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LETTER TO THE EDITOR

Convergence of finite-size scaling renormalisation techniques

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Abstract. The rate of convergence of the transfer matrix finite-size scaling (or phenomenological renormalisation) method is studied. It is shown both heuristically and numerically that the convergence of estimates for exponents, etc, is governed asymptotically by the leading irrelevant-variable scaling exponent. The more rapid apparent convergence rates observed in many practical calculations for two-dimensional lattices of widths up to ten lattice spacings are attributed to cancellation between various correction terms.

The finite-size rescaling method (or 'phenomenological renormalisation group (RG) technique') introduced by Nightingale (1979) has been used to study the critical behaviour of a variety of the $(d=2)$-dimensional lattice models. (See Nightingale (1982) for an overview and references to the literature.) This method is essentially an application of the finite-size scaling theory of Fisher (1971; Fisher and Barber 1972). Frequently, rather accurate numerical estimates for critical exponents are obtained as judged by comparison with exactly known or reliably conjectured results. The asymptotic rate of convergence of approximants for a critical exponent, say ν, follows from finite-size scaling theory (see below) and should normally be governed by the leading irrelevant bulk RG eigenvalue or scaling exponent, $\lambda_3 \equiv y_3$, which is *negative*. One thus anticipates

$$\nu_{L,L-1} = \nu[1 + CL^{y_3} + E(L)], \tag{1}$$

where $\nu_{L,L-1}$ is obtained from data for lattice strips of width L and $L-1$ lattice spacings (see below), while $E(L)$ denotes terms vanishing more rapidly than $L^{-|y_3|}$ as $L\to\infty$. However, it has been observed by Derrida and DeSeze (1982), Blöte and Nightingale (1982) and Derrida (1981) (see also references quoted in these papers) that the apparent convergence exponent, often called x, found by fitting the finite-size data for $L \lesssim 10$ to the expression

$$\nu_{L,L-1} \simeq \nu(1 + cL^{-x}), \tag{2}$$

has a value $x \gtrsim 2$ for several models for which $|y_3| \lesssim 1$ is expected! Similar effects have been noted in 'phenomenological RG' analyses of Monte Carlo (MC) data, by Binder (1981).

The work reported here attempts to understand the pattern of convergence of finite-size rescaling data and to resolve the seeming contradiction between (1) and (2). First we summarise the derivation of (1) with an emphasis on the variety of sources of corrections, arising from 'bulk' and 'finite-size' effects. Next we use a series analysis technique to estimate y_3 from finite-size data for the $q=3$ Potts model and for percolation problems in $d=2$ dimensions. Finally, we present some evidence that the abnormally large apparent convergence exponent, x, observed for these models, when $L \leqslant 10$, is due to a cancellation between the CL^{y_3} term in (1) and higher-order terms in $E(L)$. We also comment briefly on methods of extrapolating finite size data.

Consider, for illustration, the general bulk ($L=\infty$) RG transformation for the susceptibility, which may be written

$$\chi(g_t, g_h, g_u, \ldots) \approx b^{\gamma/\nu}\chi(g_t b^{y_T}, g_h b^{y_H}, g_u b^{y_3}, \ldots), \tag{3}$$

where b is the RG spatial rescaling factor, while g_t, g_h and g_u are nonlinear scaling fields which approach $t=|T-T_c|/T_c$, $h=H/k_B T$, and a constant u, respectively, in a smooth, analytic manner, when the critical point is approached. (We will comment below on further corrections.) Correspondingly, y_T, $y_H > 0 > y_3 > \ldots$ are the RG fixed point eigenvalues $(\lambda_1, \lambda_2, \lambda_3, \ldots)$ or scaling exponents. We will retain explicitly only the leading irrelevant scaling field in (3). For finite-width systems with periodic (or helical) boundary conditions Brézin (1982) has argued that (3) is still approximately valid for finite $D \equiv La \gg a$, where a is the lattice spacing, and that L can be identified as the RG flow parameter, i.e. $b \propto L$ (provided $D/b \equiv La/b \gg a$). A finite-size scaling form is thus obtained as

$$\chi(g_t, g_h, g_u, \ldots; L) = L^{\gamma/\nu} Y_\chi(g_t L^{y_T}, g_h L^{y_H}, g_u L^{y_3}, \ldots) + \Delta\chi(g_t, g_h, g_u, \ldots; L), \tag{4}$$

where one cannot *a priori* exclude the possibility that the bulk nonlinear scaling fields, $g_t, g_h, g_u, \ldots$, are themselves modified by finite-size effects so that they also depend smoothly on, say, L^{-1}: no theoretical study of this point is presently available to our knowledge. Further finite-size corrections depending on the lattice spacing a are contained in $\Delta\chi$ in (4). In general, the only information available on their form is that they become exponentially small when $L \to \infty$ at fixed *non*-critical temperatures, i.e. when $T \neq T_c$. For non-periodic, e.g. free, boundary conditions an expression of the form of (4) can also be advanced: however, the scaling function Y will then contain new arguments with L-dependent, 'surface' scaling fields which result from the generation of surface couplings by the RG transformations (see e.g. Diehl (1982) for a review of this topic and references). In addition, the exponential smallness (at $T \neq T_c$) of other corrections, if true, cannot then be demonstrated so easily. For some further discussion see Fisher (1971, 1973a), and Nakanishi and Fisher (1983).

For quantities such as the free energy or the *finite-size* longitudinal correlation length, $\xi_\parallel$, (calculated, say, from the two largest eigenvalues of the transfer matrix) the relations (3) or (4) hold, with appropriate exponents, only for the singular part, and additional additive background terms must be anticipated; these represent a further source of corrections to the leading scaling behaviour. In what follows we will concentrate on the effect of the leading *bulk* irrelevant scaling field, u. Consider, for example, the estimation of the correlation exponent ν for a ferromagnetic model from the standard expression

$$1 + 1/\nu_{L,L-1} = \ln\left[\frac{\partial\xi(\ldots; L)}{\partial T}\Big/\frac{\partial\xi(\ldots; L-1)}{\partial T}\right]_c \Big/ \ln\left(\frac{L}{L-1}\right), \tag{5}$$

where the subscript c denotes evaluation at $T=T_c$ (supposed known) and $H=0$ (Nightingale 1979). On using the scaling form

$$\xi_\parallel \approx L Y_\xi(tL^{1/\nu}, hL^{y_H}, uL^{y_3}), \tag{6}$$

(with, as usual, $\lambda_1 = y_T = 1/\nu$) and the property (Fisher 1971) that Y_ξ is differentiable any number of times at the origin where all the arguments vanish, we obtain after some algebra

$$\nu_{L,L-1} = \nu(1 + CL^{y_3} + E_1 L^{y_3-1} + E_2 L^{2y_3} + \ldots), \tag{7}$$

where the higher terms involve powers $n_3 y_3 - n_2$ with $n_2 = 0, 1, 2, \ldots$ and $n_3 = 1, 2, 3, \ldots$. (Note, we are assuming here that u is not a 'dangerous irrelevant variable' as it would be for d exceeding the upper borderline dimensionality, $d_>$ (see Fisher 1973b).) Recently, Aharony and Fisher (1983) studied the effects of the nonlinearities of scaling fields on corrections to scaling: on the basis of their analysis (§ IV) we immediately conclude that if the *exact* T_c is used in (5), only the coefficients of the correction terms in (7) will be affected by the 'bulk' (or L-independent) nonlinearities. Usually, however, T_c itself is also estimated from finite-size data; for example one can solve numerically the relation

$$\xi_\parallel(T_0, H = 0; L)/L = \xi_\parallel(T_0, H = 0; L-1)/(L-1), \tag{8}$$

to obtain an estimate, $T_{0,L}$, for T_c. If we put $t_{L,L-1} \equiv |T_{0,L} - T_c|/T_c$ then (6) gives

$$t_{L,L-1} \propto L^{y_3 - y_T} + \ldots. \tag{9}$$

Allowing for the bulk nonlinearities of the scaling fields, one can show that higher powers of L in (9) have exponents $(n_3 y_3 - n_1 y_T - n_2)$ with $n_1, n_3 = 1, 2, 3, \ldots$ and $n_2 = 0, 1, 2, \ldots$. If we use $T_{0,L}$ in place of T_c in (5), it follows from the above discussion that the general power of L appearing in $\Delta\nu_L = \nu_{L,L-1} - \nu$ is $(n_3 y_3 - n_2 - n_1 y_T)$ with $n_1, n_2 = 0, 1, 2, \ldots$ and $n_3 = 1, 2, \ldots$; this should be compared with (7). Finally, if other bulk irrelevant scaling fields are allowed (with scaling exponents $0 > y_3 > y_4 > y_5 > \ldots$) and if only *bulk* nonlinearities are allowed for, the general power of L in $\Delta\nu_L$ is

$$-n_1 y_T - n_2 + \sum_{j=3} n_j y_j, \tag{10}$$

where $n_1, n_2, \ldots = 0, 1, 2, \ldots$ but at least one of n_j for $j \geq 3$ is non-zero. This result, however, is not really definitive since we have neglected other types of corrections as discussed above in connection with the relation (4). Notice also that we have, as mentioned, assumed $d < d_>$ (=4, 6, etc) in the discussion (see also Brézin 1982) and further supposed that no special relations hold between higher-order scaling exponents which may lead to logarithmic correction factors (see Wegner 1972, and the review by Patashinskii and Pokrovskii 1977).

We proceed next to demonstrate that the L^{y_3} term can actually be detected in numerical sequences which display an apparent convergence rate with $x \simeq 2$ when fitted as in (2). Consider the estimators

$$r_L = \nu + (\nu_{L,L-1} - \nu)/L = \nu + \nu C L^{-(|y_3|+1)} + \ldots, \tag{11}$$

where (1) has been assumed. Asymptotically, the r_L converge in a way similar to that expected for ratios of coefficients constructed for a logarithmic derivative series of a function which has a confluent singularity with exponent $|y_3|$ (see further below). Since, for short series, naive ratio and Padé techniques may be misleading when confluent corrections are involved (see e.g. Baker 1975) we construct a transformed function. Thus consider the sequence

$$a_0 = 1/\nu, \qquad a_j = a_{j-1}/r_{j+1} \qquad (j \geq 1) \tag{12}$$

and the function

$$f(z)=\sum_{n=0}^{\infty} a_n z^n=(\nu-z)^{-1}[1+A(\nu-z)^{|y_3|}+D(z)], \tag{13}$$

which has a leading divergence with exponent 1 at $z_c=\nu$ and a confluent term with exponent $|y_3|$. Additional terms, denoted by $D(z)$ in (13), will, of course, be present resulting from the transformation and from higher-order corrections in (1). Hopefully, these less singular terms will have a relatively small influence on the analysis: we will, however, comment later on their potentiality for interference. The particular Padé-type method of analysis which we adopt is that proposed recently by Adler, Moshe and Privman (1982a, b) which, in brief, involves transforming the series for $f(z)$ into an expansion in powers of

$$s=1-[1-(z/\nu)]^y, \tag{14}$$

with a variable trial value y. The series for

$$G(y,s)=y(1-s)(\partial/\partial s)\ln f[z(y,s)], \tag{15}$$

is then computed and used to calculate several $[M/N]$ Padé approximants to $G(y,1)$ and thence a family of curves

$$\Gamma(y)=G^{[M/N]}(y,s=1)\simeq G(y,1), \tag{16}$$

in the (y,Γ) plane. A region of 'convergence' or 'confluence' of the $\Gamma(y)$ curves is expected close to the point $(|y_3|,1)$ in the (y,Γ) plane: see Adler *et al* (1982a, b) for details.

Consider first the $q=3$ Potts model and let us study a sequence of estimates for β/ν obtained by Hamer (1982) from the expression

$$(\beta/\nu)_{L,L-1}=(1-L)[M_L(T_c)/M_{L-1}(T_c)-1], \tag{17}$$

where $M_L(T)$ is a quantity with the critical behaviour of magnetisation which vanishes with exponent β when $L=\infty$. The exact value of β/ν is known (Den Nijs 1979, Nienhuis, Riedel and Schick 1980, Nienhuis 1982), and this exponent replaces ν in (11)–(14). (It is easy to verify that $(\beta/\nu)_{L,L-1}$ of (17) converges to β/ν with the same general pattern of corrections as for $\nu_{L,L-1}$.) In figure 1 are plotted $\Gamma(y)$ curves obtained from several near-diagonal Padé approximants. Also indicated, on the y axis, is the recent estimate, $|y_3|=0.68\pm0.13$, obtained from analysis of several low-temperature series expansions (Adler and Privman 1982); this range is consistent with earlier $|y_3|$ estimates (see Adler and Privman (1982) for references). The point with coordinates $(y=0.68, \Gamma=1)$ is marked on the plot by a cross. The $\Gamma(y)$ curves display a clear confluence close to this point: this provides a definite indication of the presence of the L^{y_3} term in the $(\beta/\nu)_{L,L-1}$ sequence. The confluence region in figure 1, if taken at face value, suggests a rather narrow $|y_3|$ range; however, the series analysed is relatively short and large systematic errors may arise in this method from background terms (see Adler *et al* 1982b). Thus it is inadvisable to propose confidence limits narrower than indicated by the original series analysis.

Consider, as a second example, the $\nu_{L,L-1}$ sequences of (5) for percolation which were calculated by Derrida and DeSeze (1982). Here only results for their longest $\nu_{L,L-1}$ sequence will be discussed: this was obtained for site percolation with helical boundary conditions. (Other $\nu_{L,L-1}$ sequences give similar results; some of the corresponding critical point, $(p_c)_{L,L-1}$, data are discussed briefly below.) The exact value of

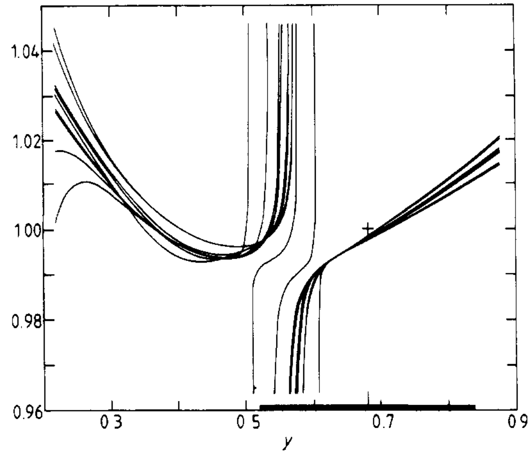

Figure 1. Plots of $\Gamma(y)$ derived from the sequence of estimates for β/ν for the $q=3$ Potts model, obtained with [2/6], [3/5], [4/4], [5/3], [6/2], [2/5], [3/4], [4/3] and [5/2] Padé approximants. The cross indicates the series estimate $|y_3|=0.68$, $\Gamma=1$; the corresponding range is shown on the axis.

ν is known (Den Nijs 1979, Nienhuis *et al* 1980, Nienhuis 1982). Several series and MC studies of the leading corrections to scaling for percolation have been reported and the results cluster in two non-overlapping ranges of y (see Adler *et al* (1982b) for a review) as obtained from the relations $y=\theta/\nu$ and $y=\Omega\beta\delta/\nu$, where θ and Ω are temperature-like and field-like bulk confluent exponents. The above relations are meaningful only for corrections due to irrelevant scaling fields. Since there is a theoretical argument (Aharony and Fisher 1983, Margolina, Djordjević, Stauffer and Stanley 1983) which suggests that the higher-value range is observed when corrections due to the nonlinearity of g_t are substantial, we concentrate on the lower range of estimates. Thus $|y_3|=0.94\pm0.11$ (Adler *et al* 1982a) is typical of both the series estimates and the MC results of Stauffer (1981). The corresponding curves $\Gamma(y)$ are plotted in figure 2 where the point ($y=0.94$, $\Gamma=1$) is marked by a cross and the quoted $|y_3|$ range is shown on the y axis. One observes a confluence region consistent with the central series estimate. Again, one should probably not be tempted to narrow the uncertainties quoted in the series analysis: indeed, systematic errors may be especially large in this case owing to a linear term, $D_1(\nu-z)$, in $D(z)$ of (13), whose presence is anticipated since it represents merely an additive constant background in $f(z)$. One may try to study the resulting interference by dividing out different terms (see Adler and Privman 1982) but the available series are too short for such analysis to be convincing. Independent evidence for the presence of both terms comes from a study of $(p_c)_{L,L-1}$ for bond percolation (where the exact value is $p_c=\frac{1}{2}$) in which two 'loose' confluences were found: one at $y\simeq1$ and another in the range of y consistent with the lower half of the range $|y_3|+1/\nu=1.69\pm0.11$ derived from series.

The above studies demonstrate that the expected leading correction term, varying as L^{y_3}, is indeed present in the finite-size sequences. There is additional convincing evidence that for $L\leqslant10$ the asymptotic form for $L\gg1$ has not been achieved in existing finite-size data. Thus several finite-size sequences vary non-monotonically (see e.g. Derrida and DeSeze 1982). Even for some monotonic sequences there are problems: thus if one determines an exponent $x\equiv x_\nu$ from an exponent sequence

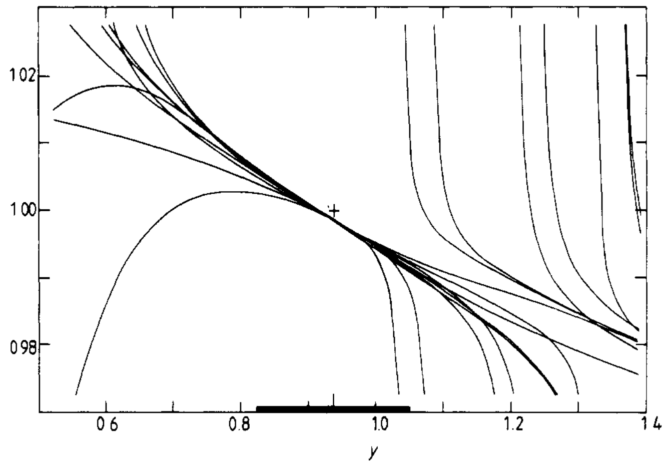

Figure 2. Plots of $\Gamma(y)$ obtained from estimates for ν for site percolation on a square lattice with helical boundary conditions (using the same Padé approximants as in figure 1). The cross indicates the series estimate $|y_3| = 0.94$, $\Gamma = 1$ with the associated range being shown on the axis.

$\nu_{L,L-1}$ and another exponent $x \equiv x_{T_c}$ from estimates for T_c as in (8), one should find $x_{T_c} - x_\nu = 1/\nu$. (Compare (7) and (9).) In practice, however, this difference takes other values (see e.g. Derrida 1981). In other cases x depends strongly on the boundary conditions (see e.g. Kinzel and Yeomans 1981). Unfortunately, the pattern of corrections to scaling in the $d = 2$ Ising spin-$\frac{1}{2}$ model, where $\nu_{L,L-1}$ is known exactly (Onsager 1944, Derrida and DeSeze 1982), is effectively 'pathological' since *all* non-analytic corrections seem to vanish identically (Aharony and Fisher 1980).

Since the sequences with $L \leqslant 10$ appear too short to fit reliably to more than one power-law term, an indirect method of estimating the relative amplitude of the contribution of L^{y_3} term has been attempted. To this end, consider

$$\tilde{\nu}_L = [L^{|y_3|}\nu_{L,L-1} - (L-1)^{|y_3|}\nu_{L-1,L-2}]/[L^{|y_3|} - (L-1)^{|y_3|}] \tag{18}$$

(where ν now denotes the exponent, etc appropriate for the particular sequence considered). The term in L^{y_3} cancels in $\tilde{\nu}_L$ which should thus approach ν as $L \to \infty$ at a rate determined by the higher powers in (7) but with modified coefficients. (In practice, one must calculate using several $|y_3|$ values based on the range of series estimates.) One finds in all the examples that $|\tilde{\nu}_L - \nu|$ usually exceeds $|\tilde{\nu}_{L,L-1} - \nu|$ while the ratio $|\tilde{\nu}_L - \nu|/|\nu_{L,L-1} - \nu|$ ranges from below 1 to 10. This suggests that there is generally some cancellation between the CL^{y_3} term in $\nu_{L,L-1}$ and one or more higher-order terms from $E(L)$ (see (1)) which leads to as much as an order of magnitude reduction in the deviation $\Delta\nu_L$ at $L \simeq 10$ over what the leading term alone would give. Such cancellation also leads fairly naturally to the observed inequality $x > |y_3|$. Notice, however, that there is probably no general underlying mechanism of cancellation, beyond fortuitous numerical coincidence, since there is at least one counter-example in which one does find x close to the expected $|y_3|$ value (Uzelac and Jullien 1981).

A related topic is the actual technique of extrapolation of the finite-size sequences to the $L \to \infty$ limit. An effective method was developed by Hamer and Barber (1981). In each iteration of their technique, a power-law correction is, ideally, cancelled. However, no effective method is known for the systematic study of exponents and the coefficients of correction terms. (The method we have used above is useful only for estimating y_3 in models with exactly known leading exponents or critical points.)

Recently, Barber (1983) proposed allowing for additional scaling fields by extending the parameter space (see also Yeomans and Fisher 1983). Although his methods are somewhat limited, in that they require prior knowledge of aspects of the phase diagram, they do seem to be a step in the right direction. Likewise, in series analysis it has proven very useful (Chen, Fisher and Nickel 1982) to allow for more variables when studying non-analytic, confluent correction terms. Basically, the idea in both cases is to fit to a multisingular scaling form like (3).

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