for a general description of this procedure). These graphs consist of single bonds (weight  $A$ ) and 'crossed bonds' (ie 4 unpaired spins, weight  $B$ ). For the zero-field susceptibility the allowed graphs must contain exactly two odd vertices. The resulting expression is

$$\chi = 1 + 2 \sum_{\{G\}} C_G A^m B^n \tag{6}$$

where  $\{G\}$  is the set of all graphs with two odd vertices,  $C_G$  is the weak lattice constant of graph  $G$ , and  $m, n$  are the numbers of single and crossed bonds in graph  $G$  respectively.

It is possible to set up a correspondence between graphs on the tetrahedron lattice and graphs on the diamond lattice formed by the centres of all tetrahedra. The advantage of this procedure is that it is much simpler to enumerate graphs on the diamond lattice. All graphs joining a particular set of tetrahedra will correspond to a particular graph, which we call the *dual graph*, joining the corresponding sites on the diamond lattice. Some examples are given in figure 2.

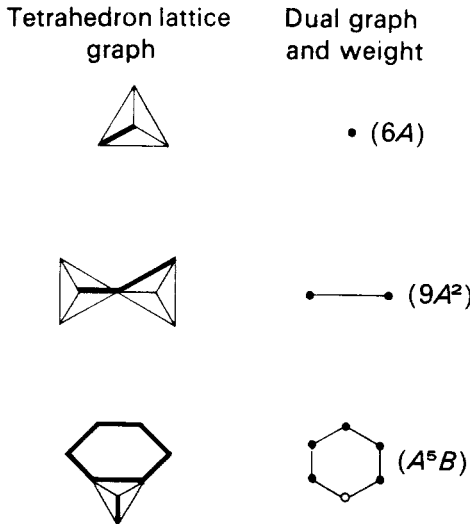
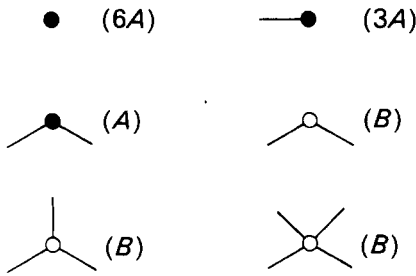
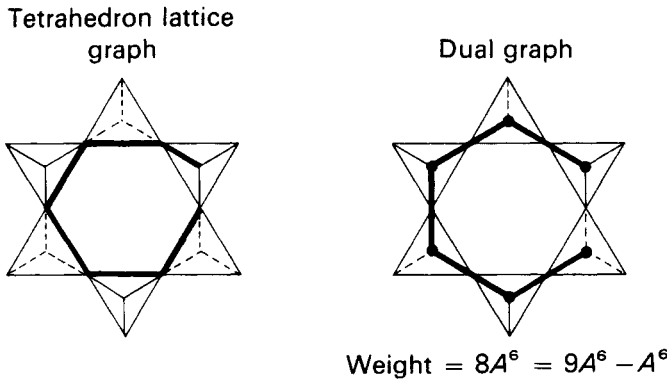


Figure 2. The correspondence between graphs on the tetrahedron lattice with dual graphs and their weights on the diamond lattice.

In order for the correspondence to be valid it is necessary to assign weights to the different vertex types for the dual graphs. The vertex types and corresponding weights are shown in figure 3. The weight for a complete graph is just the product of the vertex weights. There is one complication, namely, that when the two odd vertices of the dual graph are on nearest-neighbour sites the weight must be modified by subtracting from it the weight of the associated polygon, as shown in figure 4.



**Figure 3.** Vertex types and weights (in parentheses) for dual graphs.



**Figure 4.** An illustration of the weight correction for dual graphs with odd vertices which are nearest neighbours.

It is then necessary to enumerate all the dual graphs which correspond to configurations with two unpaired spins. This was done independently by each of us. There are many topological types and we display these in the appendix. The computation of the lattice constants for connected graphs has been carried out by computer while for disconnected graphs algebraic techniques, with various checks, have been used. The series we obtain is

$$\begin{aligned}
 \chi = & 1 + 6A + 18A^2 + 54A^3 + 162A^4 + 486A^5 + 1446A^6 + 4194A^7 \\
 & + 12234A^8 + 35442A^9 + 102522A^{10} + 294480A^{11} + 847116A^{12} \\
 & + 2427840A^{13} + 6957600A^{14} + 19878408A^{15} + 56810148A^{16} + \dots \\
 & + B(12A^5 + 72A^6 + 348A^7 + 1440A^8 + 5640A^9 + 20412A^{10} + 71028A^{11} \\
 & + 239844A^{12} + 792480A^{13} + 2552212A^{14} + \dots) + B^2(6A^7 + 54A^8 \\
 & + 414A^9 + 2106A^{10} + 10038A^{11} + 41506A^{12} + \dots) + 72A^{10}B^3 + \dots \quad (7)
 \end{aligned}$$

It is then a simple matter to expand  $\chi$  as a power series in  $v$ , using the expressions (5). We obtain

$$\begin{aligned}
 \chi = & 1 + 6v + 30v^2 + 138v^3 + 618v^4 + 2766v^5 + 12378v^6 + 55218v^7 + 245010v^8 \\
 & + 1081158v^9 + 4752054v^{10} + 20842578v^{11} + 91307598v^{12} + 399546882v^{13} \\
 & + 1745963826v^{14} + 7618990770v^{15} + 33208413570v^{16} + \dots \quad (8)
 \end{aligned}$$

The terms up to and including  $v^{10}$  agree exactly with the published series of Lambeth *et al* (1974) and confirm a small error in the tenth term of Betts and Ditzian (1968). The last six coefficients are new. Although it is possible that these coefficients may contain small errors we have taken considerable care to ensure that they are correct, re-checking our calculations several times. In § 3 we will analyse the series (8) by standard techniques and obtain estimates for the critical temperature  $v_c$  and exponent  $\gamma$ .

### 3. Series analysis and results

There are two standard methods for the analysis of series expansions such as (8), namely :

(i) the ratio method and variations;

(ii) the Padé approximant method;

and we shall use both these techniques to obtain estimates for the critical parameters  $v_c$  and  $\gamma$  for the tetrahedron lattice. Excellent reviews of these methods are available (Hunter and Baker 1973, Gaunt and Guttman 1974).

All of the analysis methods assume a particular asymptotic form for the function of interest near the singularity. For the zero-field susceptibility the dominant term is believed to be

$$\chi \sim A(1-v/v_c)^{-\gamma}, \quad v \rightarrow v_c^- \tag{9}$$

although more complex forms involving weaker confluent singularities have also been used (Sykes *et al* 1972, Saul *et al* 1975).

The ratio method is based on the fact that for a function of the form (9) the ratios  $\mu_n$  of successive coefficients of the power series expansion are given by

$$\mu_n \equiv \frac{a_n}{a_{n-1}} = \mu_c \left( 1 + \frac{\gamma-1}{n} + O\left(\frac{1}{n^2}\right) \right) \tag{10}$$

where  $\mu_c = 1/v_c$ . Thus a direct plot of  $\mu_n$  against  $1/n$  should become linear for large  $n$ , with intercept  $\mu_c$  and slope  $(\gamma-1)\mu_c$ . More accurate estimates of  $v_c$  can be obtained from the quantities

$$\mu'_n = n\mu_n - (n-1)\mu_{n-1} \simeq \mu_c \left( 1 + O\left(\frac{1}{n^2}\right) \right) \tag{11a}$$

and

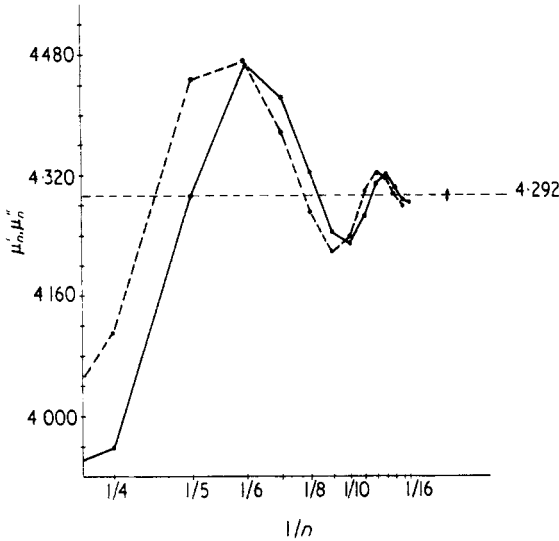
$$\mu''_n = \frac{1}{2}n\mu_n - \frac{1}{2}(n-2)\mu_{n-2} \simeq \mu_c \left( 1 + O\left(\frac{1}{n^2}\right) \right). \tag{11b}$$

Plots of  $\mu'_n$  and  $\mu''_n$  against  $1/n$  should approach the intercept  $\mu_c$  with zero slope. In figure 5 we show such plots and it can be seen that the points do appear to be approaching a horizontal line although there is a regular oscillatory behaviour indicative of the presence of other singularities near the circle of convergence. The oscillatory behaviour appears to be decreasing in a regular way and we estimate from the diagram that

$$\mu_c = 4.292 \pm 0.005$$

or

$$v_c = 0.2330 \pm 0.0003. \tag{12}$$



**Figure 5.** Ratio plots of  $\mu'_n$  (broken curve),  $\mu''_n$  (full curve) against  $1/n$  (equation (11)). The horizontal broken line and the error bar yield the estimates given by equation (12).

Having obtained an estimate of  $\mu_c$  we compute the quantities

$$\gamma_n = 1 + n \left( \frac{\mu_n}{\mu_c} - 1 \right) \tag{13}$$

which from (10) should behave like

$$\gamma_n = \gamma \left( 1 + O\left(\frac{1}{n^2}\right) \right) \tag{14}$$

so that a plot of  $\gamma_n$  against  $1/n$  should yield an estimate for  $\gamma$ . This is shown in figure 6, from which we obtain

$$\gamma = 1.250 \pm 0.003, \tag{15}$$

a result which is consistent with the ‘universality’ prediction that  $\gamma = \frac{5}{4}$  for all three-dimensional lattices. The uncertainty in (15) is due both to the oscillatory behaviour of  $\gamma_n$  in figure 6 and the uncertainty in the estimate for  $v_c$ , as indicated in figure 5.

Assuming that  $\gamma = \frac{5}{4}$  exactly we compute the quantities

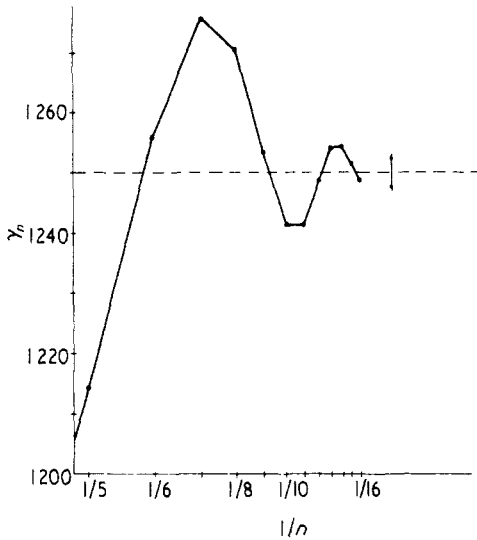
$$\beta_n = \frac{n\mu_n}{n + \frac{1}{4}} \tag{16}$$

which should behave as

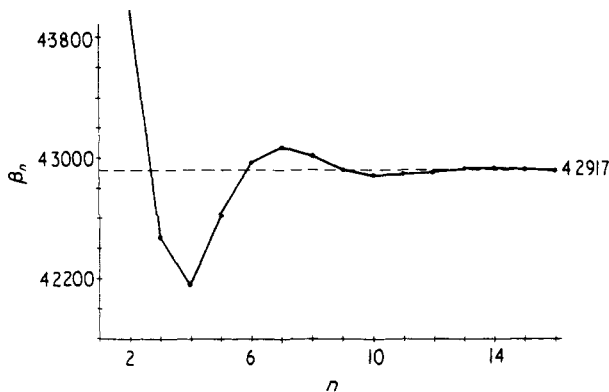
$$\beta_n \simeq \mu_c \left( 1 + O\left(\frac{1}{n^2}\right) \right). \tag{17}$$

A plot of  $\beta_n$  against  $1/n$  should approach the limit  $\mu_c$  with zero slope. In fact it is usual to plot  $\beta_n$  against  $n$  to spread out the points somewhat. This is shown in figure 7 and clearly is approaching a horizontal line. The resulting estimate of  $\mu_c$  is quite consistent with (12) but allows the confidence limits to be narrowed considerably. Our estimate from figure 7 is





**Figure 6.** Ratio plot of  $\gamma_n$  against  $1/n$  (equation (14)). The horizontal broken line and the error bar yield the estimate given by equation (15).



**Figure 7.** Plot of  $\beta_n$  against  $n$  (equation (16)). The horizontal broken line yields the refined estimates (equation (18)) for the critical temperature.

$$\mu_c = 4.2917 \pm 0.0005$$

or

$$v_c = 0.23301 \pm 0.00003.$$

(18)

The Padé approximant method attempts to represent the function as the quotient of two finite polynomials. The singularities of the function are then estimated by computing the zeros of the denominator polynomial.

The usual approach is to compute the series for the logarithmic derivative of  $\chi$ ,

$$\frac{d}{dv} \ln \chi(v) \simeq \frac{-\gamma}{v - v_c} \tag{19}$$

as this function has a simple pole at  $v = v_c$  and should be well represented by Padé approximants. In table 2 we show estimates of  $v_c$  obtained in this way. The convergence is extremely good and from the elements near to and on the diagonal we estimate

$$v_c = 0.23300 \pm 0.00005. \tag{20}$$

**Table 2.** Estimates of the critical point  $v_c$ , of the tetrahedral lattice obtained from Padé approximants to  $(d/dv) \ln \chi(v)$ .

$D \backslash N$	5	6	7	8	9	10
5	0.232451	0.233299	0.233047	0.233030	0.232984	0.233005
6	0.232911	0.233103	0.233029	0.233058	0.232997	
7	0.233184	0.233061	0.232899	0.232993		
8	0.233116	0.233015	0.233009			
9	0.232859	0.233009				
10	0.232927					

The residues in (19), evaluated at the estimated  $v_c$  values, yield the estimate

$$\gamma = 1.250 \pm 0.003. \tag{21}$$

This result again confirms the hypothesis that  $\gamma = \frac{5}{4}$  exactly. We then construct the series

$$(\chi)^{1/\gamma} \simeq \frac{v_c A^{1/\gamma}}{v_c - v}. \tag{22}$$

Forming Padé approximants to the series we obtain the results shown in table 3, from which we estimate

$$v_c = 0.23300 \pm 0.00001, \tag{23}$$

a value identical with (20) but with much reduced error estimates.

The exponent  $\gamma$  is then re-estimated from the approximants to

$$(v_c - v) \frac{d}{dv} \ln \chi(v) \tag{24}$$

**Table 3.** Estimates of the critical point  $v_c$ , of the tetrahedral lattice obtained from Padé approximants to  $(\chi(v))^{4/5}$ .

$D \backslash N$	5	6	7	8	9	10	11
5	0.2330532	0.2329667	0.2332992	0.2329978	0.2329989	0.2329986	0.2329991
6	0.2330022	0.2329862	0.2329987	0.2329992	0.2329987	0.2329988	
7	0.2329873	0.2329913	0.2329992	0.2329989	0.2329989		
8	0.2329939	0.2330056	0.2329985	0.2329989			
9	0.2329960	0.2329992	0.2329991				
10	0.2329987	0.2329991					
11	0.2329985						

evaluated at  $v = v_c$ . Using the estimates of  $v_c$  in (23) we obtain the results in table 4 from which we conclude

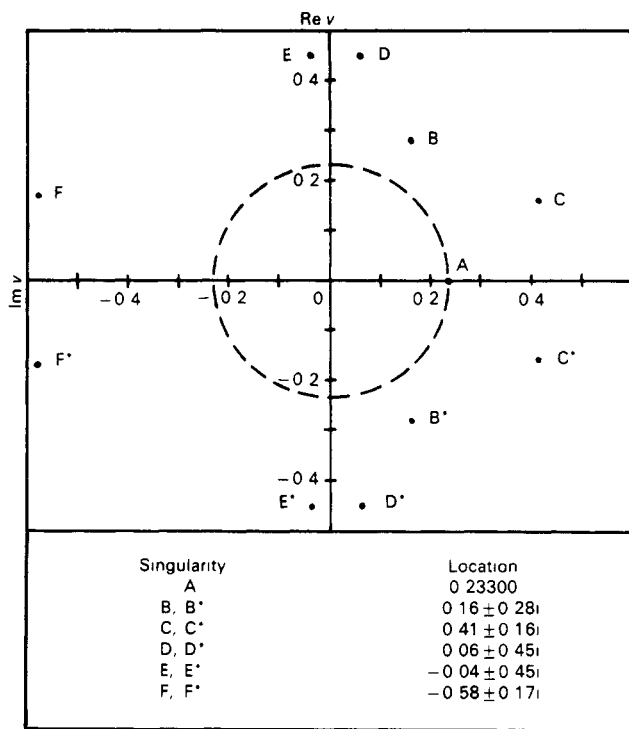
$$\gamma = 1.250 \pm 0.001. \tag{25}$$

In carrying out the Padé approximant analysis of the logarithmic derivative series (19) we noted the consistent occurrence of a number of other non-physical singularities. The approximate positions of these are shown in figure 8. We note that:

- (i) all of the non-physical singularities lie outside the circle of convergence;

**Table 4.** Estimates of the critical exponent  $\gamma$  of the tetrahedral lattice obtained from Padé approximants to  $(v_c - v)(d/dv) \ln \chi(v)$  evaluated at  $v = v_c$ .

$[N, D]$ \ $v_c$	0.23299	0.23300	0.23301
5, 10	1.2492	1.2498	1.2504
6, 9	1.2494	1.2501	1.2509
7, 8	1.2491	1.2501	1.2509
8, 7	1.2494	1.2501	1.2509
9, 6	1.2494	1.2501	1.2508
10, 5	1.2494	1.2501	1.2509
5, 9	1.2487	1.2493	1.2499
6, 8	1.2495	1.2502	1.2509
7, 7	1.2494	1.2502	1.2508
8, 6	1.2494	1.2501	1.2507
9, 5	1.2494	1.2501	1.2508



**Figure 8.** Distribution of singularities in the complex  $v$  plane obtained from Padé approximants to the series for  $(d/dv) \ln \chi(v)$ .

- (ii) there is no singularity on the negative real axis, corresponding to the impossibility of having a stable antiferromagnetic ordered state in this structure.

The oscillatory behaviour of the ratios in figure 5 can probably be attributed mainly to the singularities  $B$ ,  $B^*$  which are quite close to the circle of convergence. We have attempted to improve the rate of convergence of the ratio results by applying a conformal transformation of the form

$$v = \frac{\bar{v}}{1 - \bar{v}^2/b^2} \quad (26)$$

(Betts *et al* 1971) which has the effect of isolating the physical singularity from other singularities. Although the transformed series does indeed show much smaller oscillations in the ratios the overall estimates of  $v_c$  tend to differ slightly from the original series. The need to use transformations with caution has been noted previously by Lambeth *et al* (1974).

#### 4. Discussion and conclusions

In this paper we have generalized a transformation technique due to Gibberd (1970) and have used this to obtain a 16-term series for the high-temperature susceptibility for the spin  $\frac{1}{2}$  nearest-neighbour Ising model on a regular three-dimensional lattice which we have called the 'tetrahedron' lattice. We were motivated to carry out this work for a number of reasons.

The tetrahedron lattice is not just an artificial construct—it is the lattice made up of the  $B$  sites of the crysotobalite ( $AB_2$ ) structure and also the  $B$  sites of the spinel structure ( $AB_2X_4$ ). There are a number of important insulating ferromagnets and antiferromagnets with the spinel structure in which the magnetic ions occupy the  $B$  sites (Dwight and Menyuk 1967, 1968).

There are also a number of strong theoretical motivations for this work. According to the universality hypothesis the critical exponents of the Ising model should be the same for all three-dimensional lattices, independent of the particular lattice structure. Evidence from series expansions certainly supports this result. However for the tetrahedron lattice Lambeth *et al* (1974) found that their 10-term series was too irregular to conclude anything definite. With our longer series we are able to remove this doubt and to conclude that the exponent  $\gamma$  for this lattice is almost certainly 1.25, as predicted by universality.

Transformation techniques have been widely used in studies of the Ising model (an early discussion was given by Fisher 1959). Gibberd's transformation technique has the effect of transforming from an Ising model with pair interactions on a lattice made up of touching polyhedra to an Ising model with pair and more complex interactions on a lattice made up by the centres of the polyhedra (the dual lattice). The original technique was only applicable to the zero-field free energy. We have generalized the method to apply it to a calculation of the zero-field susceptibility. Apart from the present work it would be simple to use our method to calculate extended susceptibility expansions for other lattices, such as the 'octahedral' lattice studied by Oitmaa and Elliott (1970).

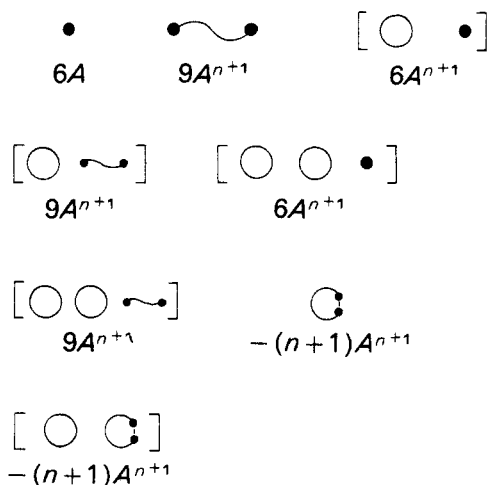
An obvious extension of our work is to include a four-spin interaction term in the original Hamiltonian, coupling the four spins at the vertices of each tetrahedron. There has been considerable interest in recent years in the effect of multiple spin interactions in the Ising model (Baxter 1971, Wu 1971, Oitmaa and Gibberd 1973, Wood and

Griffiths 1974, Baxter and Wu 1973). We have carried out calculations for the Ising model with two- and four-spin interactions in the tetrahedron lattice and the results will be presented in a subsequent paper.

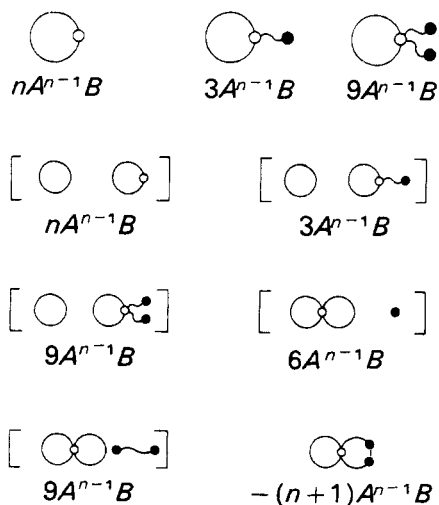
**Appendix**

In enumerating the dual graphs, as discussed in § 2, it is useful to classify them into different topological types. We list these below, together with the weights. In all cases  $n$  denotes the number of bonds in a graph and second-order vertices of the type  $\bullet$  are suppressed.

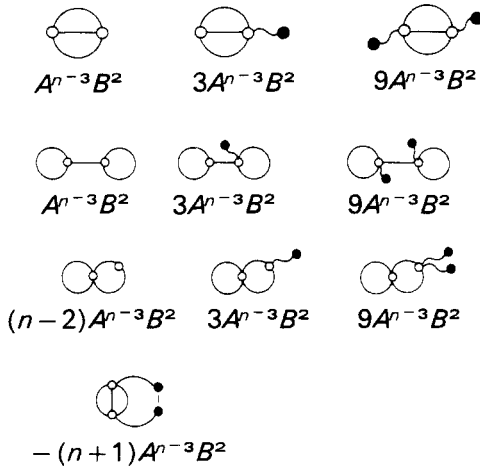
Graphs proportional to  $A^r$  ( $r \leq 16$ )



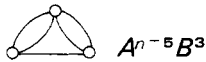
Graphs proportional to  $A^r B$  ( $r \leq 14$ )



Graphs proportional to  $A^r B^2$  ( $r \leq 12$ )



Graphs proportional to  $A^r B^3$  ( $r \leq 10$ )



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