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Critical behaviour of the Ising model along the coexistence curve and the critical isotherm

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Abstract. The basic low temperature series expansion data for the spin one-half Ising model on the hydrogen peroxide lattice are used to obtain series in $z = \exp(-2J/k_B T)$ along the coexistence curve for the specific heat C_H, the magnetization M, and its first five derivatives $\partial^l M/\partial\mu^l$, where $\mu = \exp(-2mH/k_B T)$. The same data are used to derive series in μ along the critical isotherm for M and its first five derivatives $\partial^l M/\partial z^l$. Ratio and Padé approximant analysis yield estimates of the critical exponents and critical amplitudes. On the whole the estimates of the critical exponents support scaling theory although a few of the exponent estimates are not in good agreement with scaling.

1. Introduction

The spin $\frac{1}{2}$ Ising model is of great theoretical interest as one of the simplest models exhibiting a phase transition. Experimentally the Ising model represents reasonably well several real magnetic insulators (de Jongh and Miedema 1974), binary alloys (Als-Nielsen 1969) and classical fluids (Fisher 1967) in the critical region. For further information the reader may consult recent reviews (Domb 1960, Fisher 1967, Stephenson 1971, Domb 1974) and the book by Stanley (1971).

In three dimensions no critical exponents are known exactly. The high temperature exponents γ (Sykes *et al* 1972a) and α (Sykes *et al* 1972b) are now known to high precision, but the corresponding low temperature exponents γ' and α' have until recently not been very precisely estimated. Except for δ (Gaunt and Sykes 1972) estimates of critical exponents along the critical isotherm have also suffered from lack of precision. Until recently the most extensive low temperature series expansion data have been those of Sykes *et al* (1965). These data have therefore provided the basis for studies of critical behaviour on the coexistence curve ($H = 0$, $T < T_C$) and the critical isotherm ($T = T_C$) (Essam and Hunter 1968, Guttmann *et al* 1970, Gaunt and Domb 1968, Gaunt 1967, Domb and Guttmann 1970, Gaunt and Domb 1970). As a result of these studies it had become clear that more low temperature series expansion data were required.

Sykes *et al* (1973b) in the high field expansion of the dimensionless free energy,

$$\frac{-F}{k_B T} \equiv \ln \Lambda = \sum_s L_s(z)\mu^s, \tag{1.1}$$

where $z = \exp(-2J/k_B T)$ and $\mu = \exp(-2mH/k_B T)$, have added L_{10} and L_{11} to the BCC lattice expansion, L_{12} and L_{13} to the SC lattice expansion and, most notably, L_{14},

L_{15}, L_{16} and L_{17} to the diamond lattice expansion. Simultaneously, Sykes *et al* (1973a) in the high exchange energy expansion ('temperature grouping')

$$\ln \Lambda = \sum_s \psi_s(\mu) z^s \tag{1.2}$$

have extended the data to include ψ_{28} for the BCC lattice, ψ_{20} for the SC lattice and ψ_{15} for the diamond lattice. Meanwhile Betts *et al* (1974) have found all L_s for $s < 24$ for the hydrogen peroxide lattice.

Analysis of the new data for the other lattices along the coexistence curve and the critical isotherm has been performed by Gaunt and Sykes (1972, 1973). The present paper is concerned with analysis of the low temperature expansion data for the hydrogen peroxide lattice. In § 2 we report the analysis by both ratio and Padé approximant methods of the series for the specific heat C_H, and the magnetization $\mathscr{M}$, and its first five field derivatives $\partial^l \mathscr{M}/\partial\mu^l$ all on the coexistence curve, $H = 0$ or $\mu = 1$ and $T < T_C$. The most singular parts of these thermodynamic functions are supposed to diverge as

$$\frac{C_H}{Nk_B} \sim A'\left(1 - \frac{T}{T_C}\right)^{-\alpha'} \tag{1.3}$$

and, letting $M = \mathscr{M}/Nm$,

$$\left.\frac{\partial^l M}{\partial\mu^l}\right|_{\mu=1} \sim C'_l\left(1 - \frac{T}{T_C}\right)^{-\gamma'_l}. \tag{1.4}$$

Estimates of the critical exponents α', γ'_l and the critical amplitudes, A', C'_l are sought. Note that $\gamma'_0 = -\beta$ and $\gamma'_1 = \gamma'$ in the usual notation.

In § 3 we report the analysis, again by ratio and Padé approximant techniques, of the series for the magnetization and its first five exchange energy derivatives, $\partial^l M/\partial z^l$, all evaluated at the critical temperature. Now the most singular parts of $\partial^l M/\partial z^l$ are supposed to diverge as

$$\left.\frac{\partial^l M}{\partial z^l}\right|_{z=z_C} \sim E_l\left(\frac{mH}{k_B T_C}\right)^{-\epsilon_l}. \tag{1.5}$$

Note that $\epsilon_0 = -1/\delta$ and $E_0 = D^{-1/\delta}$ in the usual notation.

In § 4 the best estimates of γ'_l and ϵ_l are used to test exponent equalities of scaling theory. The critical amplitudes could also be used to test the lattice–lattice scaling theory relations among amplitude ratios (Betts *et al* 1971) when values for the same amplitudes become available for other lattices.

The coefficients of all series used in this investigation are listed in the appendix. These coefficients have been derived from the fundamental data obtained by Betts *et al* (1974).

2. Analysis of series along the coexistence curve

Series for the spin one-half Ising model in $z = \exp(-2J/k_B T)$ and $\mu = \exp(-2mH/k_B T)$ for the specific heat at constant field $C_H(z, \mu)$ and the magnetization $\mathscr{M}(z, \mu)$ and its field derivatives $\partial^l \mathscr{M}/\partial\mu^l$ can be derived readily from the basic data for the expansion of the free energy, $F = -kT\ln\Lambda(z,\mu)$. In the case of the hydrogen peroxide lattice the high field expansion

$$\ln\Lambda = \sum_s L_s(z)\mu^s \tag{2.1}$$

has been found recently (Betts *et al* 1974) for all $s \leqslant 23$. The coefficients in the expansions along the coexistence curve ($\mu = 1$, $z < z_C$) in

$$\frac{C_H}{Nk_B(\ln z)^2} = \sum_n a_n z^n \tag{2.2}$$

and for the reduced magnetization per site, $M = \mathscr{M}/Nm$, and derivatives in

$$\frac{\partial^l M}{\partial\mu^l} = \sum_n c_n^{(l)} z^n \tag{2.3}$$

are tabulated in the appendix. It can be shown that the $L_s(z)$ for $s > 23$ contain no powers of z lower than z^{18} so that the coefficients quoted are exact.

To proceed with the analysis of the Ising model series in the low temperature (or high energy) variable z it is very helpful to have an estimate of the critical point, z_C. Leu *et al* (1969), from analysis of the high temperature expansion of the susceptibility, have estimated v_C from which one obtains $z_C = 0{\cdot}317401 \pm 0{\cdot}000010$ for the hydrogen peroxide lattice.

A standard ratio plot is given in figure 1 for the derivative of the specific heat, $(d/dz)[C_H/Nk_B(\ln z)^2]$, the derivative of the magnetization, dM/dz, and the susceptibility ($\propto \partial M/\partial\mu|_{\mu=1}$) all along the coexistence curve. Also included are lines whose

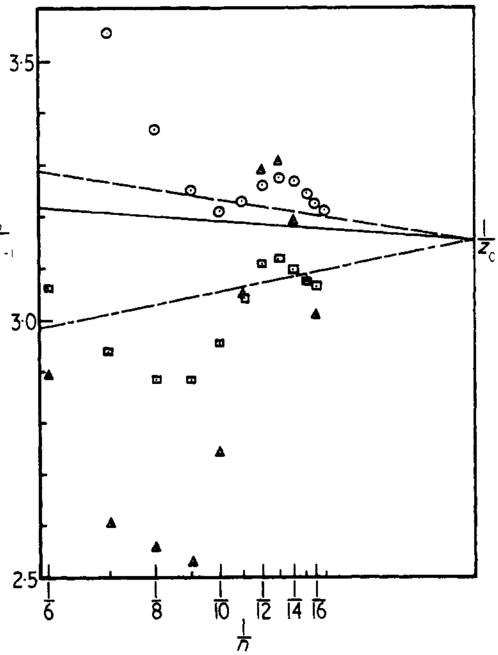

Figure 1. Ratio of coefficients a_n/a_{n-1} against $1/n$ for the following series for $H = 0$: $(d/dz)[C_H/Nk_B(\ln z)^2]$ ($\triangle$); $\chi(z)$ ($\bigcirc$) and dM/dz ($\square$). Corresponding asymptotes according to scaling theory exponent values for: (i) $\alpha'+1 = \frac{9}{8}$ (full line); (ii) $\gamma' = \frac{5}{4}$ (broken line); (iii) $1-\beta = \frac{11}{16}$ (chain line).

slope is chosen to be that given by scaling theory for the three functions. According to scaling theory the above three functions should have critical exponents $-\alpha'-1 = -\frac{9}{8}$, $\beta-1 = -\frac{11}{16}$ and $-\gamma' = -\frac{5}{4}$ respectively. It is clear that the ratios have not nearly settled down to their asymptotic behaviour. From figure 1 we obtain the almost useless estimates,

$$\alpha' = 0{\cdot}0 \pm 0{\cdot}4, \qquad \beta = 0{\cdot}3 \pm 0{\cdot}2 \qquad \text{and} \qquad \gamma' = 1{\cdot}3 \pm 0{\cdot}2.$$

To discover the specific heat exponent α', a number of series analysis techniques have been tried, none of which has been successful enough to improve noticeably the above estimate of α'. This is consistent with the findings of Gaunt and Sykes (1973) for the low temperature specific heat series on the diamond lattice. The analysis of $\partial^l M/\partial\mu^l|_{\mu=1}$ series have, however, been more successful.

One technique of analysis is to calculate poles and residues of Padé approximants to $(\mathrm{d}/\mathrm{d}z)\ln(\partial^l M/\partial\mu^l|_{\mu=1})$. The poles give estimates of z_C and the residues estimates of γ_l'. A plot of γ_l' against z_C, with a point for each Padé approximant, usually yields a smooth curve. The best estimate of γ_l' is the ordinate on the curve corresponding to the abscissa equal to the 'true' critical point, $z_C = 0{\cdot}317401$. Such a plot for the susceptibility, $\mu\partial M/\partial\mu$, is given in figure 2. From figure 2 we estimate that $\gamma' = 1{\cdot}30 \pm 0{\cdot}03$. We have repeated the calculation and made the appropriate plot for $l = 0, 1, 2, \ldots, 5$ (Chan 1974). As a result we arrive at the estimates of γ_l' given in table 1. The quoted errors in the estimates are no more than confidence limits based on inspection of the curves; our criteria can be judged from figure 2.

A more elaborate technique also used is to find poles of Padé approximants to $(\partial^l M/\partial\mu^l|_{\mu=1})^{1/\gamma_l'}$ for a set of values of γ_l'. Now each Padé approximant, $[N, D]$, yields a separate curve on a plot of z_C, the pole of the Padé approximant, against γ_l'. Again that value of γ_l' which best reproduces the known value of z_C is regarded as the best estimate of the true value.

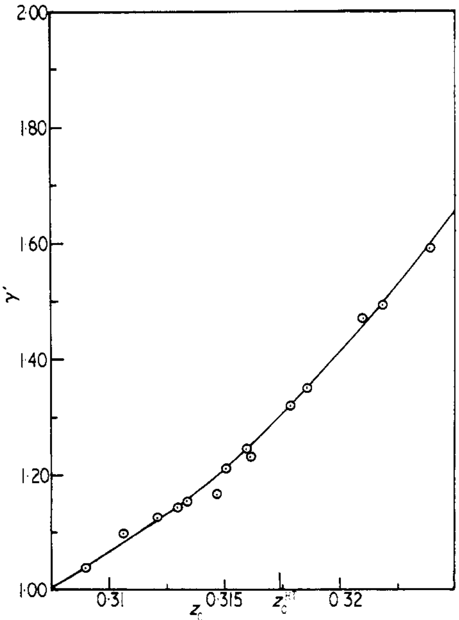

Figure 2. Estimates of z_C and γ' from poles and residues of Padé approximants to $(\mathrm{d}/\mathrm{d}z)\lg\chi(z)$.

Table 1. Estimates of critical exponents γ_l' from plots of residues against poles of Padé approximants to $(\mathrm{d}/\mathrm{d}z)\lg(\partial^l M/\partial\mu^l|_{\mu=1})$.

l	0	1	2	3	4	5
γ_l'	$-0{\cdot}309\pm0{\cdot}002$	$1{\cdot}30\pm0{\cdot}03$	$2{\cdot}82\pm0{\cdot}20$	$4{\cdot}37\pm0{\cdot}10$	$6{\cdot}0\pm0{\cdot}5$	too scattered

In practice most $[N, D]$ give nearly identical curves. Therefore, the graphical resolution is increased by plotting against γ_l' not the individual estimates $z_C([N, D])$ themselves but rather their differences, $\Delta z = z_C([N, D]) - z_0$, from a best straight line, $z_0 = a/\gamma_l' + b$ (Betts and Filipow 1972). Such a plot, again for $l = 1$, the susceptibility series, is illustrated in figure 3. From figure 3 we estimate $\gamma_l' \equiv \gamma' = 1{\cdot}295\pm0{\cdot}005$.

All series $\partial^l M/\partial\mu^l|_{\mu=1}$ for $l = 0, 1, \ldots, 5$ have also been analysed in this second way. From the resulting plots of $\Delta z([N, D])$ against $1/\gamma_l'$ we have obtained a second set of estimates of γ_l'. The results are summarized in table 2. Again the quoted errors are confidence limits; our criteria of confidence can be judged from figure 3.

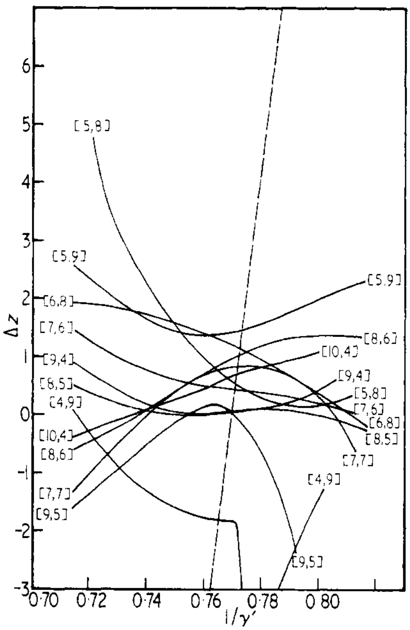

Figure 3. Deviations Δz from a standard line $z = a/\gamma' + b$, of poles of Padé approximants to $(\chi(z))^{1/\gamma'}$ against $1/\gamma'$.

Table 2. From Padé approximants to $(\partial^l M/\partial\mu^l|_{\mu=1})^{1/\gamma_l}$ estimates of critical exponents γ_l' from plots of Δz_C (see text) against $1/\gamma_l'$ and critical amplitudes C_l', from plots of residues against $1/\gamma_l'$.

l	0	1	2	3	4	5
γ_l'	$0{\cdot}310\pm0{\cdot}003$	$1{\cdot}295\pm0{\cdot}010$	$2{\cdot}86\pm0{\cdot}10$	$4{\cdot}23\pm0{\cdot}40$	$5{\cdot}74\pm0{\cdot}50$	$7{\cdot}20\pm0{\cdot}40$
C_l'	$+1{\cdot}81$	$+0{\cdot}223$	$-0{\cdot}265$	$+0{\cdot}710$	$-2{\cdot}91$	$+17{\cdot}2$

Having formed, by Padé approximant analysis, estimates for the critical exponents, it is also of interest to have estimates of critical amplitudes. Near z_C on the coexistence curve the most singular part of $\partial^l M/\partial\mu^l|_{\mu=1}$ behaves as

$$\frac{\partial^l M}{\partial\mu^l} \sim \bar{C}'_l\left(1-\frac{z}{z_C}\right)^{-\gamma'_l} \tag{2.4}$$

where the z amplitude $\bar{C}'_l$, is related to the T amplitude, C'_l, of (1.4) by

$$C'_l = \bar{C}'_l(-\ln z_C)^{-\gamma'_l}. \tag{2.5}$$

Estimates of C'_l are then obtained by plotting the residues of Padé approximants to $(\partial^l M/\partial\mu^l|_{\mu=1})^{1/\gamma'_l}$, which correspond to $z_C^{-1}(\bar{C}'_l)^{1/\gamma'_l}$, against γ'_l and choosing as best that residue corresponding to the best value of γ'_l previously determined. The resulting estimates of C'_l are also given in table 2 with their confidence limits.

Analysis of series expansions in lattice statistics is sometimes hampered by the presence of non-physical singularities. Such singularities are particularly troublesome if their location in the complex plane of the independent variable (the complex z plane here) is either (i) near to the physical singularity at z_C or (ii) nearer to the origin than z_C. Accordingly we have made estimates of the location of the important non-physical singularities in $\partial^l M/\partial z^l|_{\mu=1}$ by finding all poles of central, high degree Padé approximants to $(\mathrm{d}/\mathrm{d}z)\ln(\partial^l M/\partial z^l|_{\mu=1})$. The results are presented in table 3 in polar form.

Table 3. Estimates of location of non-physical singularities, $r\exp\mathrm{i}\theta$, of $\partial^l M/\partial\mu^l|_{\mu=1}$ in the complex z/z_C plane from poles of Padé approximants to $(\mathrm{d}/\mathrm{d}z)\ln(\partial^l M/\partial\mu^l|_{\mu=1})$.

l	0	1	2	3	4	5
$r = \lvert z\rvert/z_C$	1·23	1·08	1·13	0·96	0·78	0·70
				1·1		0·72
θ	$\pm 0{\cdot}28\pi$	$\pm 0{\cdot}29\pi$	$\pm 0{\cdot}33\pi$	$\pm 0{\cdot}27\pi$	$\pm 0{\cdot}32\pi$	$\pm 0{\cdot}35\pi$
				π		π

For all series studied ($l \leqslant 5$) there seems to be a complex conjugate pair of singularities making an angle of about 60° with the positive real axis and about the same distance from the origin as z_C. For $l = 3, 4, 5$ these non-physical singularities seem nearer to the origin than z_C and may account for the greater error we must associate with our estimates of γ'_3, γ'_4 and γ'_5 in table 2. The negative real singularity in $\partial^5 M/\partial\mu^5|_{\mu=1}$ may also be causing trouble.

Several methods exist for dealing with non-physical singularities (Gaunt and Guttmann 1974). Here we have applied the method of conformal transformation (Betts *et al* 1971 and references therein) in which a new independent variable is introduced in the series expansion via the relation

$$z = \sum_{k=1}^{m} b_k \bar{z}^k \tag{2.6}$$

where m is the maximum degree of the known terms in the original series expansion.

In particular we have used here the expansion of

$$z = \frac{\bar{z}}{1-\bar{z}}, \tag{2.7}$$

which should be effective in removing far enough from the origin a singularity on the negative real axis such as found in $\partial^5 M/\partial\mu^5|_{\mu=1}$. From poles of Padé approximants to the logarithmic derivative of the resulting transformed series we find $\gamma_5' = 7{\cdot}0 \pm 0{\cdot}4$, whereas, as we saw in table 1, we were unable to estimate γ_5' from the logarithmic derivative of the untransformed series. Again from the second method, varying the powers, we find $\gamma_5' = 7{\cdot}2 \pm 0{\cdot}2$, a slightly more precise estimate than that for γ_5' in table 2.

Another transformation has been sought which would ameliorate the effect of non-physical singularities at an angle of $\pm 60°$ to the real axis in the complex z plane. The transformation

$$z = \frac{\bar{z}}{1-27\bar{z}^3} \tag{2.8}$$

has the effect on points of distance from the origin, $|z| \simeq \frac{1}{3}$, of moving points on the rays $\arg z = 0, \pm\frac{2}{3}\pi$ radially nearer to the origin while moving points on the rays $\arg z = \pi, \pm\frac{1}{3}\pi$ radially farther from the origin. The hope is that (2.8) would be particularly helpful for $l = 4$ and $l = 5$.

We have applied (2.8) to $\partial^l M/\partial\mu^l|_{\mu=1}$ for all $l = 0, 1, \ldots, 5$. We have then plotted residues against poles of Padé approximants to $(\mathrm{d}/\mathrm{d}\bar{z})\ \ln(\partial^l M/\partial\mu^l|_{\mu=1})$ to obtain if possible γ_l' estimates improved over those of table 1. For $l = 0, 1, 2$ as expected and even for $l = 3$ little change in the estimates is observed. γ_4' becomes $5{\cdot}85 \pm 0{\cdot}10$, a distinct improvement in precision. However, the results for $l = 5$ are still too scattered to permit an estimate of γ_5'.

Series for $[(\mu\partial/\partial\mu)^l M]|_{\mu=1}$ have also been generated and analysed by the above technique (Chan 1974). The resulting estimates of critical properties are much less precise than those from $\partial^l M/\partial\mu^l|_{\mu=1}$ and so are not reported here.

3. Analysis of series along the critical isotherm

The discussion in this section is quite analogous to that of § 2. The critical isotherm is taken to be the line $z = z_C = 0{\cdot}317401$ in the (μ, z) plane. From the basic configurational data (Betts *et al* 1974), we have obtained series of degree 23 in μ for $\partial^l M/\partial z^l|_{z=z_C}$ for $l = 0, 1, \ldots, 5$. The coefficients are again quoted in the appendix, table 10. Note that the majority of coefficients depend on z_C and so are quoted to only six figures.

Our first estimates of the critical exponents ϵ_l in

$$\left.\frac{\partial^l M}{\partial z^l}\right|_{z=z_C} \sim \bar{E}_l(1-\mu)^{-\epsilon_l} \tag{3.1}$$

are obtained from the logarithmic derivative. Poles against residues of Padé approximants to $(\mathrm{d}/\mathrm{d}\mu)\ln(\partial^l M/\partial z^l|_{z=z_C})$ are plotted to yield a curve from which ϵ_l is the ordinate corresponding to $\mu = 1$. The special case of $l = 4$ is illustrated in figure 4. The remaining graphs will be found in Chan (1974). From these plots we arrive at estimates and confidence limits for ϵ_l as listed in table 4. The results for $l = 3$, however, are so scattered that no meaningful estimate of ϵ_3 can be made.

Next we have found poles and residues of Padé approximants to $(\partial^l M/\partial z^l|_{z=z_C})^{1/\epsilon_l}$ for a set of neighbouring values of ϵ_l near the best value as indicated in table 4. For each Padé approximant there is a curve of μ_C, from the pole, against ϵ_l. The best value of ϵ_l then corresponds to $\mu_C = 1$. Actually, to increase the graphical resolution, we have again used the technique of plotting against ϵ_l not μ_C but $\Delta\mu = \mu_C - a\epsilon_l - b$, the deviation

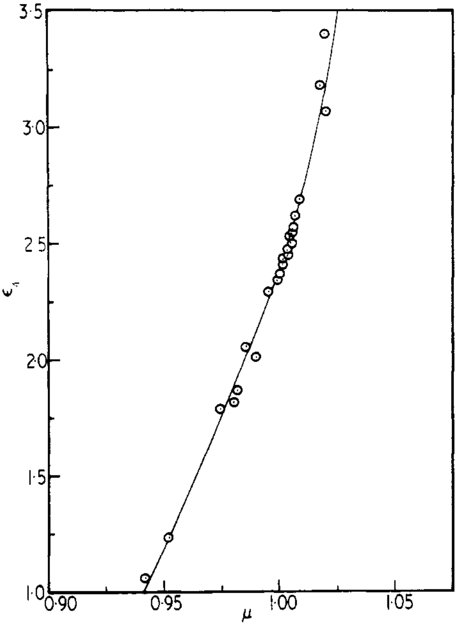

Figure 4. Estimates of μ_C and ϵ_4 from poles and residues of Padé approximants to $(d/d\mu)\ln(\partial^4 M(z,\mu)/\partial z^4|_{z_C})$.

Table 4. Estimates of critical exponents ϵ_l from plots of residues against poles of Padé approximants to $(d/d\mu)\ln(\partial^l M/\partial z^l|_{z=z_C})$ for $z_C = 0{\cdot}317401$.

l	0	1	2	3	4	5
ϵ_l	$0{\cdot}193 \pm 0{\cdot}007$	$0{\cdot}491 \pm 0{\cdot}010$	$0{\cdot}959 \pm 0{\cdot}010$		$2{\cdot}38 \pm 0{\cdot}05$	$2{\cdot}85 \pm 0{\cdot}20$

from a standard line. Figure 5 illustrates the case of $l = 4$. From this and similar plots for other l values (Chan 1974), we obtain the estimates ϵ_l with their confidence limits as listed in table 5. According to this second method also the series for $l = 3$ is too badly behaved to yield an estimate of ϵ_3. The magnetization series itself, $M(z_C, \mu)$, is also badly behaved.

If residues of Padé approximants to $(\partial^l M/\partial z^l|_{z_C})^{1/\epsilon_l}$ are plotted against ϵ_l we obtain estimates of the critical amplitudes E_l of (1.5). The 'best' value for the residue, hence $\bar{E}_l$, corresponds to the already determined best value of ϵ_l. Note that $E_l = \bar{E}_l/2^{\epsilon_l}$†. These amplitude estimates are also displayed in table 5.

To investigate further the cause of the misbehaviour for $l = 0$ and $l = 3$, we have found all the poles of high degree central Padé approximants to $(d/d\mu)\ln(\partial^l M/\partial z^l|_{z_C})$ for $l = 0, \ldots, 5$. For all l except $l = 5$, we find a second real positive pole in the complex μ plane. The poles and corresponding residues are given in table 6. No real non-physical singularity for $l = 5$ has been detected and those for $l = 2$ and $l = 4$ are sufficiently far out from the physical singularity at $\mu = 1$ as to do no harm. However, $\partial^3 M/\partial z^3|_{z_C}$ seems to have a simple zero on the real μ axis at $\mu = 0{\cdot}85$, which is disastrous for the

† The relation published by Betts and Filipow (1972) is incorrect. However they used the correct expression in their calculations so that the critical amplitudes listed in their table 3 are correct.

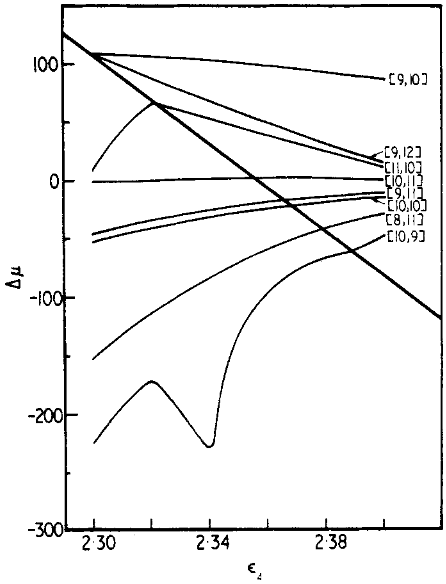

Figure 5. Deviations $\Delta\mu$ from a standard line, $\mu = a\epsilon_4 + b$, of poles of Padé approximants to $(\partial^4 M(z, \mu)/\partial z^4|_{z_C})^{1/\epsilon_4}$ against ϵ_4. The straight line corresponds to $\mu = 1$.

Table 5. From Padé approximants to $(\partial^l M/\partial z^l|_{z=z_C})^{1/\epsilon_l}$ estimates of critical exponents ϵ_l from plots of $\Delta\mu$ (see text) against ϵ_l and critical amplitudes E_l from plots of residues against ϵ_l.

l	0	1	2	3	4	5
ϵ_l	—	$0{\cdot}493 \pm 0{\cdot}010$	$0{\cdot}97 \pm 0{\cdot}02$	—	$2{\cdot}35 \pm 0{\cdot}04$	$2{\cdot}93 \pm 0{\cdot}07$
E_l	—	$-1{\cdot}06$	$-2{\cdot}47$	—	$+27{\cdot}7$	$+275$

Table 6. Estimates of real non-physical singularities μ_l, and exponents η_l from poles and residues of Padé approximants to $(\mathrm{d}/\mathrm{d}\mu)\ \ln(\partial^l M/\partial z^l|_{z_C})$.

l	0	1	2	3	4	5
μ_l	1·13	1·12	1·60	0·845	1·85	—
η_l	0·035	0·125	—	$-1{\cdot}00$	—	—

analysis of the critical behaviour of the function at $\mu = 1$. The singularities for $l = 0$ and 1 are also close enough to $\mu = 1$ to be troublesome.

For singularities of the type encountered here, on the positive real axis near the physical singularity, transformation methods cannot help. Instead we have tried to 'multiply out' the singularity. For example, instead of studying $M(z_C, \mu)$ we can study

$$M'(z_C, \mu) = (1{\cdot}13 - \mu)^{0{\cdot}035} M(z_C, \mu), \tag{3.2}$$

which should now have no competing non-physical singularity near $\mu = 1$. The multiplying out technique seems particularly helpful in conjunction with the ratio method. In figure 6 we have plotted ratios of coefficients, a_n/a_{n-1} against $1/n$ for $M(z_C, \mu)$, for

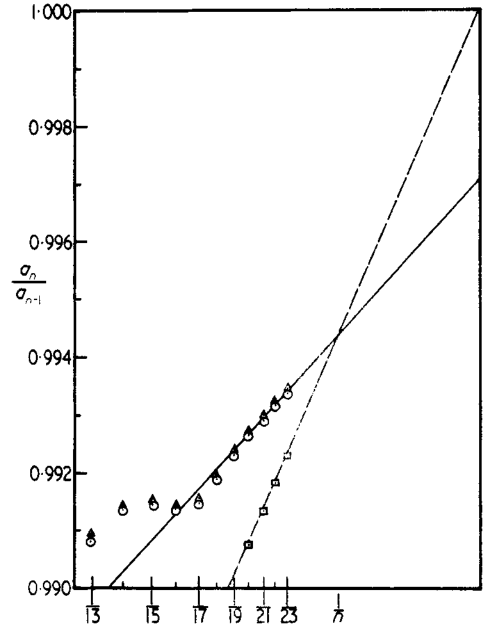

Figure 6. Ratio of coefficients, a_n/a_{n-1} against $1/n$ for the following series: $\mu(d/d\mu)M(z_C, \mu)$ (○) with $z_C = 0{\cdot}317401$; $\mu(d/d\mu)M(z_C+\Delta z, \mu)$ (△) with $\Delta z = 0{\cdot}00010$ and

$$\mu(d/d\mu)[(1{\cdot}13-\mu)^{0{\cdot}035}M(z_C, \mu)]$$

(□). The full line corresponds to $\mu_C = 0{\cdot}9971$, the broken line corresponds to $\mu_C = 1{\cdot}0000$ and $\delta = 5{\cdot}43$.

$M(z_C+\Delta z, \mu)$ where $\Delta z = 0{\cdot}00010$ and for $M'(z_C, \mu)$ as defined above. (Actually, to improve the graphical resolution we have applied the operator $\mu d/d\mu$ to each of these three series.)

The ratios for $M(z_C, \mu)$ seem to be getting nearly linear in $1/n$. However, the corresponding value of $\mu_C = 0{\cdot}9971$ is seriously in error while the corresponding value of $\delta = -1/\epsilon \simeq 11$ is completely implausible. Next, while the value of $0{\cdot}31750$ differs from the best high temperature estimate of z_C by ten times the confidence limit, the corresponding ratio plot is but little different from that for the best z_C. On the other hand, the ratios for $M'(z_C, \mu)$ have not only become quite linear, they yield the correct value of μ_C. They also yield the plausible value of $\delta = 5{\cdot}4$.

Alternatively the behaviour found for the ratios may be indicative of a more complicated singularity than (3.1) *at* $\mu = 1$. There are a great variety of more complicated forms possible, all of which would involve one or more additional parameters which makes the possibilities for analysis quite open ended. We have not explored these avenues at this time.

The 'multiplying out' technique seems less helpful to the Padé analysis. The series for $l = 3$ also seems beyond hope for any simple technique of analysis.

4. Comparison with scaling theory predictions

Scaling theory for critical phenomena (Widom 1965, Domb and Hunter 1965, Patashinskii and Pokrovskii 1966, Kadanoff 1966) makes the basic homogeneity hypothesis for the magnetization,

$$M(t, h) \sim h^{\beta/\Delta}\psi\left(\frac{t}{h^{1/\Delta}}\right) \tag{4.1}$$

where $t = (T-T_C)/T_C$ and $h = mH/k_B T_C$ and where in general ψ is an unknown function. β and Δ are basic critical exponents in terms of which the γ_l' and the ϵ_l can be expressed.

From the form (4.1) it is readily deduced that

$$\left.\frac{\partial^l M}{\partial T^l}\right|_{T=T_C} \sim h^{(\beta-l)/\Delta}$$

or

$$\left.\frac{\partial^l M}{\partial z^l}\right|_{z=z_C} \sim (1-\mu)^{(\beta-l)/\Delta} \tag{4.2}$$

This means

$$\epsilon_l = \frac{l-\beta}{\Delta}. \tag{4.3}$$

Similarly it can be shown that

$$\gamma_l' = l\,\Delta-\beta. \tag{4.4}$$

The best established estimates of critical exponents for the $s = \frac{1}{2}$ Ising model are for the high temperature susceptibility exponent γ (Sykes *et al* 1972a) and for the high temperature specific heat exponent α (Sykes *et al* 1972b). In our test of scaling theory we shall assume $\alpha = \frac{1}{8}$ and $\gamma = \frac{5}{4}$ exactly, as is strongly indicated by the investigations of the above authors. Then from the scaling relations

$$\beta = 1-\tfrac{1}{2}(\alpha+\gamma) \tag{4.5}$$

and

$$\Delta = 1+\tfrac{1}{2}(\gamma-\alpha) \tag{4.6}$$

and the relations (4.3) and (4.4) the scaling predictions for the ϵ_l and γ_l' follow.

Table 7 contains the scaling predictions for the ϵ_l and γ_l' together with the best overall estimates of the same exponents from series analysis as gleaned from §§ 2 and 3. The

Table 7. Comparison of scaling theory predictions with best estimates from series expansions for the Ising model critical exponents γ_l' of $\partial^l M/\partial H^l|_{H=0}$ and ϵ_l of $\partial^l M/\partial T^l|_{T=T_C}$.

l	0	1	2	3	4	5
γ_l' (scaling)	-0.3125	1.25	2.8125	4.375	5.9375	7.5
γ_l' (series)	-0.309 ± 0.002	1.295 ± 0.010	2.86 ± 0.10	4.37 ± 0.10	5.85 ± 0.10	7.2 ± 0.2
ϵ_l (scaling)	-0.2	0.44	1.08	1.72	2.36	3
ϵ_l (series)	-0.193 ± 0.007	0.492 ± 0.010	0.96 ± 0.02	—	2.36 ± 0.04	2.93 ± 0.07

series estimates include confidence limits which tend to increase with increasing l, confirming the wisdom of limiting investigations to small l values.

Examination of the γ_l' values in table 7 reveals agreement, within confidence limits, with scaling predictions for $l = 0, 2, 3, 4$ and 5. The notable exception is the case of the susceptibility exponent, $\gamma_1' = \gamma'$ for which the best series estimate is 4% higher than the scaling prediction.

In the only other presently available study (Gaunt and Sykes 1973) of low temperature series expansions for the three-dimensional Ising model incorporating a similarly large amount of data (for the diamond lattice) a similar value of γ' seems to be indicated. However, as the authors point out, the estimates of γ' for diamond are rather scattered and no firm conclusions can be drawn. In the present case of the susceptibility series for the hydrogen peroxide lattice, the series *seems* better behaved and *seems* to yield an estimate of γ' too high to agree with scaling.

On the critical isotherm the best series estimates of the exponents ϵ_l as given in table 7 are in agreement with the scaling predictions for $l = 0, 4$ and 5. For ϵ_3 no series estimate has been obtained. The series estimates of ϵ_1 and ϵ_2 seem to be in disagreement with scaling unless our confidence limits are much too small. Gaunt and Sykes in unpublished work have also found such discrepancy for other lattices. In their investigations the series estimates for ϵ_l agree better with the scaling results for higher coordination number, the estimates for the diamond lattice (and, by inference, *a fortiori* for the hydrogen peroxide lattice) being slow to settle down to a value in good agreement with the scaling prediction.

5. Summary and conclusion

This paper has been concerned with the analysis of low temperature series expansions for the spin $\frac{1}{2}$ Ising model on the hydrogen peroxide lattice. Estimates of critical exponents and critical amplitudes have been obtained for the magnetization and its first five field derivatives on the coexistence curve and for the magnetization and its first five derivatives with respect to $z = \exp(-J/k_BT)$ on the critical isotherm. The best overall estimates of both sets of critical exponents together with the corresponding scaling theory predictions have been given in table 7.

Along the coexistence curve all the critical exponents, γ_l' ($l = 0, 2, 3, 4, 5$), are in good agreement with prediction based on taking $\alpha = \frac{1}{8}$ and $\gamma = \frac{5}{4}$ and using scaling relations. Along the critical isotherm good agreement of the ϵ_l estimates with prediction is obtained except for the critical exponents ϵ_1 and ϵ_2. However, it was not possible to estimate ϵ_3.

How does this situation compare with the situation in two dimensions? Recent estimates of γ_l' for $l \geqslant 2$ based on recently extended low temperature series expansion data (Sykes *et al* 1973d) are not available. (Of course α', β and γ' are known exactly.) However Betts and Filipow (1972) have studied the ϵ_l on the critical isotherm for the honeycomb, square and triangular lattices, based on the data of Sykes *et al* (1973c). They found that ϵ_0, ϵ_2 and ϵ_5 could be precisely estimated and that the estimates agreed well with scaling predictions. ϵ_1 and ϵ_3 could not be so precisely estimated and ϵ_4 could not be estimated at all. The ϵ_1 estimates were in fair agreement with scaling theory while the ϵ_3 estimates were too high by an amount exceeding the confidence limits.

Qualitatively then we see that the two-dimensional and three-dimensional situations are rather similar. Most exponent estimates agree well with scaling, a few do not and a few exponents cannot be estimated. Now in two dimensions α, γ, α', β and γ' are all known exactly and satisfy scaling relations; no one seriously doubts the validity of scaling in two dimensions. But where the exponents must be estimated from series expansions, particularly on the critical isotherm, the evidence in favour of scaling is equally strong in two dimensions and in three dimensions (hydrogen peroxide lattice). Therefore we conclude that the present evidence supports thermodynamic scaling for the three-dimensional Ising model. Although we have not been able to obtain a direct estimate of the low temperature specific heat exponent, α', we hence tentatively conclude that $\alpha' = \frac{1}{8}$.

There remain in three dimensions the troublesome exceptions on the coexistence curve of the susceptibility and on the critical isotherm of the first and second derivatives of the magnetization (in two dimensions the first and third derivatives). If scaling theory is indeed valid we must conclude that a few of the low temperature expansions are still too short to reveal the true asymptotic behaviour of the functions they represent, and the apparent confidence limits are too small. These conclusions are in qualitative agreement with those of Gaunt and Sykes (1973).

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Appendix

Table 8. Coefficients of the specific heat series, $C_H/Nk_B(\ln z)^2 = \Sigma_n a_n z^n$ on the coexistence curve.

n	a_n
0	0
1	0
2	0
3	9
4	24
5	75
6	178
7	441
8	1008
9	2295
10	5250
11	13068
12	36576
13	111033
14	340746
15	1015020
16	2920032
17	8261643

Table 9. Coefficients in the series expansions on the coexistence curve for

$$\partial^l M/\partial\mu^l|_{\mu=1} = -2\Sigma_j c_j^{(l)} z^j.$$

j	$c^{(0)}$	$c^{(1)}$	$c^{(2)}$	$c^{(3)}$	$c^{(4)}$	$c^{(5)}$
0	−0·5	0	0	0	0	0
1	0	0	0	0	0	0
2	0	0	0	0	0	0
3	1	1	0	0	0	0
4	3	6	6	0	0	0
5	9	27	54	54	0	0
6	24	104	328	672	672	0
7	63	369	1638	5238	10800	10800
8	162	1242	7290	32400	103680	213840
9	415	4039	30056	174024	768240	2449920
10	1077	12978	118770	859968	4919616	21663360
11	2892	41892	459024	4028616	28624536	162932040
12	8073	136494	1749606	18158808	155382984	1094811600
13	23151	446841	6581550	79255710	798024240	6748932240
14	67041	1459590	24399822	336086568	3912915384	38830791600
15	193862	4737428	89125914	1389067290	18448456560	211173474720
16	558582	15277500	321297396	5616301896	84165825384	1096344816480
17	1610073	49071243	1146225822	22297505670	373577513976	5476646132280

Table 10. Coefficients of $\partial^l M/\partial z^l|_{z_C} = \Sigma_n d_n^{(l)}\mu^n$ for $z_C = 0{\cdot}317401$.

n	$d^{(0)}$	$d^{(1)}$	$d^{(2)}$	$d^{(3)}$	$d^{(4)}$	$d^{(5)}$
0	1	0	0	0	0	0
1	−0·0639524	−0·604462	−3·80882	−12	0	0
2	−0·0527159	−0·612801	−4·81771	−15·0087	146·142	1828·23
3	−0·0417026	−0·562168	−5·09322	−13·2927	394·675	5717·82
4	−0·0334756	−0·507041	−5·10493	−9·51146	710·037	11520·0
5	−0·0274116	−0·457447	−5·01673	−5·00340	1067·94	19052·4
6	−0·0228616	−0·414762	−4·89428	−0·433923	1452·43	28168·5
7	−0·0193713	−0·378373	−4·76538	3·87211	1852·96	38763·4
8	−0·0166371	−0·347293	−4·64181	7·76505	2262·50	50766·1
9	−0·0144547	−0·320589	−4·52816	11·1866	2676·26	64128·6
10	−0·0127914	−0·300104	−4·47647	13·4903	3090·75	79020·8
11	−0·0114881	−0·283831	−4·45656	15·4096	3522·25	95805·4
12	−0·0104273	−0·270145	−4·44549	17·3700	3976·47	114535
13	−0·00953663	−0·258120	−4·43294	19·4955	4452·03	135106
14	−0·00877872	−0·247452	−4·42022	21·6997	4944·82	157410
15	−0·00812313	−0·237808	−4·40515	23·9951	5453·16	181387
16	−0·00754964	−0·229013	−4·38855	26·3212	5973·90	206956
17	−0·00704498	−0·220997	−4·37283	28·5986	6504·46	234084
18	−0·00659960	−0·213722	−4·36002	30·7826	7044·06	262803
19	−0·00620413	−0·207088	−4·34948	32·9070	7593·90	293174
20	−0·00585053	−0·200995	−4·34020	35·0038	8154·52	325217
21	−0·00553246	−0·195367	−4·33177	37·0826	8725·68	358920
22	−0·00524492	−0·190148	−4·32403	39·1452	9306·96	394272
23	−0·00498373	−0·185288	−4·31675	41·1957	9898·00	431262

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