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Correction to scaling exponents and critical properties of the n-vector model with dimensionality > 4

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Abstract. A perturbation calculation is given which implies that the susceptibility of the five and six-dimensional n-vector models can be written $\chi \sim At^{-1}(1+Bt^{1/2})$ and $\chi \sim At^{-1}(1+Bt \ln t)$ respectively, independent of n. For $n=0$ and 1 it is shown that series analysis techniques can extract the above 'correction-to-scaling' exponents, and that estimates of the critical temperatures and critical amplitudes can also be obtained. The correction-to-scaling exponents found are in agreement with those known to exist in the case of the spherical model.

1. Introduction

In a recent paper (Guttmann 1978) a technique was described whereby estimates of the exponent of the confluent logarithmic term which arises in the susceptibility (and other thermodynamic properties) at the critical dimension could be obtained. For the n-vector model, which is representable by a ϕ^4 field theory, the critical dimension is of course $d=4$. With this technique it was possible to use existing series expansions, derived some time ago by Fisher and Gaunt (1964), to obtain estimates of the confluent logarithmic exponent, which were in good agreement with those obtained from ϕ^4 field theory (Brézin 1975). Unlike the field theoretical calculation, the series analysis also yielded estimates of the critical temperature and critical amplitudes.

For $d > d_c = 4$ the leading susceptibility exponent is a simple pole as predicted by mean field theory, but the correction terms are expected to be non-classical. The form of these correction terms is mentioned by Pfeuty and Toulouse (1977) as an unsolved problem, though Joyce (1972) has obtained the correction terms for the spherical model, and finds

$$kT\chi/m^2 \sim Ct^{-1} + Dt^{-1/2} + E + Ft^{1/2} + \dots, \qquad (d=5) \qquad (1.1a)$$

$$kT\chi/m^2 \sim Ct^{-1} + D \ln t + t(E + F \ln t + G \ln^2 t) + \dots, \qquad (d=6) \qquad (1.1b)$$

$$kT\chi/m^2 \sim Ct^{-1} + D + Et^{1/2} + \dots, \qquad (d=7) \qquad (1.1c)$$

where $kT\chi/m^2$ is the reduced isothermal susceptibility and $t = 1 - T/T_c$ is the reduced temperature. Thus the 'correction-to-scaling' exponent is $\frac{1}{2}$ for $d=5$ and 1 for $d=6$. For the five- and six-dimensional self-avoiding walk (SAW) problem and the Ising model, Fisher and Gaunt (1964) obtained the first 11 terms of the susceptibility expansion. It seemed worthwhile to see whether these series could be analysed to give both the form of the correction term and estimates of the critical parameters. It was also of interest to see whether the form of the susceptibility found by Joyce for the spherical model was applicable to other realisations of the n-vector model.

A heuristic argument due to Fisher (1978, private communication) suggests that this is so. Renormalisation group arguments suggest that there should be a singular part of the free energy satisfying the hyperscaling relation $d\nu = 2 - \alpha_s$, even for $d > 4$. Setting $\nu = \frac{1}{2}$ for all n, with $d > 4$, and extracting the dominant mean-field specific heat term t^2, we obtain a contribution to the correction-to-scaling terms of the form $t^{(d-4)/2}$. This is consistent with the spherical model results obtained by Joyce.

I am indebted to the referee for the following remark: One knows from a simple ϵ-expansion that for $d = 4 + |\epsilon|$ the correction-to-scaling exponent is independent of n. This is additional evidence for the results obtained here.

In the next section the method of series analysis is described, and applied to the series expansions obtained by Fisher and Gaunt. In § 3 an explicit calculation is outlined which, while not rigorous, implies that the correction-to-scaling exponent is indeed of the form $t^{(d-4)/2}$, and the final section comprises a conclusion.

2. Analysis of series

Several methods are, in principle, capable of analysing for the assumed asymptotic form. The principal methods are the method of Baker and Hunter (1973), whereby the series is transformed in such a manner that the exponents become poles of Padé approximants, the recurrence relation method (Guttmann and Joyce 1972), whose natural generalisation to the case of confluent singularities has recently been described by Rehr *et al* (1980), and the method introduced by Saul *et al* (1975) in which one fits the series to the assumed asymptotic form

$$f(v) = \sum_{n \geq 0} a_n v^n \sim A(1-\mu v)^{-\gamma} + B(1-\mu v)^{-\beta} \qquad \text{as } v \to 1/\mu^-. \tag{2.1}$$

None of these methods is directly applicable to the present problem, due to the loose-packed nature of the hypercubic lattices, which have 'antiferromagnetic' singularities at $v = 1/\mu$ if the ferromagnetic singularity is at $v = 1/\mu$. For the Ising model in any dimension this follows from consideration of the graphs which contribute to the specific heat expansion, which are all of even degree, while the analogous result for the SAW problem has been obtained by Guttmann and Whittington (1978).

Using the Baker–Hunter method, we found that the effects of the antiferromagnetic singularity masked the confluent singularity. Using an Euler transformation to map the antiferromagnetic singularity to infinity appeared to distort the complex plane, to the extent that the transformed series failed to behave smoothly when analysed by the Baker–Hunter method.

The recurrence relation method was also comparatively unsuccessful, due to both the presence of the antiferromagnetic singularity and the comparatively short length of the series. One feature of the recurrence relation method is that comparatively long series are often required to obtain reliable estimates of the critical parameters.

The Saul–Wortis method, in which successive quintets of coefficients are used to estimate the critical parameters A, B, μ, α and β, also requires modification for loose-packed lattices. For close-packed lattices the equations, though nonlinear, are cubic or quadratic polynomials and can be readily solved. For loose-packed lattices it is appropriate (Gaunt and Guttmann 1974) to consider every second coefficient, and this has the unfortunate effect of distinctly increasing the complexity of the equations. Accordingly, we must solve systems of nonlinear equations by any one of a number of standard numerical analysis techniques.

It is this method we choose to pursue, as the only one that gives convergent estimates for the critical parameters. The numerical algorithm used is a generalisation of Newton's method, and is available as FORTRAN subroutine NS01A in the Harwell Scientific Subprogram Library.

Any iterative procedure requires an initial estimate, and in this analysis we have used as our starting point the value of μ given by Fisher and Gaunt. We have also used the fact that the dominant singularity is known to be a simple pole ($\gamma = 1$), so that we only require estimates of four unknowns A, B, μ and β.

The numerical algorithm is such that its performance is best if all the unknown parameters are of the same magnitude. For this reason, since γ is fixed at 1, we have normalised the series to a critical point of approximately 1 by dividing the coefficient of v^n by μ^n. Finally, to make the leading amplitude A approximately equal to 1, we have multiplied the series by a constant C. That is, given the series (2.1), $f(v) = \Sigma_{n\geq 0}\, a_n v^n$, we have constructed the series $F(v) = C\, \Sigma_{n\geq 0}\, a_n (v/\mu)^n = \Sigma_{n\geq 0}\, b_n v^n$, where C is chosen so that each $b_n \approx 1$. Then, setting $\gamma = 1$, we have used successive quartets of coefficients $\{b_n, b_{n-2}, b_{n-4}, b_{n-6}\}$ with $n = 6, 7, \ldots, n_{\max}$ (where $n_{\max}$ is the power of the highest available coefficient) to estimate the critical parameters A, B, μ and β in (2.1).

For the five-dimensional SAW model, denoting μ^* as our estimate of the true value μ, and choosing $1/\mu^* = 0{\cdot}113\,230$ (Fisher and Gaunt 1964) and $C = 7/\mu^*$ as our starting estimates, we find that the coefficients b_n slowly increase from 0·79 to 0·97.

Analysing as stated above, we obtain the sequence of estimates shown in table 1. The estimates of μ/μ^* are slowly decreasing, and appear to be approaching a value around 1·0007 or 1·0008. If the correct value of μ^* had been chosen, this sequence would approach 1. Notice that alternate estimates of β are increasing regularly. We next choose a range of values of μ^* consistent with the above estimates, that is, our range of μ^* is 0·07–0·08% lower than that used above, and, holding μ constant at this value, use successive triples of alternate terms $\{b_n, b_{n-2}, b_{n-4}\}$ to estimate A, B and β. In table 2 we show the result of this analysis for three values of μ^* in the range obtained from the preceding analysis. From this analysis it can be seen that, for $1/\mu^* = 0{\cdot}113\,150$, alternate values of both β and AC are steadily increasing, while for $1/\mu^* = 0{\cdot}113\,145$ the rate of increase is much slower, and indeed the last two even estimates are steady. For $1/\mu^* = 0{\cdot}113\,140$ the odd estimates are increasing and the last two even estimates are decreasing. For a wider spread of values (not shown) this pattern of behaviour continues. For $1/\mu^* > 0{\cdot}113\,150$ the estimates of β and AC

Table 1. Five-dimensional SAW generating function. Estimate of critical parameters assuming $\gamma = 1$ and $C = 7/\mu^*$.

n	μ/μ^*	β	AC	B
8	1·001 69	0·253	0·974 9	−0·507
9	1·001 38	0·218	0·979 7	−0·702
10	1·000 89	0·472	1·005 0	−0·308
11	1·000 96	0·362	0·995 8	−0·429
12	1·000 75	0·526	1·015 1	−0·288

Table 2. Five-dimensional SAW generating function. Estimate of critical parameters with critical point fixed and assuming $\gamma = 1$, $C = 7/\mu^*$.

	$1/\mu^* = 0{\cdot}113\ 140$			$1/\mu^* = 0{\cdot}113\ 145$			$1/\mu^* = 0{\cdot}113\ 150$		
n	β	AC	B	β	AC	B	β	AC	B
6	0·366	0·942	−0·393	0·371	0·995	−0·390	0·376	0·996	−0·387
7	0·321	0·947	−0·502	0·328	0·996	−0·493	0·335	0·997	−0·485
8	0·495	1·010	−0·300	0·505	1·012	−0·298	0·515	1·014	−0·295
9	0·411	1·003	−0·386	0·423	1·005	−0·376	0·437	1·008	−0·368
10	0·509	1·001	−0·293	0·525	1·015	−0·288	0·541	1·018	−0·284
11	0·437	1·001	−0·360	0·457	1·009	−0·347	0·476	1·012	−0·336
12	0·502	1·010	−0·297	0·525	1·015	−0·288	0·547	1·019	−0·281

increase more and more rapidly as $1/\mu^*$ increases, while for $1/\mu^* < 0{\cdot}113\ 140$ estimates of β and AC decrease more and more rapidly. Since the estimates should be steady at the correct value of μ^*, we can make the estimate $\mu = 0{\cdot}113\ 14 \pm 0{\cdot}000\ 01$, $\beta = 0{\cdot}50 \pm 0{\cdot}1$, $AC = 1{\cdot}01 \pm 0{\cdot}02$, $BC = -0{\cdot}30 \pm 0{\cdot}04$. These estimates are made on the basis that the even estimates are the most obviously convergent, while the odd estimates are changing more rapidly. Though more attention has been paid to the even estimates, the above values are nevertheless consistent with the apparent limits of both odd and even sequences.

For the five-dimensional Ising model the same analysis was performed. As before, we set $C = 7/\mu^*$, with the initial estimate $\mu^* = 0{\cdot}113\ 54$. In order to save space, the detailed results are not shown. However the behaviour of the series was qualitatively similar to the SAW generating function series, though slightly better behaved. Following the method of the previous paragraph, we were able to make the estimate $1/\mu = v_c = 0{\cdot}113\ 427 \pm 0{\cdot}000\ 007$, $\beta = 0{\cdot}50 \pm 0{\cdot}05$, $AC = 1{\cdot}041 \pm 0{\cdot}007$, $BC = -0{\cdot}38 \pm 0{\cdot}02$. Despite the apparent reasonableness of these results, we found some difficulty in applying the above method of analysis to the series. The reason for this was that estimates of β are quite small, with $|\beta| \lesssim 0{\cdot}1$. As a consequence, we found poor convergence of the numerical procedure for estimating the critical parameters. Recall that one of the conditions for rapid convergence is that the different parameters should be of the same size. In this case, however, we have $|\gamma/\beta| \gtrsim 10$, which gives rise to poor convergence. However, this difficulty can be circumvented by differentiating the series. This increases both γ and β by 1, but now the ratio $\gamma/\beta \approx 2$, and the numerical procedure is once again quite stable. From table 3 it appears that $\mu/\mu^* \approx 1{\cdot}0007$, and

Table 3. Six-dimensional Ising model susceptibility series. Estimate of critical parameters assuming $\gamma = 1$, $C = 7/\mu^*$, $\mu^* = 0{\cdot}0921$.

n	μ/μ^*	β	AC	B
8	1·000 39	0·278	0·760 1	−0·271
9	1·000 66	0·011	0·752 0	−8·528
10	1·000 73	0·154	0·753 2	−0·477
11	1·000 69	0·042	0·752 1	−2·104
12	1·000 67	0·175	0·754 3	−0·422

so a three-parameter fit to alternate terms of the *differentiated* series was made, with μ^* held constant and γ held at 2·0. A range of values of μ^* around 0·092 04 was used, as suggested by the results of a four-parameter fit, and C was chosen to be $0{\cdot}643/\mu^*$. A set of results is shown in table 4 for $\mu^* = 0{\cdot}092\,033$, which is the central estimate of μ. Repeating this procedure for a range of values of μ^* gives rise to the estimates $\mu = 0{\cdot}092\,033 \pm 0{\cdot}000\,007$, $\beta = 1{\cdot}02 \pm 0{\cdot}05$, $AC = 0{\cdot}751 \pm 0{\cdot}005$, $BC = -0{\cdot}78 \pm 0{\cdot}02$, where the critical parameters refer to the differentiated series.

Table 4. Six-dimensional *differentiated* Ising model susceptibility series. Estimate of critical parameters assuming $\gamma = 2$, $C = 0{\cdot}643/\mu^*$ and $\mu^* = 0{\cdot}092\,033$.

n	β	AC	B
5	1·057	0·755 8	−0·758 4
6	1·039	0·753 0	−0·775 1
7	1·042	0·752 9	−0·767 4
8	1·032	0·751 9	−0·780 8
9	1·036	0·752 0	−0·773 8
10	1·027	0·751 4	−0·786 5
11	1·029	0·751 3	−0·782 2

A similar analysis of the six-dimensional differentiated SAW generating function gives $\mu = 0{\cdot}091\,922 \pm 0{\cdot}000\,008$, $\beta = 1{\cdot}02 \pm 0{\cdot}05$, $AC = 0{\cdot}745 \pm 0{\cdot}005$ and $B = -0{\cdot}77 \pm 0{\cdot}02$.

The critical parameters are summarised in table 5. For the six-dimensional series we have been unable to estimate the subdominant amplitude B, as the differentiation mixes in a contribution from the dominant amplitude A, and these two contributions cannot subsequently be separated.

From the estimates of β for both the five- and six-dimensional lattices, it appears that the correction-to-scaling exponent is constant as n, the dimensionality of the spin space, changes. In the next section we give a perturbation analysis that implies that this is indeed the case.

Table 5. Estimates of critical parameters fitting to the form $f(x) = A(1-\mu x)^{-1} + B(1-\mu x)^{-\beta}$. * see text.

	Five dimensions				Six dimensions			
	$1/\mu$	β	A	B	$1/\mu$	β	A	B
SAW generating	0·113 14	0·50	1·27	−0·38	0·091 922	0·02	1·158	*
function	±0·000 01	±0·10	±0·02	±0·05	±0·000 008	±0·05	±0·008	
Ising	0·113 427	0·50	1·311	−0·48	0·092 033	0·02	1·168	*
susceptibility	±0·000 007	±0·05	±0·009	±0·03	±0·000 007	±0·05	±0·008	

3. Calculation of correction terms

In this section we show that a straightforward perturbation calculation taking into account just the one-loop and two-loop graphs yields the desired correction-to-scaling exponents. We use the notation of Wallace (1976), and write the inverse susceptibility $r = \chi^{-1}$ as

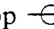
$$r_0(T) = r + \Sigma(q = 0, r). \tag{3.1}$$

At the critical temperature r vanishes, so that

$$r_0(T_c) = 0 + \Sigma(q = 0, 0). \tag{3.2}$$

Since r_0 is assumed to be analytic in temperature, subtracting these two equations yields

$$T - T_c = r + [\Sigma(q = 0, r) - \Sigma(q = 0, 0)].$$

The two lowest-order graphs contributing to the self energy are the one-loop  and two-loop  diagrams. In five dimensions only the one-loop diagram needs to be retained, as it gives a contribution proportional to $r^{3/2}$. The second diagram gives a leading term proportional to r, which just modifies the constant multiplying this term in the previous equation. Higher-order contributions are of lower order than the $r^{3/2}$ term. Thus this diagram can (in hindsight) be neglected in the five-dimensional case. In six dimensions we require both diagrams. Retaining only the leading-order terms, we find that

$$\begin{aligned} T - T_c &= A_0 r + A_1 r^{3/2} + \ldots \qquad & d = 5 \\ T - T_c &= A_0 r + A_1 r^2(\ln r + B_0) \qquad & d = 6. \end{aligned} \tag{3.3}$$

Reverting these equations, we find the desired results

$$\chi \sim C_0 t^{-1}(1 + C_1 t^{1/2} + \ldots) \qquad \text{and} \qquad \chi \sim D_0 t^{-1}(1 + D_1 t \ln t + \ldots). \tag{3.4}$$

These results are independent of n, the dimensionality of the spin space, and accordingly are in agreement with the existing results for the $n \to \infty$ limit, which is the spherical model. Note that the contributions of the two diagrams considered are n-dependent, but for $d > 4$ this dependence affects only the amplitudes of the correction terms (C_1 and D_1 in (3.4)). For $d < 4$, where infrared divergences occur, the requirement that the renormalised vertex functions must remain finite as the lattice spacing vanishes has the consequence that these terms exponentiate, and hence the n dependence moves into the exponents. For $d = 4$ the n dependence manifests itself in the exponent of the confluent logarithmic term.

There are several gaps in the foregoing analysis, which makes it far from rigorous. For that reason we give the derivation with appropriate terseness, but have every confidence in the correctness of the results.

4. Conclusion

We have obtained by perturbation analysis results that imply that the five- and six-dimensional n-vector model has 'correction-to-scaling' terms independent of n, and have explicitly obtained these exponents. Series analysis of susceptibility series for $n = 0$ and 1 (the SAW problem and the Ising model) enable estimates of critical amplitudes and critical temperatures to be made, and incidentally give correction to scaling exponent estimates in agreement with those found by exact calculation. Much worthwhile work remains to be done in making rigorous the somewhat sketchy perturbation analysis presented above, and—following a suggestion of Fisher (1978, private communication)—extending the analysis to include a full discussion of the equation-of-state correction terms.

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