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LETTER TO THE EDITOR

On the variation of the critical exponent γ with spin

J L Gammel and D C Power†

Physics Department, Saint Louis University, St Louis, Missouri 63103, USA

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Abstract. The rational approximation method is used to examine estimates for the first and second derivatives of the critical exponent of the Ising model with respect to a variable related to the spin on the three-dimensional body centred cubic lattice. 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 support the concepts of universality of γ with respect to the spin.

In a recent publication (Gammel and Power 1983, hereafter referred to as I) we examined the behaviour of the estimates for the critical exponent γ of the Ising model for four three-dimensional lattices, the face centred cubic, the body centred cubic, the simple cubic, and the diamond. We presented evidence which supported the concept of universality with respect to the coordination number, q. In particular, we examined the difference in the estimates for the face centred and body centred cubic, and the simple and body centred cubic lattices and found them to be tending toward zero. We found that the estimates for the diamond lattice were consistent with the other lattices, but contained oscillations as a function of the parameter $(1/n)$ which precluded inclusion in the detailed analysis.

In this paper we investigate the behaviour of successive estimates of the first and second derivatives of γ with respect to a variable related to the spin on the body centred cubic lattice. As in I we use a method we call the 'self renormalised critical point' technique and the rational approximation method. To briefly outline the method, consider two series

$$f(x)=\sum f_n x^n \sim (x-x_0)^{-\alpha}, \qquad g(x)=\sum g_n x^n \sim (x-x_0)^{-\beta} \qquad \text{for } x\sim x_0; \tag{1}$$

then the series

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

We use the general spin susceptibility series $\chi(K)$ as the function $g(x)$ and its logarithmic derivative as $f(x)$. The resulting series $h(x)$ diverges with exponent $(2-\gamma)$ allowing a direct estimate of γ.

Standard Padé analysis of the logarithmic derivative of $h(x)$ indicates, in addition to the singularity at $x=1$, a branch point at $x=-1$, and a cut extending to $x=-\infty$ along the negative real axis. According to the rational approximation method, we place orthogonal polynomials along the image of this cut in the reciprocal plane ($t=x^{-1}$). Specifically, we place Tchebycheff polynomials on the interval $-1\leqslant t\leqslant 0$,

† Current address: McDonnell Aircraft Co, PO Box 516, St Louis, Missouri 63166, USA.

and calculate approximants according to the formula

$$l_n = -(2-\gamma)_n = H_n/p_n(1) \tag{2}$$

where p_n is the nth-order Tchebycheff polynomial and H_n is the coefficient of x^n of the quantity $(1-x)p_n(x)\,(\mathrm{d}/\mathrm{d}x)\ln h(x)$.

Consider the form of the general spin susceptibility series

$$\chi(S,K) = 1 + \sum_n K^n \sum_{m=1}^{n} [1-3/4S(S+1)]^{m-1} A_n^m. \tag{3}$$

Since these are explicitly functions of the quantity $s=[S(S+1)]^{-1}$, we use s as the independent variable rather than S.

Using equation (2) to obtain estimates for $\gamma_n(s)$, we approximate $\mathrm{d}\gamma_n/\mathrm{d}s$ and $\mathrm{d}^2\gamma_n/\mathrm{d}s^2$ by the finite difference formulae

$$\begin{aligned}\frac{\Delta\gamma_n}{\Delta S} &= \frac{\gamma_n(S+\Delta S)-\gamma_n(S-\Delta S)}{2\Delta S},\\ \frac{\Delta^2\gamma_n}{\Delta S^2} &= \frac{\gamma_n(S+\Delta S)-2\gamma_n(S)-\gamma_n(S-\Delta S)}{\Delta S^2},\end{aligned} \tag{4}$$

and the chain rule for differentiation

$$\begin{aligned}\frac{\mathrm{d}\gamma_n}{\mathrm{d}s} &= \frac{\mathrm{d}S}{\mathrm{d}s}\frac{\Delta\gamma_n}{\Delta S} = -\frac{S^2(S+1)^2}{2S+1}\frac{\Delta\gamma_n}{\Delta S},\\ \frac{\mathrm{d}^2\gamma_n}{\mathrm{d}s^2} &= \frac{\mathrm{d}^2S}{\mathrm{d}s^2}\frac{\Delta\gamma_n}{\Delta S} + \frac{\mathrm{d}S^2}{\mathrm{d}s}\frac{\Delta^2\gamma_n}{\Delta S^2}.\end{aligned} \tag{5}$$

Since the finite difference expressions (4) are valid approximations for $\mathrm{d}\gamma_n/\mathrm{d}S$ and $\mathrm{d}^2\gamma_n/\mathrm{d}S^2$ only in the limit $\Delta S \to 0$, we examined their behaviour for increasingly small values of ΔS. Some of the results are given below.

$|\Delta\gamma_n/\Delta S|$ $(S=1)$

ΔS	$n=19$	$n=17$	$n=15$
0.005	0.020 405 01	0.021 478 86	0.022 751 77
0.010	0.020 406 64	0.021 479 69	0.022 752 65
0.020	0.020 409 78	0.021 483 01	0.022 756 18
0.040	0.020 422 35	0.021 498 28	0.022 770 28

Based on these results we used $\Delta S = 0.010$ and believe that $\Delta\gamma_n/\Delta S$ calculated in this way is an approximation to $\mathrm{d}\gamma_n/\mathrm{d}S$ accurate to approximately four to five decimal places.

Another question relating to our method is the form of the convergence of successive estimates as a function of $(1/n)$. It can be shown quite generally (Baumel *et al* 1982) that the approximants obtained using the rational approximation method converge as

$$\alpha_n = \alpha_0 + A/n^p \tag{6}$$

to leading order in the presence of confluent singularities, where α is a generic critical exponent, and p is not necessarily an integer. The sequences of estimates we obtain are smooth enough to allow an estimation of the value of p using the equation

$$-(p_n+1)/n = (\alpha_{n+1} - 2\alpha_n + \alpha_{n-1})/(\alpha_{n+1} - \alpha_{n-1})/2. \tag{7}$$

We plot successive estimates for p_n, for the quantity $\mathrm{d}\gamma_n/\mathrm{d}s$ as a function of n^{-1} in figure 1. It appears that the estimates are settling down to a value in the range $0.3 \leq p \leq 0.7$ but an accurate extrapolation is clearly not possible. Therefore we choose $p = 0.5$ and proceed with the caution that precise quantitative predictions will depend on this choice. We therefore restrict ourselves to observation of trends in the remainder of the paper.

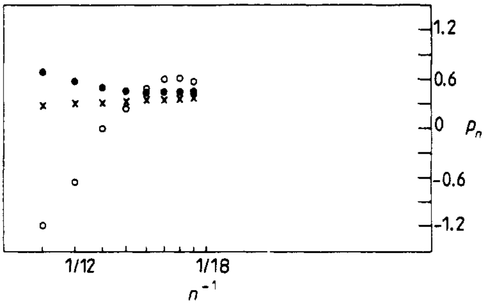

Figure 1. Successive estimates for the exponent of convergence, p_n, plotted as a function of n^{-1}. The open circles represent values obtained from the $\mathrm{d}\gamma_n/\mathrm{d}s$ sequence at $S = \frac{1}{2}$. The full circles and crosses represent $\mathrm{d}\gamma_n/\mathrm{d}s$ at $S = 1$ and $S = 2$ respectively.

From (6) it is clear that plots of $\mathrm{d}\gamma_n/\mathrm{d}s$ and $\mathrm{d}^2\gamma_n/\mathrm{d}s^2$ will be asymptotically linear if plotted against n^{-p}, if p has been correctly chosen. Figures 2 and 3 are plots of these quantities against $n^{-0.5}$. From these plots it appears that the derivatives are decreasing in magnitude steadily and may be approaching linearity. Although precise extrapolations are not possible, we believe that a value of zero for both $\mathrm{d}\gamma/\mathrm{d}s$ and $\mathrm{d}^2\gamma/\mathrm{d}s^2$ is consistent with our results, and with the universality assumption.

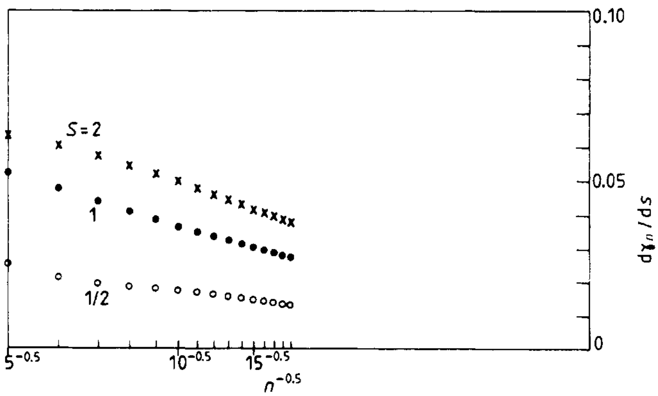

Figure 2. Successive estimates for the first derivative of $\mathrm{d}\gamma_n/\mathrm{d}s$ with respect to $s = [S(S+1)]^{-1}$, plotted against $n^{-0.5}$.

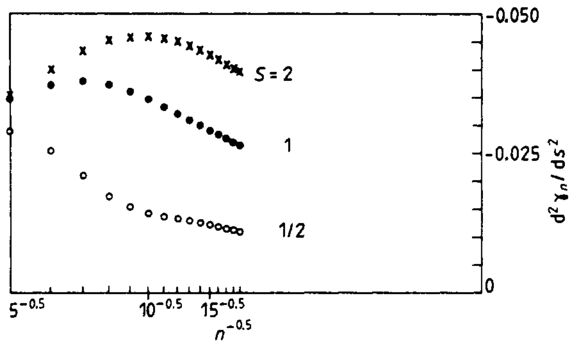

Figure 3. Successive estimates for the second derivative of $d^2\gamma_n/ds^2$ with respect to $s=[S(S+1)]^{-1}$, plotted against $n^{-0.5}$.

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