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ADDENDUM

The Ising model on the tetrahedron lattice II. Amplitudes and confluent singularities

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Abstract. We have carried out a further analysis of the recently derived 16 term high temperature susceptibility series for the spin 1/2 Ising model on the tetrahedron lattice (crystobalite or B-site spinel lattice). We have found convincing evidence for the asymptotic form

$$\chi = C_0\left(1-\frac{K}{K_c}\right)^{-5/4}+C_1\left(1-\frac{K}{K_c}\right)^{-1/4}+X_0+C_2\left(1-\frac{K}{K_c}\right)^{3/4}+\ldots$$

and have obtained estimates for the amplitudes C_0, C_1, C_2 and X_0. We have also used recent lattice–lattice scaling hypotheses to calculate the specific heat and magnetization amplitudes.

All of the available evidence indicates that the high temperature susceptibility of the spin 1/2 Ising model on all three-dimensional lattices has the asymptotic form

$$\chi = \left(1-\frac{K}{K_c}\right)^{-5/4}C(K)+X(K) \tag{1}$$

where the functions $C(K)$, $X(K)$ are analytic in the disc $|K|\leqslant K_c$. Expanding these functions around K_c leads to the asymptotic form

$$\chi = C_0\left(1-\frac{K}{K_c}\right)^{-5/4}+C_1\left(1-\frac{K}{K_c}\right)^{-1/4}+X_0+C_2\left(1-\frac{K}{K_c}\right)^{3/4}+\ldots. \tag{2}$$

Sykes *et al* (1972) and Guttmann (1975) have attempted to fit existing series for the common three-dimensional lattices to the form (2), with limited success. They find that only the leading amplitude C_0 can be estimated with confidence. We too have attempted to analyse the face-centred cubic lattice series using Padé approximants and have found it impossible to obtain consistent results for the amplitudes or exponents of the higher-order terms in (2).

In a recent paper (Ho-Ting-Hun and Oitmaa 1975, to be referred to as I), we obtained a 16 term high temperature susceptibility series for the spin 1/2 Ising model on a particular three-dimensional lattice which we named the tetrahedron lattice. This is the lattice made up of the B-sites of the crystobalite or spinel structure. It has proved

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possible to analyse the tetrahedron lattice series by means of standard Padé approximant (PA) techniques and the results provide convincing support for the correctness of the asymptotic form (2).

The leading amplitude C_0 can be estimated by forming the PA to the series for $(K-K_c)\chi^{4/5}$ and evaluating these at $K=K_c=0{\cdot}23736$ (the value obtained in I). Some results are shown in table 1, and we make the overall estimate

$$C_0=1{\cdot}1790\pm0{\cdot}0005. \tag{3}$$

Table 1. Estimates of the amplitudes from Padé approximants, as explained in the text.

(N, D)	C_0	C_1	X_0	C_2
(10, 6)	1·1802	−0·1232	−0·0020	−0·0521
(9, 7)	1·1790	−0·1232	−0·0023	−0·0509
(8,8)	1·1790	−0·1232	−0·0020	−0·0518
(7, 9)	1·1790	−0·1232	−0·0026	−0·0534
(6, 10)	1·1794	−0·1233	−0·0023	−0·0517
(9, 6)	1·1789	−0·1232	−0·0026	−0·0586
(8, 7)	1·1790	−0·1232	−0·0024	−0·0526
(7, 8)	1·1789	−0·1231	−0·0025	−0·0522
(6, 9)	1·1789	−0·1231	−0·0025	−0·0523

Note that it is also possible to obtain estimates of C_0 from the PA to $\chi(1-K/K_c)^{5/4}$. This gives results consistent with (3). Throughout the analysis we have used a number of different methods such as this to check the consistency of the results.

The difference series

$$\chi_1\equiv\chi-1{\cdot}179\left(1-\frac{K}{K_c}\right)^{-5/4} \tag{4}$$

should, according to (2), show a singularity at K_c with exponent $-1/4$. In table 2 we show estimates of the position of the singularity and of the exponent obtained from the PA to the logarithmic derivative of the χ_1 series. The results provide strong confirmation of the expected behaviour. Estimates of the amplitude C_1 can be obtained from the PA

Table 2. Estimates of the position of the singularity and the exponent for the second and third most singular terms, as explained in the text.

	Series χ_1		Series χ_3	
(N, D)	Position	Exponent	Position	Exponent
(9, 6)	0·2379	−0·253	0·2374	0·895
(8, 7)	0·2382	−0·252	0·2371	0·898
(7, 8)	0·2372	−0·252	0·2371	0·896
(6, 9)	0·2372	−0·252	0·2337	0·894
(8, 6)	0·2389	−0·255	0·2375	0·895
(7, 7)	0·2386	−0·252	0·2370	0·895
(6, 8)	0·2366	−0·252	0·2378	0·894
Expected	0·23736	−0·25	0·23736	0·75

to $(K-K_c)\chi_1^4$ evaluated at $K=K_c$. The results are shown in table 1. The overall estimate is

$$C_1=-0{\cdot}123\pm0{\cdot}001. \quad (5)$$

We then 'subtract off' this term, i.e. we form the series for

$$\chi_2\equiv\chi-1{\cdot}179\left(1-\frac{K}{K_c}\right)^{-5/4}+0{\cdot}123\left(1-\frac{K}{K_c}\right)^{-1/4}=X_0+C_2\left(1-\frac{K}{K_c}\right)^{3/4}. \quad (6)$$

The constant term X_0 can be estimated from the PA to this series, evaluated at $K=K_c$. The results, shown in table 1, are somewhat irregular. We make the overall estimate

$$X_0=-0{\cdot}002\pm0{\cdot}0005. \quad (7)$$

Finally we subtract off the constant term. The remaining series

$$\chi_3\equiv\chi-1{\cdot}179\left(1-\frac{K}{K_c}\right)^{-5/4}+0{\cdot}123\left(1-\frac{K}{K_c}\right)^{-1/4}+0{\cdot}002=C_2\left(1-\frac{K}{K_c}\right)^{3/4} \quad (8)$$

should show a singularity at K_c with exponent 3/4. From the PA to the logarithmic derivative series we obtain the results shown in table 2. The position of the singularity is given accurately but the exponent at about 0·89 is higher than expected. However, these results are quite sensitive to the choice of values for C_1 and particularly X_0. By varying these within the error estimates quoted it is possible to fit the exponent values to 0·75 at the expense of a worse fit to K_c. From the PA to $(K-K_c)\chi_3^{-4/3}$ we obtain estimates of the amplitude C_2. These are shown in table 1 and our overall estimate is

$$C_2=-0{\cdot}052\pm0{\cdot}005. \quad (9)$$

The lattice–lattice scaling hypothesis (Betts *et al* 1971) enables one to relate the critical amplitudes of systems in the same universality class, e.g. for any two three-dimensional Ising lattices X and Y. In particular the susceptibility amplitudes are related by

$$\frac{C_X}{C_Y}=\frac{n_X}{n_Y}\left(\frac{g_X}{g_Y}\right)^{-5/4} \quad (10)$$

and the specific heat amplitudes by

$$\frac{A_X}{A_Y}=\frac{n_Y}{n_X}\left(\frac{g_X}{g_Y}\right)^{15/8} \quad (11)$$

where n_X, g_X, n_Y and g_Y are the universality scale factors. Using (10) and the one-scale-factor universality hypothesis (Betts and Ritchie 1975), we obtain the results

$$\frac{g_X}{g_Y}=\left(\frac{C_X}{C_Y}\right)^4\left(\frac{q_XK_{cX}}{q_YK_{cY}}\right)^6\left(\frac{\rho_X}{\rho_Y}\right)^2 \quad (12)$$

and

$$\frac{n_X}{n_Y}=\left(\frac{C_X}{C_Y}\right)\left(\frac{g_X}{g_Y}\right)^{5/4} \quad (13)$$

where the q are coordination numbers and the ρ are geometrical density factors.

We take as our reference lattice the face-centred cubic (F) so that $n_F = g_F = 1$ and use the estimate $C_F = 0{\cdot}972$ (Domb 1974) and our amplitude value (3). This yields the results

$$g_T = 1{\cdot}336, \qquad n_T = 1{\cdot}742 \tag{14}$$

for the universality scale factors of the tetrahedron lattice (T). Equation (11) then gives

$$A_T = 1{\cdot}076 \tag{15}$$

using the value $A_F = 1{\cdot}089$ (Domb 1974), for the specific heat amplitude of the tetrahedron lattice.

A 19 term specific heat series for the tetrahedron lattice was derived by Gibberd (1970). If we assume the asymptotic form

$$C_T = A\left(1 - \frac{K}{K_c}\right)^{-1/8} + a \tag{16}$$

we can then subtract off the singular term, and obtain estimates for the constant term a. We have done this and find that

$$a = -1{\cdot}09 \pm 0{\cdot}01. \tag{17}$$

We have also used the lattice–lattice scaling hypothesis results to obtain values for the amplitudes B and D in the expressions for the magnetization in zero field $m = B[1-(T/T_c)]^{\beta}$ and along the critical isotherm $m = D^{-1/\delta}h^{1/\delta}$. Using the values $B_F = 1{\cdot}487$, $D_F = 0{\cdot}715$ (Domb 1974) we find

$$B_T = 1{\cdot}628 \qquad D_T = 0{\cdot}410. \tag{18}$$

An extension of lattice–lattice scaling to apply to the second most singular part of the Ising model susceptibility (Guttmann 1974, Ritchie and Betts 1975) appears to be valid for a number of two-dimensional lattices, but has not been conclusively tested in three dimensions. If this hypothesis were valid it would relate the amplitudes of the second most singular terms according to

$$C_{1T} = C_{1F} n_T g_T^{-1/4}$$

which, using the value $C_{1F} = 0{\cdot}1968$ given by Sykes *et al* (1972) yields a value $C_{1T} = 0{\cdot}319$ compared with our direct estimate $C_{1T} = -0{\cdot}123 \pm 0{\cdot}001$. It is thus clear that this 'extended universality', at least in its present form, is not in general valid for the three-dimensional Ising model.

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