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Critical temperatures of the $d = 3$, $s = \frac{1}{2}$ Ising model; the effect of confluent corrections to scaling

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Abstract. Much attention has been paid to the $d = 3$, $s = \frac{1}{2}$ Ising model on the BCC lattice in recent years because the best high-temperature series expansions were available for this lattice. However, in order to compare series estimates of critical exponents and temperatures with independent evaluations via the Monte Carlo method, lattices of lower coordination number must be considered, since Monte Carlo studies are usually made on these. In this paper a study of extant susceptibility series on the FCC, SC, diamond and tetrahedron lattices is reported on and some comments are made on aspects of recent Monte Carlo analyses of the $d = 3$, $s = \frac{1}{2}$ Ising model on the SC and diamond lattices.

1. Introduction

There has been renewed interest in the literature concerning the technique of exact series expansions in critical phenomena during the last few years, because following the pioneering work of Nickel (1981), it has become clear that any apparent disagreement between series and renormalisation group (RG) estimates of critical exponents (or disagreement over the validity of hyperscaling) is removed when the hypothesis of non-analytic confluent corrections to dominant exponents is invoked in the analysis of series expansions. This hypothesis (which is an integral part of RG theory (Wegner 1972)) replaces the assumed critical behaviour of, for example, the susceptibility χ,

$$\chi \sim (v - v_c)^{-\gamma}[1 + b_1(v - v_c) + \ldots] \tag{1}$$

by

$$\chi \sim (v - v_c)^{-\gamma}[1 + a_1(v - v_c)^{\Delta_1} + b_1(v - v_c) + \ldots] \tag{2}$$

where $v = \tanh K$ is the high-temperature series expansion variable, b_1 is the amplitude of the first analytic correction term, and a_1 is the amplitude of the first confluent non-analytic correction term. Analyses which invoke and justify this hypothesis to remove hyperscaling violations for the $d = 3$, $s = \frac{1}{2}$ Ising model on the BCC lattice include Chen *et al* (1982), Zinn-Justin (1981), Roskies (1981b) and Adler *et al* (1982b). Similar studies have been made for the FCC lattice, (McKenzie 1979), but most recent studies of the $s = \frac{1}{2}$ model on the SC diamond and tetrahedron lattices predate Nickel (1981) and imply $a_1 = 0$ in the susceptibility series for $s = \frac{1}{2}$ (Gaunt and Sykes 1979, Oitmaa and Ho-Ting-Hun 1979, Gaunt 1982). Two exceptions are the calculations of Zinn-Justin (1979) and Roskies (1981a). Zinn-Justin (1979) obtained partial agreement with hyperscaling (see table 2), but Roskies (1981a), who studied a short second moment series on the SC lattice using field theoretic methods and accepted the possibility that $a_1 \neq 0$, still found hyperscaling violation, and we shall discuss this below.

In the case where $a_1 = 0$ (see table 1) (McKenzie 1975, Sykes *et al* 1972, Gaunt and Sykes 1973, 1979, Ho-Ting-Hun and Oitmaa 1975), analysis of the susceptibility series leads to v_c values of 0.10173 ± 0.00001 (FCC), 0.21813 ± 0.00001 (SC), 0.15612 ± 0.00003 (BCC), 0.35381 ± 0.00003(diamond) and 0.23300 ± 0.00001 (tetrahedron). We denote the central v_c values for the case $a_1 = 0$ as $v_c(0)$, and note (see § 2) that invocation of the hyopthesis that $a_1 \neq 0$ led to downward revision of $v_c(0)$ for the BCC and FCC lattices. A slight downward trend was also observed by Zinn-Justin (1979) (see table 2) for the SC and diamond lattices. We examine v_c in the case that $a_1 \neq 0$ for all these lattices in § 3 below.

Table 1. Series estimates of v_c and γ for 3D lattices ($a_1 = 0$).

Lattice	BCC	FCC	SC	Diamond	Tetrahedron
Susceptibility series derivation[1]	Sykes *et al* (1972)	McKenzie (1975)	Gaunt and Sykes (1979)	Gaunt and Sykes (1973)	Ho-Ting-Hun and Oitmaa (1975)
No of terms	15	15	19	22	16
Analysis[2]	Sykes *et al* (1972)	McKenzie (1975)	Gaunt and Sykes (1979)	Gaunt and Sykes (1973)	Oitmaa and Ho-Ting-Hun (1979)
v_c	0.156 12 ± 0.000 03	0.101 73 ± 0.000 01	0.218 13 ± 0.000 01	0.353 81 ± 0.000 03	0.233 00 ± 0.000 01
γ	1.25 ± 0.003	1.246 ± 0.005	1.25 ± 0.003	1.25 ± 0.003	1.250 ± 0.001

(1) We quote the authors of the most recent terms only.
(2) We quote $\nu = 0.638\ ^{+0.002}_{-0.001}$ from Gaunt (1982).

It is perhaps prudent to enquire at the outset why one would be concerned with further series studies on other lattices (and in particular with loose packed lattices) when arguments of universality predict that critical exponents will take the same values on all lattices. This is a valid consideration, however, since critical temperatures are not lattice independent and since it has been common practice in Monte Carlo (MC) calculations to use series estimates of v_c as a starting point (e.g. Knak Jensen and Mouritsen 1982) or point of reference (e.g. Blöte and Swendsen 1980), it appears desirable that reliable series estimates of v_c be available for loose packed lattices. The series estimates were used in the MC studies because they were supposedly more accurate; we shall demonstrate below that this accuracy is spurious and that the v_c obtained in a series analysis is a function of whether the confluent singularity hypothesis is invoked or not.

In § 2 we shall discuss previous work on the BCC lattice and present evidence for the dependence of v_c on the acceptance/rejection of the confluent hypothesis. We shall indicate the dependence observed on the BCC lattice and also discuss the FCC study of McKenzie (1979) and the SC calculation of Gaunt (1982). Section 3 will include a presentation of new results of the FCC, SC, diamond and tetrahedron lattices and a discussion of general trends. In § 4 comments will be made on the above mentioned Monte Carlo calculations and a discussion of the implications of the present work will be made in § 5. Comprehensive tables of v_c and exponent values obtained by various authors are also presented.

2. Previous studies on the BCC, FCC and SC lattices

All the above cited analyses of Nickel's 21-term susceptibility series lead to similar conclusions, *videlicit* $\gamma \sim 1.238$ and $\Delta_1 \sim 0.5$ in agreement with RG predictions and consistent with hyperscaling. These analyses use many different types of techniques including ratio (Zinn-Justin 1981), partial differential Padé approximants (Chen *et al* 1982), and Padé Roskies transformation (Roskies 1981b, Nickel and Dixon 1981, Adler *et al* 1982b). The virtues and deficiencies of these methods have been discussed elsewhere (Adler *et al* 1983, Guttmann 1983) and we only note that the strong agreement between the different methods is most pleasing.

Let us re-examine the analyses. Two of them (Chen *et al* 1982 and Nickel and Dixon 1981) do not consider the $s=\frac{1}{2}$ Ising model directly but work on models that interpolate between the $s=\frac{1}{2}$ Ising model and the Gaussian model. They concentrate on a particular choice of model parameters for which $a_1=0$ and estimate γ at this point. These γ values ($\gamma = 1.2385 \pm 0.0015$ and $\gamma = 1.23 \pm 0.003$ respectively) are then transferred to the Ising limit. The Chen *et al* (1982) calculation is independent of v_c choice, whereas in the Nickel–Dixon (1981) study the exponent γ is a function of v_c (the above estimate corresponds to $v_c \sim 0.156\,086$ whereas $\gamma = 1.240$ corresponds to $v_c \sim 0.156\,090$). The ratio study of Zinn-Justin (1981) also gives exponent estimates that are independent of v_c choice, but he notes that in a biased study a relative variation of 10^{-5} in $\tanh^{-1} v_c$ leads to an error of 1.2×10^{-3} at the 20th ratio estimate. This independent ratio study is made possible by the existence of two long series (susceptibility and correlation length) for the BCC lattice.

We note that the dependence of γ on the choice of v_c is not peculiar to the above calculations. It was observed earlier (Baker and Hunter 1973) for shorter Ising model and test series, and in fact many exponent results are quoted in terms of uncertainties in critical temperatures (e.g. Essam 1980).

We now consider the question of temperature dependence of γ on v_c in detail. The Nickel–Dixon (1981) study is a Padé analysis which uses the Roskies (1981b) transformation to a new variable $y = 1-(v/v_c - 1)^{1/2}$ to eliminate the effect of a non-analytic term with exponent $\Delta_1 = \frac{1}{2}$ exactly. Roskies (1981b) developed this transformation and applied it to the $s=\frac{1}{2}$ BCC series where the temperature dependence of γ on v_c also appears. Adler *et al* (1982a, b) have generalised the transformation to $y = 1-(v/v_c - 1)^{\Delta}$ and find that estimates of γ, v_c and Δ_1 are all interrelated. We found that the best convergence (see § 3 below) is given for $0.156\,086 \leqslant v_c \leqslant 0.156\,090$, $\gamma = 1.238 \pm 0.003$ and $\Delta_1 = 0.49 \pm 0.08$.

Zinn-Justin (1981) previously noted that γ estimates depend on Δ_1 input values and the general trend observed in all these studies is that γ and Δ_1 decrease as v_c decreases. In particular the 'old' (Sykes *et al* 1972, Gaunt and Sykes 1979) estimates of $\gamma \sim 1.250 \pm 0.003$, and $v_c \sim 0.156\,12 \pm 0.000\,03$, are replaced by $\gamma \sim 1.24$ and $v_c \sim 0.156\,09$, the v_c estimate just touching the old value and the γ estimate outside the old range. The variation in Δ_1 is very slow and estimates of Δ_1 are all quite wide.

We now consider the FCC lattice. McKenzie (1979) found that $\gamma = 1.241$ and $\Delta_1 = 0.496$ correspond to $K_c = 0.102\,07$, whereas $\gamma = 1.25$ and $\Delta_1 = \frac{1}{2}$ correspond to $K_c = 0.102\,08$ and $\gamma = 1.25$ and $a_1 = 0$ (no confluent singularity) yield $K_c = 0.102\,09$.

Table 2. Series estimates[1] of v_c, γ, Δ, and ν for 3D lattices ($a_1 \neq 0$)

Lattice	BCC	SC	FCC	Diamond	Tetrahedron
Susceptibility series derivation	Nickel (1981)	← As in table 1 →			
No of terms	21				
Second moment series derivation	Nickel (1981)	Roskies (1981a)	Moore *et al* (1969)		
No of terms	21	15	12		
Series analyses[1],[2]	Zinn Justin (1981) $\gamma = 1.2385 \pm 0.0025$ $\nu = 0.6305 \pm 0.0015$	Zinn Justin (1979) $\gamma = 1.245 \pm 0.003$ $v_c = 0.218\,11$	Zinn Justin (1979) $\gamma = 1.245 \pm 0.003$ $v_c = 0.101\,73$ $\nu = 0.638$	Zinn-Justin (1979) $\gamma = 1.245 \pm 0.003$ $v_c = 0.353\,74$	
	Nickel (1981) $\gamma = 1.239 \pm 0.002$ $\nu = 0.631 \pm 0.003$	Gaunt (1982)[3] ($\gamma = 1.241, \Delta_1 = 0.496$) $v_c = 0.218\,10 \pm 0.000\,01$	McKenzie (1979) ($\gamma = 1.241, \Delta_1 = 0.496$) $v_c = 0.101\,72$		
	Roskies (1981) $v_c = 0.15609$ $\gamma = 1.2400 \pm 0.0002$ $\nu = 0.6303 \pm 0.0008$				

	Nickel–Dixon (1981) $\gamma = 1.237 \pm 0.003$ $\nu = 0.630 \pm 0.003$ $(v_c = 0.156\,086)$				
	Chen *et al* (1982) $\gamma = 1.2385 \pm 0.0015$ $\Delta_1 = 0.54 \pm 0.05$				
	Adler *et al* (1982b) $\gamma = 1.238 \pm 0.003$ $\nu = 0.629 \pm 0.002$ $\Delta_1 = 0.49 \pm 0.08$ $0.156\,086 \leqslant v_c \leqslant 0.156\,090$				
This work[4]		$0.218\,09 \leqslant v_c \leqslant 0.218\,10$ $\gamma = 1.239 \pm 0.003$ $\Delta_1 = 0.51 \pm 0.08$ $\nu = 0.631 \pm 0.004$	$0.101\,719 \leqslant v_c \leqslant 0.101\,722$ $\gamma = 1.239 \pm 0.003$ $\Delta_1 = 0.48 \pm 0.08$	$0.353\,74 \leqslant v_c \leqslant 0.353\,79$	$0.232\,90 \leqslant v_c \leqslant 0.232\,99$

(1) Quantities in brackets are input values.
(2) Details of these analyses are given in § 2.
(3) This value (D S Gaunt, private communication) can be read off the graph.
(4) Error bounds on v_c values are $\pm 0.000\,03$ at the extrema of the ranges or values given here.

Again there is a decrease in Δ_1 and γ as v_c decreases, small changes in K_c are irrelevant and the best convergence is found for $K_c = 0.10207$ ($v_c \sim 0.101\,72$), outside the old range.

A ratio analysis similar to the above has been carried out for the SC lattice by Gaunt (1982). Assuming $\gamma = 1.241$ and $\Delta_1 = 0.496$ he found $K_c = 0.221\,66 \pm 0.000\,01$, although no clear preference for these values over the old ones was expressed. The difference between the BCC and FCC studies noted above and this latter work is that in the former works clear indications of better convergence near the RG estimates were found. A summary of the results presented in this section can be found in table 2. In § 3, we aim to obtain equally clear indications for the SC diamond and tetrahedron lattices.

3. New results

We present below new results for the FCC, SC, diamond and tetrahedron lattices obtained using the methods of Adler *et al* (1982a, b). The FCC lattice is close packed (coordination number 12) and is generally considered to be the best lattice for series analyses. In the case of the $d = 3$, $s = \frac{1}{2}$ Ising model however, the series (15 terms) is much shorter than that for the BCC lattice so that the BCC has been more thoroughly investigated. The SC, diamond and tetrahedron lattices are all loose packed (with coordination numbers of 6, 4 and 6 respectively) and are thus well suited for Monte Carlo calculations. The susceptibility series (from Gaunt and Sykes 1979, 1973, Ho-Ting-Hun and Oitmaa 1975) are 19, 22 and 16 terms long respectively, and although the diamond lattice series is not particularly well behaved, the others are quite suitable for Padé analysis. We note that of all the methods successfully applied to the $s = \frac{1}{2}$, BCC lattice only Roskies' (1981b) and our generalisation of it, can be applied to these four lattices, since no long pair-correlation and no extensive series interpolating to the Gaussian model are available in the literature to the best of the author's knowledge. We mention that the method utilised by Bessis *et al* (1980) and Moussa (1982) which is a modification of the Baker–Hunter transform is applicable; however, since no stability for the subdominant indices was found for the $s = \frac{1}{2}$, BCC lattice we do not consider this technique further here.

We caution that in view of the evidence accrued from other methods of analysis the reliability of the Baker–Hunter transform for spin-$\frac{1}{2}$ Ising susceptibility series appears questionable; perhaps this method needs to be applied to a wider range of v_c values to obtain results that are consistent with those of other methods.

From the preceding discussion we can expect that if the confluent singularity hypothesis is invoked the γ value will move downwards, and the v_c value may well change. We follow the procedure of Adler *et al* (1982a, b) and transform the χ series to one in $y = 1 - (v/v_c - 1)^{\Delta}$ and analyse

$$G\Delta(y) = \Delta(y-1)(\mathrm{d}/\mathrm{d}y)(\ln\chi(y)) \doteqdot -\gamma_{\mathrm{output}}(\Delta)$$

for various input Δ and v_c values. For each Δ and v_c choice several highest- and nearest-diagonal Padé approximants to $-\gamma_{\mathrm{output}}(\Delta)$ are obtained and we plot surfaces in the three-dimensional (Δ, γ, v_c) space by looking at (Δ, γ) planes for certain choices of v_c (see figure 1). Since an analytic b_1 term is always present, the plane $\Delta = 1$ corresponds to $a_1 = 0$ or no confluent singularity with $\Delta_1 < 1$ and the γ value for this plane at $v_c(0)$ corresponds to the result of ordinary Padé analysis (Adler *et al* 1982a,

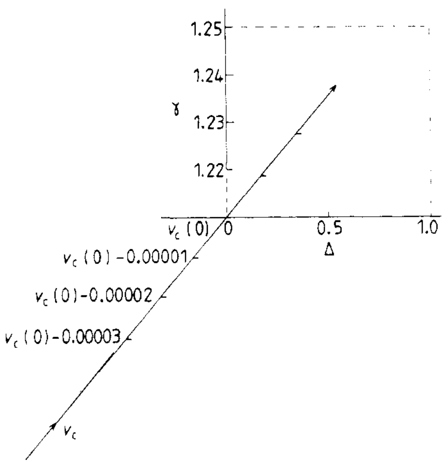


Figure 1. The (Δ, γ, v_c) space in which we search for a point of optimal convergence of surfaces traversed by different biased Padé approximants to the function $\Delta(y-1)(d/dy)\times[\ln \chi(y)]$, where $y=1-(v/v_c-1)^{\Delta}$.

1983) at $v_c(0)$. However, the presence of a confluent singularity with $a_1 \neq 0$ and $\Delta_1 < 1$ introduces systematic errors into this γ evaluation since $G_\Delta(y)+\gamma_{\text{output}}(\Delta)$ is non-analytic; these errors are similar for different lattices. When one invokes the confluent singularity hypothesis and expects a singularity with $a_1 \neq 0$ and some $\Delta_1 < 1$, one may search in the region near this Δ_1, and since $G_\Delta(y)+\gamma_{\text{output}}$ will now be a linear function proportional to $|\Delta-\Delta_1|$ near this Δ_1, there will now be a point (Δ_1, γ) where all these surfaces intersect. Higher-order confluent terms will smear this point into a 'convergence region'. For the BCC lattice this region coincides with estimates of Δ_1 and γ from other series studies as well as with renormalisation group estimates (Baker *et al* 1976, 1978, Le Guillou and Zinn-Justin 1980) and experiment (Sengers 1982). It is of interest to see whether a similar picture emerges for other lattices.

Since our method of searching involves examining successive (Δ, γ) planes, the convergence region within the plane leads quite naturally to error bounds for Δ_1 and γ estimates. The question of error bounds on v_c is more complex, and we quote below ranges of v_c values for which stable convergence is obtained. An extra $\pm 0.000\,03$ at either extremum should be understood as a possible inherent systematic error on the method.

We consider firstly the SC lattice. In figure 2(*a*) we present the (Δ, γ) plane at $v_c(0)$, and in figure 2(*b*) we present this plane for $v_c = 0.218\,100$, just at the bottom limit of the old v_c range. We feel that this v_c value is at the upper end of acceptable choices and in figure 2(*c*) we illustrate the same plane for $v_c = 0.218\,097$. Below $v_c \sim 0.21809$ the structure disappears. Boxes corresponding to our (Adler *et al* 1982b) BCC estimates and those of Chen *et al* (1982) are superimposed on the figures, the results being in close agreement in 2(*b*) and 2(*c*). We retain the BCC γ and Δ_1 estimates (although perhaps γ is a little higher here) and propose $0.218\,09 \leqslant v_c \leqslant 0.218\,10$ for the SC lattice. This corresponds to $0.221\,65 \ll K_c \ll 0.221\,66$. This compares favourably with one of the values ($K_c = 0.221\,66 \pm 0.000\,01$) obtained by Gaunt (1982). In our case however, clear evidence of convergence to a value *below* the old range is apparent.

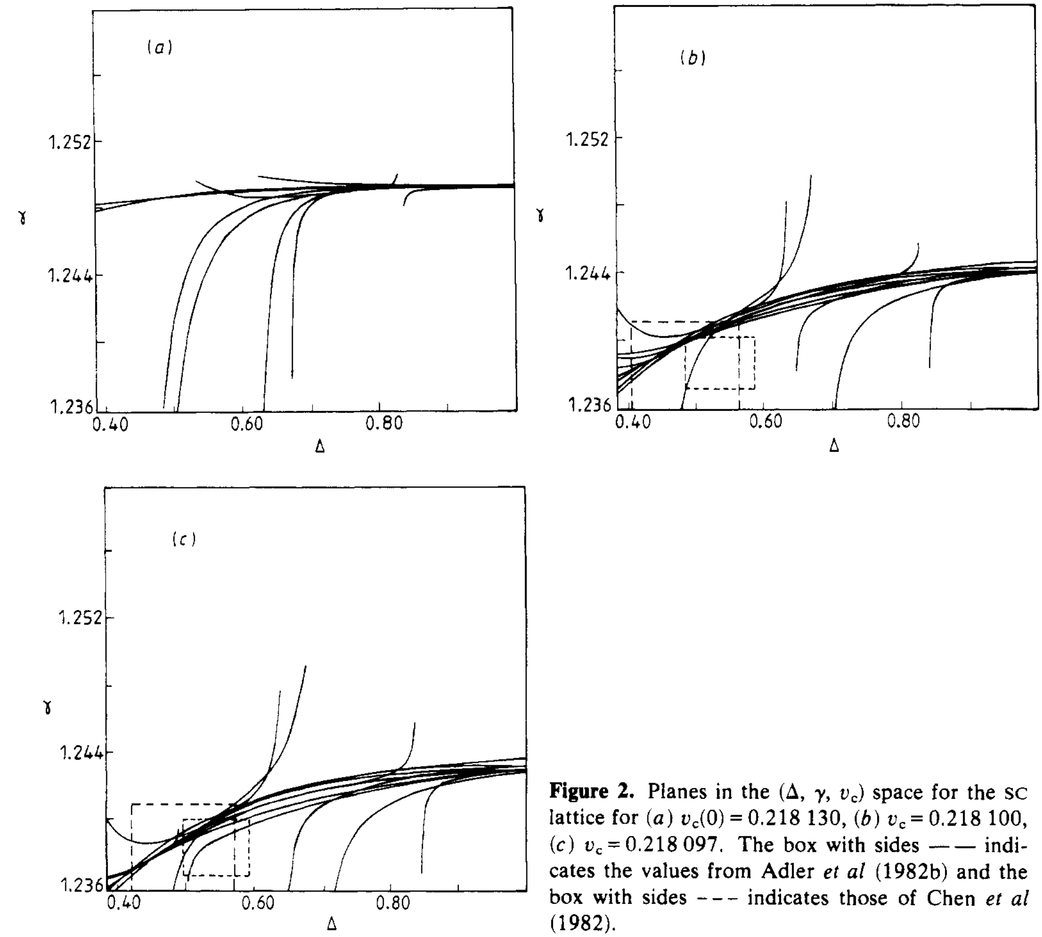
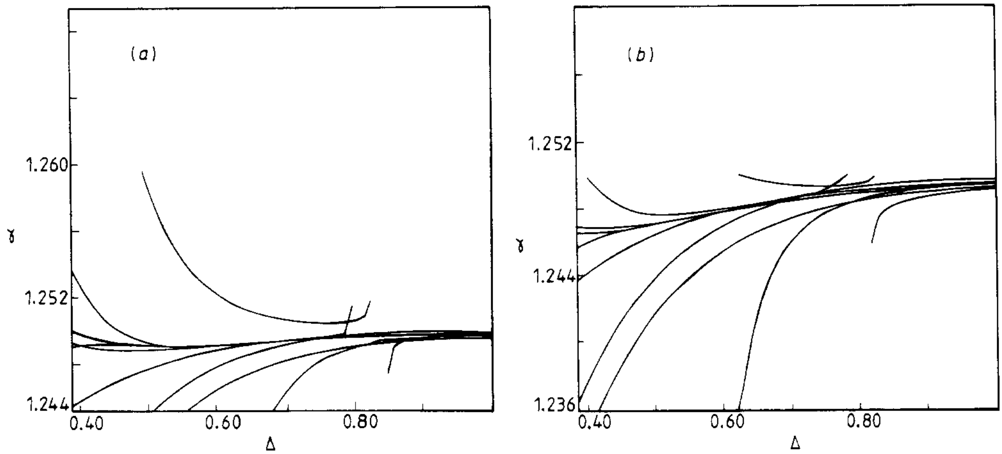


Figure 2. Planes in the (Δ, γ, v_c) space for the SC lattice for (*a*) $v_c(0) = 0.218\,130$, (*b*) $v_c = 0.218\,100$, (*c*) $v_c = 0.218\,097$. The box with sides —— indicates the values from Adler *et al* (1982b) and the box with sides - - - indicates those of Chen *et al* (1982).

The situation with the tetrahedron lattice is somewhat different. This is a rather interesting lattice since although it has a low coordination number, the series seem to be very regular (Oitmaa and Ho-Ting-Hun 1979). The lattice is made up of either the magnetic (B) ions in the spinel AB_2X_4 structure or the B sublattice of crystobalite AB_2. The susceptibility series was obtained (Ho-Ting-Hun and Oitmaa 1975) via a generalisation of Gibberd's (1970) transformation of a diamond lattice free energy series to the tetrahedron lattice. In figure 3(*a*) we present the (Δ, γ) plane at $v_c(0)$ and note the strong similarity to 2(*a*). In 3(*b*) this plane is shown for $v_c = 0.232\,99$, the bottom of the old limit; we observe that there is no approach to the boxed area. In 3(*c*) ($v_c = 0.232\,94$), there is overlap with the boxes, similar behaviour being observed for $v_c = 0.232\,94 \pm 0.000\,01$. By $v_c = 0.232\,93$ there is no longer any overlap with the boxed region although some structure persists with an apparent $\Delta_1 \sim 0.7$. This lattice seems to present a higher Δ_1 estimate than the Adler *et al* (1982) BCC calculation and we conclude $0.232\,90 \leqslant v_c \leqslant 0.232\,99$. It is not possible to place too much emphasis on the Δ_1 estimate since the series is relatively short.

We now consider the diamond lattice. The lattice is known to be problematic for many methods of analysis, and in applications of this method to percolation (Adler



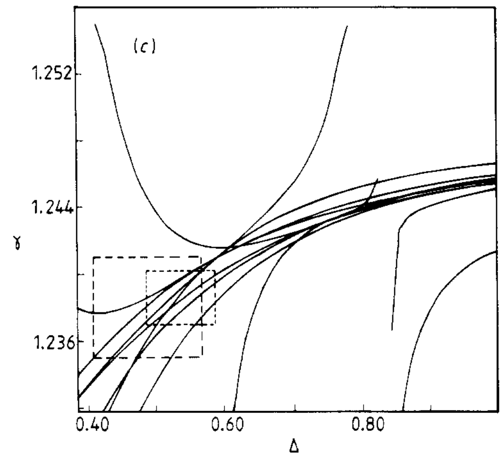


Figure 3. Planes in the (Δ, γ, v_c) space for the tetrahedron lattice for (a) $v_c(0) = 0.233\,00$, (b) $v_c = 0.232\,99$, (c) $v_c = 0.232\,94$. The box with sides — — indicates the values from Adler *et al* (1982b) and the box with sides - - - indicates those of Chen *et al* (1982).

et al 1982a, 1983) the analogous two-dimensional lattice (honeycomb) was problematic. Here again intersection regions are minimal; however, we can study v_c. Again (figure 4(a)) the $v_c(0)$ plane exhibits the now familiar flat behaviour of γ as a function of Δ_1 and the erroneous $\gamma \sim 1.25$. For $v_c \sim 0.353\,76$ there is movement into the boxed region (4(b)); below $v_c \sim 0.353\,74$ this disappears. We estimate $0.353\,74 \leqslant v_c \leqslant 0.353\,79$.

Finally we come to the FCC lattice. Here at a first glance the $v_c(0)$ plane (figure 5(b)) appears similar to the BCC and SC cases. However, unlike the three lattices studied above, the value of γ for $\Delta > 0.7$ is well below 1.25. In fact in the original analysis of the 15-term series (McKenzie 1975) a value of $\gamma = 1.246$ was quoted although this was claimed to converge to the then expected value of $\gamma = 1.25$. For $v_c = 0.101\,72$ (figure 5(c)) the results are very similar to the BCC results at $v_c = 0.156\,09$; the intersection regions exactly overlap. The structure disappears before $v_c = 0.101\,71$ and thus the lower half of the $v_c(0)$ estimate seems to be quite accurate.

As noted above McKenzie (1979) suggests that for the FCC lattice the exponent $\gamma \sim 1.241$, $\Delta_1 \sim 0.496$ imply a v_c of $\sim 0.101\,72$, in general agreement with the above.

We can conclude that for both the SC and FCC lattices the ratio studies indicate values of v_c near the bottom of the old Padé ranges (using $\gamma \sim 1.241$ as input), whereas

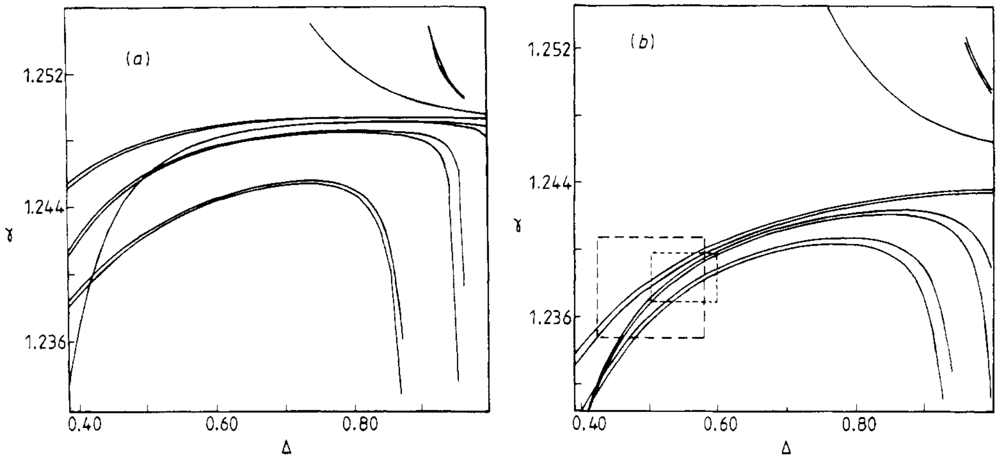
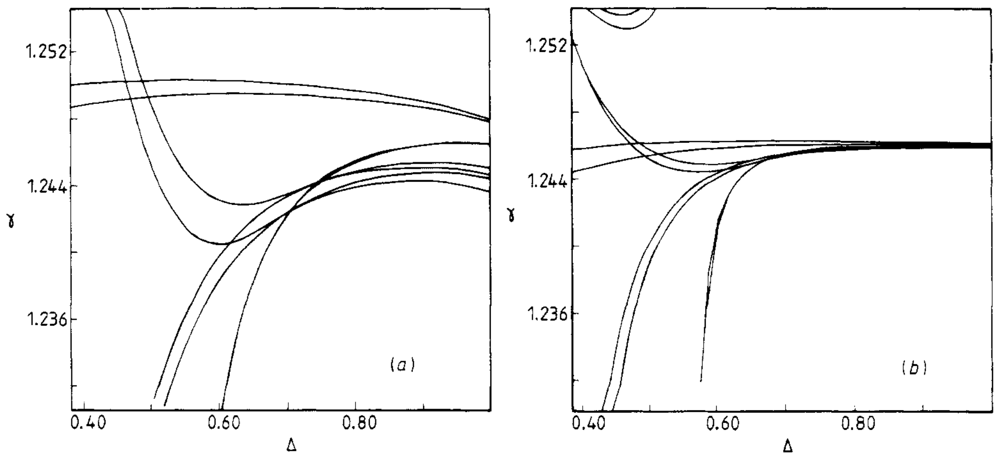


Figure 4. Planes in the (Δ, γ, v_c) space for the diamond lattice for (*a*) $v_c(0) = 0.353\,80$, (*b*) $v_c = 0.353\,76$. The box with sides — — indicates the values from Adler *et al* (1982b) and the box with sides - - - indicates those of Chen *et al* (1982).



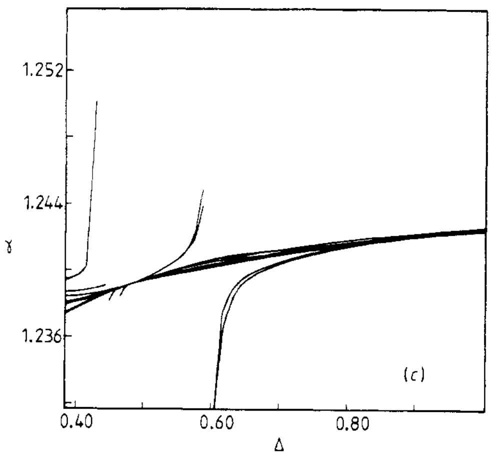
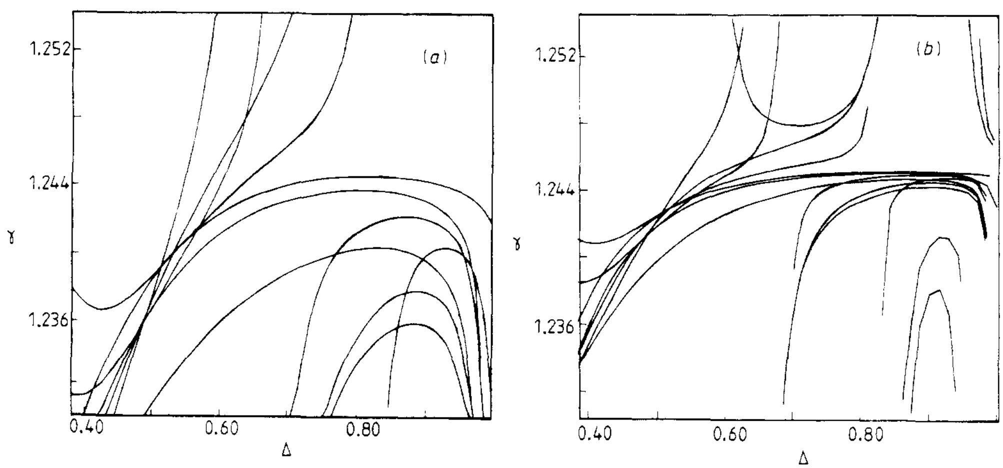


Figure 5. Planes in the (Δ, γ, v_c) space for the FCC lattice for (*a*) $v_c = 0.101\,75$, (*b*) $v_c(0) = 0.101\,73$, (*c*) $v_c = 0.101\,72$.

we find values centring below the old range and $\gamma \sim 1.238$ in agreement with Chen *et al* (1972).

We have also considered the region above the old estimates. Near the top of the $v_c(0)(\sim 0.101\,75)$ estimate we observe some very interesting (figure 5(*a*)) effects, notably a very loose intersection region near $\gamma \sim 1.243$ and $\Delta \sim 0.65$. Thus if one were to consider at which points in the (Δ, γ, v_c) space consistent estimates of $\gamma \sim 1.243$ and $0.4 < \Delta < 0.7$ appeared one could not *a priori* exclude this v_c value. However, the looseness of the intersection region indicates that such a choice is unlikely.

To investigate further this second 'convergence' at v_c values greater than $v_c(0)$ we have carried out some further studies on the BCC lattice. In the region near the top of the $v_c(0)$ estimate $v_c \sim 0.156\,12$ (figure 6(*a*)) we see this loose convergence and in figure 6(*b*) we show behaviour that is intermediate between this and the behaviour of the type shown in figures 2(*a*), 3(*a*) and 5(*b*). While we think (and this is the case in $d=2$ percolation (Adler *et al* 1982a) where p_c is known exactly)) that the true convergence is exhibited below $v_c(0)$, we cannot exclude this region near the top of the $v_c(0)$ error range on either the FCC or BCC lattices. We can, however, exclude values way above the $v_c(0)+0.000\,03$ estimates for both lattices.



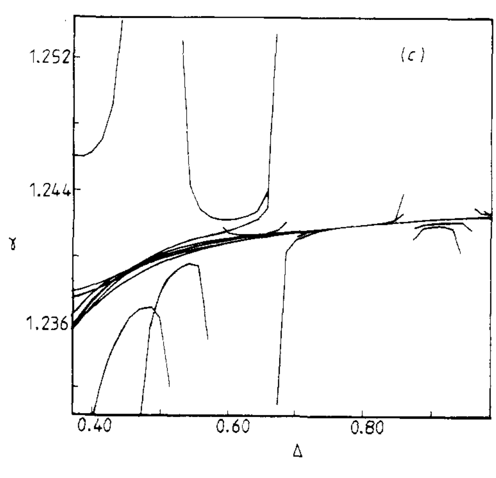


Figure 6. Planes in the (Δ, γ, v_c) space for the BCC lattice for (*a*) $v_c = 0.156\,12$, (*b*) $v_c = 0.156\,10$, (*c*) $v_c = 0.156\,09$.

There is some independent evidence for our conclusions from Monte Carlo renormalisation group (MCRG) work (Friedman and Felsteiner 1977) on the SC lattice. This calculation is a real space RG method and can be expected to give good K_c values. By looking at K_c as a function of increasing cell size (where the cell side is of length L), convergence to the exact limit for the $d = 2$, $s = \frac{1}{2}$ Ising model on the square lattice was observed. However, the value of K_c that corresponds to $v_c(0)$ is obtained for the SC lattice already at cell size $9\times9\times9$ and thus extrapolation to $L = \infty$ should give $K_c < 0.2217$, since in both cases K_c decreases as L increases. This is in agreement with our conclusion and was in fact a partial motivation for the investigation discussed herein. There is another MCRG study (Blöte and Swendsen 1980) that confirms the series estimate to within 1%. This is consistent with the above.

It does of course seem desirable to study the dependence of v_c and a_1 on each other via series methods for quantities other than the susceptibility χ. This has been done for the M_2/χ series on the BCC lattice (Adler *et al* 1982b, Nickel and Dixon 1981) and similar behaviour is found. We note that a second (15-term) M_2/χ series is available for the SC lattice. This series (Roskies 1981a) gives similar values to the BCC ones of Adler *et al* (1982b) and Nickel and Dixon (1981), *videlicet* $0.628 < \nu < 0.633$ and $0.38 < \Delta_1 < 0.56$, and convergence is most clearly apparent near $v_c \sim 0.218\,097$ in agreement with the susceptibility results above. Near $v_c(0)$, $\nu \sim 0.64$ which is in agreement with the old series estimates. We illustrate the $(2\nu, \Delta)$ plane at $v_c = 0.218\,097$ in figure 7. These results for the M_2/χ series are an improvement on those of Roskies (1981a) who found $\nu = 0.6423 \pm 0.0008$ as compared with the RG value $\nu \sim 0.630$ and confirm the dependence of the observation or otherwise of a confluent term with amplitude not equal to zero on the critical temperature.

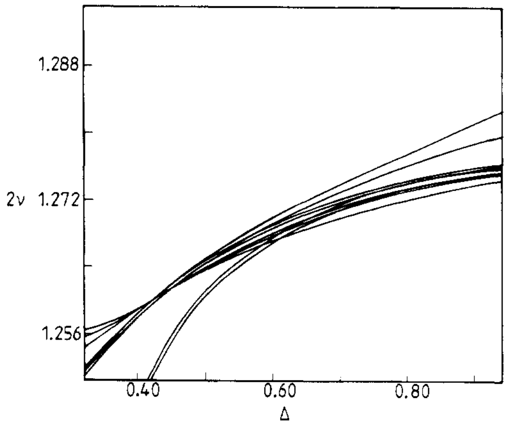


Figure 7. A plane in the $(\Delta, 2\nu, v_c)$ space for $v_c = 0.218\,097$ (SC lattice).

At this point of time all the indications seem to point to a downward revision of $v_c(0)$ estimates for the BCC, FCC, SC, diamond and tetrahedron lattices. These new estimates are presented in table 2. It is clear that the old $v_c(0)$ values no longer constitute an unquestionable standard for comparison with the results of other methods. It is also clear that very small changes in $v_c(0)$ lead to very rapid changes in γ estimates and thus the question is a delicate one. Two possibilities present themselves for validating the downward temperature revisions, one being a large MC study that does not assume an old $v_c(0)$ value and the other an extension of the Bessis *et al* (1980) calculation, using the Baker–Hunter method, to v_c values outside the old range. Preliminary results from the Santa Barbara Monte Carlo processor (Toussaint and Pearson 1983) indicate $v_c = 0.218\ 11 \pm 0.000\ 02$ in pleasing agreement with this work.

4. Comments on some recent Monte Carlo studies

We now consider the implications of the results of § 3. In most cases the v_c estimates barely overlap the old $v_c(0)$ values. The old values correspond to an absence of a confluent correction term with $\Delta_1 < 1$ and thus their use in MC studies means that one may well be excluding, *a priori*, any possibility of observing confluent singularities. We note that it is quite feasible to observe corrections to scaling via MC (Chakraborti *et al* 1981, Havlin and Ben Avraham 1982).

The first study that we wish to comment on is the heat capacity analysis of Knak Jensen and Mouritsen (1982). Actually, they consider the energy which we may write as

$$E \sim E_c + E_a(t-t_c) + E^+(t-t_c)^{1-\alpha}(1 + a_1^+(t-t_c)^{\Delta_1} + b_1^+(t-t_c) + a_2^+(t-t_c)^{2\Delta_1} + c_1^+(t-t_c)^{\Delta_2} + \ldots) \qquad \text{for } t > t_c$$

and similarly $(t \to t_c,\ t_c \to +,\ a^+ \to a^-)$ for $t < t_c$. They set b_1 and $c_1 = 0$ but make full acknowledgement of the existent of a confluent singularity, allowing either (i) a_1 or (ii) a_2 to be non-zero. In the former case, they do not find agreement with ε-expansion dominant singularity ratios for their choice of t_c. For the latter case $(a_1 = 0)$ they claim agreement at their t_c; however, the exponent of the a_2 term $(2\Delta_1)$ is equal to 0.986 and thus could easily be confused with the analytic (b_1) term in a MC study. They ignore the possibility of a second confluent term with $\Delta_2 \sim 0.9$ (Rehr 1979 and references therein) which is distinct from $2\Delta_1$; we have looked for this term in the BCC series and find some evidence for a term with $\Delta_2 \sim 0.78$. The justification given for setting $a_1 = 0$ is the results of Camp *et al* (1976); however, as discussed in the introduction, this study is now outdated. At first sight agreement between their $a_1 = 0$ results and the expansion amplitude ratios seems surprising. However, in view of the fact that incorrect effective critical exponents obey scaling relations (Aharony and Ahlers 1980) and that amplitude variations may be small, such agreement may well occur.

We suggest that the reason for their contradictory results is their choice of t_c. They consider the estimates of Sykes *et al* (1972) for the SC and Gaunt and Sykes (1973) for the diamond, which we have quoted in § 3 above. We have shown the (γ, Δ) plane at the centre of these estimates in figures 2(*a*) and 4(*a*) respectively and noted that at $v_c(0)$ corresponding to their t_c, it does indeed seem that $a_1 = 0$ and $b_1 \neq 0$; the distinction between an analytic (b_1) term and a confluent (a_2) term with exponent $2\Delta_1 \sim 0.986$ is very fine, and at any rate we study susceptibility series and they look at energy series and thus relative amplitudes may vary. However, it does seem quite possible that they are merely observing an analytic term and that their results do not correspond to any non-analytic correction term. Thus their results are quite consistent with ours at $v_c(0)$ (It is of course also possible that at $v_c(0)$ the second confluent singularity at $2\Delta_1$ dominates the singularity at Δ_1 and we have seen this rather than the analytic term but this seems unlikely.) We propose that their results reduce to $a_1 = 0$ and $b_1 \neq 0$ at $v_c(0)$, and the reason they do not find consistent results for $a_1 \neq 0$ is because they are considering an incorrect t_c for the model. Further, by choosing the old t_c estimates with their spurious apparent accuracy Knak Jensen and Mouritsen exclude *a priori* any possibility of observing the correct confluent structure.

An interesting question is what effect a change in t_c would have on their results. They state that the uncertainty of t_c is not important in the interval covered by the data; however, they do not seem to consider what happens beyond the old v_c estimates. We think that v_c is outside the old limits for both the SC and diamond lattices, and thus it would be of interest to see what results they would find if they considered t_c values in the ranges suggested by our § 3. In this range $a_1 \neq 0$ from our study, and it would be interesting to see if this would be confirmed by MC results.

The second MC study that we shall consider is the renormalised coupling constant study of Freedman and Baker (1982). These authors claim that a small violation of hyperscaling is observed, and in their MC analysis they mention the old high-temperature series critical temperature on the SC lattice, but do not indicate what effect a change in v_c would have on their conclusions. They compare their MC results with series estimates (Baker and Kincaid 1981) that are made under the assumption that no confluence is present near the Ising limit of the continuous spin mode. (This assumption was verified by application of the Baker–Hunter transformation, which as above is apparently problematical for the BCC spin-$\frac{1}{2}$ Ising model; for this lattice there is independent evidence of a confluent structure and thus it is not at all certain that negative results from application of the Baker–Hunter transformation are confirmation of the absence of confluent terms.) It is not surprising that when Baker and Kincaid (1981) ignore confluent effects they find that their series results violate hyperscaling. The strong similarity between the series and MC results suggests that acknowledgment of the confluent corrections may well be missing in the MC study as well.

5. Conclusions

We have demonstrated in §§ 2 and 3 that the observation or otherwise of non-analytic confluent singularities in the $d = 3$, $s = \frac{1}{2}$ Ising model appears to be a function of the critical temperature chosen. We have shown that there is strong evidence that the v_c at which $a_1 \neq 0$ is below the v_c for which $a_1 = 0$ for the BCC, FCC, SC, diamond and tetrahedron lattices and that choosing to use $v_c(0)$ in a MC study is tantamount to setting $a_1 = 0$. We suggest that this idea be pursued further by showing the effect of the change of v_c on the results of MC calculations; certainly the high accuracy of the old v_c estimates now appears spurious!

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Note added in proof. Recent MCRG results from the ICL Distributed Array Processor at Edinburgh (G S Pawley, R H Swendsen, D J Wallace and K G Wilson, to be published) give a K_c value for the SC lattice of $0.221\,656 \pm 0.000\,005$, in excellent agreement with § 2 of this work.

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