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On hyperscaling in the Ising model in three dimensions

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Abstract. The spin-$\frac{1}{2}$ Ising model high-temperature series are re-examined by an analysis that parallels the method used to analyse the continuum ϕ^4 spin model. Our results for the Ising model in three dimensions do not agree with results in the literature based on more conventional methods of analysis. We cannot decide, using only the series terms presently available, which of the methods is to be preferred. We conclude that previous error assessments are unduly optimistic and that the three-dimensional, spin-$\frac{1}{2}$, Ising model may satisfy hyperscaling in agreement with the continuum results. An attempt is made to estimate the number of additional high-temperature series terms necessary to resolve the hyperscaling question.

1. Introduction

Exponent estimates for the Ising model have conventionally been obtained by a direct analysis of the series expansions of correlation functions in inverse temperature or variable analytically dependent on the temperature. (For a review see Gaunt and Guttmann (1974). Some more recent analyses are those of Saul *et al* (1975), Camp and Van Dyke (1975), Camp *et al* (1976) and Baker (1977).) Inherent in these methods is the assumption that the singularity structure of the correlation functions in the complex temperature plane is sufficiently non-pathological that the first few available terms in the power-series representation already contain the information necessary for the description of the critical behaviour. Padé analysis of the series is then expected to extract efficiently the details of the critical behaviour from the remaining information. In certain cases other analyses such as ratio test, Neville table extrapolation, or temperature renormalisation may be preferable, but the advantages can only be marginal as all these methods have in common the temperature plane 'smoothness' assumption.

Quite distinct from these standard methods is another scheme in which the assumption is made that correlation functions are relatively smooth functions of other observables such as, for example, the correlation length. There is no *a priori* reason to prefer either one or the other of these two assumptions. Because Ising model series are derived as functions of temperature, temperature analysis has always been treated as more natural. On the other hand, field-theoretic or continuum model expansions are

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typically given as expansions in the renormalised mass, i.e. correlation length, and coupling constant and hence analysis in terms of these variables is the obvious choice.

In this paper we examine the application of the field-theoretic methods to the analysis of the Ising model high-temperature series with the specific aim of testing the apparent failure of hyperscaling in three dimensions. (See the recent calculation of Baker (1977) and the references therein.) We define a variable that is the analogue of the renormalised coupling constant in the continuum ϕ^4 model and manipulate the known high-temperature series to express the correlation length as a power series in this coupling constant analogue. We then attempt to establish by Padé analysis whether the correlation length diverges as the coupling constant approaches a finite value as is predicted by hyperscaling. There are clear indications of such a divergence for the body-centred cubic lattice and we estimate a critical renormalised coupling constant that differs by only 2% from the continuum ϕ^4 model estimate (Le Guillou and Zinn-Justin 1977, Baker *et al* 1978). The results of our analysis of the simple cubic and face-centred cubic lattice are in agreement with the body-centred lattice result but cannot be considered as strong independent evidence for hyperscaling. In the simple cubic case, the critical value of the coupling constant analogue is close to the radius of convergence of the series, and as a consequence our estimate is not precise. The series for the face-centred lattice appears to be better with regard to competition from unphysical singularities but only nine terms, as compared with thirteen for the other lattices, are available.

Our procedure can be viewed as a mapping of the complex temperature plane onto the complex coupling constant plane, but it is crucial to note that this is qualitatively different from the analytic transformations that have been used on occasion in the conventional analysis. The coupling constant is not an analytic function of temperature in the vicinity of the critical point and the mapping will therefore produce a *qualitative* change in the singularity structure of the correlation functions to be analysed. Whether this change is an improvement can only be determined empirically from the series analysis. Since we obtain relatively stable Padé approximants with few defects (see, for example, Baker 1975) in both schemes we cannot, with the series terms presently available, decide in favour of one or the other.

In an attempt to understand the source of the discrepancy between the coupling constant and temperature plane analysis we have made explicit comparisons of the correlation functions predicted by the two methods. We find that implicit in the temperature plane analysis, indicating violation of hyperscaling by an amount $3\nu+\gamma-2\Delta \simeq 0{\cdot}03$ (Baker 1977) is the prediction of cross-over behaviour at a correlation length to lattice spacing ratio $\xi/a \simeq 10$. Since the available series only sample the lattice to a distance approximately equal to $10a$, the prediction of the cross-over, and by implication hyperscaling violation, must be treated with some scepticism. On the other hand, we argue that because the apparent cross-over length is *only* $10a$, the question of the validity of hyperscaling may very likely be resolved by the extension of the available series by a few more terms.

In the following section we describe the series manipulations necessary for a coupling constant analysis and present our Padé results for the three cubic lattices. In § 3 we compare the coupling constant and temperature plane predictions for the body-centred cubic lattice and attempt to estimate the additional number of series terms needed to resolve the discrepancies. In the last section we present the results of analysis of two- and four-dimensional Ising systems and comment on the application of our methods to systems with order parameter dimension greater than one.

2. Coupling constant analysis

We will restrict ourselves to a discussion of the usual spin-$\frac{1}{2}$ Ising model in spatial dimension d. The partition function is

$$Z = \sum_{\{S_i=\pm 1\}} \exp\Big(K \sum_{nn} S_i S_j + \sum_i h_i S_i\Big) \tag{1}$$

where K is the ferromagnetic coupling between nearest-neighbour spins and h_i is an external field at the lattice site i. Cumulant averages in zero magnetic field are defined by

$$\langle S_i S_j \ldots S_l\rangle_c = \frac{\partial}{\partial h_i}\frac{\partial}{\partial h_j}\ldots\frac{\partial}{\partial h_l}\ln Z|_{\{h_i=0\}}. \tag{2}$$

We use the second-moment definition of the correlation length ξ and, for convenience in the following, define the dimensionless parameter

$$x = \xi^2/a^2 = (2d)^{-1}\Big(\sum_i (r_i/a)^2 \langle S_0 \ S_i\rangle_c\Big)\Big(\sum_i \langle S_0 \ S_i\rangle_c\Big)^{-1} \tag{3}$$

where a is the nearest-neighbour spin separation and r_i is the distance from the origin to the site i. For small K, $x = qK/(2d) + O(K^2)$ where q is the coordination number of the lattice. In the vicinity of the critical point x diverges as $(1-K/K_c)^{-2\nu}$.

The assumption of hyperscaling in the critical region is just the assumption that a single correlation length ξ sets the scale for the variation of all correlation functions and that the divergence of ξ as one approaches the critical point is responsible for the singular behaviour of all thermodynamic functions. Although the validity of this assumption remains unproven, it can at least be made plausible by renormalisation group calculations (see, for example, reviews by Wilson and Kogut 1974, Wilson 1975, Ma 1976, Domb and Green 1976) that are generalisations of the original block spin picture of Kadanoff (1966). The specific consequence of the hyperscaling assumption that we are concerned with here is the prediction for the behaviour of the dimensionless ratio of cumulant averages $\langle(\Sigma_i S_i)^{2n+2}\rangle_c/\langle(\Sigma_i S_i)^2\rangle_c^{n+1}$. Note that this ratio does not depend on the particular normalisation chosen for the spin variable S_i. Also, this ratio does not depend *explicitly* on the lattice spacing in the critical region since whenever the spin correlations are long range we may use the continuum approximation $\langle(\int d^d r\, S(r))^{2n+2}\rangle_c/\langle(\int d^d r\, S(r))^2\rangle_c^{n+1}$. The hyperscaling assumption then states that the only remaining microscopic dependence is the *implicit* dependence through the correlation length ξ. Since each cumulant average is extensive and hence proportional to the volume V of the system, we deduce that the ratio is proportional to $\xi^{dn}V^{-n}$. The $n=1$ ratio is conventionally used to define the dimensionless renormalised coupling constant

$$u \equiv -V\xi^{-d}\Big\langle\Big(\sum_i S_i\Big)^4\Big\rangle_c \Big\langle\Big(\sum_i S_i\Big)^2\Big\rangle_c^{-2} \tag{4}$$

which is expected to approach a constant u^* in the limit that the correlation length diverges. Furthermore, if we assume universality in addition to hyperscaling, then the constant u^* should be the same for all models with scalar order parameter. In the case $d=3$, we have the accurate continuum-model (cf equation (12)) estimate (Le Guillou and Zinn-Justin 1977, Baker *et al* 1978)

$$3u^*/16\pi = 1{\cdot}415 \pm 0{\cdot}003, \tag{5}$$

but this is not consistent with the results of conventional temperature plane analysis of the spin-$\frac{1}{2}$ model where u appears to vanish as $(1-K/K_c)^{d^*\nu}$ with the anomalous dimension $d^* = 3-(2\Delta-\gamma)/\nu \simeq 0{\cdot}044 \pm 0{\cdot}005$ (Baker 1977). In the following we investigate whether an analysis of the spin-$\frac{1}{2}$ model that parallels the method used to obtain (5) can change this conclusion.

We rewrite the expression (4) for the coupling constant as

$$u = 2(V/N)a^{-d}x^{-d/2}\Big\langle -\tfrac{1}{2}\sum_{i,j,k} S_0S_iS_jS_k\Big\rangle_c \Big\langle \sum_i S_0S_i\Big\rangle_c^{-2} \tag{6}$$

where V/N is the volume per lattice site, and note that as $K \to 0$ each average $\langle\ \rangle_c$ approaches unity but u diverges because $x \propto K$. Hence it is advantageous to define

$$u \equiv 2(V/N)a^{-d}y^{-d/2} \tag{7}$$

$$y = x\bigg(\Big\langle -\tfrac{1}{2}\sum_{i,j,k} S_0S_iS_jS_k\Big\rangle_c \Big\langle \sum_i S_0S_i\Big\rangle_c^{-2}\bigg)^{-2/d} \tag{8}$$

where now y has a Taylor expansion in K. Because of the linear relationship between x and K for small K, the second-moment series (3) can be reverted order-by-order and the result used to express (8) as a series in x. Finally, because of the linear relationship between y and x for small x, (8) can be reverted to obtain x as a series in y. The validity of hyperscaling is then simply tested by determining whether x diverges as y approaches some critical value y^*. We make the standard asymptotic assumption

$$y \simeq y^* - C(a/\xi)^{\omega} \qquad a/\xi \to 0, \tag{9}$$

where ω is the (universal) exponent characterising the leading corrections to scaling and C is a model-dependent constant (Wegner 1972). If (9) is correct, then we obtain

$$\gamma(y) \equiv \left(\frac{\partial}{\partial y}\ln x\Big|_a\right)^{-1}$$
$$\simeq \tfrac{1}{2}\omega(y^*-y) \qquad y \to y^*. \tag{10}$$

That is, we expect the inverse logarithmic derivative $\gamma(y)$ to have a zero at $y = y^*$ with negative slope $-\frac{1}{2}\omega$. From the definitions (3) and (7) we see that (10) can be rewritten as

$$\frac{\gamma(y)}{y} = \frac{\partial \ln y}{\partial \ln x}\bigg|_a = -\frac{1}{d}\frac{\partial \ln u}{\partial \ln \xi}\bigg|_a \tag{11}$$

and the last expression in (11) can be related directly to the Callan–Symanzik function as conventionally defined in the continuum model (see, for example, Brezin *et al* 1976). Before proceeding with the series analysis of (10) we digress to discuss this connection with the continnuum model in more detail.

To make the discussion concrete we introduce the continuum model defined by the partition function

$$Z = \Big(\prod_q \int d\sigma_q\Big) \exp\Big(-\frac{1}{2V}\sum_q (m_0^2+q^2+q^4/\Lambda^2)\sigma_q\sigma_{-q}$$
$$-\frac{\lambda}{4!\,V^3}\sum_{q_1q_2q_3} \sigma_{q_1}\sigma_{q_2}\sigma_{q_3}\sigma_{-q_1-q_2-q_3}\Big) \tag{12}$$

where $\sigma_q = \int d^d r \exp(-i\boldsymbol{q}\cdot\boldsymbol{r}) S(\boldsymbol{r})$ is the Fourier transform of a continuous spin distribution and the momenta $\boldsymbol{q}$ are restricted to the usual discrete set allowed by periodic boundary conditions in a volume V. The calculations leading to (5) were based on the model (12) in the limit that the momentum cut-off $\Lambda \to \infty$. For the convenience of the reader we list below quantities defined in those calculations and of relevance here. First, the renormalised mass was defined by the relation

$$m^{-2} \equiv -\frac{\partial}{\partial q^2} \langle \sigma_q \sigma_{-q} \rangle_c \big|_{q^2=0} \langle \sigma_0^2 \rangle_c^{-1}$$
$$= (2d)^{-1} \int d^d r\, r^2 \langle S(\boldsymbol{r}) S(0) \rangle_c \left(\int d^d r\, \langle S(\boldsymbol{r}) S(0) \rangle_c \right)^{-1} \tag{13}$$

so that in the critical region where a continuum approximation may be used for (3), the definitions for ξ and m^{-1} are in agreement. Strictly speaking, of course, $\xi \neq m^{-1}$ since the definitions (3) and (13) refer to different models; however, since in the following it will be obvious from the context which model is under consideration, we will not make this distinction and simply set $\xi = m^{-1}$. Similarly, the renormalised coupling constant λ_R is given by

$$\lambda_R \equiv -V m^4 \langle \sigma_0^4 \rangle_c \langle \sigma_0^2 \rangle_c^{-2}$$
$$= \lambda - \tfrac{3}{2}\lambda^2 \int \frac{d^d q}{(2\pi)^d} (m^2 + q^2 + q^4/\Lambda^2)^{-2} + O(\lambda^3)$$
$$\equiv m^{4-d} u \tag{14}$$

and the *dimensionless* coupling constant u defined by (14) agrees with the definition (4) for the Ising model. Finally, we note that in the limit $\Lambda \to \infty$, u defined by (14) is a function of the dimensionless factor λm^{d-4} only and as a result, in the calculation leading to (5), the Callan–Symanzik function could be written in various equivalent ways. For example,

$$\frac{\beta(u)}{u} \equiv (d-4) \frac{\partial \ln u}{\partial \ln \lambda}\bigg|_m = \frac{\partial \ln u}{\partial \ln m}\bigg|_\lambda = -\frac{\partial \ln u}{\partial \ln \xi}\bigg|_\lambda . \tag{15}$$

On comparing (11) and (15) we see that both γ and β measure the rate at which the coupling constant approaches its fixed-point value as the correlation length diverges while the remaining microscopic length parameters are held fixed. We define

$$\gamma(y)/y \equiv d^{-1} \beta(u)/u \tag{16}$$

and view (7) and (16) as a convenient set of relations for comparing the continuum and spin-$\frac{1}{2}$ Ising model systems. In this regard, one particular point should be noted. In the Ising model the numerical evidence in three dimensions suggests that u is a monotonic decreasing function of ξ and hence approaches u^* from above. In the continuum model with $\Lambda = \infty$, it appears that u is a monotonic increasing function of ξ and approaches u^* from below. Thus if u^* is the same for the two models the functions β or γ are never defined on the same interval. This somewhat surprising behaviour is presumably related to the dramatic microscopic differences in the two models. We note that if, in three dimensions, λ and Λ are both finite, then (12) can be viewed as an approximation to the lattice model defined by

$$Z = \left(\prod_i \int dS_i \right) \exp\left(\sum_{nn} S_i S_j - K_4 \sum_i S_i^4 + K_2 \sum_i S_i^2 \right) \tag{17}$$

where S_i is a continuous spin variable on the lattice site i, K_4 is of order λ/Λ and K_2 plays the same role as m_0^2 in (12) or K in (1). If in (17) we take the limit $K_4 = K_2/2K \to \infty$ for fixed K, the Ising model (1) is obtained. Clearly there is a complete reversal of the roles of λ and Λ; the Ising model is the limit $\lambda/\Lambda \to \infty$ whereas the model leading to the estimate (5) is the limit $\lambda/\Lambda \to 0$.

If we accept the renormalisation group picture as a valid description of the critical region, and in addition assume that the limiting procedures discussed above do not invalidate any of the renormalisation group arguments, then we expect $\gamma(y)$ for the continuum model and Ising model to be zero at the same $y = y^*$. Also, if the coefficient of the leading correction term to scaling does not vanish in either model, we expect the function $\gamma(y)$ to have the same slope at $y = y^*$. There is no direct evidence that the constant C in (9) vanishes for the Ising system since previous temperature plane analyses have excluded the existence of a finite y^*. However, it is worrying that the analysis of the Ising susceptibility and correlation length series separately does indicate that the leading confluent correction terms vanish for spin-$\frac{1}{2}$ (Saul *et al* 1975, Camp and Van Dyke 1975, Camp *et al* 1976). If the analysis of $\gamma(y)$ as given below is correct, then there should have been confluent corrections with detectable amplitude in at least one of the functions χ, M_2, or $\partial^2\chi/\partial h^2$.

From the available high-temperature series expansions (Essam and Hunter 1968, Moore *et al* 1969) we determine $\gamma(y)$, the analogue of the Callan–Symanzik function, for the three cubic lattices as given below.

(*a*) Simple cubic:

$$\begin{aligned}\gamma = y &- 8y^2 + 24y^3 - 112y^4 + 469\tfrac{1}{3}y^5 - 896y^6 - 2880y^7 \\ &+ 46563\tfrac{5}{9}y^8 - 159466\tfrac{2}{3}y^9 - 512960y^{10} + 5772583\tfrac{41}{81}y^{11} \\ &- 16377353\tfrac{13}{27}y^{12} - 53100416y^{13} + \ldots,\end{aligned} \tag{18a}$$

(*b*) body-centred cubic:

$$\begin{aligned}\gamma = y &- 8y^2 + 14y^3 - 90y^4 + 596\tfrac{7}{12}y^5 - 1306\tfrac{2}{3}y^6 + 298\tfrac{11}{16}y^7 \\ &+ 28704\tfrac{275}{576}y^8 - 170850\tfrac{331}{4608}y^9 + 347985\tfrac{9}{512}y^{10} \\ &+ 1627103\tfrac{318641}{331776}y^{11} - 18348011\tfrac{388783}{1327104}y^{12} \\ &+ 77485833\tfrac{2330613}{2654208}y^{13} + \ldots,\end{aligned} \tag{18b}$$

(*c*) face-centred cubic:

$$\begin{aligned}\gamma = y &- 8y^2 + 4y^3 + 16y^4 + 59\tfrac{1}{3}y^5 + 238\tfrac{2}{3}y^6 + 777y^7 \\ &+ 1539\tfrac{5}{9}y^8 - 371\tfrac{13}{36}y^9 + \ldots.\end{aligned} \tag{18c}$$

We have analysed these series by Padé approximant methods and tables 1 to 3 give our results for the apparent zero y^* and the slope $\gamma'(y^*)$. For the simple cubic lattice the higher-order Padé approximants show singularities in the complex y plane in the neighbourhood of $-0{\cdot}10 \pm 0{\cdot}17i$ and $0{\cdot}14 \pm 0{\cdot}20i$. Because of the interference from these singularities the estimate of y^* is not precise and the behaviour of $\gamma(y)$ for $y \gtrsim 0{\cdot}25$ is quite uncertain. For the body-centred cubic lattice the dominant singularities in γ appear at $y \simeq -0{\cdot}14 \pm 0{\cdot}16i$; the behaviour of $\gamma(y)$ for $y \gtrsim 0{\cdot}22$ is uncertain but the apparent zero in this case lies well within the estimated radius of convergence of the series and hence is actually better defined. The series for the face-centred cubic lattice

Table 1. Central block of Padé estimates of $\gamma(y)$ giving zero y^* (upper number) and slope $\gamma'(y^*)$ (lower number) for the simple cubic lattice. A blank denotes no positive axis zero and asterisks denote defects, i.e. Padé estimates with a close pole-zero pair.

D \ N	4	5	6	7	8	9	10
3	0·17988	0·18803	0·180*	0·19910	0·196*	0·17282	0·18697
	−0·724	−0·553	−0·71	−0·328	−0·41	−1·701	−0·649
4	0·18340	0·175*	—	0·19218	0·18816	0·18918	
	−0·666	−0·75	—	−0·492	−0·602	−0·570	
5	0·185*	—	0·18418	0·18996	0·18907		
	−0·64	—	−0·678	−0·548	−0·573		
6	0·18959	0·19134	0·18868	0·18939			
	−0·556	−0·521	−0·582	−0·563			
7	0·19087	0·19028	0·18918				
	−0·531	−0·544	−0·570				
8	0·18962	0·185*					
	−0·560	−0·77					
9	0·18869						
	−0·585						

is too short to enable us to even predict the existence of a zero with any certainty. Actual plots of $\gamma(y)$ for the three lattices are shown in figure 1. Included in these figures are error estimates obtained by extrapolation of small-y errors as suggested by Hunter and Baker (1973). The errors grow sufficiently rapidly with increasing y that for the simple cubic lattice the $\gamma(y)$ curve only dips below zero by an amount approximately three times the apparent error. For the body-centred lattice the negative value of γ is as much as six times the apparent error. Thus in the body-centred lattice we can be reasonably confident that $\gamma(y)$ actually has a zero; the evidence from the simple cubic lattice is marginal. On the other hand, if we assume the existence of a zero at $y = y^*$, then we obtain the following estimates.

Table 2. As table 1 for the body-centred cubic lattice.

D \ N	4	5	6	7	8	9	10
3	0·15210	0·16239	0·16151	0·15964	0·15960	0·160*	0·15936
	−0·783	−0·481	−0·512	−0·578	−0·580	−0·58	−0·589
4	0·15494	0·16148	0·163*	0·15957	0·160*	0·15951	
	−0·718	−0·513	−0·47	−0·581	−0·58	−0·583	
5	0·15569	0·15913	0·15932	0·15937	0·15937		
	−0·701	−0·598	−0·591	−0·589	−0·589		
6	0·15759	0·15935	0·15940	0·15937			
	−0·652	−0·590	−0·588	−0·589			
7	0·15822	0·15939	0·15937				
	−0·633	−0·588	−0·589				
8	0·15860	0·15937					
	−0·621	−0·589					
9	0·15893						
	−0·609						

Table 3. As table 1 for the face-centred cubic lattice.

D \ N	3	4	5	6	7
2	0·15367 −0·457	0·15587 −0·379	0·155* −0·41	0·14829 −0·693	0·15048 −0·590
3	0·15818 −0·289	0·155* −0·41	0·156* −0·36	0·15089 −0·571	
4	0·15264 −0·504	0·14793 −0·713	0·15084 −0·573		
5	0·15089 −0·573	0·15035 −0·596			
6	0·15053 −0·588				

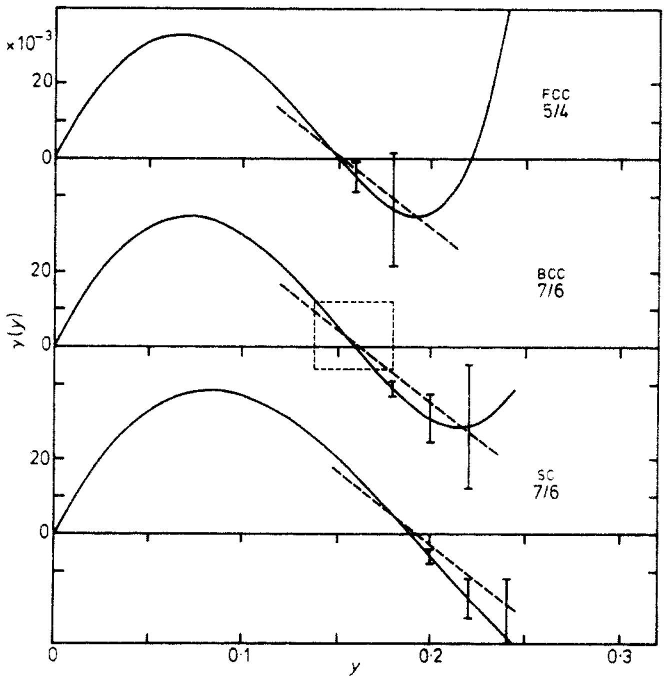

Figure 1. The full curves are estimates of the spin-$\frac{1}{2}$ Ising model $\gamma(y)$ based on the m/n Padés as indicated for the three cubic lattices. The broken lines are continuum model $\gamma(y)$ estimates obtained using (7) and (16) and a Padé Borel–Leroy estimate of $\beta(u)$. An enlargement of the small box region in the body-centred lattice graph is shown in figure 2.

(*a*) Simple cubic:

$$y^* = 0{\cdot}189 \pm 0{\cdot}002 \qquad \gamma'(y^*) = -0{\cdot}56 \pm 0{\cdot}04 \qquad 3u^*/16\pi = 1{\cdot}45 \pm 0{\cdot}02; \tag{19a}$$

(*b*) body-centred cubic:

$$y^* = 0{\cdot}1594 \pm 0{\cdot}0008 \qquad \gamma'(y^*) = -0{\cdot}59 \pm 0{\cdot}03 \qquad 3u^*/16\pi = 1{\cdot}444 \pm 0{\cdot}01; \tag{19b}$$

(*c*) face-centred cubic:

$$y^* = 0{\cdot}151 \pm 0{\cdot}005 \qquad \gamma'(y^*) = -0{\cdot}6 \pm 0{\cdot}2 \qquad 3u^*/16\pi = 1{\cdot}44 \pm 0{\cdot}07. \tag{19c}$$

Thus the different lattice estimates are completely consistent and yield a u^* that is about 2% above the continuum estimate (5). The correction to the scaling exponent $\omega = -2\gamma' \simeq 1{\cdot}18$ is some 50% above the continuum estimate of $\omega \simeq 0{\cdot}79$. Were it not for the conflicting temperature plane analysis results we would conclude that the spin-$\frac{1}{2}$ Ising model satisfies scaling, but that it does not lie in the same universality class as the continuum model.

In an attempt to clarify this rather unsatisfactory situation we have made certain comparisons as described in the following section. These comparisons include new error estimates of temperature plane analysis results that are consistent with the exponent uncertainties obtained by Baker (1977) but are more directly related to those obtained here and shown in figure 1.

3. Coupling constant against temperature plane analysis

To present a direct visual comparison of coupling constant and temperature plane analyses we have replotted a small region of figure 1 for the body-centred cubic lattice in figure 2. Different portions of the spin-$\frac{1}{2}$ $\gamma(y)$ curve are distinguished by values of the dimensionless correlation length $\xi/a = \sqrt{x}$ which were obtained by numerical integration of the Padé estimate of $\gamma(y)$. Also replotted from figure 1 is $\gamma(y)$ for the continuum model as determined from Borel–Leroy Padé estimates of the β function and the transformations (7) and (16). In this case the curve is labelled by the dimensionless correlation length $3\lambda\xi/16\pi$ where $\xi = m^{-1}$. From (14) we see that in three dimensions the expansion for u begins as

$$u \simeq \lambda\xi(1 - 3\lambda\xi/16\pi + \ldots) \tag{20}$$

so that in some sense $3\lambda\xi/16\pi \leqslant O(1)$ represents a weak coupling region and $3\lambda\xi/16\pi \geqslant O(1)$ is strong coupling. Error bars on the spin-$\frac{1}{2}$ $\gamma(y)$ curve are Hunter–Baker (1973) estimates exactly as in figure 1. The error estimate in (5) is the larger of the two estimates given by Le Guillou and Zinn-Justin (1977) and Baker *et al* (1978); the y estimate corresponding to (5) is $y^* = 0{\cdot}1616 \pm 0{\cdot}0002$ and the uncertainty is negligible on the scale shown in figure 2.

To obtain the comparison with temperature plane analysis we determined the functions $x(v)$ and $y(v)$ for the body-centred cubic lattice by integrating numerically Padé approximant estimates of $f = (v_c - v)(d/dv)\ln(x/v)$ and $g = (v_c - v)(d/dv)\ln(y/x)$. Here $v = \tanh K$ and the critical value $v_c = 0{\cdot}1561093\ldots$ was determined from the 7/7 Padé of the logarithmic derivative of the susceptibility series (Sykes *et al* 1972). Straightforward manipulations of $x(v)$ and $y(v)$ then yield $\gamma(v)$.

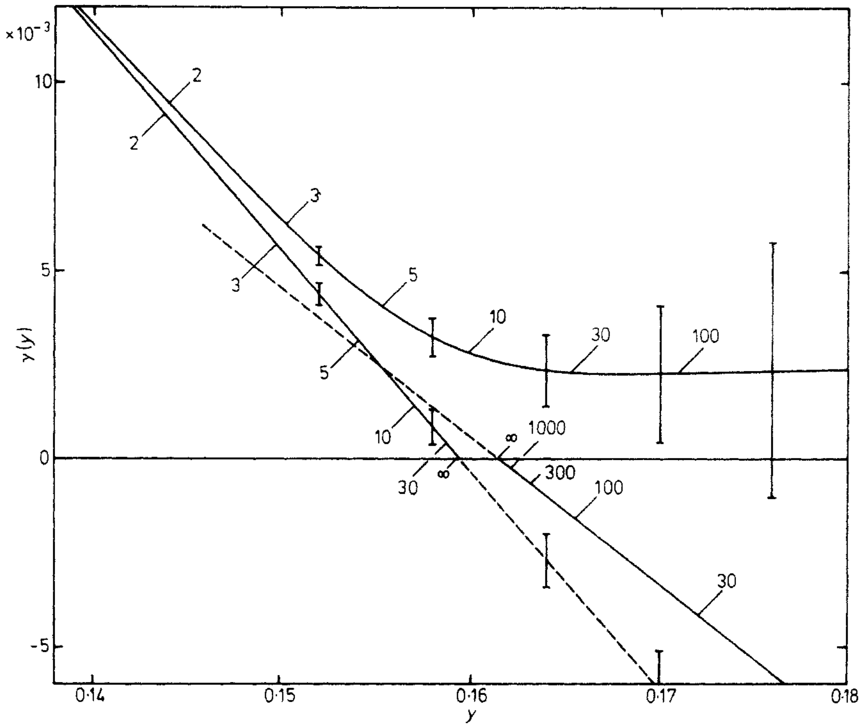

Figure 2. Comparison of $\gamma(y)$ obtained by temperature plane (upper full curve) and direct y-plane Padé analysis (lower full curve for $y<0{\cdot}16$) of the spin-$\frac{1}{2}$ Ising model on the body-centred cubic lattice, and Padé Borel–Leroy analysis (lower full curve for $y>0{\cdot}16$) of the continuum model. Spin-$\frac{1}{2}$ Ising curves are labelled by ξ/a ratios; the continuum curve is labelled by values of $3\lambda\xi/16\pi$.

One particular but representative result, based on the diagonal 5/5 Padé for f and the 5/6 for g, is plotted in figure 2. Again, a number of values of ξ/a are shown on the $\gamma(y)$ curve. Since temperature plane analysis predicts that the coupling constant u vanishes as $(1-K/K_c)^{d^*\nu}$ and x diverges as $(1-K/K_c)^{-2\nu}$, we obtain immediately from (7) and (11) that in the asymptotic regime y diverges and

$$\gamma(y)/y \simeq d^*/d \qquad y\to\infty. \tag{21}$$

Thus implicit in the temperature analysis is the cross-over behaviour in $\gamma(y)$ so evident in figure 2. Furthermore, the length scale ξ at which cross-over occurs is directly related to the magnitude of the anomalous dimension d^*. The error estimates on the $\gamma(y)$ curve based on temperature plane analysis were obtained by the Hunter–Baker (1973) method of extrapolating the small-y error estimates. Exactly the same analysis applied to f and g leads to the estimate

$$3\nu+\gamma-2\Delta = 0{\cdot}025\pm0{\cdot}004 \tag{22}$$

to be compared with Baker's (1977) estimate $0{\cdot}029\pm0{\cdot}005$ for the body-centred lattice. The small differences are not significant because the present analysis is carried out in the tanh K plane whereas Baker used a renormalised T_c approach.

To show that hyperscaling fails we must show that $\gamma(y)$ approaches yd^*/d for large y as given by (21); the evidence for such a straight line in figure 2 is not compelling. This situation is reminiscent of what we found in the y-plane analysis. Because of the rapid growth of errors the existence of a zero of $\gamma(y)$ was not definitely proved but by assuming a zero exists we could make the quantitative estimate (19*b*). Similarly, by temperature plane analysis we have not proved that hyperscaling fails, but again, by assuming that $\gamma(y)$ approaches yd^*/d we can make the quantitative estimate (22).

The obvious discrepancy between the central estimates obtained by coupling constant and temperature plane analysis as shown in figure 2 is not so surprising when one distinguishes those sections of the $\gamma(y)$ curves that are based largely on extrapolation and, in addition, one makes a plausible guess as to the true behaviour of $\gamma(y)$. To take an extreme view, we note that the second moment of the pair correlations is represented approximately by an integral proportional to $\int r^2(\exp(-r/\xi)/r)r^2\,dr$ and hence its value is dominated by the region $r \simeq 3\xi$. Since the available series only extend to 12 terms and thus to a distance $12a$, we can argue that only the region $\xi/a \leqslant 4$ is based on hard evidence and that the region $\xi/a \geqslant 4$ is determined by the implicit assumptions built into the series analysis methods. If the correct $\gamma(y)$ is almost a straight line with slope $-0{\cdot}6$ in the region $y \leqslant 0{\cdot}15$ and a curve in the region $0{\cdot}15 \leqslant y \leqslant 0{\cdot}16$ so as to match the continuum model slope of $-0{\cdot}4$ for $y \geqslant 0{\cdot}16$, then the two distinct Padé estimates are quite reasonable. In the present scheme one assumes 'smoothness' in the coupling constant and hence the Padé attempt to fit the true curve with the best straight, or nearly straight, line. In the temperature analysis scheme curvature is easily accommodated by a finite anomalous dimension d^*; no *internal* inconsistency is apparent because the straight line portion $\gamma(y) = d^*y/d$ only applies for ξ/a ratios well beyond those directly accessible from the available series.

We remark, as an aside, that similar uncertainty arguments could be applied to the continuum model curve in figure 2. This curve has been labelled by the dimensionless product $3\lambda\xi/16\pi$ and one would naively have expected the strong coupling region $3\lambda\xi/16\pi \gg \mathrm{O}(1)$ to be inaccessible by perturbation theory. The error assignment in (5) is realistic only if one assumes that $\beta(u)$ is completely structureless, that is, no new physics develops for large values of the dimensionless correlation length. Renormalisation group calculations such as those begun by Golner and Riedel (1975) should therefore prove extremely valuable in providing independent estimates of the behaviour of the continuum model.

We conclude this section with an attempt to estimate the additional number of body-centred lattice, high-temperature, series terms needed to decide between the two curves in figure 2. Two specific calculations are described in which we explore what we believe are the 'weak links' in the coupling constant and temperature plane analyses. We first investigate to what extent hyperscaling is forced into, rather than derived from, the coupling constant plane analysis. Thus, although in principle Padé analysis in the y plane could reproduce the $\gamma(y)$ curve for a model in which hyperscaling failed, in practice the number of terms required might be so large as to make the calculation impossible. To test this possibility, we have obtained y-plane Padé analysis estimates of the temperature plane $\gamma(y)$ curve shown in figure 2. Specifically, we treated as exact the 5/5 Padé estimate of $f = (v_c - v)(\mathrm{d}/\mathrm{d}v)\ln(x/v)$ and the 5/6 estimate of $g = (v_c - v)(\mathrm{d}/\mathrm{d}v)\ln(y/x)$ where $v = \tanh K$ and $v_c = 0{\cdot}156\ldots$ as before. Instead of obtaining $x(v)$, $y(v)$ and $\gamma(v)$ by numerical integration we obtained the Taylor series expansions of these functions in v. Straightforward manipulation of these series yielded $\gamma(y)$. The first 13 terms of course agree with the exact series (18*b*). Our results for the Padé analysis of this 'possible' $\gamma(y)$ are shown in table 4. Essentially all the Padés based on anywhere from 14 to 18 terms contain defects which we interpret as evidence that

Table 4. Estimates of $\gamma(y)\times 10^3$, $y=0\cdot15937$, as given by $(n+l)/n$ Padé. The number of terms in the $\gamma(y)$ series on which each Padé is based is $N=2n+l$. Coefficients up to $N=13$ are exact; coefficients for $N\geq 14$ were obtained from tanh K plane Padé estimates as described in the text. Asterisks denote Padé estimates with defects. Numbers in brackets give the positive axis pole position for those estimates which do not have a zero near $y=0\cdot16$ but curve upwards and diverge rather dramatically.

N \ l	−2	−1	0	1	2	3
9		−2·604*		1·095		1·110
10	−1·161		−0·145		1·600	
11		−0·013		−0·032		0·115
12	0·012		0·017		0·002	
13		0·003		≡0		−0·000
14	0·01*		0·02*		0·00*	
15		−0·01*		−0·03*		0·11*
16	−2·56*		−0·15*		1·81 (0·182)	
17		−0·83*		−3·55*		−2·51*
18	−1·49*		1·12		5·83* (0·165)	
19		2·33 (0·177)		2·01 (0·184)		2·19 (0·180)
20	3·51 (0·169)		5·92 (0·164)		2·61 (0·174)	
21		2·96 (0·171)		2·74 (0·173)		2·76 (0·173)
⋮						
26	4·16 (0·166)		4·17 (0·166)		4·17 (0·166)	
⋮						
			Exact = 2·939			

the behavior of $\gamma(y)$ is different from its assumed behaviour based on 13 terms. Padés based on 19 or more terms clearly indicate $\gamma(y)$ has no zero. We find this extremely encouraging in that extension of the available series by even a few terms would be useful and that extension by six terms is likely to be definitive in demonstrating whether or not the coupling constant plane analysis will show a zero near $y\simeq 0\cdot16$.

For our second analysis we assume that the available terms only determine the correlation length correctly for $\xi/a\leq 4$ as discussed earlier. Since such a small ξ/a ratio may not be representative of the critical region, we treat the 5/6 v-plane Padé estimate of $g=(v_c-v)(\mathrm{d}/\mathrm{d}v)\ln(y/x)$ and the 7/6 y-plane estimate of $\gamma(y)$ as exact and determine from these an extrapolated series for $x(v)$. Padé estimates of $f=(v_c-v)(\mathrm{d}/\mathrm{d}v)\ln(x/v)$ based on the exact 12 terms yield the exponent $\omega=0\cdot638$, estimates based on 13 to 18 terms contain defects and estimates based on 20 or 21 terms yield $\nu\simeq 0\cdot634$. This is disappointingly slow convergence to the exact scaling value of 0·6292 for this model series, but is not so surprising since the point $v=v_c$ is a confluent singularity. We conclude that unless sophisticated methods of analysis that handle confluent singularities can be made to work, six additional terms will not be adequate to establish, by temperature plane analysis, precise exponent estimates that verify the y-plane results. The best one can hope for is the negative information deduced from the presence of a large number of defects in the temperature plane Padé tables.

Work on extending the body-centred lattice susceptibility and correlation length series by the linked cluster method as developed by Wortis and co-workers (Moore *et al* 1969, Wortis 1974) is being started. An enormous simplification that has not, to our knowledge, been used before is possible because of the particular form of the nearest-neighbour coupling on this lattice, namely only free embedding constants on a one-dimensional chain need be evaluated. We expect that a considerable extension of the available series will be possible and since all graphs that contribute to the body-centred lattice or its hypercubic generalisations also contribute to the linear chain and simple quadratic lattice we can virtually guarantee the correctness of the new terms. It is not obvious to us what method is to be preferred for generating higher-order terms for the second field derivative of the susceptibility, but we hope that the present analysis will motivate others to examine the feasibility of extending this series.

4. Other systems

Although our major interest has been in resolving the question of hyperscaling in three dimensions, we have also analysed the spin-$\frac{1}{2}$ high-temperature series for the two-dimensional square and triangular lattices and the four-dimensional hypercubic lattice.

For the simple quadratic lattice hyperscaling is not in doubt and hence $\gamma(y)$ must have a nontrivial zero. To estimate y^* we have used all the terms available for $\partial^2\chi/\partial h^2$ (Essam and Hunter 1968) and this required an extension of the known series for M_2 (Fisher and Burford 1967). From the work of Wu *et al* (1976) one can obtain explicit expansions for both χ and M_2 in which, for $T > T_c$, the terms of order $(2n+1)$ are given as $2n$-dimensional integrals over elementary functions. By expanding the integrands as high-temperature series and performing the necessary integrations numerically we have obtained

$$\chi^{(1)}+\chi^{(3)} = \ldots + 150660388v^{19} + 377009364v^{20} + 942106116v^{21} + \ldots \tag{23}$$

and

$$\begin{aligned} M_2^{(1)}+M_2^{(3)} = \ldots &+ 3185188v^{11} + 9468480v^{12} + 27729316v^{13} \\ &+ 80168352v^{14} + 229179140v^{15} + 648697984v^{16} \\ &+ 1820052468v^{17} + 5066498144v^{18} + 14004100644v^{19} \\ &+ 38461119936v^{20} + 105017024900v^{21} + 285226504608v^{22} + \ldots . \end{aligned} \tag{24}$$

The terms in $\chi^{(1)}+\chi^{(3)}$ up to order v^{19} agree with the expansion of χ given by Sykes *et al* (1972). Since we find $\chi^{(5)}$ and $M_2^{(5)}$ first contribute respectively at order v^{24} and v^{29}, the results (23) and (24) also give the total χ and M_2. The expansion of $\gamma(y)$ is

$$\begin{aligned} \gamma = y - 8y^2 + 8y^3 - 32y^4 - 16y^5 + 480y^6 + 1344y^7 - 128y^8 - 800y^9 \\ + 14112y^{10} - 233728y^{11} - 2923840y^{12} - 17714048y^{13} - 95329280y^{14} \\ - 559149248y^{15} - 3197866176y^{16} - \ldots , \end{aligned} \tag{25}$$

and from a Padé analysis of (25) we estimate

$$y^* = 0{\cdot}1361 \pm 0{\cdot}0002 \qquad \gamma'(y^*) = -0{\cdot}94 \pm 0{\cdot}04 \qquad 3u^*/8\pi = 1{\cdot}754 \pm 0{\cdot}003. \tag{26}$$

The higher-order Padés show $\gamma(y)$ has singularities in the complex y plane near $y \simeq 0{\cdot}19 \pm 0{\cdot}04\mathrm{i}$ and, although this suggests that y^* may be the beginning of a branch cut rather than a simple zero of $\gamma(y)$, we have not been able to verify this by other methods of analysis.

The estimate (26) for u^* is consistent with the estimate $3u^*/8\pi = 1{\cdot}754 \pm 0{\cdot}001$ we obtain from an analysis of a nine-term $\gamma(y)$ series for the triangular lattice and also with the value $1{\cdot}751 \pm 0{\cdot}005$ obtained by Baker (1977) by temperature plane analysis. The value for the correction to the scaling exponent $\omega = -2\gamma' = 1{\cdot}88 \pm 0{\cdot}08$ for the simple quadratic and $2{\cdot}00 \pm 0{\cdot}02$ for the triangular lattice is surprising and not understood. The corrections to the susceptibility are known (Wu *et al* 1976) to contain terms proportional to $K_c - K$ and $(K_c - K)^{7/4}$ so that we would naively have expected $\omega = 1$ or, if the coefficient of the leading correction term in y vanished, $\omega = 1{\cdot}75$.

For the four-dimensional hypercubic lattice there is no evidence for a zero in $\gamma(y)$ in the range $y \leqslant 0{\cdot}26$ and for larger y the uncertainty in $\gamma(y)$ is too large for any definitive conclusion.

It is difficult to see how the $\gamma(y)$ analysis could be extended to systems with order parameter dimension $n > 1$. One of the key but unstated assumptions in the y-plane analysis described in this paper is that $y(x)$ is monotonic and hence the inverse $x(y)$ is single-valued. If instead $y(x)$ had a maximum $\tilde{y}$ for some finite x, then $\gamma(y)$ would have a square-root branch point at $y = \tilde{y}$ and the critical region $y \simeq y^*$ would not be accessible by Padé analysis. For the spin-$\frac{1}{2}$ Ising model a monotonic $y(x)$ is reasonable since the discrete nature of the spins means the fluctuations are always very non-gaussian and hence the coupling constant u, which measures deviations from the gaussian, can be expected to be large. However, for systems with $n > 1$, the dominant fluctuations near the critical point are very likely transverse; hence the discrete nature

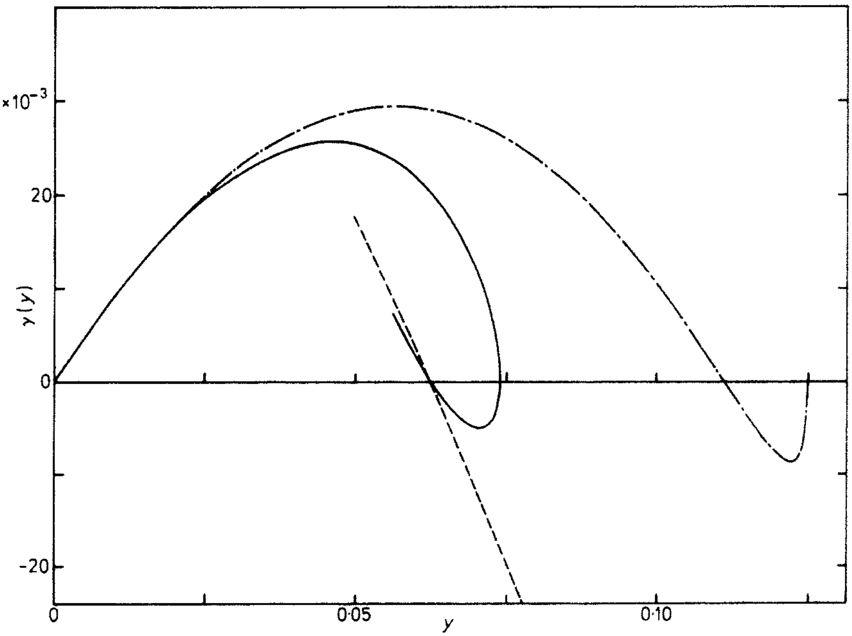

Figure 3. Linear chain $\gamma(y)$. The chain curve is the result (27) for the Ising model; the full curve is (34) for the spherical model. The broken line is $\gamma(y)$ for the continuum $(\phi^2)^2$ spherical model.

of the spin magnitude is irrelevant and the system can be expected to behave like a continuum model. In this case y will approach y^* from above and so $y(x)$ *must* have a maximum. The situation for the nearest-neighbour, discrete length, spin model in one spatial dimension is worked out below and one can indeed show that for all $n > 1$ y approaches y^* from above. On the other hand, for the spin-$\frac{1}{2}$ Ising model

$$\gamma(y) = \tfrac{1}{2}[1 - 8y - (1-6y)(1-8y)^{1/2}] \tag{27}$$

and the plot of this γ in figure 3 is seen to be qualitatively similar to the three-dimensional results shown in figure 1.

For arbitrary order parameter dimension n we define our model by the partition function

$$Z = \left(\prod_i \int d^n S_i\, \delta(S_i^2 - 1)\right) \exp\left(K \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \sum_i h_i S_i^0\right). \tag{28}$$

We maintain $x = \xi^2/a^2$ as the second moment of the correlations but for numerical convenience modify the normalisation of y so that (8) now reads

$$y = x\left(\left\langle -\tfrac{1}{6}(n+2) \sum_{i,j,k} S_0^0 S_i^0 S_j^0 S_k^0 \right\rangle_c \left\langle \sum_i S_0^0 S_i^0 \right\rangle_c^{-2}\right)^{-2}. \tag{29}$$

Fisher's (1964) calculation for the linear chain classical Heisenberg model can be easily extended to treat both higher-order correlations and arbitrary n. We find

$$\begin{aligned} x &= \lambda_1(1-\lambda_1)^{-2} \\ y &= \lambda_1\left(1 - \lambda_1 + \frac{4\lambda_1}{1+\lambda_1} + \frac{2\lambda_2(1-\lambda_1)}{1-\lambda_2} + \frac{2n(\lambda_1^2 - \lambda_2)}{(1+\lambda_1)(1-\lambda_2)}\right)^{-2} \end{aligned} \tag{30}$$

where

$$\begin{aligned} \lambda_1 &= \langle \boldsymbol{S}_i \,.\, \boldsymbol{S}_{i+1} \rangle = I_{n/2}(K)/I_{n/2-1}(K) \\ \lambda_2 &= \langle n(\boldsymbol{S}_i \,.\, \boldsymbol{S}_{i+1})^2 - 1\rangle/(n-1) = I_{n/2+1}(K)/I_{n/2-1}(K) \end{aligned} \tag{31}$$

with I_ν the modified Bessel function. For arbitrary n, (30) must be handled numerically but for both $n = 1$ and $n \to \infty$ simplifications occur. In the Ising limit, $n = 1$, (30) reduces to

$$y = \lambda_1(1+\lambda_1)^2(1 + 4\lambda_1 + \lambda_1^2)^{-2} = x(1+4x)(1+6x)^{-2}, \tag{32}$$

from which we obtain the explicit expression (27) for $\gamma(y)$. In the spherical model limit we find

$$\begin{aligned} &\lim_{n\to\infty} n(\lambda_1^2 - \lambda_2) = 2\lambda_2(1-\lambda_2)/(1+\lambda_2) \\ &\lim_{n\to\infty} y = \lambda_1(1+\lambda_1^2)^2(1+\lambda_1)^{-6} = x(1+2x)^2(1+4x)^{-3} \end{aligned} \tag{33}$$

and

$$\begin{aligned} &\lim_{n\to\infty} \gamma(y) = y(2\cos\phi - 1)(4\cos\phi - 1)/(2\cos\phi + 1) \\ &\cos 3\phi = 1 - 27y \qquad \cos\phi = (1+x)/(1+4x). \end{aligned} \tag{34}$$

The result (34) is plotted in figure 3. It is qualitatively similar to $\gamma(y)$ for arbitrary $n \neq 1$ and illustrates our contention that y^* cannot be obtained by a direct series analysis of γ.

To illustrate another point, we have also plotted $\gamma(y)$ for the continuum $(\phi^2)^2$ spherical model. Although the values of y^* are in agreement the slopes $\gamma'(y^*)$ differ and reflect that in the continuum model the leading corrections are proportional to m^3/λ compared with a^2/ξ^2 in the lattice model. This is an 'accidental' feature of the continuum model because a high momentum cut-off Λ has not been included; finite Λ would lead to corrections proportional to m^2/Λ^2.

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