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The calculation of critical indices by the rational approximation method†

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Abstract. A new method of calculating critical indices from series expansions is given. The method involves rational approximation with a denominator chosen so that the effect of singularities other than the critical one is minimised. The method suggests that the index for the low-temperature spontaneous magnetisation in the spin-$\frac{1}{2}$ Ising model may be 0.323 ● 0.003 for both BCC and FCC lattices.

1. Introduction

The determination of critical indices for Ising model ferromagnets from low-temperature series has proved to be more difficult than the corresponding problem in the high-temperature case, although generally more terms are known in the low-temperature expansions. The reason for this is the presence of (complex) singularities of each thermodynamic function nearer to the origin than the singularity associated with the critical point. Padé and related methods have been introduced to overcome this difficulty, but the results are not completely satisfactory on account of the erratic nature of successive estimates. (An explanation of this behaviour is given in § 2.) Padé approximants, as well as other procedures (Guttmann 1969), have however produced a reasonably accurate idea of the location of the additional singularities, and this information forms the basis for a new method for estimating critical indices, particularly in the low-temperature case. An alternative procedure, using conformal transformations, has been described by Pearce (1978).

The new method, which we call the rational approximation method, is based on the work of Baumel *et al* (1981) and involves approximating the function whose expansion we are given by the ratio of two polynomials. The denominator is chosen to be much larger near the critical point than at the other singularities and the numerator is then calculated in the usual Padé manner. The effect is to focus attention on the critical point and a smooth, converging sequence of estimates results.

In § 2 we discuss Padé methods and in § 3 explain the new method. Some initial results from the method are given and analysed in § 4.

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2. Padé methods

Since Padé approximants were first introduced into the study of critical indices, a good deal of progress has been made in understanding their asymptotic behaviour. In particular, it seems likely (Nuttall 1980) that most of the poles of high-order diagonal or near-diagonal Padé approximants to a function with branch points approach an appropriate set of minimum capacity containing the branch points. (It is assumed that we are expanding about the point at infinity.) The density of poles is proportional to the density of charge when the minimum capacity set is a conductor.

As an example, we have shown in figure 1 the poles of the [12/12] and [14/14] Padé approximants to the spin-$\frac{1}{2}$ BCC spontaneous magnetisation $I(u)$, $u = \exp(-4J/kT)$ using the series given by Sykes *et al* (1965, 1973). The poles are plotted in the t plane, $t = u^{-1}$. The results seem to be consistent with an approach to the minimum capacity set containing three points $t \approx t_c = u_c^{-1} = (0.532\,853)^{-1}$ (corresponding to the critical point) and $t \approx a, a^*$, $a = -1.58 + 2.06\mathrm{i}$. Notice the increase in density of poles near these three points which corresponds to the inverse square root behaviour of the charge density near an arc end of the set.

Similar results are obtained for the BCC low-temperature specific heat (actually $C_H/(\ln u)^2$) and susceptibility, indicating that all three functions probably have the same branch points. These results are consistent with those of Guttmann (1969).

A technique that has often been used to determine critical indices is known as the dlog Padé method (Baker 1961). For example, if near $u = u_c$

$$I(u) \sim (u - u_c)^{\beta} h(u),$$

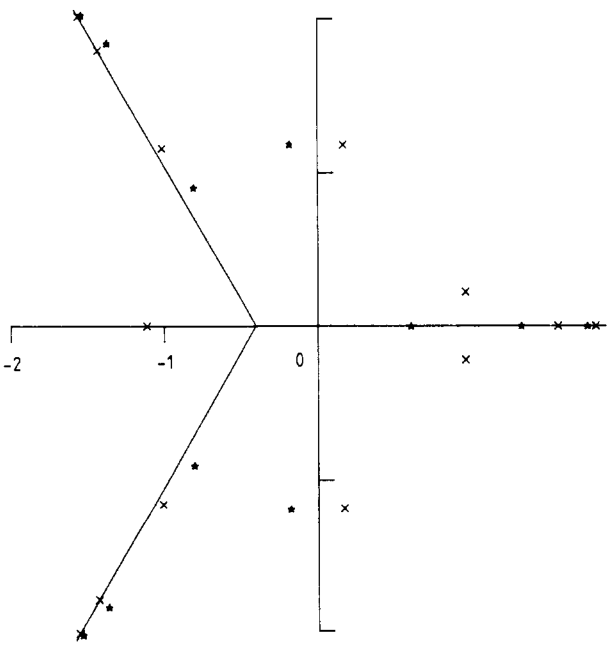

Figure 1. Poles of the [12/12] (marked by a star) and [14/14] (×) Padé approximants to the BCC spontaneous magnetisation $I(u)$. One spurious pole has been omitted in each case. The set of minimum capacity joining a, a^* and t_c is shown.

then it is expected that Padé approximants to I'/I will have a pole near u_c of residue near β. On the basis of recent ideas, we think that, if $h(u)$ is analytic near u_c, then these estimates of β will converge exponentially and most of the remaining poles of the approximants will approach a minimum capacity set containing all singularities of I except u_c. Figure 2 shows the poles of [12/12] and [13/13] to I'/I. These poles are distributed in much the same way as in figure 1, which suggests that $h(u)$ has a branch point at or near to u_c. In addition the estimates of β do not appear to be converging exponentially (Essam and Fisher 1963), which supports the conclusion that u_c is a confluent or near-confluent singularity of I. The same situation appears to apply to the specific heat and susceptibility.

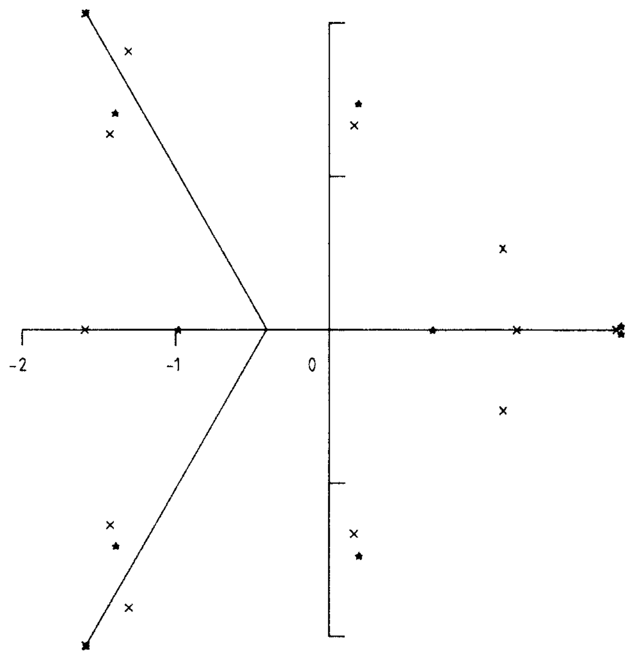

Figure 2. Poles of the [12/12] (marked by a star) and [13/13] (×) Padé approximants to I'/I. Two spurious poles have been omitted from the [12/12]. The set of minimum capacity is shown as in figure 1.

It sometimes occurs that poles of the Padé approximant appear nowhere near the set of minimum capacity. The location and number of such poles changes in an apparently irregular manner as the degree of approximation is increased. Such poles are almost cancelled by zeros of the numerator and are often called spurious poles. An understanding is now developing about the location of these poles (Nuttall and Singh 1977, Nuttall 1982). The asymptotic behaviour of the numerator and denominator polynomials is given by the solution of a Hilbert problem, and, if the minimum capacity set has more than two branch points, there will be at least one spurious pole. The spurious poles appear as the solution of the Jacobi inversion problem on the two-sheeted Riemann surface $y^2 = X(t)$, where $X(t)$ is a polynomial whose zeros are the branch points plus other points where arcs of the minimum capacity set meet.

The simplest non-trivial case is when there are three branch points, as could well be the situation for the BCC functions discussed above. $X(t)$ is of degree four, for there is one point where the three arcs of the minimum capacity set meet. The elliptic integral of the first kind maps the Riemann surface $y^2 = X$ onto the complex plane which may be covered by a grid of period parallelograms. Each parallelogram is a copy of the Riemann surface. As n increases the spurious pole of $[n/n]$ moves in equal steps along a line in this plane. The corresponding motion in the original plane appears to be erratic. Other quantities, such as estimates of β, include a similar erratic component. This type of behaviour was first observed by Dumas (1908) and later in more general cases by Akhiezer (1960) and Nuttall and Singh (1977).

Recent work Nuttall (1982) has generalised these ideas to Hermite–Padé approximants, such as those used by Fisher and Au-Yang (1979), and the same erratic behaviour, which is smooth if viewed in the correct space, is to be expected.

3. Rational approximation method

Let us assume that u_c is known from high-temperature analyses. Then the index β may be written as $g(u_c)$, where

$$g(u) = (u - u_c)I'(u)/I(u).$$

We approximate $g(u)$ by

$$g(u) \approx Q(u)/P(u)$$

where $P(u)$ is a chosen polynomial of degree n and $Q(u)$ is a degree-n polynomial given by

$$Q(u) = P(u)g(u) + O(u^{n+1}).$$

As in Baumel *et al* (1981) it is easy to show that

$$Q(u_c)/P(u_c) = \beta + (2\pi i p(t_c))^{-1} \int dt'\, p(t')G(t')(t' - t_c)^{-1} \tag{1}$$

where

$$p(t) = t^n P(t^{-1}), \qquad G(t) = g(t^{-1}) - \beta.$$

In (1), the integral is taken round any closed contour including the singularities of $g(t^{-1})$, assuming, as appears to be the case in this example, that $I(u)$ has no zeros in the plane cut along the set of minimum capacity S.

We now choose $P(u)$ in such a way that $p(t)$ is much larger near $t = t_c$ than near the other branch points of $G(t)$. Thus we could choose $p(t)$ to be a Chebychev polynomial with the argument linearly transformed so that ± 1 become a, a^*, i.e. $p(t) = \exp[n\phi(t)] + \exp[-n\phi(t)]$ where

$$\exp[\phi(t)] = x + (x^2 - 1)^{1/2}, \qquad x = \frac{t - \operatorname{Re} a}{i \operatorname{Im} a}.$$

The square root is chosen so that $|\exp \phi| \geqslant 1$.

In fact our argument does not require $P(u)$ to be a polynomial, so we have made the simpler choice

$$p(t) = \exp[n\phi(t)]. \tag{2}$$

Along the line joining a, a^*, $|\exp \phi| = 1$, and, at $t = t_c$, $|\exp \phi| = 3.6314$. If we choose the contour in (1) to surround closely the set of minimum capacity, then for larger n the dominant contribution to the integral will come from those values of t' nearest to t_c, and we can write

$$Q(u_c)/P(u_c) - \beta \approx (2\pi i p(t_c))^{-1} \int_d^{t_c} dt' \, p(t') \Delta G(t')(t' - t_c)^{-1} \tag{3}$$

where ΔG is the discontinuity of G across the cut ending at t_c, and $d < t_c$. What is omitted in (3) decreases exponentially, and in particular, the contribution from branch points at or near a, a^* will be negligible in the present case for the higher values of n available. (There are 29 terms known in the series for I.)

If there is no confluent singularity at t_c, then $G(t)$ will not be singular there and the error in our approximation will decrease exponentially. It is more likely, however, that $G(t)$ has a branch point at $t = t_c$. If we suppose that the dominant part of $G(t)$ is given by

$$G(t) \sim A(t - t_c)^{\theta}, \qquad t \approx t_c,$$

then standard asymptotic analysis (Bender and Orszag 1978) will give

$$\begin{aligned} Q(u_c)/P(u_c) - \beta &\sim A\pi^{-1} \sin \pi\theta \int^{t_c} dt' \exp[n\phi'(t_c)(t' - t_c)](t_c - t')^{\theta - 1} \\ &\sim A\pi^{-1}\Gamma(\theta) \sin \pi\theta \, (n\phi'(t_c))^{-\theta} \end{aligned} \tag{4}$$

as the leading term in the error for large n.

In practice u_c is not known exactly. A straightforward analysis shows that if $\bar{Q}$ is obtained as a result of using a value $\bar{u}_c$, then

$$\bar{Q}(\bar{u}_c)/Q(u_c) = (\bar{u}_c/u_c)^{n+1}$$

so that the effect of a change in u_c on our estimate of β is easily determined. Thus, in the example discussed above, if u_c is increased by 0.0001, the estimate of β for $n = 27$ is increased by a factor 1.0018, less for smaller n.

4. Results and discussion

With the method described in § 3 we obtain a sequence of estimates β_n for the BCC spontaneous magnetisation β which are given in table 1. It is seen that they vary much more smoothly than typical Padé results. We must extrapolate the sequence to $n = \infty$. From (4) we see that, if β_n is plotted against $n^{-\theta}$, the resulting curve should approach $n = \infty$ linearly, but of course we do not know θ. In figure 3, β_n is plotted against n^{-1} and it is seen that for larger n the resulting curve is remarkably straight with a limiting value near $\beta = 0.323$. If we have reached the region of validity of the asymptotic expansion (4), then this is probably close to the correct value. On the other hand, if θ is not near to 1 and we are still at a stage where other terms must be added to (4), then β might have a different value.

The FCC spontaneous magnetisation can be treated in a similar way. In this case Padé analysis shows that $I(u)$ has four singularities in addition to the critical point at $u_c = 0.664\,73$. We have taken these singularities to be at $t = u^{-1} = -1.6 \pm i$, $0.24 \pm 1.8i$, in agreement with the work of Guttmann (1969). (It is probably just a coincidence

Table 1. Estimates β_n for the BCC lattice.

n	β_n
3	0.081 617 397 546 45
4	0.137 724 081 103 47
5	0.176 298 627 352 45
6	0.207 298 118 015 37
7	0.232 359 967 295 91
8	0.251 360 594 351 03
9	0.265 427 338 700 03
10	0.275 688 572 084 38
11	0.283 137 135 326 81
12	0.288 583 646 025 30
13	0.292 639 126 268 31
14	0.295 733 451 636 29
15	0.298 155 855 471 26
16	0.300 097 411 238 67
17	0.301 685 411 865 97
18	0.303 007 478 318 29
19	0.304 126 660 742 51
20	0.305 090 056 469 96
21	0.305 933 477 825 71
22	0.306 684 062 306 22
23	0.307 361 978 783 32
24	0.307 981 798 863 61
25	0.308 553 735 702 75
26	0.309 084 770 743 71
27	0.309 579 629 101 30

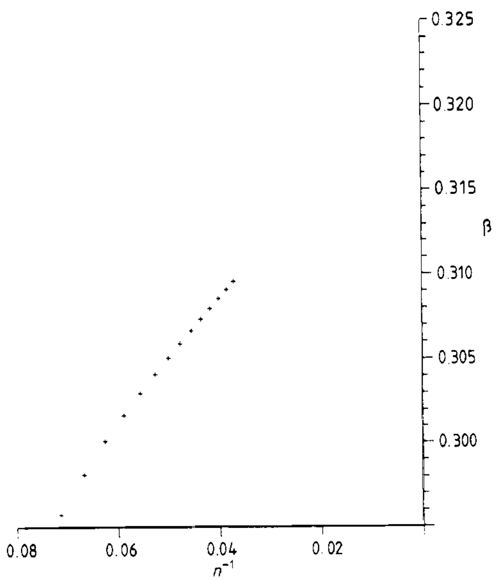

Figure 3. Values of β_n for the BCC lattice plotted against n^{-1}.

Table 2. Estimates β_n for the FCC lattice.

n	β_n
5	0.155 155 348 787 62
6	0.185 804 650 137 40
7	0.205 543 925 966 74
8	0.218 277 182 833 82
9	0.220 202 759 543 50
10	0.247 425 305 271 67
11	0.259 111 749 755 37
12	0.268 761 601 149 90
13	0.274 636 790 409 95
14	0.279 424 287 765 40
15	0.285 171 718 065 67
16	0.289 740 781 377 90
17	0.293 036 009 195 10
18	0.295 544 484 184 01
19	0.297 623 068 059 87
20	0.299 576 914 295 43
21	0.301 109 030 430 28
22	0.302 393 723 021 61
23	0.303 460 052 100 25
24	0.304 354 680 449 08
25	0.305 129 928 350 14
26	0.305 834 700 777 77
27	0.306 450 805 580 95
28	0.306 992 933 043 74
29	0.307 484 534 285 06
30	0.307 950 269 400 46
31	0.308 376 575 887 97
32	0.308 774 338 883 59
33	0.309 148 685 460 35
34	0.309 502 359 384 74
35	0.309 833 453 917 14
36	0.310 150 843 736 46
37	0.310 450 037 651 87
38	0.310 731 184 662 29
39	0.310 995 518 762 30

that the uncertainty in our knowledge of these five points is such that we cannot rule out the possibility that in the t plane they form the vertices of a regular pentagon. It is probably also a coincidence that the corresponding three points for the BCC lattice might form an equilateral triangle, which accounts for the fact that the three arms of the minimum capacity set are virtually straight lines.) Next we define the set Σ in the complex t plane to consist of rays joining the origin to the four singularities. In place of the definition (2) we now choose $p(t) = p_n(t)$ where $p_n(t)$ are polynomials orthogonal on Σ, i.e.

$$\int_{\Sigma} |\mathrm{d}t| p_n(t) p_n^*(t) = \delta_{nm}.$$

Away from Σ, for large n, it is known (Widom 1969) that these polynomials have the behaviour

$$|p_n(t)| \sim \exp[n\psi(t)]$$

where $\psi(t)$ is a harmonic function which vanishes on Σ and approaches $\ln|t|$ at ∞. Thus, as before, for large n, $|p_n(t_c)| \gg |p_n(t)|$, $t \in \Sigma$, and a similar analysis applies. However the situation is not now as favourable as before. For $n = 39$, we find

$$p_n(t_c)\left(\int_{\Sigma} |\mathrm{d}t| |p_n(t)|^2\right)^{-1/2} = 773.$$

Results for this method applied to $I(u)$ for the FCC spontaneous magnetisation are given in table 2. The estimates β_n are plotted against n^{-1} in figure 4. Again we observe a linear behaviour for larger n with an apparent limit near $\beta = 0.323$.

In figure 5, β_n for the FCC case is plotted against $n^{-0.75}$ and this graph suggests a value of β nearer to 0.325. The BCC results are similar. An even higher value would be indicated if θ were less than 0.75.

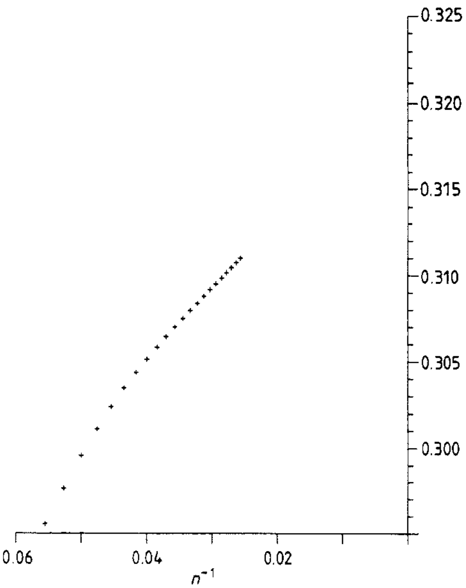

Figure 4. Values of β_n for the FCC lattice plotted against n^{-1}.

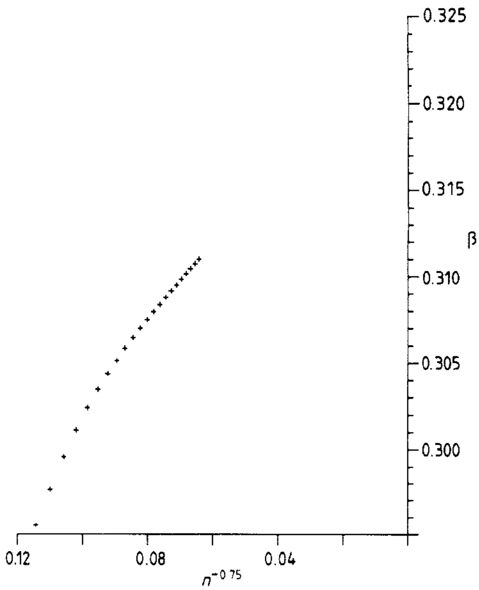

Figure 5. Values of β_n for the FCC lattice plotted against $n^{-0.75}$.

The rational approximation method seems to be superior to methods which have previously been applied to the analysis of low-temperature critical indices. There is scope for numerous modifications and other applications, including the high-temperature case, and work continues.

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