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LETTER TO THE EDITOR

Low temperature Ising model series and the ratio method

C J Pearce† and M J Buckingham
University of Western Australia, Nedlands, Western Australia, 6009

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Abstract. A transformation is applied to low temperature series for the FCC Ising model, which enables the ratio method to be used in their extrapolation, and apparently more precise estimates to be made of the critical exponents than hitherto. These estimates are consistent with the scaling value of $\alpha' = 1/8$, and strongly favour the value of $\gamma' = 5/4$ over the previous estimates of around 1·28; they thus counter previous evidence for a possible violation of scaling in this model.

The low temperature series for the three-dimensional Ising model have long presented difficulty in extrapolation. An outline of the problems involved is given in, for example, the article by Guttmann *et al* (1970). No direct ratio analysis is possible because the series do not in general converge up to the physical singularity, and Padé analysis has suggested values of the critical exponents which appear to be at variance with scaling predictions. In particular, for the cubic lattices the Padé estimates for the susceptibility exponent γ' lie typically in the range $1{\cdot}28 \pm 0{\cdot}03$ instead of around the expected scaling value of 1·25, and the estimates for the specific heat exponent α' are generally about 0·2 or higher, as against the accepted scaling value of 0·125. Clearly an alternative means of estimating the exponents is desirable. Guttmann *et al* (1970) applied various transformations to the series and were successful in obtaining new series which converged up to the critical singularity; unfortunately the non-physical singularities were too close to the circle of convergence for the coefficients to be extrapolated by the ratio method.

We report a new analysis based on a systematic choice of the transformation function. We have developed a method for such choice (Pearce 1975) which makes full use of the details of the singularity distribution of the original function (so far as this can be determined from Padé analysis). Using this method we obtain transformed series which are apparently dominated by the physical singularity and yield smooth ratio sequences. We here confine our attention to the low temperature series for the FCC lattice since the published series for this lattice are sufficiently long for the asymptotic behaviour of the coefficients to be fairly well determined.

The expansion variable for the low temperature Ising series is $z = \exp(-4J/kT)$ where J is the spin–spin interaction energy, k Boltzmann's constant and T the temperature. An indication of the distribution of singularities in the z-plane for the thermodynamic functions may be obtained from Padé analysis, and was calculated by Guttmann (1969) who used the method of N-point fits. The physical singularity occurs

† Present address: Wheatstone Physics Laboratory, King's College, Strand, London WC2R 2LS, UK.

at $z_c \simeq 0{\cdot}6647$ and the non-physical singularities at $z_a, z_a^* \simeq a$, $a^* = 0{\cdot}0725 \pm 0{\cdot}533\mathrm{i}$ and at $z_b, z_b^* \simeq b$, $b^* = -0{\cdot}446 \pm 0{\cdot}28\mathrm{i}$. In the present approach the transformation to a new variable $u = u(z)$ was chosen so as to have the following properties: $|u(z)|$ large in the neighbourhoods of z_a, z_a^*, z_b, z_b^*; $u(z)$ real and monotonically increasing from zero along the positive real axis; and $u(z)$ analytic with $\mathrm{d}u/\mathrm{d}z$ non-zero for all z within the contour in the z-plane defined by $|u(z)| = u(z_c)$ and which encloses the origin. The function chosen was

$$u = z/[(1-z/a)(1-z/a^*)(1-z/b)(1-z/b^*)]^{1/5}.$$

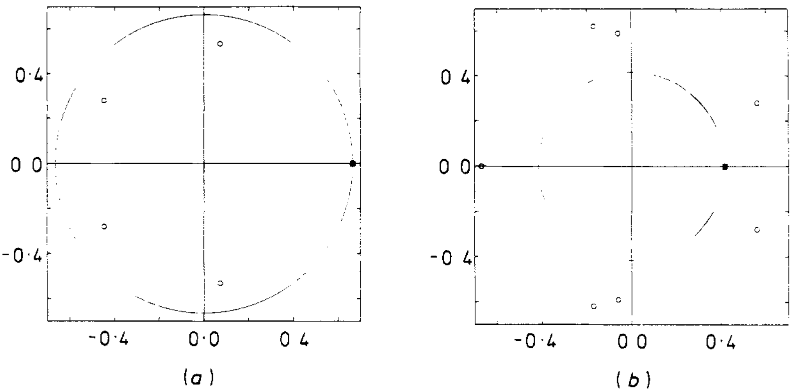

Figure 1. Distribution of singularities in the complex plane of the expansion variable: (*a*) before and (*b*) after the transformation. ■ indicates the physical singularity and ⊙ a non-physical singularity. The circle indicates the so called 'physical disc'.

Given the uncertainties in the locations of the non-physical singularities, it is possible to say only that these singularities are mapped somewhere outside the circle $|u| = 2{\cdot}0$ in the u-plane. The inverse function $z(u)$ will also have a number of singularities in this plane, the approximate locations of which are most conveniently determined by Padé analysis. It is found that these are a distance from the origin comparable to (but larger than) that of u_c: thus the transformation effectively replaces the original non-physical singularities with a set arising from the transformation function itself. The physical singularity is mapped to $u_c \simeq 0{\cdot}416$, the next-nearest singularity in the u-plane being at a distance of approximately $1{\cdot}4u_c$ from the origin, which suggests that the ratio method might be usefully employed. The singularity distributions before and after the transformation are shown in figure 1. For this transformation $(\mathrm{d}u/\mathrm{d}z)_{z_c} \simeq 0{\cdot}33$, and the dominant singular form of the physical singularity is preserved. Both the susceptibility and specific heat series, taken from Sykes *et al* (1965, 1973), begin with z^6, and the actual series transformed were those for

$$z^{-6}\chi(z)/4 \qquad \text{and} \qquad z^{-6}C_H(z)/k(\ln z)^2.$$

Since z_c is known from the high temperature series to a much greater precision than that obtainable from the present series, we have plotted for the transformed series sequences of exponent estimates rather than the ratios. Specifically we have used (see Hunter and Baker 1973)

$$\gamma_n'(r) = 1 + n(u_c r_n - 1) = \gamma' + \mathrm{O}(1/n)$$

and the corresponding quantity $\alpha_n'(r)$ for the specific heat exponents, where r_n are the ratios of successive coefficients. In addition, a sequence of exponent estimates was obtained from the logarithmic derivative of the transformed series:

$$\gamma_n'(\mathrm{ld}) = b_n u_c^{n+1}$$

where b_n are the coefficients of this series. The exponent estimate sequences are given for $n \geq 10$ in table 1, and are shown plotted against $1/n$ in figure 2.

Table 1. Sequences of exponent estimates $\alpha_n'(r)$, $\alpha_n'(\mathrm{ld})$, $\gamma_n'(r)$ and $\gamma_n'(\mathrm{ld})$ with $n \geq 10$ for the specific heat and the susceptibility.

n	$\alpha_n'(r)$	$\alpha_n'(\mathrm{ld})$	$\gamma_n'(r)$	$\gamma_n'(\mathrm{ld})$
10	1·1403	0·6322	1·7893	1·2988
11	0·3403	0·5672	1·1911	1·2844
12	0·2226	0·5078	1·1309	1·2735
13	0·2470	0·4614	1·2174	1·2824
14	0·2063	0·3983	1·2349	1·2453
15	0·0275	0·3719	1·1612	1·2457
16	−0·0038	0·3459	1·1792	1·2451
17	−0·0273	0·3260	1·2032	1·2496
18	−0·0771	0·3068	1·2042	1·2454
19	−0·1348	0·2946	1·1992	1·2485
20	−0·1560	0·2833	1·2100	1·2517
21	−0·1787	0·2745	1·2174	1·2558
22	−0·2058	0·2666	1·2194	1·2578
23	−0·2276	0·2605	1·2219	1·2615
24	−0.2382	0·2554	1·2269	1·2656
25	−0·2480	0·2513	1·2302	1·2694
26	−0·2563	0·2475	1·2323	1·2726
27	−0·2603	0·2445	1·2347	1·2759
28	−0·2603	0·2419	1·2372	1·2790
29	−0·2593	0·2395	1·2389	1·2815
30	−0·2567	0·2373	1·2402	1·2833
31	−0·2521	0·2353	1·2414	1·2849
32	−0·2462	0·2334	1·2425	1·2859
33	−0·2398	0·2316	1·2431	$1{\cdot}2863_4$
34	−0·2326	0·2299	1·2437	$1{\cdot}2863_8$

Comparison with published results (see for example Gaunt and Sykes 1973) shows that the values of $\alpha_n'(\mathrm{ld})$ and $\gamma_n'(\mathrm{ld})$ are similar to those of Padé estimates for α' and γ' obtained using the same number of terms; in particular, the last few values of $\gamma_n'(\mathrm{ld})$ are nearly level at 1·28, but their trend suggests that this is a maximum and that the values will decrease again for larger n. The ratio estimates for α' can at best be said to be consistent with the value of $1/8$ (and rather more so than with $\alpha' = 0$), but those for γ' unequivocally favour the scaling value of $5/4$, in preference to the other rational value, mentioned in the literature, of $21/16$ (1·3125). This work therefore gives no support to the apparent discrepancy, based on earlier studies, between the values of γ and γ'. It appears furthermore that, at least for the susceptibility, the final asymptotic behaviour of the series coefficients is displayed; the subsequent assumption of the value $\gamma' = 5/4$ then enables information to be obtained directly about higher-order contributions to the critical singularity. Details of this will be given in a subsequent publication.

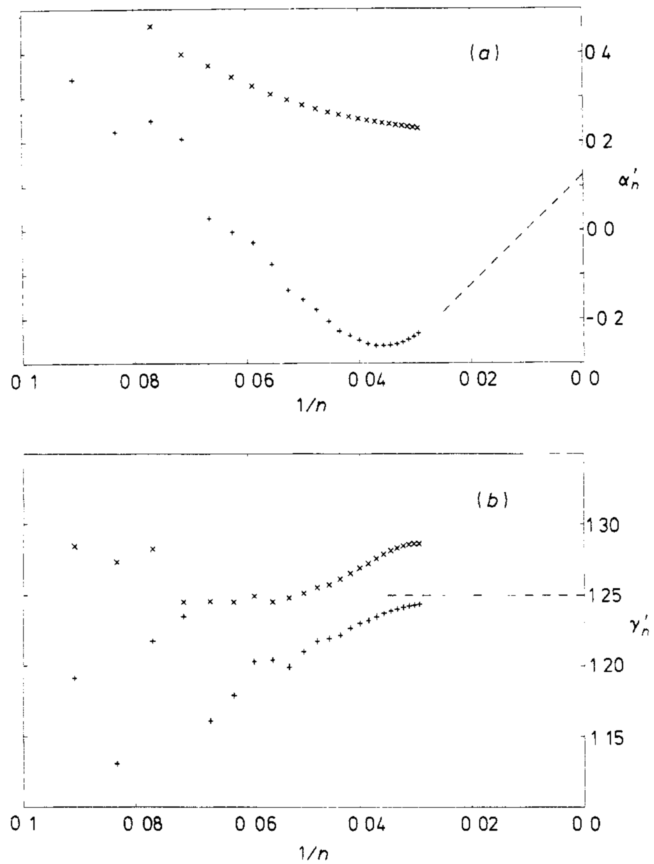

Figure 2. Sequences of exponent estimates calculated from the ratios (+) and from the logarithmic derivative series (×). (*a*) Specific heat exponent α'; (*b*) susceptibility exponent γ'. The broken lines indicate likely asymptotes for the ratio sequences.

As further coefficients in the transformed series are obtained, the effect of the non-physical singularities is expected to decrease exponentially, and the accuracy of the exponent estimates to improve correspondingly. Thus on the basis of the present work it appears to be worthwhile extending the series to higher terms. In addition, a few more terms in the specific heat series would greatly strengthen the evidence on the final asymptotic singular behaviour, and in the susceptibility series would establish whether the γ_n'(ld) values do in fact decrease smoothly from the apparent maximum at approximately 1·286. A full account of the present approach to series transformations, together with details of transformations corresponding to other series will be given in a later publication.

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References

Gaunt D S and Sykes M F 1973 *J. Phys. A: Math., Nucl. Gen.* **6** 1517–26
Guttmann A J 1969 *J. Phys. C: Solid St. Phys.* **2** 1900–7
Guttmann A J, Thompson C J and Ninham B W 1970 *J. Phys. C: Solid St. Phys.* **3** 1641–51
Hunter D L and Baker G A Jr 1973 *Phys. Rev.* B **7** 3346–76
Pearce C J 1975 *PhD Thesis* University of Western Australia
Sykes M F, Essam J W and Gaunt D S 1965 *J. Math. Phys.* **6** 283–98
Sykes M F, Gaunt D S, Essam J W and Elliott C J 1973 *J. Phys. A: Math., Nucl. Gen.* **6** 1507–16