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Series expansions for the zero-temperature transverse Ising model

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Abstract. Series expansions are presented for the magnetisation, susceptibility, magnetic field derivatives of the susceptibility and 'specific heat' of the zero-temperature transverse Ising model. Coefficients in these series have been calculated to tenth order in λ^2 (where λ is the transverse field) for the linear chain, to eighth order for the square lattice and to seventh order for the triangular lattice. These series yield estimates of the low-temperature critical exponents α', β, γ' and Δ' of the two- and three-dimensional Ising models. They provide good evidence for the symmetry of exponents above and below the critical point, e.g. $\gamma' = \gamma$.

1. Introduction

There exists a correspondence between the d-dimensional transverse Ising model at zero temperature and the $(d+1)$-dimensional Ising model (Pfeuty 1970, Suzuki 1976). This correspondence is well known for spin-$\frac{1}{2}$ and has been extended by Oitmaa and Coombs (1981) to the spin-1 case. For spin-$\frac{1}{2}$ the relation between the two models is most clearly seen by considering the transfer matrix of the Ising model in an extremely anisotropic limit of the exchange couplings (Kogut 1979). The ground-state energy, E_0, of the quantum mechanical system is related to the free energy of the $(d+1)$-Ising system. In addition, the mass gap of the quantum model (the difference in energy between the first excited state and the ground state) is related to the inverse correlation length of the Ising model. This is an example of a more general correspondence between a statistical mechanical system and an appropriate quantum model which is discussed in Kogut (1979).

The spin-$\frac{1}{2}$ transverse Ising model is described by the Hamiltonian

$$H = \sum_{\langle ij \rangle} (1 - \sigma_i^z \sigma_j^z) + h \sum_i (1 - \sigma_i^z) + \lambda \sum_i \sigma_i^x \qquad (1)$$

where the σ_i^α are Pauli spin operators and $\langle ij \rangle$ denotes nearest-neighbour bonds. At finite temperature this model has a number of physical applications (Stinchcombe 1972) but this work is concerned only with the zero-temperature limit. At $T = 0$ the ground state has two phases: a broken symmetry phase at small λ and a disordered phase for large λ. There is a second-order phase transition between the two regimes at $\lambda = \lambda_c$. In one dimension the ground-state energy and magnetisation are known exactly (Pfeuty 1970). The transition occurs at $\lambda_c = 1$. This zero-temperature phase transition

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has also been studied in one and two dimensions by series methods (Pfeuty and Elliott 1971, Elliot *et al* 1970, Yanase *et al* 1976) and the real space renormalisation group (Jullien *et al* 1978, Penson *et al* 1979).

The inclusion of a parallel magnetic field in (1) facilitates the calculation of the magnetisation, $M=-\mathrm{d}E_0/\mathrm{d}h|_{h=0}$, susceptibility $\chi=\mathrm{d}^2E_0/\mathrm{d}h^2|_{h=0}$ and further field derivatives. The 'specific heat' is given by $-\mathrm{d}^2E_0/\mathrm{d}y^2$ (where $y=\lambda^{-1}$) as suggested by Barber (Hamer and Kogut 1979). Series expansions for these quantities are presented for the linear chain and the square and triangular lattices.

Series for the mass gap are not presented because the method of derivation uses a linked cluster expansion which restricts the study to extensive quantities. In one dimension the mass gap is known to be simply proportional to $(1-\lambda)$ as shown by Hamer *et al* (1979). The mass gap series has also been calculated for general d by Pfeuty and Elliott (1971) and Sobel'man (1980).

In the following section the method of calculation is outlined. Section 3 discusses the results in one dimension and §4 is concerned with the series for the two-dimensional lattices.

2. Derivation of the series

Series expansions for the zero-temperature spin-$\frac{1}{2}$ transverse Ising model may be obtained using perturbation theory (Pfeuty and Elliott 1971, Hamer and Kogut 1979). In addition high-temperature series for the susceptibility have been calculated which can treat both the finite-temperature and zero-temperature transitions, thus investigating the crossover behaviour (Elliott *et al* 1970, Yanase *et al* 1976).

The new feature employed in this work is a linked cluster expansion (Nickel 1980). In generating the series expansion for the ground-state energy, E_0, in the ordered regime, terms arise from one spin flip, two spin flips, etc. The expression for E_0 may be rearranged as an expansion of the form

$$E_0=\sum_{m=1}^{N}\sum_{\alpha_m} C_{m,\alpha_m}\varepsilon_{m,\alpha_m} \tag{2}$$

where the C_{m,α_m} are constants and ε_{m,α_m} is the ground-state energy of m spins in configuration α_m. The perturbation expression for each ε_{m,α_m} contains at least one power of $\lambda\sigma_i^x$ for every site i in the cluster g_{m,α_m}. Further, for any finite cluster

$$E_0^{i,\alpha_i}=\sum_{j=1}^{i}\sum_{\alpha_j} C_{j,\alpha_j}^{i,\alpha_i}\varepsilon_{j,\alpha_j}. \tag{3}$$

If a graph, g_{p,α_p}, consists of two disconnected pieces containing q and r spins then $H_{p,\alpha_p}=H_{q,\alpha_q}\oplus H_{r,\alpha_r}$ and $E_0^{p,\alpha_p}=E_0^{q,\alpha_q}+E_0^{r,\alpha_r}$. There is then no contribution to ε_{p,α_p} and only connected graphs need be included in the expressions of (2) and (3).

The C_{m,α_m} and $C_{j,\alpha_j}^{i,\alpha_i}$ are lattice constants. The form of the perturbation in (1) requires that they be the strong embedding constants. They are given by the number of ways in which a graph, g_{m,α_m}, may be embedded on the lattice under consideration subject to the constraint that sites in the cluster can only be nearest neighbours when embeddded if they are also neighbours in the free cluster. For convenience the C_{m,α_m} are defined per site. To give an example, the strong embedding constant for a chain of four spins embedded on the square lattice is 14. In terms of graph theory (Domb 1974a)

$$C_{m,\alpha_m} = [g_{m,\alpha_m}; \mathscr{L}]$$
$$C^{i,\alpha_i}_{j,\alpha_j} = [g_{j,\alpha_j}; g_{i,\alpha_i}] \tag{4}$$

where $\mathscr{L}$ is the lattice. These graphs and lattice constants are also used to determine the density expansions for an Ising model in a field (Domb 1974b). Reproduction of those series served as a check on the calculation.

The Hamiltonian matrix for a given cluster has a tridiagonal form if the basis is chosen to be the unsymmetrised set of states with zero spin flips, one flip, two flips etc from the unperturbed ground state with all spins aligned. For a cluster of m spins it has the form

$$\begin{pmatrix} 0 & \lambda V_1 & & & \\ \lambda V_1^{\perp} & U_1 & \lambda V_2 & & \\ & \lambda V_2^{\perp} & U_2 & & \\ & & & \ddots & \\ & & & & U_m \end{pmatrix} \tag{5}$$

The U_j are diagonal matrices with entries of the form $a + bh$. Each entry in V_j is either 0 or 1. The perturbed ground-state energy is obtained by recursion, for which the U_j^{-1} are required. At this point only L powers of h are retained. The U_j are stored in a linear array with dimension $(2^m - 1)(L + 1)$. The array for the V_j has dimension $m \times 2^{m-1}$. Series are thus generated for the E_0^{i,α_i} to λ^{2N} where N is defined in (2). It follows from the structure of (5) that the series are even in λ. The series expansion for E_0 is then obtained using (2) and (3). The coefficients of this series in $x = \lambda^2$ are themselves expansions in h to h^L. Series expansions for C, M, χ, and $\mathrm{d}^n\chi/\mathrm{d}h^n$ $(n \leqslant L-2)$ are thus generated which yield estimates of the low-temperature critical exponents for the Ising model in $d+1$.

In the disordered, large λ, regime the ground-state energy is even in h, odd in λ. A linked cluster expansion may be used to generate an expansion for E_0 in λ^{-1}. The graphs considered in (2) and (3) would then contain m bonds and the constants in those expansions would become the *weak* embedding constants. The form of the Hamiltonian matrix for a cluster in this perturbation scheme is somewhat different from (5) and the calculation of E_0^{i,α_i} by recursion more complex.

3. One dimension (1+1)

In one dimension (3) reduces to the simple form

$$E_0^p = \sum_{i=1}^{p} (p - i + 1)\varepsilon_i \tag{6}$$

and to order x^j: $E_0 = E_0^j - E_0^{j-1}$. The series have been calculated to tenth order in x. To this order, the expansions for E_0 (and hence C) and M agree with the exact expressions of Pfeuty (1970).

The expansions for χ and its first and second derivative with respect to h are given in table 1. Ratio analyses of these series are shown in figures 1 and 2. The ratio method (for a review, see Gaunt and Guttmann 1974) assumes that the function approximated

Table 1. Series expansion coefficients for one dimension. The expansion parameter is $x = \lambda^2$, with λ defined in (1).

Order	χ	$-d\chi/dh$	$d^2\chi/dh^2$
0	0.125 000 E0	0.187 500 E0	0.375 000 E0
1	0.203 125 E0	0.867 188 E0	0.428 906 E1
2	0.271 484 E0	0.224 561 E1	0.201 211 E2
3	0.334 412 E0	0.450 101 E1	0.630 992 E2
4	0.393 572 E0	0.779 133 E1	0.156 578 E3
5	0.449 886 E0	0.122 611 E2	0.333 135 E3
6	0.503 931 E0	0.180 447 E2	0.635 557 E3
7	0.556 104 E0	0.252 689 E2	0.111 773 E4
8	0.606 690 E0	0.340 538 E2	0.184 545 E4
9	0.655 904 E0	0.445 146 E2	0.289 722 E4

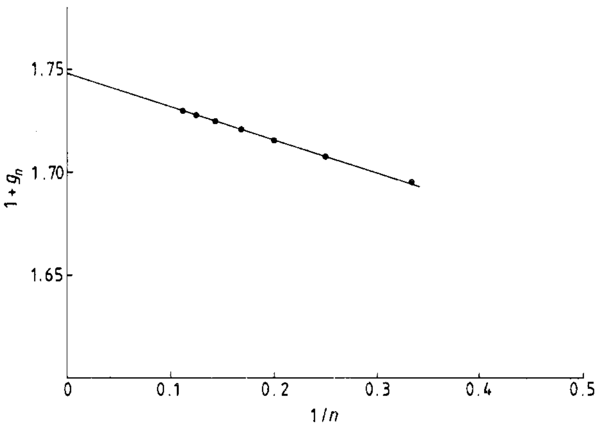

Figure 1. Plot of $1+g_n$ against $1/n$ for the series for χ in one dimension.

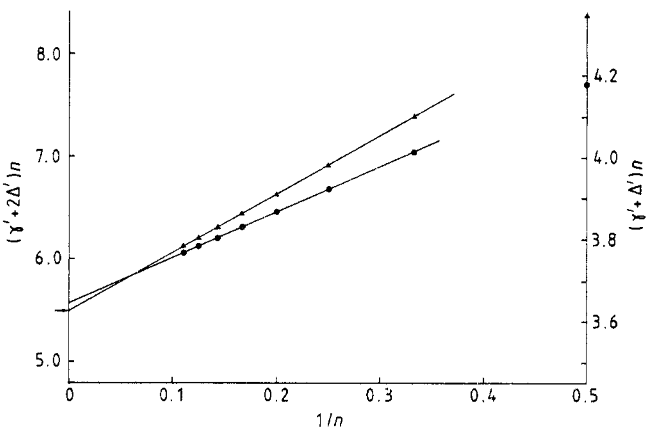

Figure 2. Plots of $1+g_n$ against $1/n$ for the $d\chi/dh$ and $d^2\chi/dh^2$ series in one dimension, represented by closed circles and triangles respectively.

by the power series

$$F_s(x)=\sum_{n=0}^{N} b_n x^n \tag{7}$$

has a power law form

$$F(x)=A(x-x_c)^{-\gamma} \tag{8}$$

from which it follows that the ratio of successive coefficients will be

$$R_n=\frac{b_n}{b_{n-1}}=\frac{1}{x_c}\left(1+\frac{\gamma-1}{n}+O(n^{-2})\right). \tag{9}$$

The sequence

$$g_n=n(R_n x_c-1) \tag{10}$$

then provides estimates to $\gamma-1$ if x_c is known.

The ratio plot for γ' shown in figure 1 uses (10) and the value of the critical point, $x_c=\lambda_c^2=1$. The extrapolation gives an estimate of $\gamma'=1.748\pm0.002$. Similar ratio plots for the exponents of $d\chi/dh$ and $d^2\chi/dh^2$ are shown in figure 2. The field derivatives of the susceptibility are believed to diverge from below the critical point as

$$\frac{d^n\chi}{dh^n}\sim(x-x_c)^{-\gamma'-n\Delta'} \tag{11}$$

where Δ' is the low-temperature gap exponent (Essam and Hunter 1968). The ratio plots in figure 2 yield the estimates: $\gamma'+\Delta'=3.63\pm0.01$; $\gamma'+2\Delta'=5.50\pm0.02$. The arrow marks the intercept expected if the scaling form of equation (11) were satisfied with $\Delta'=1.875$, $\gamma'=1.750$.

The method of Padé approximants is widely used in the determination of critical points and exponents. For a function of the form of $F(x)$ in (8), the Dlog Padé approximant

$$\frac{1}{F_s}\frac{dF_s}{dx}=\frac{P_N(x)}{Q_M(x)}=[N/M] \tag{12}$$

provides an estimate of $-\gamma/(x-x_c)$ from the series $F_s(x)$. $P_N(x)$ and $Q_M(x)$ are polynomials of degree N and M respectively. These approximants may also be biased with the known value of x_c. The $[N/M]$ Padé approximants to $(x-x_c)(1/F)\,dF/dx$, with $F=\chi$, $d\chi/dh$ and $d^2\chi/dh^2$, are given in tables 2–4. The convergence is extremely

Table 2. $[N/M]$ biased Dlog Padé approximants to the series for χ on the linear chain.

$N\backslash M$	1	2	3	4	5	6	7
2	1.7418	1.7436	1.7465	1.7476	1.7483	1.7487	1.7490
3	1.7436	1.7353	1.7478	1.7493	1.7489	1.7496	
4	1.7463	1.7478	1.7486	1.7490	1.7491		
5	1.7474	1.7492	1.7490	1.7500			
6	1.7482	1.7489	1.7491				
7	1.7486	1.7495					
8	1.7490						

Table 3. As table 2 for $d\chi/dh$. An asterisk indicates a defect.

$N\backslash M$	1	2	3	4	5	6	7
2	3.6295	3.6345	3.6252	3.6252	3.6251	3.6251	3.6251
3	3.6345	3.6313	3.6252	3.6252*	3.6251	3.6251	
4	3.6256	3.6251	3.6251	3.6251	3.6250		
5	3.6251	3.6251	3.6252	3.6251			
6	3.6251	3.6251	3.6251				
7	3.6251	3.6251					
8	3.6251						

Table 4. As table 2 for $d^2\chi/dh^2$.

$N\backslash M$	1	2	3	4	5	6	7
2	5.8466	5.4204	5.5175	5.4955	5.5016	5.4998	5.5000
3	5.3588	5.4989	5.4995	5.5002	5.5002	5.5000	
4	5.5550	5.4995	5.4964	5.5002	5.5003*		
5	5.4776	5.5003	5.5002	5.5000			
6	5.5097	5.5002	5.5003*				
7	5.4962	5.5000					
8	5.5015						

good, yielding the estimates

$$\gamma' = 1.750 \pm 0.001$$

$$\gamma' + \Delta' = 3.6250 \pm 0.0001$$

$$\gamma' + 2\Delta' = 5.5000 \pm 0.0002$$

and hence

$$\Delta' = 1.875 \pm 0.001.$$

The agreement with the value of 1.87 ± 0.01 found for Δ, the high-temperature gap exponent, by Essam and Hunter (1968), is excellent. These estimates and the exact value for β of 0.125 provide good evidence for the scaling relations

$$\Delta' = \Delta \qquad \gamma' = \gamma \qquad \Delta' = \beta + \gamma'.$$

4. Two dimensions (2+1)

It is convenient to calculate the series in two dimensions from the Hamiltonian

$$H = \frac{1}{4} \sum_{\langle ij \rangle} (1 - \sigma_i^z \sigma_j^z) + \frac{h}{2} \sum_i (1 - \sigma_i^z) + \lambda \sum_i \sigma_i^x. \tag{13}$$

The series obtained for the square lattice are given in table 5. The first four terms of the magnetisation series were previously calculated by Pfeuty and Elliott (1971). They are somewhat less regular than those obtained in one dimension. In particular the ratios

Table 5. Series expansion coefficients for the square lattice. The expansion parameter is $x=\lambda^2$, with λ defined in (10).

Order	C	M	χ	$-d\chi/dh$	$d^2\chi/dh^2$
0	0.300 000 E1	0.500 000 E0	0.250 000 E0	0.375 000 E0	0.750 000 E0
1	0.833 333 E0	−0.250 000 E0	0.606 481 E0	0.227 546 E1	0.950 540 E1
2	0.437 500 E0	−0.173 611 E0	0.108 464 E1	0.738 256 E1	0.510 040 E2
3	0.942 708 E0	−0.146 701 E0	0.222 461 E1	0.223 647 E2	0.221 627 E3
4	0.613 644 E0	−0.202 286 E0	0.387 519 E1	0.557 043 E2	0.755 279 E3
5	0.168 294 E1	−0.225 083 E0	0.746 816 E1	0.137 719 E3	0.238 096 E4
6	0.939 918 E0	−0.348 168 E0	0.126 702 E2	0.303 987 E3	0.661 903 E4
7	0.406 439 E1	−0.416 851 E0	0.242 430 E2	0.689 220 E3	0.179 347 E5
8	—	−0.719 441 E0	—	—	—

show considerable fluctuations which can be attributed to the presence of an antiferromagnetic singularity. The analysis of these series is thus based on the method of Padé approximants.

The estimates for β and x_c found from the $[N/M]$ Dlog Padé approximants are given in table 6. The approximants clearly favour a value of 0.578 for x_c. Padé approximants to the other series in table 5 do not have such convergent behaviour. There exists an independent estimate of x_c from the susceptibility series calculated by Yanase *et al* (1976). Their ratio analysis indicates a value for x_c close to 0.579. Figure 3 shows the variation with x_c of the estimates of α', β and γ' obtained from the highest-order biased Dlog Padé approximants. If the Rushbrooke relation between the exponents

$$\alpha'+2\beta+\gamma'\geqslant 2 \tag{14}$$

is used to determine x_c, then the estimates in figure 3 indicate a value of 0.580 at which the equality in (14) is satisfied. The critical point is thus estimated as being

$$x_c=0.579\pm0.001.$$

Taking the band of estimates of figures 3 and 4 in this more limited region gives the

Table 6. $[N/M]$ Dlog Padé approximants to the series for the magnetisation on the square lattice. The first entry is the estimate for β, the second the estimate for x_c.

N\M	1	2	3	4	5	6
1	0.362	0.299	0.298	0.301	0.312	0.311
	0.619	0.574	0.573	0.574	0.578	0.578
2	0.233	0.298	0.299	0.296*	0.311	
	0.534	0.573	0.573	0.572	0.578	
3	0.393	0.301	0.296*	0.300*		
	0.609	0.574	0.572	0.574		
4	0.230	0.311	0.310			
	0.547	0.578	0.578			
5	0.455	0.310				
	0.613	0.578				
6	0.193					
	0.542					

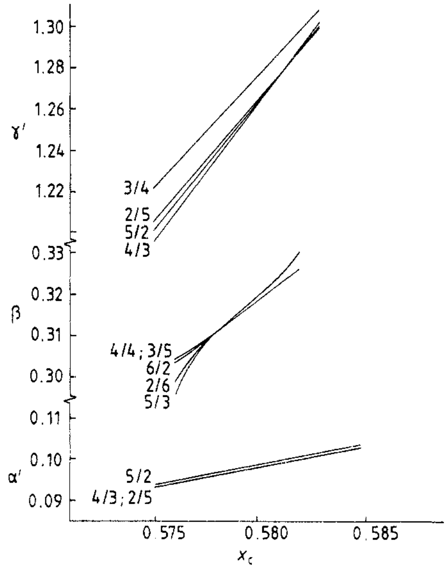

Figure 3. Highest-order Padé approximant exponent estimates from the C, M and χ series on the square lattice. They are plotted against the value of x_c used to bias the approximant.

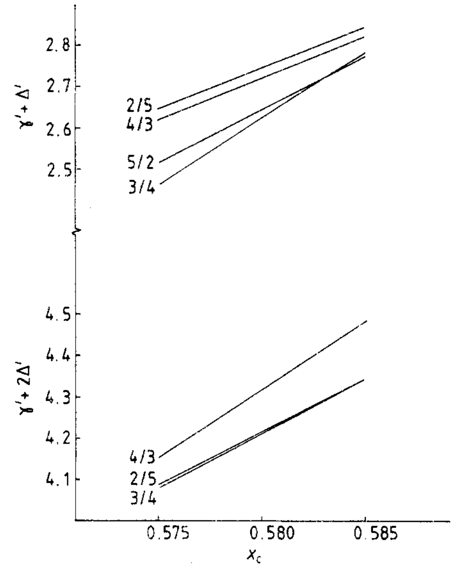

Figure 4. As figure 3 from the series for $d\chi/dh$ and $d^2\chi/dh^2$ on the square lattice.

following exponent estimates:

$$\alpha' = 0.097 \pm 0.001 \qquad \beta = 0.315 \pm 0.005 \qquad \gamma' = 1.25 \pm 0.02$$

$$\gamma' + \Delta' = 2.65 \pm 0.10 \qquad \gamma' + 2\Delta' = 4.24 \pm 0.10.$$

The last two estimates are consistent with

$$\Delta' = 1.5 \pm 0.2.$$

Series expansions have been calculated for the triangular lattice to seventh order in x (see table 7). (The number of graphs required is approximately ninety, which is similar to the number required for the square lattice series to eighth order.) These series appear to be better behaved; they do not have an antiferromagnetic singularity due to the close packed nature of the lattice. They are not as well behaved as those for the

Table 7. As table 5 for the triangular lattice.

Order	C	M	χ	$-d\chi/dh$	$d^2\chi/dh^2$
0	0.200 000 E1	0.500 000 E0	0.740 741 E-1	0.740 741 E-1	0.987 654 E-1
1	0.148 148 E0	−0.111 111 E0	0.596 543 E-1	0.147 305 E0	0.400 298 E0
2	0.671 605 E-1	−0.251 852 E-1	0.487 608 E-1	0.209 663 E0	0.921 627 E0
3	0.290 448 E-1	−0.107 437 E-1	0.373 911 E-1	0.244 223 E0	0.155 690 E1
4	0.151 504 E-1	−0.507 865 E-2	0.280 505 E-1	0.254 847 E0	0.219 445 E1
5	0.835 498 E-2	−0.263 893 E-2	0.207 222 E-1	0.247 442 E0	0.274 286 E1
6	0.522 291 E-2	−0.144 522 E-2	0.153 204 E-1	0.230 120 E0	0.316 573 E1
7	—	−0.838 931 E-3	—	—	—

linear chain, though, as is most clearly seen from the series for $\mathrm{d}\chi/\mathrm{d}h$. Hence the analysis of these series is also based on the Padé approximant method.

The estimates for β and x_c on the triangular lattice are shown in table 8. Figure 5 shows a plot of α', β and γ' obtained from biased Dlog Padé approximants and their variation with the value of x_c chosen. The susceptibility series of Yanase *et al* (1976) for the triangular lattice suggests a value for x_c of 1.4195 from ratio analysis and 1.4206 from a Padé analysis. Thus

$$x_c = 1.420 \pm 0.001.$$

Equation (14) is satisfied for x_c greater than 1.420. Estimates for the exponents may then be read from figure 5 as before. They are

$$\alpha' = 0.098 \pm 0.003 \qquad \beta = 0.315 \pm 0.002 \qquad \gamma' = 1.250 \pm 0.012.$$

A similar analysis of the series for $\mathrm{d}\chi/\mathrm{d}h$ yields

$$\Delta' + \gamma' = 2.70 \pm 0.15.$$

Table 8. As table 6 for the triangular lattice.

N \ M	1	2	3	4	5
1	0.285 1.377	0.300 1.403	0.314 1.419	0.324 1.426	0.312* 1.418
2	0.307 1.412	0.311 1.416	0.321 1.424	0.315* 1.420	
3	0.310 1.416	0.326 1.390	0.312* 1.418		
4	0.315 1.420	0.311* 1.417			
5	0.302 1.410				

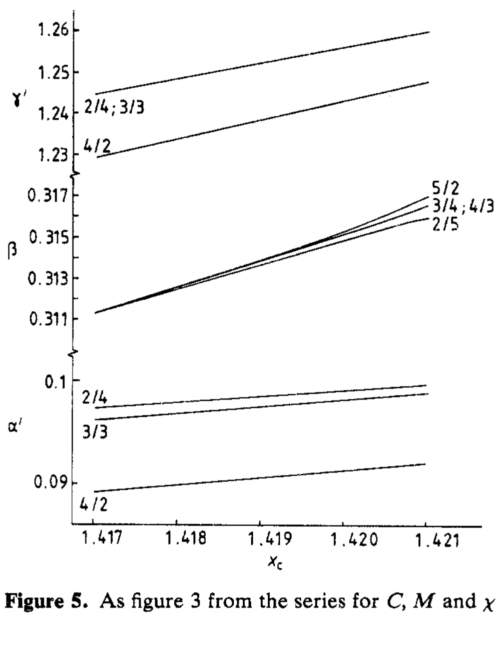

Figure 5. As figure 3 from the series for C, M and χ on the triangular lattice.

The consistency of these values with the estimates from the series on the square lattice is very encouraging. It should be noted though that, as shown for the magnetisation series in table 8, almost all the highest-order approximants have defects.

5. Conclusions

High-temperature series for the Ising model have yielded quite accurate determinations of the critical exponents. The low-temperature series, however, are quite irregular and do not give exponents to the same accuracy (for a review, see Domb 1974b). The symmetry of the critical exponents above and below the critical point has thus been in question. The results here presented provide good evidence for such a symmetry, in particular

$$\gamma' = \gamma \qquad \Delta' = \Delta.$$

The accurate determination of critical exponents by the renormalisation group method (Le Guillou and Zinn-Justin 1977) assumes this symmetry.

The series presented are also of interest as they may be investigated using the ratio method. Ratio plots for the series on the two-dimensional lattices have not been presented. They require a change of variable to $z = x/(x+a)$, an Euler transformation, where a is some constant. The results from these plots are consistent with the Padé approximant analysis but somewhat less accurate.

The estimates presented for α' require a further comment. Analysis of series for d^2E_0/dx^2 on the two-dimensional lattices, which should also diverge at the critical point with exponent α', suggest a value close to 0.2. This may be explained by the presence of a background term which is implicitly generated and which considerably affects the estimate of such a small exponent. This type of series may be analysed by a generalisation of the Padé approximant method (Fisher and Au-Yang 1979). Unfortunately a sufficient number of coefficients is not presently available.

The series expansions presented for the derivatives of the susceptibility support the conclusions of Essam and Hunter (1968). The two-dimensional Ising gap exponent is now known to somewhat better accuracy. The estimate for the three-dimensional Ising exponent Δ' is lower than the value found for Δ by Essam and Hunter. Their estimate for Δ' was on the high side with a similar error to that quoted here.

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