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1983 J. Phys. A: Math. Gen. 16 L359

(http://iopscience.iop.org/0305-4470/16/11/004)

J. Phys. A: Math. Gen. 16 (1983) L359–L363. Printed in Great Britain

LETTER TO THE EDITOR

On the critical exponent γ for four common three-dimensional lattices

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Received 12 May 1983

Abstract. The rational approximation method is used to examine the critical exponent for the susceptibility in the $S = \frac{1}{2}$ Ising model on the face centred cubic (FCC), body centred cubic (BCC), simple cubic (SC) and diamond lattices. A variation of the method of critical point renormalisation is used to eliminate bias due to uncertainty in the location of the critical point. The results are in agreement with the renormalisation group and with recent series analysis of the BCC series.

There has been a tremendous increase in recent years in efforts to calculate precise values of the critical exponents for the Ising model. The situation in 1979 was marked by small but disturbing discrepancies between estimates calculated by 'traditional' means, i.e. ratio and/or Padé, and those using the renormalisation group approaches. Regarding the exponent γ which characterises the divergence of the reduced susceptibility χ_0, Gaunt and Sykes (1979) presented convincing evidence that $\gamma \sim 1.250$ for the four common three-dimensional lattices (FCC, BCC, SC and diamond). The renormalisation group estimate was considerably lower, $\gamma \sim 1.241$ (Baker *et al* 1978, Le Guillou and Zinn-Justin 1980). McKenzie (1979) presented an analysis of the FCC lattice which indicated a preference for the renormalisation group value, but her approach was to assume a value for γ and consider the rates of convergence of other quantities, such as critical points and amplitudes.

The dramatic extension and analysis of the BCC high temperature series (Nickel 1981) and subsequent analyses of this series have provided estimates for γ which are closer to, but usually slightly lower than, the renormalisation group. These recent estimates are $\gamma \sim 1.2385$ (Chen *et al* 1982 and references therein) with one exception (Gammel *et al* 1983) $\gamma \sim 1.241$. It has been assumed that, given additional series coefficients, the other lattices would provide estimates in agreement with the BCC results as a consequence of universality.

This letter presents an analysis of the four three-dimensional lattices using the newly developed rational approximation method (Baumel *et al* 1982, Gammel *et al* 1983). The results indicate good agreement with the renormalisation group and with our previous results for the BCC lattice.

The series analysed are derived from the high temperature series in the variable $v = \tanh K$ which are available elsewhere (McKenzie 1975 (FCC), Sykes *et al* 1972 and Nickel 1981 (BCC), Sykes *et al* 1972 and Gaunt and Sykes 1979 (SC), Gaunt and Sykes 1973 (diamond)). Since the critical point of the Ising model on these lattices

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is not known exactly, some method is required to eliminate any biases due to its location from entering the analysis. Gaunt and Sykes, and Nickel, used the unbiased ratio method, in which the critical point is estimated using a Neville type extrapolation. This is inaccurate because the use of an extrapolation of this type assumes that the critical point estimates are converging linearly with $1/N$ without accounting for higher-order corrections. In the presence of confluent singularities, which are believed to be present in this case, the ratio estimates of the critical points converge more nearly as

$$\mu_N = a_{N+1}/a_N \sim \mu_c + (A_0/N)[1+(A_1/N^p)] \tag{1}$$

where a_n is the coefficient of v^n in the series; $\mu_c = 1/v_c$, and $0 \leqslant p < 1$. For finite values of N, the correction terms can be significant, considering the degree of precision for which one strives.

To avoid this difficulty a different method, introduced by Sheludyak and Rabinovitch (1979), is used here. The method of critical point renormalisation allows the estimate of the difference between two exponents if series are available with the same critical point. That is, given series

$$f(x) = \sum f_n x^n \sim (x-x_c)^{-\alpha} \qquad \text{and} \qquad g(x) = \sum g_n x^n \sim (x-x_c)^{-\beta}$$

the series

$$h_1(x) = \sum (f_n/g_n) x^n \sim (x-1)^{-1-(\alpha-\beta)}.$$

The two series used are the susceptibility, in the role of $g(x)$, and its logarithmic derivative, in the role of $f(x)$. Since the logarithmic derivative has a simple pole at the critical point, the self-renormalised function $h_1(x)$ formed in the above manner diverges with exponent $-(2-\gamma)$, allowing a direct estimation of γ. Reversing the roles of the susceptibility and its logarithmic derivative produces a function which we define as $h_2(x)$ which diverges with exponent γ. It is likely that the functions $h_1(x)$ and $h_2(x)$ contain confluent singularities. Unfortunately, the values of their sub-dominant exponents do not appear to be simply related to the values of the sub-dominant exponent of the susceptibility series. Therefore, to demonstrate the method, we analyse an exactly known case, the two-dimensional susceptibility. With $h_1(x)$ and $h_2(x)$ defined, any of the series analysis techniques can be used to analyse them. We use the rational approximation method.

The rational approximation method is based on the placement of orthogonal polynomials on the branch cuts, in the reciprocal plane, of the function being approximated. To determine the location of the branch of $h_1(x)$ and $h_2(x)$ we analysed them using Dlog Padé approximants. In the case of the loose packed lattices (simple quadratic, honeycomb, SC, BCC and diamond) it appears that the antiferromagnetic point at $v=-v_c$ is transformed to the point $x=-1$, although no analytical proof of this has been found. In the case of the honeycomb lattice, branch points were also indicated at the points $x=\pm\mathrm{i}$ which we believe correspond to the well known interfering singularities at $v=\pm\mathrm{i}/\sqrt{3}$ (Domb 1974). Due to limitations in our computer code, these additional singularities prevented our analysing the honeycomb lattice. The rational approximation method, however, has worked well in situations similar to this one (Baumel *et al* 1982). For the remaining loose packed lattices, Tschebysheff polynomials were placed on the interval $-1 \leqslant t \leqslant 0$ ($t = x^{-1}$). For the triangular and FCC lattices there is no apparent branch line on which to place the polynomials. It has proven effective in previous studies of the FCC specific heat to place the polynomials at the origin of the reciprocal plane (the point at infinity in the normal plane). Therefore, the degenerate polynomials $p_n(t) = t^n$ were used for the analysis of the series for the close packed lattices. The approximants were calculated for all lattices according to the formula

$$G_N = -H_N/p_N(1) \tag{2}$$

where H_N is the Nth term of the series for $H(x) = p_N(x)(\mathrm{d}/\mathrm{d}x)\ln h_i(x)$, and G_N represents $-(2-\gamma)$ in the case of $h_1(x)$ and γ in the case of $h_2(x)$.

The results of the analysis of $h_2(x)$ on the two-dimensional lattices are presented in figure 1. Convergence to the exact value $\gamma = 1.75$ is rapid. The oscillations in the simple quadratic case are large, but are very regular and rapidly decaying. The

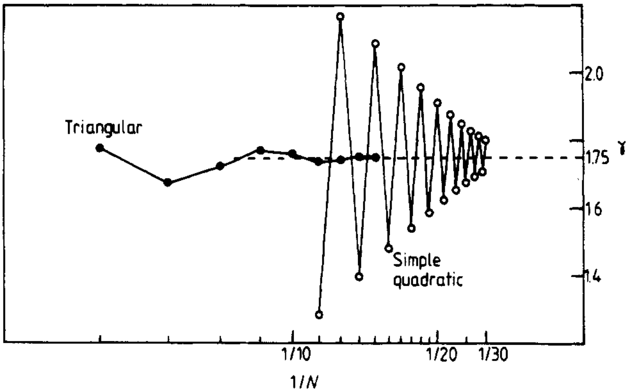

Figure 1. Successive estimates for γ against $1/N$ obtained using the rational approximation method for the triangular and simple quadratic lattices.

estimates from the triangular lattice contain oscillations of longer period, but these are nearly decayed by $N = 14$, the last approximation available. The analysis of $h_1(x)$ for the two-dimensional lattices provides a sequence of approximants which is very smooth, but slowly converging. We believe that there are two reasons for this, the first being that the exponent $-(2-\gamma) = -0.25$ is small. All known series analysis techniques converge slowly for such small exponents. It may be that other techniques, such as ratios, may be better suited to the analysis of $h_1(x)$ on the two-dimensional lattices, but we have not pursued this possibility. The second reason for the slow convergence is the likelihood that the subdominant exponent has a value in the range $0 \leqslant p < 1$. Since we expect our estimates for G_N to converge as

$$G_N = G_0 + (B/N^p) \tag{3}$$

such a value for p would dramatically slow convergence. Using the approximants obtained from $h_1(x)$ we estimate $\frac{1}{3} \leqslant p \leqslant \frac{1}{2}$ using the formula

$$-\frac{p_N + 1}{N} = \frac{(G_{N+1} - 2G_N + G_{N-1})}{(G_{N+1} - G_{N-1})/2}. \tag{4}$$

The three-dimensional results for the analysis of $h_1(x)$ are shown in figure 2. The BCC and FCC results are very nearly straight lines, while the SC displays slightly

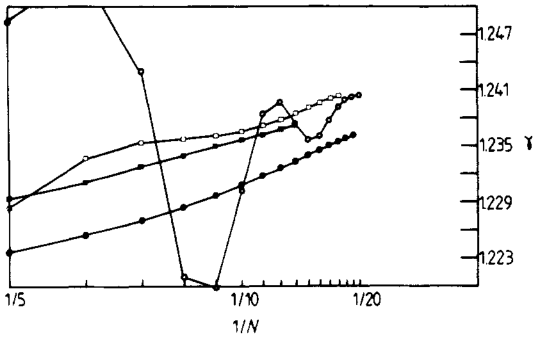

Figure 2. Successive estimates for γ against $1/N$ obtained from the rational approximation method for the three-dimensional lattices. ■ denotes FCC, □ denotes SC, ● denotes BCC and ○ denotes diamond.

oscillatory behaviour. The diamond lattice results are more erratic but generally are not inconsistent with the other lattices. We use a plot of $1/N$ because we estimate $p \sim 0.9–1.0$ from the BCC and FCC curves.

To investigate the issue of a common limit for the curves, we plot in figure 3 the differences between the approximants. That is, we calculate $D = (G_N^{\mathrm{FCC}} - G_N^{\mathrm{BCC}})$ (the full circles) and $D = (G_N^{\mathrm{SC}} - G_N^{\mathrm{BCC}})$ (the open circles), and plot against $1/N$. If a common limit exists, these curves should approach the origin. It appears that the FCC–BCC case is converging nicely to zero. The SC–BCC case apparently turns away from the origin at $N \sim 12$, but may be turning back by $N \sim 16$ or 17. Further coefficients in the SC and BCC series may decide this issue. We conclude that upper limits of

$$D = |\gamma_{\mathrm{FCC}} - \gamma_{\mathrm{BCC}}| < 0.0005 \qquad D = |\gamma_{\mathrm{SC}} - \gamma_{\mathrm{BCC}}| < 0.005$$

are consistent with our results. We provide no better estimate of γ_{BCC} than we have previously given, i.e. $\gamma = 1.241 \pm 0.001$ (Gammel *et al* 1983).

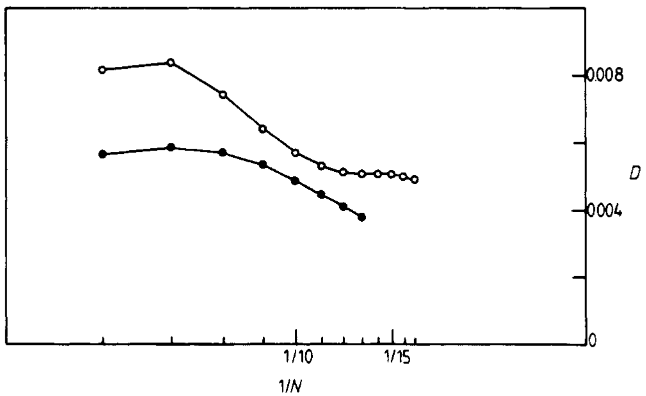

Figure 3. Successive estimates for the differences between the susceptibility exponents for the FCC–BCC (full circles) and SC–BCC (open circles) lattices, derived from the data plotted in figure 2.

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