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LETTER TO THE EDITOR

Series expansion analysis of corrections to scaling in the three-state Potts model

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Abstract. Several extant series for the $d=2$, $q=3$ Potts model are analysed with a method suggested recently that explicitly accounts for the effect of confluent corrections to scaling. Excellent agreement with the conjectured exponents for this model is found, as well as confirmation of renormalisation group estimates of the sub-leading eigenvalue.

The three-state ($q=3$) Potts model (for a review, see Wu 1982) with Hamiltonian

$$-\beta\mathscr{H} = K \sum_{\langle ij\rangle} \delta_{S_i S_j}$$

where i and j are neighbouring sites with variables S_i and S_j which can each take one of three values, is known (Baxter 1973, Baxter *et al* 1978) to have a continuous (second-order) phase transition at $d=2$. The critical exponents are not known exactly, but plausible conjectures for the thermal eigenvalue $y_{\mathrm{T}}^{(q=3)} = \frac{6}{5}$ (den Nijs 1979) and the magnetic eigenvalue $y_{\mathrm{H}}^{(q=3)} = \frac{28}{15}$ (Nienhuis *et al* 1980, Pearson 1980a) of the $d=2$ Potts model lead to exponent predictions. For the exponents of the specific heat C_{v} ($\sim|T-T_{\mathrm{c}}|^{-\alpha}$), magnetisation M ($\sim|T-T_{\mathrm{c}}|^{\beta}$) and susceptibility χ ($\sim|T-T_{\mathrm{c}}|^{-\gamma}$) these are $\alpha = 2-d/y_{\mathrm{T}} = \frac{1}{3}$, $\beta = (d-y_{\mathrm{H}})/y_{\mathrm{T}} = \frac{1}{9}$ and $\gamma = (2y_{\mathrm{H}}-d)/y_{\mathrm{T}} = \frac{13}{9}$, respectively.

Confirmation of these conjectures from the results of numerical calculations is, in general, tolerable but not outstanding. In particular, the β estimates listed by Wu (1982) all fall below 0.109. The 'best' (closest to the conjectured) results for α are from the Kadanoff variational renormalisation group (RG) calculations ($\alpha = 0.3365$ (Burkhardt *et al* 1976) and $\alpha = 0.326$ (Dasgupta 1977)), and from some Hamiltonian series for the Z_3 model ($\alpha = 0.320 \pm 0.004$ (Elitzur *et al* 1979)). The usual (partition function) series results for α are either very bad (Zwanzig and Ramshaw 1977) or exhibit slow convergence (Enting 1980).

Recently, there has been considerable interest in series analysis methods which explicitly account for the influence of the leading confluent singularities on critical exponent estimates. Much attention has been paid to the $d=3$ Ising (or $q=2$ Potts) model, where correct treatment of the leading non-analytic confluent term has been shown to remove discrepancies between series and RG results (Roskies 1981, Zinn-Justin 1981, Chen *et al* 1982, Adler *et al* 1982b, and references therein).

If we consider a (q, d) plane of Potts models (figure 1) with q values on the abscissa and d values on the ordinate we may look along the line of fixed $q=2$ (Ising model) and varying d, and observe that the next to leading eigenvalue, which is marginal at $d=4$ (causing logarithmic corrections, Wegner 1972), governs the non-analytic

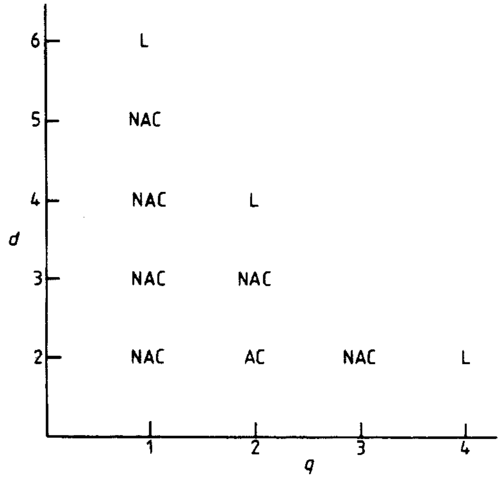

Figure 1. The (q, d) plane of Potts models. L indicates leading logarithmic corrections to scaling, NAC indicates leading non-analytic power law confluent corrections and AC indicates leading analytic confluent corrections. References for $d = 2$ and all $q = 2$ are in the text, and the $q = 1$ results are quoted from Houghton *et al* (1978), Aharony (1980), and Adler *et al* (1982c).

confluent corrections to scaling at $d = 3$ (Wegner 1972). In the $d = 2$ Ising model the leading correction to scaling term is analytic and is attributed to nonlinear scaling fields (Aharony and Fisher 1980).

A similar picture arises if we look along the line of fixed $d = 2$. The $q = 4$ Potts model (for which agreement between the y_T and y_H conjectures and the results of numerical calculation is even worse than for $q = 3$ (Wu 1982)) has logarithmic corrections at $d = 2$ caused by the marginality of the next to leading eigenvalue y' (Nauenberg and Scalapino 1980, Rebbi and Swendsen 1980). These explain the slow convergence of both Monte Carlo RG and series work for this model. At $q = 3$ this next to leading eigenvalue causes non-analytic corrections to scaling and the critical behaviour is of the form (considering C_v as an example)

$$C_v \sim \text{constant}|T - T_c|^{-\alpha}(1 + a_c|T - T_c|^{\Delta_1} + b_c|T - T_c| + \ldots) \tag{1}$$

where a_c is the coefficient of the non-analytic correction to scaling ($\Delta_1 = y'/y_T$ is universal (Wegner 1972)) and b_c is the coefficient of the first analytic term which is always present. The case of $q = 2$ (Ising model) was mentioned above and in the case $q = 1$ (bond percolation) non-analytic corrections to scaling are again present ($\Delta_1 > 1$, Adler *et al* 1982a, and references therein). Here again proper treatment of these corrections removes discrepancies between conjectures and series results and thus it seems reasonable to expect that series for the $q = 3$ Potts model should be analysed with the assumed critical behaviour of the type of equation (1). (We note that logarithmic corrections should not occur for any $q \neq 4$ at $d = 2$ (Adler and Privman 1981).)

Various methods of evaluating Δ_1 from series expansions have been developed (see the references listed above for the $d = 3$ Ising model). In the present letter, we shall apply the method introduced by Adler *et al* (1982a) to several series for the $q = 3$ Potts model, and shall show that improved exponent estimates are obtained, as well as results for y' that are in agreement with the RG predictions.

We restrict our attention to the case of the square lattice (where T_c is exactly known from duality arguments (Potts 1952, Hintermann *et al* 1978)). We consider the low-temperature series of Enting (1980, 1982) for the magnetisation

$$M = 1 - \sum_{k=4}^{35} b_k u^k + O(u^{36})$$

and the partition function

$$Z = 1 + \sum_{k=4}^{35} a_k u^k + O(u^{36}),$$

where $u \equiv e^{-K}$ and $u_c = (\sqrt{3}-1)/2$. The second series is transformed to a series for $E_s = (1 - 1/\sqrt{3}) - u(\mathrm{d}\ln Z/\mathrm{d}u)$, where E_s has exponent $1-\alpha$. We also consider the 'quantum Hamiltonian' series of Pearson (1980b, 1982) for the magnetisation

$$M = \sum_{n=0}^{15} m_n x^n + O(x^{16}),$$

the susceptibility

$$\chi/x^2 = \sum_{n=0}^{13} \chi_n x^n + O(x^{14})$$

and the ground-state energy

$$\varepsilon_0 = \sum_{n=0}^{15} e_n x^n + O(x^{16})$$

which have $x_c = 1$ (x is a temperature-like variable). We take two derivatives of the last (ε_0) series to obtain a series for C_v.

The method introduced by Adler *et al* (1982a) involves transforming a series in the variable t with leading critical behaviour of the form

$$f(t) \approx \mathrm{constant}(t_c - t)^{-h}[1 + a_f(t_c - t)^{\Delta_1} + \ldots] \qquad (2)$$

to an expansion in powers of $y = 1 - (1 - t/t_c)^{\Delta}$ where $y_c = y(t_c) = 1$ (a restricted form of this transformation with $\Delta = \Delta_1$ was studied by Roskies (1981)). The function

$$F_\Delta(y) = f(t(y)) \approx \mathrm{constant}\ t_c^{-h}(1-y)^{-h/\Delta}[1 + a_f t_c^{\Delta_1}(1-y)^{\Delta_1/\Delta} + \ldots]$$

is studied for various input values of Δ, using the biased Dlog Padé method. (An exact t_c value is important although this analysis is possible when t_c is unknown (Adler *et al* 1982b).) Different Padé approximants to the function

$$h_{\mathrm{out}}(\Delta) = \{\Delta(1-y)[\mathrm{d}(\ln F_\Delta(y))/\mathrm{d}y]\}_{y=1}$$

define a family of $h = h_{\mathrm{out}}(\Delta)$ curves in the (Δ, h) plane. When the input $\Delta = 1$, evaluation of $h_{\mathrm{out}}(\Delta)$ is equivalent to the usual Dlog Padé, and the confluent term in equation (2) may introduce systematic errors in the h_{out} values, but in the case that the input Δ is close to the correct Δ_1, the influence of the confluent term is to change the relative *slopes* of different $h_{\mathrm{out}}(\Delta)$ curves (see Adler *et al* 1982a for details). Ideally, $h_{\mathrm{out}}(\Delta)$ curves should intersect at the correct (Δ_1, h), however due to other finite series effects, one usually obtains a region of convergence (with a large number of intersections) of different $h_{\mathrm{out}}(\Delta)$ curves (see Adler *et al* 1982a, b for examples and further discussion).

In figures 2 and 3 we present the results for the magnetisation series in the usual (Enting 1980, 1982) and 'quantum Hamiltonian' (Pearson 1980b, 1982) cases, respectively. The different $-\beta(\Delta)$ curves in figures 2 and 3 were obtained by evaluating nine central Padé approximants to each series. In both cases we observe clear regions of 'convergence' of different $-\beta(\Delta)$ curves, delineated by broken-line boxes. Critical exponent estimates from the usual (figure 2) and Hamiltonian (figure 3) magnetisation series are

$$\beta = 0.1110 \pm 0.0007 \qquad \text{and} \qquad \Delta_1 = 0.63 \pm 0.19$$

$$\beta = 0.1111 \pm 0.0006 \qquad \text{and} \qquad \Delta_1 = 0.54 \pm 0.14$$

respectively. Our β values are in excellent agreement with the conjectured $\beta = \frac{1}{9} = 0.11111\ldots$. Inspection of figures 2 and 3 shows that input $\Delta = 1$ corresponds to $\beta \lesssim 0.110$, thus correct treatment of the leading confluent term removes a small systematic deviation of β values. We shall discuss Δ_1 values below.

In both figures 2 and 3 there is the second region of convergence of $-\beta(\Delta)$ curves at $\Delta \sim 1$. This structure may be attributed to the analytic ($\Delta_1 \equiv 1$) correction term (b in equation (1)) or to higher non-analytic terms. In either case, presence of such an additional confluent term of non-negligible amplitude may introduce residual systematic errors in estimates from the first regions of convergence. In order to understand the origin of the second convergence region, and to study its possible influence on β (and Δ_1) estimates, we used a method suggested by Aharony (1982). This method involves analysing the F_Δ series derived from $f/[1 + b(t_c - t)]$ with varying input b values. The effect of this division is to change the amplitude of the leading analytic term (equation (1)). A scan of different input b values shows that while the first

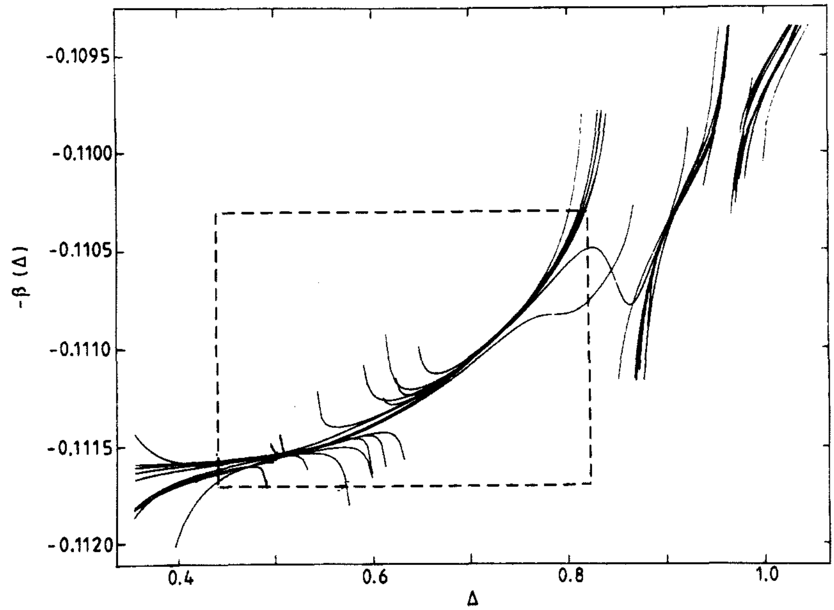

Figure 2. $-\beta(\Delta)$ curves for the M series of Enting (1980, 1982) obtained using [15, 19], [16, 18], [17, 17], [18, 16], [19, 15], [15, 18], [16, 17], [17, 16] and [18, 15] Padé approximants.

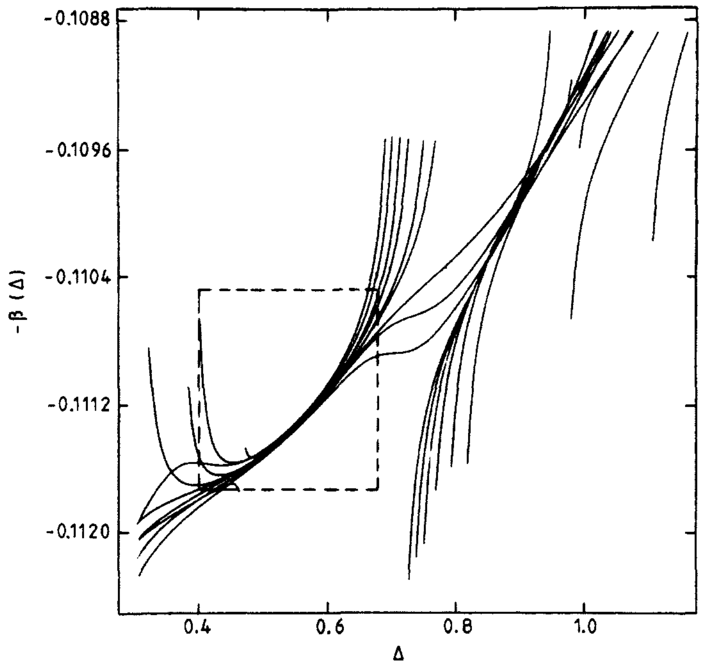

Figure 3. $-\beta(\Delta)$ curves for the M series of Pearson (1980b, 1982) obtained using [5, 9], [6, 8], [7, 7], [8, 6], [9, 5], [5, 8], [6, 7], [7, 6] and [8, 5] Padé approximants.

convergence region is not appreciably influenced, both the position and the structure of the second region depend strongly on the input b value. We did not succeed in finding b values such that the second region disappears, but using the present method and a different method (also mentioned in Adler *et al* (1982a) as an extension of the method of Adler *et al* (1981) and not discussed here in detail because the method which we consider here usually gives more stable results) we were able to estimate (for both M series) that the order of magnitude of $b_M \sim -(0.1 \div 0.2)$. As an illustration, we present the $-\beta(\Delta)$ curves obtained for the Hamiltonian $M/[1+b(t_c-t)]$ series with input $b=-0.1$ in figure 4. One clearly observes the change in the position and the structure of the second region (cf figure 3), while the first convergence region is only slightly changed, the new ranges of β and Δ_1 values being

$$\beta = 0.1113 \pm 0.0012 \qquad \text{and} \qquad \Delta_1 = 0.54 \pm 0.12.$$

In figures 5 and 6 we present the result for the E_s series (derived from the Z series of Enting (1980, 1982)) and for the Hamiltonian C_v series (derived from the ε_0 series of Pearson (1980b, 1982)), respectively. The α and Δ_1 estimates from the regions of convergence of different $\alpha(\Delta)-1$ curves (in the E_s case) and $\alpha(\Delta)$ curves (in the C_v case), which are enclosed in the broken-line boxes of figures 5 and 6, are (for E_s and C_v series, respectively)

$$\alpha = 0.348 \pm 0.008 \qquad \text{and} \qquad \Delta_1 = 0.56 \pm 0.14 \tag{3}$$

$$\alpha = 0.331 \pm 0.009 \qquad \text{and} \qquad \Delta_1 = 0.65 \pm 0.12. \tag{4}$$

The second convergence region at $\Delta \sim 1$ in the E_s case (figure 5) and some structure at $\Delta \sim 1$ in the C_v case (figure 6) are again due to the analytic b term (equation (1)).

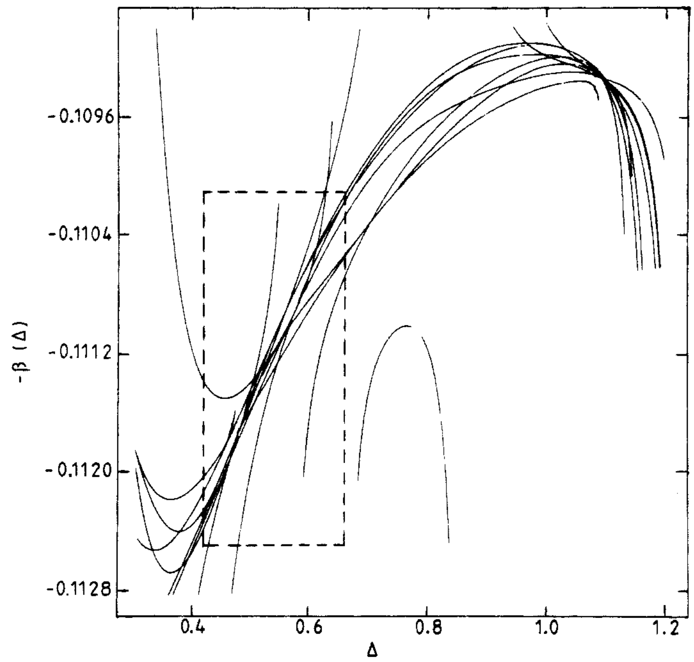

Figure 4. $-\beta(\Delta)$ curves obtained from the series of $M/[1+b(x_c-x)]$, with $b=-0.1$. The M series is that studied in figure 3.

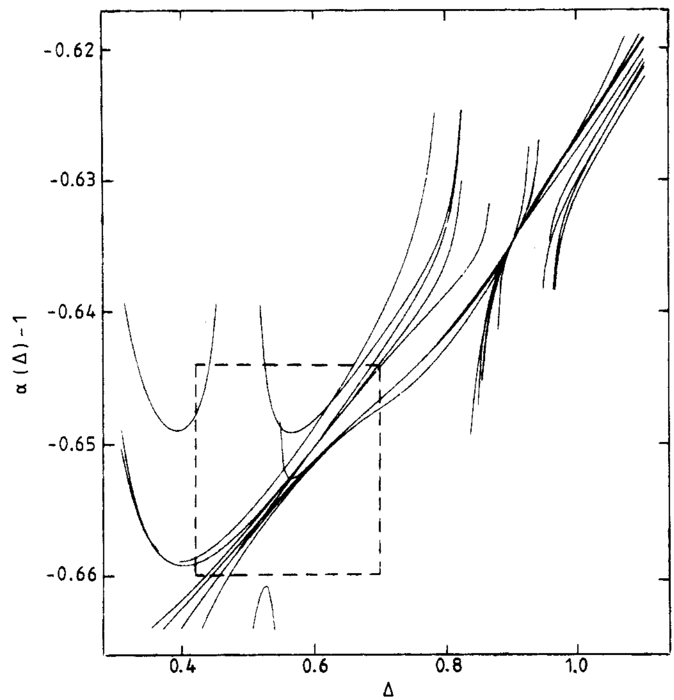

Figure 5. $\alpha(\Delta)-1$ curves for the E_s series (derived from Z series of Enting (1980, 1982)) obtained using [15, 19], [16, 18], [17, 17], [18, 16], [19, 15], [15, 18], [16, 17], [17, 16] and [18, 15] Padé approximants.

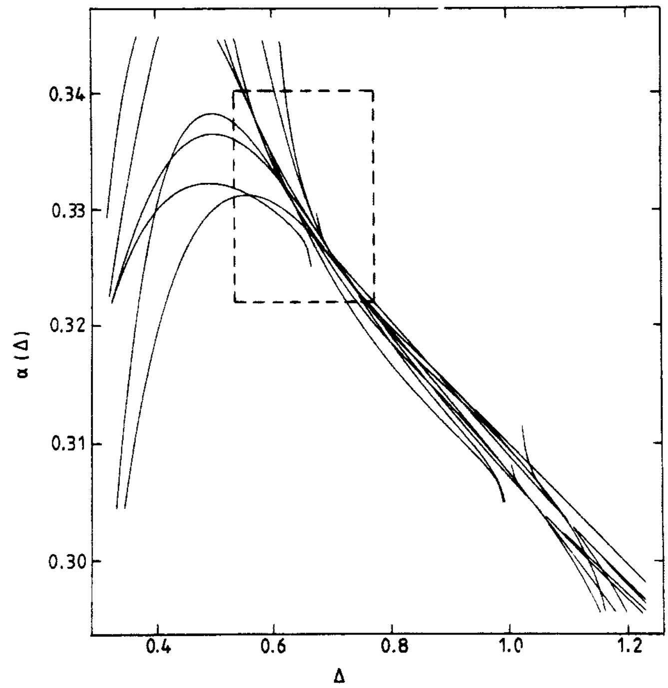

Figure 6. $\alpha(\Delta)$ curves for the C_v series (derived from the ε_0 series of Pearson (1980b, 1982)) obtained using [4, 8], [5, 7], [6, 6], [7, 5], [8, 4], [4, 7], [5, 6], [6, 5] and [7, 4] Padé approximants.

We have verified this with the same method as for the M-series case, but the situation here is less clear, and we did not determine the order of magnitude of b_{E_s} or b_{C_v}. The first convergence region is rather stable with respect to changing the amplitude of the analytic term.

The conjectured α value is $\alpha = \frac{1}{3} = 0.3333\ldots$, and is apparently outside the range of equation (3). It must be stressed, however, that our error estimates based on the 'boxes' enclosing the convergence regions are rather subjective, and overestimation of the accuracy of the results, due to their apparent stability, is possible. Typical α values at $\Delta \sim 1$ (see figures 5 and 6) are $\alpha \approx 0.31$ for the C_v series and $\alpha \approx 0.37$ for the E_s series (the last α value is a typical one obtained in the usual Padé analysis (see Enting 1980)). Thus a correct treatment of the leading confluent term reduces the 'discrepancy' between the series α estimates and the conjectured value by an order of magnitude. There still remains a possibility that the residual deviation of the central values of equations (3) and (4) from the conjectured $\alpha = \frac{1}{3}$ is due to a systematic error induced by higher correction terms.

We also analysed the (relatively short) Hamiltonian χ series of Pearson (1980b, 1982). In this case we found evidence for an analytic (b of equation (1)) term of large amplitude. The first convergence region is difficult to locate (we do not present the details of the analysis here). We were able to determine for γ and Δ_1 the following rather wide ranges:

$$\gamma = 1.449 \pm 0.027 \qquad \text{and} \qquad \Delta_1 = 0.53 \pm 0.18.$$

Note that the conjectured γ value is $\gamma = \frac{13}{9} = 1.4444\ldots$, and that typical γ values obtained from the usual Padé analysis are $\gamma \gtrsim 1.49$.

Our overall Δ_1 estimate is an average of the ranges quoted above of Δ_1 values as well as of the results of the analysis for different series when the analytic term of varying amplitude is divided out. We propose

$$\Delta_1 = 0.57 \pm 0.13.$$

Assuming the conjectured $y_T = \frac{6}{5}$, we can obtain an estimate of the absolute value of the leading irrelevant RG eigenvalue

$$y' = \Delta_1 y_T = 0.68 \pm 0.16. \tag{5}$$

Estimates of y' have been made in several real-space RG studies of the $q = 3$ Potts model (as a special case of the Blume–Emery–Griffiths model by Berker and Wortis (1976), ($y' = 0.52$), Burkhardt *et al* (1976), ($y' = 0.46$) and Adler *et al* (1978), ($y' = 0.6$) and as a Potts lattice gas with vacancies by Rebbi and Swendson (1980), ($y' = 0.7$)). Nienhuis (1982) has recently provided analytic support for Burkhardt's (1980) conjecture that $y' = \frac{4}{5} = 0.8$ (at $q = 3$). The first term of an expansion in powers of $\varepsilon = (4-q)^{1/2}$ (Cardy *et al* 1980) gives $y' \approx 2/\pi \approx 0.64$. Finally, Pearson (1980a) has conjectured that $y' = \frac{2}{3} \approx 0.67$. Our range of y' includes most of these predictions, though Pearson's (1980a) conjecture and the Monte Carlo RG results (Rebbi and Swendsen 1980) are the closest to our central value.

We are unaware of experimental results available for comparison with y' or Δ_1 but the results of Bretz (1977) for helium adsorbed on graphite which is in the $q = 3$ Potts universality class suggest $\alpha = 0.35 \pm 0.02$. It is interesting to speculate whether a Δ_1 value could be obtained from such an experiment (as has been done for superfluid helium (Ahlers 1980)) and whether an analysis of the data with the scaling form of equation (1) would alter the α value, as occurs in the series analysis.

In summary, we have found that the inclusion of a correction to scaling term with the exponent Δ_1 consistent with the results of several RG calculations, leads to series analysis values of the critical exponents α, β and γ which agree with the conjectured 'exact' values.

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