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The critical index of the magnetic susceptibility of 3D Ising models

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Abstract. Series expansions for certain thermodynamic variables have been computed for various standard model lattices. The high-temperature series for the magnetic susceptibility of the Ising model of three-dimensional SC, BCC and FCC lattices allows estimates of the critical index γ of each series to be made. Dramatic progress in this direction was made by the Padé Dlog method, and here a similar technique is introduced. Estimates of γ from row sequences of generalised inverse vector-valued Padé approximants are made. The results point to the conclusion that $\gamma = 1.2406 \pm 0.0017$ is the critical index common to all three lattices.

1. Introduction

Power series expansions for the magnetic susceptibility χ for the three-dimensional Ising model on several different lattices are available. For the BCC lattice, for example (Nickel 1982),

$$\chi(v) = 1 + 8v + 56v^2 + 392v^3 + \ldots + 199\,518\,218\,638\,233\,896v^{21} + \ldots \tag{1}$$

where $v = \tanh(J/kT)$ is the usual variable for high-temperature power series. Equation (1) indicates that the coefficients of v^j in $\chi(v)$ are known up to $j = 21$. A comprehensive review of the data for these series, the methods of analysing them and their present status has been provided by Gaunt (1982) and Nickel (1982). A conspicuous feature in any such review is the Padé Dlog method (Baker 1961). It is generally assumed that the behaviour of $\chi(v)$ near the Curie point v_C (and corresponding temperature T_C) is modelled by

$$\chi(v) \simeq C_1(v_C - v)^{-\gamma} \simeq C_2(T - T_C)^{-\gamma}. \tag{2}$$

Therefore

$$f(v) := D\log\chi(v) = \frac{\chi'(v)}{\chi(v)} \simeq \frac{-\gamma}{v - v_C}. \tag{3}$$

We see that estimates of γ, v_C can be obtained from suitably chosen Padé approximants of $f(v)$ using the data of (1). For the two-dimensional SQ lattice, the values of γ and v_C are known to be 1.75 and $\sqrt{2} - 1$ respectively (Fisher 1959, Domb 1974). Estimates of γ based on near-diagonal Padé approximants converge impressively (Gaunt and Guttmann 1976) but from below. This implies that estimation of γ based on averages over neighbouring approximants does not produce an estimate of γ better than that of the best individual approximant in this case. It also indicates that some form of extrapolation of the estimates of γ is required for the SQ lattice. In this spirit, estimates of γ for the SC lattice based on the $[l/3]$ and $[l/4]$ row sequences of Padé approximants were computed, and the results are shown in figure 1. The folly of naive extrapolation to $l=\infty$ of these estimates is obvious from this figure.

Of course, the erratic behaviour of the estimates of γ based on sequences of Padé approximants to $f(v)$, as given by (1) and (3), is notorious, and there are rules for deciding the error estimate (Essam and Hunter 1968). It is sometimes said that series such as (1) are noisy, but this is not so: its coefficients are known integers, and it is the estimates of γ which are noisy. A proper analysis of such series should incorporate the values of the coefficients exactly, and smooth the estimates of the critical constants in some fashion. To this end, simultaneous approximation of several series was investigated.

The vector function $\boldsymbol{f}(v)$ is defined as

$$\boldsymbol{f}(v)=(f_1(v),f_2(v),\ldots,f_d(v)) \tag{4}$$

where the first component of $\boldsymbol{f}(v)$ is

$$f_1(v):=f(v)=c_0+c_1v+c_2v^2+\ldots+c_Nv^N+\ldots \tag{5a}$$

and from it the other components of $\boldsymbol{f}$ are defined by

$$\begin{aligned} f_2(v)&:=c_1 \quad +c_2v+c_3v^2 \quad +\ldots+c_{N+1}v^N+\ldots \\ &\vdots \\ f_d(v)&:=c_{d-1}+c_dv+c_{d+1}v^2+\ldots+c_{N+d-1}v^N+\ldots. \end{aligned} \tag{5b}$$

If the coefficients of $f(v)$ are known up to v^n, the coefficients of $\boldsymbol{f}(v)$ are known up to v^{n-d+1}.

The method of generalised inverse Padé approximants (GIPA) provides rational approximants of $\boldsymbol{f}(v)$ which have pole positions which are common to all of its components. For the case of the model of equation (3), we expect that

$$\boldsymbol{f}(v)\simeq\left(\frac{-\gamma}{v-v_C},\frac{-\gamma/v_C}{v-v_C},\ldots,\frac{-\gamma/v_C^{d-1}}{v-v_C}\right). \tag{6}$$

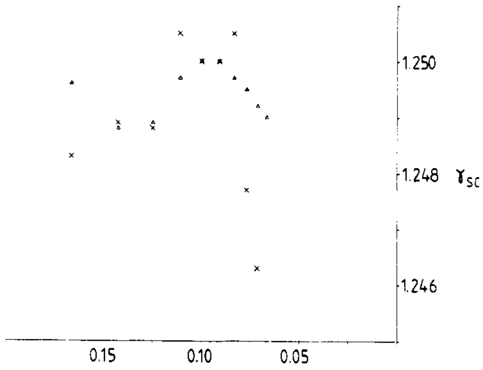

Figure 1. The estimates of the critical index γ_{SC} for the three-dimensional SC lattice, obtained using $[l/m]$-type Padé approximants in the rows $m=3$ ($\triangle$), $m=4$ ($\times$) are plotted against l^{-1}.

In approximating $f(v)$, d (usually different) estimates γ_j of γ are obtained from the jth component of the GIPA, and these form the components of $\boldsymbol{\gamma}$. The significance of this point is that the error in the prediction of the critical index γ can be assessed from the internal consistency of the components of $\boldsymbol{\gamma}$. In fact, the use of GIPA permits imposition of a consistency requirement on the various estimates of γ, and we obtain not only an estimate of γ but also an internal error estimate for it.

2. Construction and application of GIPA

These approximants grew from the continued fractions containing vector elements introduced by Wynn (1963). A GIPA of type $[n/2k]$ is a set of d rational fractions with a common denominator of degree $2k$, numerators of degree n at most, and which match d given power series up to order z^n inclusively. The full axiomatic definition is given by Graves-Morris and Jenkins (1986). A GIPA is a kind of Padé approximant for vector-valued functions. If, for example, all the components of (4) are the same, so that $f_1 = f_2 = \ldots = f_d$, the components of the GIPA of type $[n/2k]$ to $f(v)$ are the Padé approximants of type $[n-k/k]$ to $f_1(v)$.

The coefficients of a GIPA of type $[n/2k]$ for a power series having the generic form

$$f(z) = c_0 + c_1 z + c_2 z^2 + \ldots + c_n z^n + \ldots \tag{7}$$

are found by the following method (Graves-Morris and Jenkins 1987). Define the elements $\{M_{ij}\}_{i,j=0}^{n}$ of the matrix M by

$$M_{ij} = \sum_{l=0}^{j-i-1} c_{l+i+n-2k+1} \cdot c^{*}_{j-l+n-2k} \qquad j>i \tag{8a}$$

$$M_{ij} = 0 \qquad j=i \tag{8b}$$

$$M_{ij} = -\sum_{l=0}^{i-j-1} c_{l+j+n-2k+1} \cdot c^{*}_{i-l+n-2k} \qquad j<i. \tag{8c}$$

In equation (8), we have assumed that $c_j := \mathbf{0}$ for $j<0$ and that scalar multiplication is defined by

$$a \cdot b := \sum_{i=1}^{d} a_i b_i \qquad \text{for } a, b \in \mathbb{C}^d.$$

The set of equations

$$\begin{bmatrix} 0 & M_{01} & M_{02} & \ldots & M_{0,2k} \\ M_{10} & 0 & M_{12} & \ldots & M_{1,2k} \\ \vdots & \vdots & \vdots & & \vdots \\ M_{2k,0} & M_{2k,1} & M_{2k,2} & \ldots & 0 \end{bmatrix} \begin{bmatrix} q_{2k} \\ q_{2k-1} \\ \vdots \\ q_0 \end{bmatrix} = 0 \tag{9}$$

is a consistent set of homogeneous equations, and has a non-trivial solution for $q_0, q_1, \ldots, q_{2k}$. In non-degenerate cases, we may take $q_0 = 1$ and obtain the denominator polynomial

$$q(z) := \sum_{i=0}^{2k} q_i z^i.$$

The numerator vector polynomial $\boldsymbol{p}(z)$ is defined by cross-multiplication and truncation, using Nuttall's notation (Nuttall 1970), as

$$\boldsymbol{p}(z) := [\boldsymbol{f}(z)q(z)]_0^n. \tag{10}$$

From (10) it is obvious that the GIPA $\boldsymbol{r}(z)$ satisfies the accuracy-through-order condition

$$\boldsymbol{r}(z) := \frac{\boldsymbol{p}(z)}{q(z)} = \boldsymbol{f}(z) + \mathrm{O}(z^{n+1}). \tag{11}$$

Convergence of row sequences of Padé approximants of functions meromorphic in a disk is well understood, and similar results for GIPA have been established by Graves-Morris and Saff (1987). These results suggest (but do not prove) that row sequences of GIPA converge for functions of the type shown in (5) within the appropriate disk of meromorphy.

From a practical viewpoint, it is not advisable to form GIPA to the series (5) to obtain the estimates of γ shown in (6). Because the denominators of GIPA are real and non-negative on the real axis, it turns out that a GIPA can only have a simple pole of the type (6) if each component of its numerator has a common simple zero, and its denominator has a double zero at the same point. To avoid numerical simulation of this awkward mathematical occurrence, it is preferable to use the variable $u := v/i$, and the vector function

$$\boldsymbol{F}(u) := (F_1(u), F_2(u), \ldots, F_d(u)) \tag{12}$$

where

$$\begin{aligned}
F_1(u) &:= c_0 \quad + \mathrm{i}c_1 u - c_2 u^2 \quad + \ldots + \mathrm{i}^N c_N u^N + \ldots \\
F_2(u) &:= c_1 \quad + \mathrm{i}c_2 u - c_3 u^2 \quad + \ldots + \mathrm{i}^N c_{N+1} u^N + \ldots \\
&\;\;\vdots \qquad\qquad \vdots \\
F_d(u) &:= c_{d-1} + \mathrm{i}c_d u - c_{d+1} u^2 + \ldots + \mathrm{i}^N c_{N+d-1} u^N + \ldots.
\end{aligned} \tag{13}$$

Because each GIPA of $\boldsymbol{F}(u)$ has a simple pole at $u \simeq -\mathrm{i}v_\mathrm{C}$, estimates of γ are easily obtained from its d residues. All GIPA have poles at conjugate positions, and this property is useful for present purposes. The pole at $u \simeq \mathrm{i}v_\mathrm{C}$ occurs near the Néel point; this pole and others on $[\mathrm{i}v_\mathrm{C}, \mathrm{i}\infty)$ represent the associated cut of $\boldsymbol{F}(u)$. Likewise, poles on $(-\mathrm{i}\infty, -\mathrm{i}v_\mathrm{C}]$ other than the one at $u \simeq -\mathrm{i}v_\mathrm{C}$ represent the cut of $\boldsymbol{F}(u)$ starting at the Curie point. This kind of minimal analytic structure has been assumed as a working hypothesis previously (Gammel *et al* 1984); convergence of the approximants is assumed to occur in much the same way that Padé approximants converge to Hamburger functions (Baker 1975, Baker and Graves-Morris 1981).

The previous remarks make an essential difficulty of principle more noticeable. The difficulty is that the assumptions (2) and (3) are too vague to permit determination of γ, unless further information is available about the discontinuity of $\chi(u)$, and hence that of $F_1(u)$ across its cut along $[\mathrm{i}v_\mathrm{C}, \mathrm{i}\infty)$. The value of γ obtained from Padé and Padé-like approximants surely derives from an aggregate of the point discontinuity of $F_1(u)$ at the Curie point,

$$\Delta(u) := 2\pi\mathrm{i}\gamma_0\delta(u + \mathrm{i}v_\mathrm{C}) \tag{14}$$

and the unknown continuum discontinuity near the Curie point. For this reason, some limiting procedure or extrapolation to high order may be essential to obtain the true value of γ_0.

Despite appearances, the method described thus far is not really free from unknown parameters. Each component of $\boldsymbol{F}(u)$ can be multiplied by an arbitrary complex constant, and the value of γ obtained depends on the choice made. To settle this indeterminacy, the following procedure was adopted. A scaling parameter λ is introduced which is initially arbitrary, but is subsequently fixed. The values of the coefficients of the series (1), for example, are used to obtain the power series coefficients of $\chi(\lambda w)$, and from this we define

$$\tilde{f}(w) := \frac{\mathrm{d}}{\mathrm{d}w} \log \chi(\lambda w). \tag{15}$$

The power series coefficients $\{\tilde{c}_i\}$ of $\tilde{f}(w)$ are defined by the equation

$$\tilde{f}(w) = \tilde{c}_0 + \tilde{c}_1 w + \tilde{c}_2 w^2 + \ldots \tag{16}$$

which is the scaled version of (5*a*). In passing, note that critical exponents computed by the Padé Dlog method are invariant under this scaling. Following (12) and (13), we define $u := w/i$ and

$$\tilde{\boldsymbol{F}}(u) := (\tilde{F}_1(u), \tilde{F}_2(u), \ldots, \tilde{F}_d(u)) \tag{17}$$

where

$$\begin{aligned}
\tilde{F}_1(u) &:= \tilde{c}_0 \quad + \mathrm{i}\tilde{c}_1 u - \tilde{c}_2 u^2 \quad + \ldots + \mathrm{i}^N \tilde{c}_N u^N + \ldots \\
\tilde{F}_2(u) &:= \tilde{c}_1 \quad + \mathrm{i}\tilde{c}_2 u - \tilde{c}_3 u^2 \quad + \ldots + \mathrm{i}^N \tilde{c}_{N+1} u^N + \ldots \\
&\vdots \\
\tilde{F}_d(u) &:= \tilde{c}_{d-1} + \mathrm{i}\tilde{c}_d u - \tilde{c}_{d+1} u^2 + \ldots + \mathrm{i}^N \tilde{c}_{N+d-1} u^N + \ldots .
\end{aligned} \tag{18}$$

If the simple approximation in (3) is made,

$$\tilde{f}(w) \simeq \frac{\gamma\lambda}{v_{\mathrm{C}} - \lambda w} \tag{19}$$

and

$$\tilde{F}_j(u) \simeq \frac{\gamma\lambda}{v_{\mathrm{C}} - \mathrm{i}\lambda u}\left(\frac{\lambda}{v_{\mathrm{C}}}\right)^{j-1} \qquad j = 1, 2, \ldots, d. \tag{20}$$

From (20), we see how to use an estimate of the position of the dominant pole of $\tilde{\boldsymbol{F}}(u)$ and its d residues to obtain d estimates of γ. Let γ_j be the estimate of γ obtained from the jth component of a GIPA for $\tilde{\boldsymbol{F}}(u)$, and let

$$\boldsymbol{\gamma} := (\gamma_1, \gamma_2, \ldots, \gamma_d). \tag{21}$$

From the values $\{\gamma_j\}_{j=1}^{d}$, find their average $\bar{\gamma}$, their standard deviation σ and the slope $m(\boldsymbol{\gamma})$ of the regression of γ_j against j. Since each component of $\boldsymbol{F}(u)$ should ideally lead to the same value of γ_j as indicated by (19) and (20) and should not correlate with j, the value of λ leaving $m(\boldsymbol{\gamma}) = 0$ is selected. This method provides (i) internal consistency of the prediction of γ, (ii) an internal estimate σ of the error of γ and (iii) extrapolation of the residues to a value independent of j (as described by (21) *et seq*).

The method described by (15)-(21) *et seq* is numerically stable: scaling with the parameter λ equilibrates the equations.

3. Test results

The fundamental aim of this paper is the extrapolation of values of the critical index γ (for various 3D Ising models) obtained using a row sequence of rational approximants. In § 4, we describe the numerical results obtained using 3D Ising model series, whereas in this section we describe how the procedure developed works on test series for which the indices are known *a priori*. Two of our test series are Maclaurin expansions of the mathematical functions in (22) and (28), and the third test series is the Ising series for the 2D SQ lattice. Since we aim to analyse series for which only about 20 coefficients are known explicitly, we restrict our attention to results obtainable using coefficients of v^j up to $j=20$ in the series expansions of $\chi(v)$.

3.1. Model 1

The mathematical model of the susceptibility which we consider first is based on a formula of Sykes *et al* (1972) and is

$$\chi_1(v)=(1-v)^{-1.25}+0.5(1+v)^{-0.875}. \tag{22}$$

This model has a 'Curie point' at $v=1$, a 'Néel point' at $v=-1$ and a 'critical exponent' $\gamma=1.25$. Using the procedure described by (14) *et seq*, d-dimensional GIPA of types $[n/4]$ and $[n/6]$ were computed for this series with $d=4$ and $d=6$. The maximum degree allowed for the GIPA numerator for the Dlog series is $20-d$. A suitable value of the scaling parameter λ was found for the components of about 50% of the GIPA, which allows them to be extrapolated to $m(\gamma)=0$. The results for γ are shown in figure 2, along with results from the $[l/2]$ and $[l/3]$ rows of the Padé table for Dlog $\chi_1(v)$ for comparison. From (11), we see that we should take $n=l+m$ to make a fair comparison of GIPA with ordinary Padé approximants. Some values of n are plotted

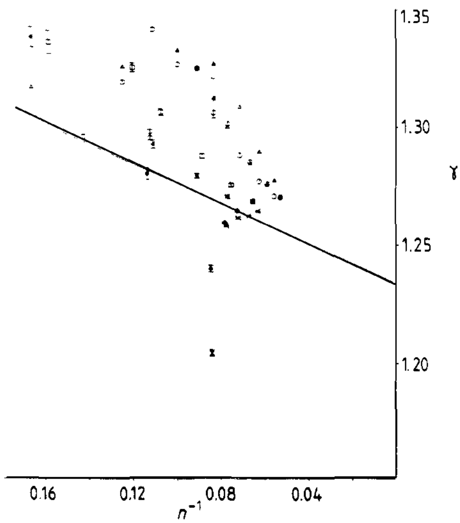

Figure 2. Values of the critical exponent and their internal errors are shown for model 1. The values are calculated for GIPA of type $[n/2k]$ and a linear fit is shown. Comparative results using Padé approximants of order $[l/m]$ are also shown. □, $2k=4$, $d=4$; $*$, $2k=4$, $d=6$; $\times$, $2k=6$, $d=4$; $\diamond$, $2k=6$, $d=6$; $\bigcirc$, $m=2$; $\triangle$, $m=3$.

slightly off-set from their true integer values in figures 2–11 for clarity of presentation only.

The straight line shown in figure 2 is a weighted least-squares regression line for the GIPA results, based on the hypothesis that

$$\gamma(n) \simeq \gamma_0 + \theta/n. \tag{23}$$

Figure 2 shows that the estimates of γ depend on n, despite extrapolation to $m(\gamma)=0$ by scaling. The fit in figure 2 is not very good. Using the standard statistical analysis for linear regression and weighted data (Dunn and Clark 1974), the result for γ_0 is

$$\gamma_0 = 1.2337 \pm 0.0645. \tag{24}$$

The error quoted in (24) measures the likely effect of the actual spread of the results from the GIPA shown in figure 2. The error is based on (23) as a hypothesis and it is purely statistical in character. Knowing the 'correct' answer for γ_0 from (22), we conclude that (23) is an incorrect hypothesis.

By considering the order of magnitude of the power series coefficients of (22), and recalling the formula

$$\lim_{n\to\infty} n^{b-a}\frac{\Gamma(n+a)}{\Gamma(n+b)} = 1 \tag{25}$$

(Abramowitz and Stegun 1965, section 6.1.46), it is tempting to speculate that

$$\gamma(n) \simeq \gamma_0 + \theta n^{-2.125} \tag{26}$$

provides a better parametrisation than (23). This is confirmed in figure 3, where the same results are plotted against $n^{-2.125}$. Under the hypothesis (26), we find that

$$\gamma_0 = 1.2503 \pm 0.0243 \tag{27}$$

which is entirely satisfactory.

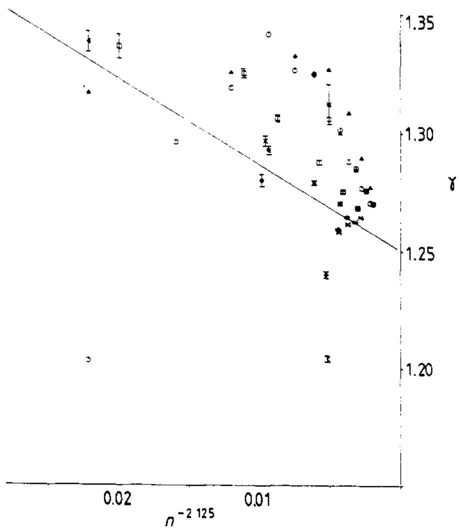

Figure 3. The same data as in figure 2, but plotted against $n^{-2.125}$.

3.2. *Model 2*

It is widely believed that confluent singularities are present at the Curie point, and that they have the effect of biasing estimates of γ. To investigate their effect on the numerical procedures we are analysing, we use the model

$$\chi_2(v) = (1-v)^{-1.25} + 0.1\,(1-v)^{-0.75} \tag{28}$$

for the susceptibility. The results for γ derived from the Padé Dlog analysis previously described are shown in figure 4. Results from the row sequences of $[n/4]$ and $[n/6]$ type GIPA of dimensionality $d=4$ and $d=6$ are shown. For this model, the estimates of γ obtained from each component of the GIPA (after extrapolation to $m(\gamma)=0$) are virtually identical in the cases shown, and so the internal errors are almost zero. Clearly, the internal errors of model 2 are unrealistic and they are neither shown nor used. Extrapolation to $m(\gamma)=0$ could not be made for the [6/6], [7/6] and [10/6] GIPA with $d=4$, and so there are no results for these cases. A linear fit of the form (23) was made to the 37 remaining estimates of γ, which were weighted equally. This fit led to the result

$$\gamma_0 = 1.2459 \pm 0.0027$$

which is an unsatisfactory estimate of the exponent in (25). Comparative results from the row sequences of $[l/2]$ and $[l/3]$ Padé approximants are also shown in figure 4. A simple analysis of the determinants occurring in the explicit formulae for the denominators of Padé approximants (Baker 1975 ch 11, Baker and Graves-Morris 1981 ch 6) indicates that the error in γ is $O(n^{-1/2})$. This conclusion suggests that the same behaviour could hold for GIPA, for which no such analysis has yet been developed. To test this conjecture, the same results were plotted against $n^{-1/2}$ as shown in figure 5. The linear fit takes the form

$$\gamma(n) = \gamma_0 + \theta n^{-1/2} \tag{29}$$

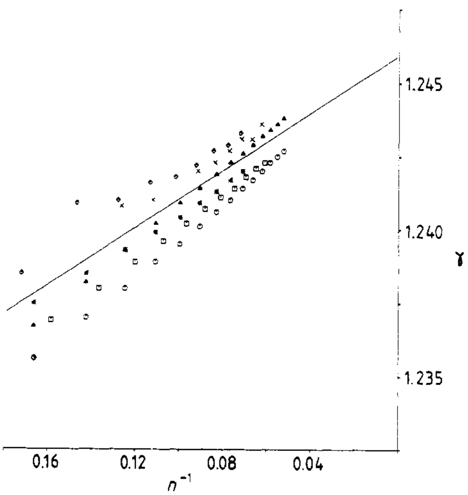

Figure 4. Values of the critical exponent for model 2. The values are calculated from GIPA of type $[n/2k]$, and a linear (unweighted) fit to them shown. Comparative results derived using Padé approximants are also shown. The symbols are as in figure 2.

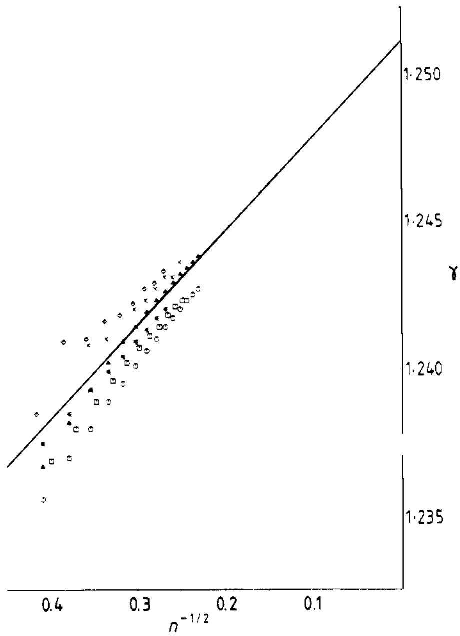

Figure 5. The same data as shown in figure 2, but plotted against $n^{-1/2}$.

and the value of γ_0 obtained using the GIPA results for γ is

$$\gamma_0 = 1.2511 \pm 0.0054.$$

This value is entirely compatible with (28) and the fit to the data in figure 5 looks reasonable.

3.3. *Model 3*

Data from the SQ lattice are analysed using the method previously described. The series for $\chi(v)$ from the 2D Ising model provides a much more realistic test of the method, because the coefficients are not smoothly varying, and the equivalent Padé estimates cannot easily be extrapolated to $n=\infty$. The method worked satisfactorily for $[n/6]$- and $[n/8]$-type GIPA, with $d=4$ and $d=6$. Many of the GIPA allowed by the constraints

$$n \leqslant 20-d \qquad 2k=6, 8 \qquad d=4, 6$$

were unacceptable. About 30% we rejected because no value of λ was found for which $m(\gamma)=0$. Around 30% of the remaining GIPA were rejected because they had poles in the disk $|u|<1.5u_C$, but not on the known cuts $(-i\infty, -iv_C]$ and $[iv_C, i\infty)$ in the u plane, and these GIPA were deemed to have spurious singularities. The remaining GIPA were used to produce the results for the SQ lattice shown in figure 6. There is no perceptible regression of γ against n, and so an L_2-weighted mean of indices was computed, leading to a weighted mean value

$$\gamma = 1.7497 \pm 0.0005.$$

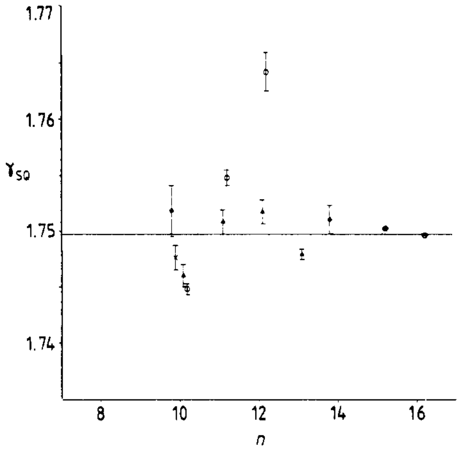

Figure 6. The estimates of the critical index γ_{SQ} and its internal error for the two-dimensional SQ lattice, obtained using $[n/2k]$-type GIPA of dimensionality 4, 6 in the rows $2k=6$, 8 are plotted against n. The line shows the weighted mean value $\gamma_{SQ}=1.7497$. $\times$, $2k=6$, $d=4$; $\diamond$, $2k=6$, $d=6$; $\bigcirc$, $2k=8$, $d=4$; $\triangle$, $2k=8$, $d=6$.

Because the exact result $\gamma = 1.75$ is known *a priori* (Fisher 1959), we observe from the figure that the internal errors do provide an indication of the precision of each GIPA. It is clear that the internal error estimates are too small by a factor of about five, and that the errors need to be rescaled to be realistic estimates of the actual error. Assignment of errors, and thereby weights, to an individual approximant is a vital ingredient of a satisfactory procedure for reliable extrapolation of Padé-like approximants in this context. It is obvious that some Padé approximants provide much better estimates of γ than others (see table 3 of Gaunt and Guttmann (1974)), but hitherto it has not been possible to characterise the better Padé approximants nor to assess the likely precision of each one.

4. 3D Ising models

The same procedure as that described for the SQ lattice was followed for the SC, BCC, FCC and D lattices. A greater proportion of the approximants were unacceptable by the previous criteria, and so the row sequence with $2k=4$ was included (but the conclusions were scarcely altered). The values of γ and its error from the $[n/2k]$-type GIPA are shown in figures 7 and 8 for the SC and BCC lattices. The estimated errors for the points in figure 9 for the FCC lattice are absurdly small, and they are not shown. Similar vanishingly small errors were also found in model 2, which has no antiferromagnetic singularity. It correlates well with the fact that antiferromagnetism is frustrated in the FCC lattice and that $\chi(v)$ is analytic at $v=-v_C$ (Domb 1974). No satisfactory results were found for the diamond lattice. It is evident that the values of γ obtained for the SC, BCC and FCC lattices depend on n (despite extrapolation to $m(\gamma)=0$), and these results appear to be compatible with the formula

$$\gamma(n) \simeq \gamma_0 + \theta/n. \qquad (30)$$

No fundamental *a priori* justification of (30) is offered. The parametrisation has been used previously in this context (e.g. Nickel 1982) and it looks reasonable for the data

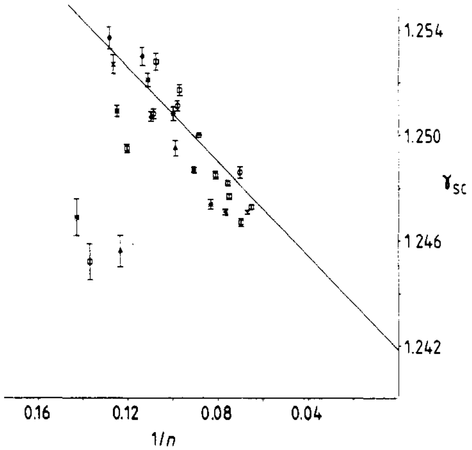

Figure 7. The estimates of the critical index γ_{SC} and its internal error for the three-dimensional SC lattice, obtained using $[n/2k]$-type GIPA of dimensionality 4 and 6 in rows $2k=4, 6, 8$ are plotted against $1/n$. The straight line shows the linear regression. □, $2k=4$, $d=4$; $*$, $2k=4$, $d=6$; $\times$, $2k=6$, $d=4$; ◇, $2k=6$, $d=6$; ○, $2k=8$, $d=4$; △, $2k=8$, $d=6$.

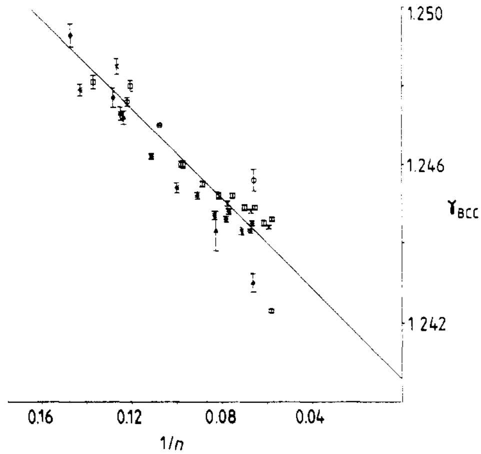

Figure 8. The estimates of the critical index γ_{BCC} and its internal error for the three-dimensional BCC lattice obtained using $[n/2k]$-type GIPA of dimensionality 4 and 6 in rows $2k=4$, 6 and 8 are plotted against $1/n$. The straight line shows the linear regression. Symbols are as in figure 7.

shown. It is envisaged that

$$\chi(v)=A(v)(1-v)^{-\gamma_0}+B(v)(1+v)^{\gamma_a}+C(v) \tag{31}$$

where $A(v)$, $B(v)$ and $C(v)$ are analytic in a domain including the closed disc $|z|\leq 1$, $\gamma_a > -\gamma_0+1$ and $A'(1)\neq 0$. From the analysis of models 1 and 2, it is reasonable to expect that the hypothesis (31) leads to the leading behaviour in (30), with a non-zero value of θ corresponding to the non-zero value of $A'(1)$. In this sense, (30) is the hypothesis of maximum simplicity. The value of γ_0 obtained using (30) is taken as the estimate of the true critical index.

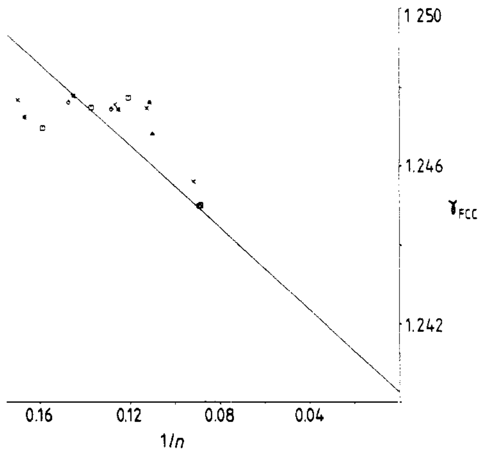

Figure 9. The estimates of the critical index γ_{FCC} for the three-dimensional FCC lattice, obtained using $[n/2k]$-type GIPA of dimensionalities 4 and 6 in rows $2k=4$, 6 and 8 are plotted against $1/n$. The straight line shows the (unweighted) linear regression. Symbols are as in figure 7.

The following values of γ_0, namely

$$\begin{aligned} \gamma_{SC} &= 1.2418 \pm 0.0064 \\ \gamma_{BCC} &= 1.2406 \pm 0.0020 \\ \gamma_{FCC} &= 1.2403 \pm 0.0033 \end{aligned} \tag{32}$$

were obtained using the procedures previously described. The results of models 1 and 2, depicted in figures 2–5, serve as a reminder that the errors quoted are only statistical and they depend on the validity of the hypothesis (30). If we assume that the values in (32) are all estimates of the same universal index, the combined estimate is

$$\gamma = 1.2406 \pm 0.0017. \tag{33}$$

Nowadays, there is a widespread belief that a sub-dominant singularity $(1-v)^{-\gamma_0+\delta}$, with $\delta = \frac{1}{2}$, contributes to $\chi(v)$, and so we consider an alternative to (30). If there is such a sub-dominant singularity controlling convergence, we would expect that

$$\gamma(n) \simeq \gamma_0 + \theta n^{-1/2} \tag{34}$$

on the basis of the results of models 1 and 2. The same data as shown in figures 7 and 8 are shown in figures 10 and 11, but the data are plotted against $n^{-1/2}$. The corresponding results (for all three lattices) are

$$\begin{aligned} \gamma_{SC} &= 1.2334 \pm 0.0118 \\ \gamma_{BCC} &= 1.2357 \pm 0.0037 \\ \gamma_{FCC} &= 1.2341 \pm 0.0073. \end{aligned} \tag{35}$$

(If these are estimates of the same index, it would be $\gamma = 1.2351 \pm 0.0031$, again showing consistency with universality.)

The quality of the fit corresponding to (34) shown in figures 10 and 11 is obviously much the same as the quality of the fit corresponding to (30) and shown in figures 7

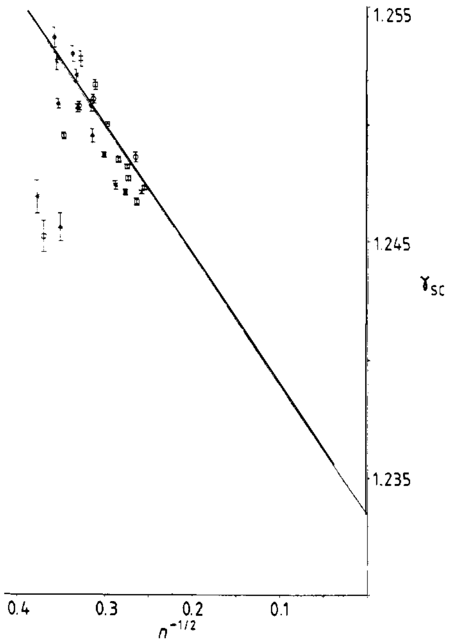

Figure 10. The same data as shown in figure 7, but plotted against $n^{-1/2}$.

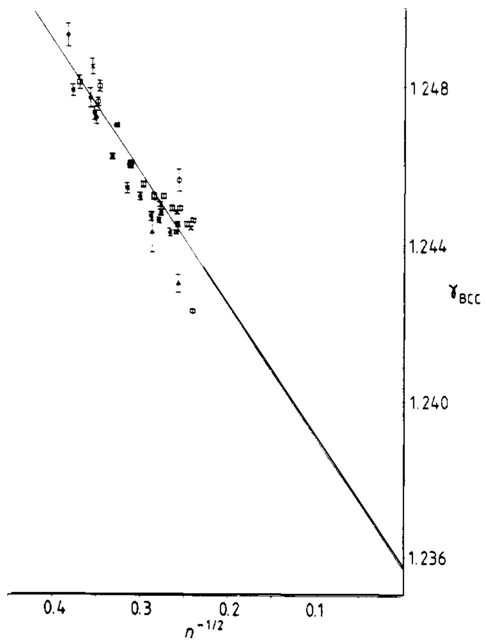

Figure 11. The same data as shown in figure 8, but plotted against $n^{-1/2}$.

and 8. The differences in the standard deviations of the fits (not the standard deviations of γ_0) are small, and so one cannot discriminate between (30) and (34) using the data, nor should one try to estimate the subdominant exponent from the data. We decide between (32), (35) and similar possibilities by opting for the hypothesis of minimal complexity, namely (30), and hence for the set of results in (32).

5. Conclusion

The values for the critical indices obtained in (32) are quite different from those obtained using the best (i.e. diagonal) Padé approximants. Of course, the difficulties of using Padé approximants in this context are well known (see table 6 in Baker and Hunter (1973)). The empirical technique described here stabilises the results of Padé-like calculations of the critical index of the high-temperature series of the magnetic susceptibility of the 3D Ising models. The results expressed in (32) and (33) are not at variance with the renormalisation group predictions of Le Guillou and Zinn-Justin (1977) nor with those of Fisher and Chen (1985). Deduction based on empirical numerical convergence is notoriously hazardous. No firm conclusions should be drawn from the evidence presented in this paper unless further analysis of the method corroborates its validity in the present context.

No doubt the main objectives of this paper can be achieved in other ways, not necessarily involving GIPA, and it will be interesting to see what are the essential ingredients for stable extrapolation of the exponents of the high-temperature series.

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