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Ising model susceptibility amplitudes II. Three-dimensional lattices

A J Guttmann

Department of Applied Mathematics, Research School of Physical Sciences and
The Computer Centre, Australian National University, Canberra, ACT 2600, Australia
and
Department of Mathematics, University of Newcastle, New South Wales 2308, Australia

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Abstract. Amplitudes for a number of three-dimensional Ising model series have been estimated from recently extended series expansions. The amplitudes have then been used to re-estimate the field and temperature scaling parameters that are fundamental to the Generalized Law of Corresponding States. These new scaling parameters have been used (i) to estimate the amplitudes of the next most singular term in the high-temperature susceptibility for the four common three-dimensional lattices, and (ii) to show that an earlier conjecture, that the field scaling parameter n_X is the same for the Ising and spherical models, is unlikely to hold.

1. Introduction

In this paper we continue the investigation started in the preceding paper (Guttmann 1975, to be referred to as I). In that paper we studied the susceptibility amplitudes of the two-dimensional Ising model, while in this paper our attention is directed to the three-dimensional Ising model.

For the three-dimensional Ising model, unlike its two-dimensional counterpart, we have no exact knowledge of critical points, critical exponents or any non-trivial thermodynamic functions, but only an extensive body of numerical information. We will now summarize the contemporary extensions to this body of information.

Recently the three-dimensional high-temperature susceptibility series have been extended by Sykes *et al* (1972a) for the simple cubic (SC), body-centred cubic (BCC) and face-centred cubic (FCC) lattices, and by Gaunt and Sykes (1973) for the diamond (D) lattice. Using these extended series those authors were able to make more accurate estimates of the critical temperatures. Their results for the critical temperatures are summarized in table 1. They also obtained more accurate estimates of the ferromagnetic susceptibility amplitudes, C_0^+ in the notation of I, for the SC, BCC and FCC lattices. For the diamond lattice no new determination of C_0^+ has been published, so we have estimated this, as described in § 2. The amplitudes C_0^+ are also given in table 1.

The amplitudes of the critical isotherm series have also been extended and re-examined by Gaunt and Sykes (1972). This amplitude is defined by

$$1-\exp(-2mH/kT) \sim DM_c^\delta \qquad T = T_c, \qquad H \to 0^+. \tag{1.1}$$

Gaunt and Sykes found $\delta = 5$, within 1%, and obtained the estimates of D quoted in table 1.

Table 1. Critical temperature and critical amplitude estimates for the three-dimensional Ising model.

Critical parameter \ Lattice	D	SC	BCC	FCC
$v_c = \tanh(J/kT_c)$	0.353806 ± 0.000012	0.21813 ± 0.00001	0.15612 ± 0.00003	0.101740 ± 0.000005
$K_c = J/kT_c$	0.369787 ± 0.000015	0.22169 ± 0.00001	0.15741 ± 0.00003	0.102093 ± 0.000005
$u_c = e^{-4K_c}$	0.227831 ± 0.000013	0.411985 ± 0.00002	0.53278 ± 0.00006	0.664731 ± 0.000017
C_0^+	1.1717 ± 0.0007	1.0582 ± 0.001	0.985 ± 0.003	0.971 ± 0.002
D	0.390 ± 0.015	0.535 ± 0.015	0.66 ± 0.02	0.715 ± 0.015

For the spontaneous magnetization, extended series have been published by Sykes *et al* (1973), and the critical behaviour studied by Gaunt and Sykes (1973). They reaffirmed the generally accepted result $\beta = \frac{5}{16}$ where β is the exponent characterizing the vanishing of the spontaneous magnetization as $T \to T_c^-$, for all three-dimensional lattices, though the low-temperature susceptibility exponent γ' as $T \to T_c^-$ has still not been unambiguously determined. For this reason we have not attempted a re-determination of the low-temperature susceptibility amplitudes, since estimates of these depend on the value of γ'. However, using the value $\beta = \frac{5}{16}$ and the values of the critical temperatures given in table 1, we have been able to obtain new estimates of the spontaneous magnetization amplitudes B from the extended series of Sykes *et al* (1973).

Given the estimates of C_0^+ and D in table 1 and combining them with the newly determined estimates of C_0^+ for the diamond lattice and B for all lattices, we re-examine the Generalized Law of Corresponding States as it applies to the three-dimensional Ising model. In the notation of I we have estimated the temperature and field scaling parameters g_X and n_X respectively. With our more precise estimates of the various critical amplitudes, the tighter confidence limits on n_X suggest that an earlier conjecture of Betts *et al* (1971), which suggested that n_X is the same for the three-dimensional Ising model and the spherical model, does not hold.

From these estimates of n_X and g_X we have estimated the amplitude of the *next* most singular term in the susceptibility, C_1^+, and compared this to the series analysis predictions (where available). We have also estimated the specific heat high-temperature amplitudes, A_0^+, and compared these to series analysis predictions. Reasons are given for preferring these estimates to those from series expansions.

2. Amplitude estimations

Using the critical temperature quoted in table 1, the generally accepted high-temperature susceptibility critical exponent $\gamma = \frac{5}{4}$ and the 22-term susceptibility expansion

$$kT\chi_0(v)/m^2 = \sum_{n \geq 0} a_n v^n$$

given by Gaunt and Sykes (1973), we have estimated the high-temperature susceptibility amplitude of the diamond lattice from the sequence $b_n = v_c^n a_n / |\binom{-5/4}{n}|$. The last 10 terms in this sequence, $b_{13} - b_{22}$, are 1·049306, 1·048573, 1·048838, 1·048450, 1·048771, 1·048380, 1·048566, 1·048293, 1·048475, 1·048227. These form an oscillatory decreasing sequence due to the presence of additional singularities at $-v_c$ and $\pm iv_c$. However, alternate terms may be linearly extrapolated and in this way we estimate the limit to be $1{\cdot}0476 \pm 0{\cdot}0006$, from which follows

$$C_0^+ = 1{\cdot}1717 \pm 0{\cdot}0007, \tag{2.1}$$

as entered in table 1.

For the spontaneous magnetization series $I_0(u) = \Sigma_{n\geqslant 0} c_n u^n$ on the D, SC, BCC and FCC lattices, we have proceeded by forming Padé approximants to $(u_c - u)(I_0(u))^{-1/\beta}|_{u=u_c}$, with $\beta = \frac{5}{16}$ and u_c as given in table 1. The Padé tables so obtained for the four lattices are shown in tables 2, 3, 4 and 5 for the D, SC, BCC and FCC lattices respectively. The table entries appear to be converging to the following limits:

$$\begin{array}{llll} 0{\cdot}0655 \pm 0{\cdot}0002 & (\text{D}) & 0{\cdot}086333 \pm 0{\cdot}00005 & (\text{SC}) \\ 0{\cdot}0905 \pm 0{\cdot}0002 & (\text{BCC}) & 0{\cdot}0764 \pm 0{\cdot}0002 & (\text{FCC}) \end{array} \tag{2.2}$$

Table 2. Padé approximants to $(u_c - u)(I_0(u))^{-1/\beta}|_{u=u_c}$ for the diamond lattice.

N	$[N-1/N]$	$[N/N]$	$[N+1/N]$
3	0·06712	0·06648	0·06606
4	0·06526	0·06584	0·06584
5	0·06584	0·06584	0·06548
6	0·06573	0·06565	0·06563
7	0·06562	0·06563	0·06563
8	0·06560		

Table 3. Padé approximants to $(u_c - u)(I_0(u))^{-1/\beta}|_{u=u_c}$ for the simple cubic lattice.

N	$[N-1/N]$	$[N/N]$	$[N+1/N]$
4	0·087719	0·087494	0·087146
5	0·087249	0·087688	0·075673
6	0·085738	0·086844	0·086346
7	0·086490	0·086367	0·086364
8	0·086364	0·086368	0·086355
9	0·086337	0·086333	0·086333
10	0·086333	0·086333	

Table 4. Padé approximants to $(u_c - u)(I_0(u))^{-1/\beta}|_{u=u_c}$ for the body-centred cubic lattice.

N	$[N-1/N]$	$[N/N]$	$[N+1/N]$
5	0·0907503	0·0915790	0·0911674
6	0·0913031	0·0924668	0·0907657
7	0·0909911	0·0908736	0·0908123
8	0·0915583	0·0906341	0·0905512
9	0·0905738	0·0905955	0·0905318
10	0·0905700	0·0906285	0·0906834
11	0·0907157	0·0907090	0·0907889
12	0·0907139	0·0906770	0·0905498
13	0·0907743	0·0904836	0·0906395
14	0·0902933	0·0904236	

Table 5. Padé approximants to $(u_c - u)(I_0(u))^{-1/\beta}|_{u=u_c}$ for the face-centred cubic lattice.

N	$[N-1/N]$	$[N/N]$	$[N+1/N]$
10	0·0767222	0·0769014	0·0765348
11	0·0765860	0·0755407	0·0763631
12	0·0763977	0·0763037	0·0765198
13	0·0756710	0·0762123	0·0762825
14	0·0763216	0·0762740	0·0762791
15	0·0762842	0·0762591	0·0763059
16	0·0763472	0·0763608	0·0765510
17	0·0763409	0·0763894	0·0763764
18	0·0763797	0·0763878	0·0764184
19	0·0760977	0·0763687	0·0761595
20	0·0763338	0·0773160	

from which we calculate the amplitudes B_0 as

$$\begin{array}{llll} B = 1{\cdot}6684 \pm 0{\cdot}0016 & (\text{D}) & B = 1{\cdot}5696 \pm 0{\cdot}0003 & (\text{SC}) \\ B = 1{\cdot}5059 \pm 0{\cdot}0010 & (\text{BCC}) & B = 1{\cdot}4861 \pm 0{\cdot}0013 & (\text{FCC}). \end{array} \qquad (2.3)$$

The confidence limits in (2.3) include errors due to the imprecise knowledge of the critical temperature. In § 3 we use these amplitudes to estimate the scaling parameters n_X and g_X as used in the Generalized Law of Corresponding States (see I and Betts *et al* 1971).

3. Scaling parameters

The temperature scaling parameter g_X is given for lattice X in terms of a standard lattice—for which we choose the FCC lattice—by $(B_X/B_F)^{1/\beta}$ or equivalently by $(D_F C^+_{0,F}/D_X C^+_{0,X})^{1/\gamma}$ (see I and Betts *et al* 1971). Using the amplitudes in table 1, those in § 2 and the values $\beta = \frac{5}{16}$ and $\gamma = \frac{5}{4}$, we obtain the estimates of g_X shown in table 6. As can be seen for each lattice, agreement between the two estimates is good, though the estimates obtained from the spontaneous magnetization amplitudes are about an order of magnitude more accurate than those obtained from the magnetization and susceptibility amplitudes. This reflects the difficulty in precisely determining the magnetization amplitudes D, as discussed by Gaunt and Sykes (1972).

Turning now to the field scaling parameter n_X, this is given in terms of the standard FCC lattice by the expressions $n_X = (C^+_{0,X}/C^+_{0,F})(B_X/B_F)^4$ and equivalently by $n_X = D_F/D_X$. These are also shown in table 6 and again we find that the estimate obtained from the

Table 6. Field and temperature scaling parameters for the three-dimensional lattices.

	FCC	BCC	SC	D
$g_X = (B_X/B_F)^{16/5}$	1	1·043 ± 0·005	1·191 ± 0·004	1·448 ± 0·008
$g_X = (D_F C^+_{0,F}/D_X C^+_{0,X})^{4/5}$	1	1·05 ± 0·07	1·18 ± 0·07	1·40 ± 0·06
$n_X = (C^+_{0,X}/C^+_{0,F})(B_X/B_F)^4$	1	1·070 ± 0·011	1·356 ± 0·010	1·917 ± 0·009
$n_X = D_F/D_X$	1	1·08 ± 0·06	1·34 ± 0·07	1·83 ± 0·11
n_X for spherical model	1	1·0655670	1·3945666	2

in-field magnetization series is less accurate than the other estimate though not as markedly so as for the parameter g_X. Agreement between the two estimates is again seen to be satisfactory.

Using less accurate amplitude estimates than those quoted here, it was conjectured by Betts *et al* (1971) that n_X for the Ising model and for other three-dimensional lattice models of the same class should be equal to n_X for the spherical model. We have listed the spherical model n_X values in table 6 also (these are exact), and it can be seen that the error bars for one n_X estimate for the SC lattice and for both n_X estimates for the diamond lattice clearly exclude the spherical model values. It thus appears that the conjecture does not hold and that, in general, n_X for the Ising model is slightly less than the corresponding spherical model value.

Using the most accurate values of g_X and n_X from table 6, we estimate further critical amplitudes in § 4 by assuming the validity of lattice–lattice scaling.

4. Amplitude predictions

Using the recently extended high-temperature specific heat series for the FCC lattice as given by Sykes *et al* (1972b), we have attempted to estimate the amplitude by following the technique of Sykes *et al* (1972a) and fitting the series to the Darboux form:

$$C_{H=0} = a(1-v/v_c)^{-\alpha}+b(1-v/v_c)^{1-\alpha}+c(1-v/v_c)^{2-\alpha} \qquad (4.1)$$

with $\alpha = \frac{1}{8}$ and v_c as given in table 1. Only the estimates of 'a' are regular enough to allow extrapolation, the last seven estimates being 1·11257, 1·11487, 1·10110, 1·09046, 1·08516, 1·08310, 1·08226. We estimate $a = 1{\cdot}079 \pm 0{\cdot}002$, from which follows $A_0^+ = 1{\cdot}080 \pm 0{\cdot}002$. From lattice–lattice scaling it follows (Betts *et al* 1971) that the amplitude for the other lattices $A_{0,X}^+$ will be given by

$$A_{0,X}^+ = A_{0,FCC}^+ g_X^{15/8}/n_X, \qquad (4.2)$$

so from the n_X and g_X values in table 6 and the above result for $A_{0,FCC}^+$ we find

$$\begin{aligned} A_0^+ &= 1{\cdot}09 \pm 0{\cdot}02 && (\text{BCC}) \\ A_0^+ &= 1{\cdot}105 \pm 0{\cdot}015 && (\text{SC}) \\ A_0^+ &= 1{\cdot}128 \pm 0{\cdot}017 && (\text{D}). \end{aligned} \qquad (4.3)$$

It was found by Sykes *et al* (1972b) that estimates for the specific heat amplitudes on these lattices were not readily extrapolable, the values they gave being derived from the last available coefficient. Thus while they were able to construct good mimic functions, the true amplitudes are probably more accurately given by (4.3).

Turning now to the high-temperature susceptibility series, the leading amplitudes C_0^+ are given in table 1 with the results for the FCC, BCC and SC lattices as quoted by Sykes *et al* (1972a), and that for the diamond lattice as obtained in § 2. In order to attempt to estimate the amplitude of the next most singular term, C_1^+ in the notation of I, we first turn to the FCC lattice. We follow the analysis of Sykes *et al* (1972a) by fitting the susceptibility series to the Darboux form:

$$\frac{kT\chi_0(v)}{m^2} = a(1-v/v_c)^{-\gamma}+b(1-v/v_c)^{1-\gamma}+c(1-v/v_c)^{2-\gamma}. \qquad (4.4)$$

Since the calculation by Sykes *et al* using 13 terms of the susceptibility series, one further term has been added by Rapaport (1974). The resulting estimates of the parameters a, b and c are shown in table 7 using the full 14-term series. The value of v_c quoted in table 1

Table 7. Fitting the FCC susceptibility series to Darboux form (equation (4.4)).

n	a	b	c
7	0·964672	0·11890	0·1329
8	0·964405	0·13225	0·1797
9	0·964047	0·15304	0·2663
10	0·963760	0·17197	0·3578
11	0·963565	0·18640	0·4372
12	0·963442	0·19648	0·4993
13	0·963371	0·20285	0·5428

has been used along with the value $\gamma = \frac{5}{4}$. Linear extrapolants of the 'a' column confirm the estimate of Sykes *et al* (1972a) that $a = 0{\cdot}963 \pm 0{\cdot}002$, while linear extrapolants of the 'b' column suggest $b = 0{\cdot}22 \pm 0{\cdot}02$. These results yield, in the notation of I,

$$C_0^+ = 0{\cdot}971 \pm 0{\cdot}002 \qquad C_1^+ = 0{\cdot}21 \pm 0{\cdot}02. \tag{4.5}$$

Now from the generalized law of corresponding states, assuming it to hold for the next most singular term for the three-dimensional lattices, as it does for the regular two-dimensional lattices, the following (equivalent) results follow:

$$\frac{C_0^+}{C_1^+} = \frac{\text{constant}}{B^{1/\beta}}; \qquad g_{\mathrm{X}}\frac{C_{0,\mathrm{X}}^+}{C_{1,\mathrm{X}}^+} = g_{\mathrm{FCC}}\frac{C_{0,\mathrm{FCC}}^+}{C_{1,\mathrm{FCC}}^+} \tag{4.6}$$

where B is the spontaneous magnetization amplitude. From (4.5) we find the constant in (4.6) to be $16{\cdot}4 \pm 1{\cdot}8$. For the two-dimensional lattices the corresponding constant is exactly 64. If the constant is an integer in the three-dimensional case also, 16 is the most likely contender. However, we see no compelling reason why it *should* be an integer. From the second relation in (4.6) we can estimate the amplitudes C_1^+ for the remaining lattices, and find

$$C_1^+ = 0{\cdot}22 \pm 0{\cdot}03 \ (\text{BCC}), \qquad 0{\cdot}27 \pm 0{\cdot}03 \ (\text{SC}), \qquad 0{\cdot}37 \pm 0{\cdot}04 \ (\text{D}). \tag{4.7}$$

If we write the susceptibility in terms of the usual high-temperature variable $v = \tanh(J/kT)$, so that

$$\frac{kT\chi_0(v)}{m^2} = c_0(1-v/v_c)^{-\gamma} + c_1(1-v/v_c)^{1-\gamma}, \tag{4.8}$$

the amplitudes in (4.7) translate to

$$c_1 = 0{\cdot}25 \pm 0{\cdot}03 \ (\text{BCC}), \qquad 0{\cdot}33 \pm 0{\cdot}04 \ (\text{SC}), \qquad 0{\cdot}55 \pm 0{\cdot}06 \ (\text{D}). \tag{4.9}$$

Now Sykes *et al* (1972a) have obtained a sequence of estimates for c_1 for the BCC and SC lattices, which they state are not sufficiently well converged to establish their limit. Now that we have an estimate of the limit in (4.9), it is instructive to study these sequences. For the BCC lattice the last seven estimates of c_1 are 0·1210, 0·1430, 0·1444, 0·1613, 0·1651, 0·1784, 0·1826. The limit quoted in (4.9) seems quite attainable. For the SC lattice, however, the sequence is considerably more erratic, the last eight estimates being

0·0405, 0·0345, 0·0443, 0·0429, 0·0518, 0·0519, 0·0587, 0·0590. These seem to increase in pairs and are clearly well away from the limit quoted in (4.9). This is possibly due to the more prominent effect of the antiferromagnetic singularity or, perhaps, to other singularities lying outside the physical disc $|v| \leqslant v_c$ or it may even be that the generalized law of corresponding states does not hold for the next most singular term for the three-dimensional lattices.

5. Conclusions

We have studied a number of three-dimensional series and made several new amplitude estimates. These have in turn been used to provide new estimates for the field and temperature scaling parameters which form the basis of the Generalized Law of Corresponding States. An earlier conjecture of Betts *et al* (1971) has been shown to be unlikely. The next most singular Ising susceptibility amplitudes and the specific heat amplitudes have been estimated for the common three-dimensional lattices.

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