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1994 J. Phys. A: Math. Gen. 27 6987

(http://iopscience.iop.org/0305-4470/27/21/014)

J. Phys. A: Math. Gen. 27 (1994) 6987–7005. Printed in the UK

# Low-temperature series expansions for the spin-1 Ising model

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Received 14 May 1994

**Abstract.** The finite-lattice method of series expansion has been used to extend low-temperature series for the partition function, order parameter and susceptibility of the spin-1 Ising model on the square lattice. A new formalism is described which uses two distinct transfer-matrix approaches in order to significantly reduce computer memory requirements and which permits the derivation of the series to 79th order. Subsequent analysis of the series clearly confirms that the spin-1 model has the same dominant critical exponents as the spin-$\frac{1}{2}$ Ising model. Accurate estimates for both the critical temperature and non-physical singularities are obtained. In addition, evidence for a non-analytic confluent correction with exponent $\Delta_1 = 1.1 \pm 0.1$ is found.

## 1. Introduction

Low-temperature expansions for the spin-1 Ising model were first obtained by Fox and Guttmann (1973), who gave a 26-term series for the square lattice, of which only the first 24 terms were correct. The method used to obtain the series was a generalization of the code method of Sykes *et al* (1965). Series on other lattices, both two- and three-dimensional, were also obtained. Subsequently the finite-lattice method of series expansions (de Neef 1975, de Neef and Enting 1977) has proved to be an extremely powerful technique for deriving series expansions for a range of two-dimensional models. The formalism is applicable in higher dimensions but the technique becomes progressively less efficient (Guttmann and Enting 1993). Adler and Enting (1984) used the finite-lattice method to extend low-temperature expansions for the zero-field partition function, the magnetization and the zero-field susceptibility of the spin-1 Ising model to order $u^{45}$. As we have noted elsewhere, developments in computing over the last decade, notably faster computers with more memory, have allowed larger finite-lattice calculations to be made. By re-running the program used by Adler and Enting we easily extended the series to 65 terms. We have, however, recently implemented a revised algorithm that removes much of the memory-size requirement that has previously limited our finite-lattice calculations. This involves using two different ways of calculating finite-lattice partition functions. A preliminary analysis of the formalism was given by Enting (1990). In this paper we use this new formalism

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0305-4470/94/216987+19$19.50 

to calculate low-temperature spin-1 Ising series to order $u^{78}$. Using a rather cumbersome correction method described in the appendix we also obtained the coefficients of $u^{79}$. We have also substantially extended the spin-$\frac{1}{2}$ low-temperature susceptibility series.

The layout of the paper is as follows. In section 2 we describe the finite-lattice method of series expansions. The various expansions are detailed in section 3. The results of the series analysis, with the emphasis on the new extended spin-1 series, are presented in section 4. Finally, section 5 contains a short summary and discussion of our results.

## 2. Series expansions from the finite-lattice method

As in the study by Adler and Enting (1984), the series expansions are derived from

$$Z \approx \prod_{m,n} Z_{mn}^{a_{mn}} \qquad \text{with} \quad m \leqslant n \quad \text{and} \quad m+n \leqslant k \tag{2.1}$$

where $Z$ is the infinite-lattice partition function and the $Z_{mn}$ are the partition functions of the $m \times n$ lattices. The weights, $a_{mn}$ are derived from the expressions given by Enting (1978), modified to exploit the rotational symmetry of the lattice. The difference from Enting and Adler is that we use a larger cut-off, $k$, which leads to longer series.

The finite-lattice method relies on efficient techniques for evaluating the $Z_{mn}$. We use what are known as 'transfer-matrix' techniques. These work by moving a boundary through the lattice and constructing a partial sum of Boltzmann weights for each possible configuration of the boundary. The traditional form of transfer-matrix calculation involves moving the boundary one column at a time. For a system with $q$ states per site, evaluating $Z_{mn}$ involves $n$ iterations of $q^{2m}$ operations on series. It is more efficient to move the boundary by adding one site at a time. Evaluating $Z_{mn}$ involves $m \times n$ iterations of $q^{m+1}$ series operations. The 'one-site-at-a-time' algorithm seems to have been rediscovered independently a number of times. Our use of the technique derives from unpublished work by Baxter.

The new procedure proposed by Enting (1990) and adopted here is to use (2.1) as before but to use two different techniques for calculating the $Z_{mn}$. We define a cut-off parameter $b_{\max}$ so that, for a $q$-state system, the maximum vector size is $q^{b_{\max}}$. In evaluating $Z_{mn}$ (and considering only $m \leqslant n$ because of our use of symmetry), if $m \leqslant b_{\max}$ we use our original procedure of building up the lattice column by column with each column built up one site at a time. Evaluating $Z_{mn}$ requires $mnq^{m+1}$ series operations but the evaluation of $Z_{mn}$ enables us to determine $Z_{mp}$ for $p < n$ with little extra computation. For square (or nearly square) lattices we evaluate the partition functions by a technique in which the boundary pivots about a central point. The general principle is based on unpublished work by Baxter.

The 'pivoting' transfer-matrix approach uses three integers, $a$, $b$ and $c$ (with $c = b$ or $c = b - 1$) to specify the rectangles. The rectangles are of size $m = (a + b)$ by $n = (b + c + 1)$. We refer to sites by integer coordinates $(x, y)$ with $1 - a \leqslant x \leqslant b$ and $-c \leqslant y \leqslant b$. The partition function is a sum over the $q^a$ conditional lattice sums in which the $a$ sites $(x, 0)$ with $x \leqslant 0$ are fixed. Transfer-matrix techniques are used to calculate the lattice sum conditional on the state of the fixed sites.

The algorithm outlined below requires space for $2q^b$ series and takes time $\propto m \times n \times q^{(a+b)}$.

We consider two alternative forms of 'cut-off'.

*Space-limited.* If the execution time was not limiting, then the smallest rectangle that could not be computed by pivoting would be a square of size $(2b + 2) \times (2b + 2)$. Thus we use

$$m + n \leqslant k = 4b_{\max} + 2 \,. \tag{2.2}$$

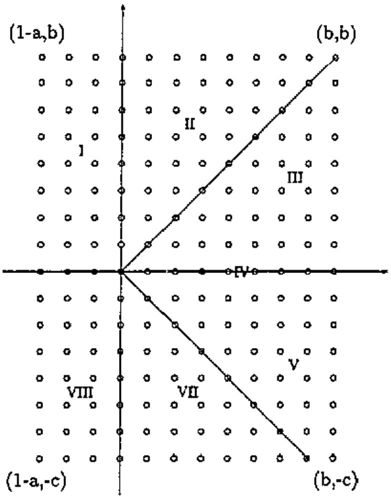


**Figure 1.** The various regions of the lattice numbered according to the order in which they are traversed in the pivoting algorithm. The $a$ spins on the full circles are fixed. In the case of this $12 \times 16$ lattice we have $a = 4$, $b = 8$ and $c = 7$.

We use the original transfer-matrix technique for $m \leqslant b_{\max}$ and use the pivoting algorithm for rectangles of size $m = (b + c + 1)$ by $n = (a + b)$ for $b, c \leqslant b_{\max}$. For $m = b_{\max} + 1$ the longest rectangle is of length $n = a + b = 3b_{\max} + 1$, so that in terms of the cut-off, $k$, the time requirement grows as $q^{3k/4}$.

*Time-limited.* If we wish to restrict the growth in the time requirement to the $q^{k/2}$ that applies to our original technique, then we use the cut-off

$$m + n \leqslant k = 3b_{\max} + 2\,. \tag{2.3}$$

Again we use our original technique for $m \leqslant b_{\max}$ and use the pivoting algorithm for rectangles of size $m = (a + b)$ by $n = (2b + 1)$ for $a + b$ from $b_{\max} + 1$ to $\lfloor k/2 \rfloor$.

In the work presented here we have used the 'time-limited' form. The algorithm for evaluating finite lattices by 'pivoting' is:

- For each of the $q^a$ states of the fixed line (the full circles in figure 1):
  - Construct the conditional lattice sum.
  - Multiply the conditional sum by the internal weight of the fixed line.
  - Add the product to the running total for the finite-lattice partition function.

    The procedure for building up the conditional sum is:
    * For each $x$ from $1 - a$ to 0, build up the lattice sum for the column $(x, y)$ for $y$ from 1 to $b$ (region I of figure 1).
    * For each $x$ from 1 to $b$, build up the lattice sum for the partial column $(x, y)$ for $y$ from $b$ to $x$ (region II of figure 1).
    * For each $y$ from $b - 1$ to 1, build up the lattice sum for the partial row $(x, y)$ for $x$ from $b$ to $y$ (region III of figure 1).
    * Build up the lattice sum for the row $(x, 0)$ for $x$ from $b$ to 1 (IV).
    * For each $y$ from $-1$ to $1 - b = -c$, build up the lattice sum for the partial row $(x, y)$ for $x$ from $b$ to $-y$ (region V in figure 1).
    * If $b = c$, build up the lattice sum for the diagonal $(x, -x)$ for $x$ from $b$ to 1 (not present in figure 1).
    * For each $x$ from $b - 1$ to 1, build up the lattice sum for the partial row $(x, y)$ for $y$ from $-b$ to $-x$ (region VII of figure 1).

* For each $x$ from 0 to $1-b$, build up the lattice sum for the partial column $(x, y)$ for $y$ from $-b$ to $-1$ (region VIII of figure 1).

Another new feature of our calculations is the choice of a machine (Cray YMP–EL) which emphasizes processing speed rather than large memory. The fact that most of our basic operations in the transfer-matrix approach are actually operations on truncated series means that we can readily utilize the vector capabilities of such a machine by ensuring that the series operations are performed in vector mode. We note that the pivoting algorithm also permits a high degree of parallel operation since each of the sums for a given centre line can be evaluated independently of the others.

In order to deal with the large integer coefficients in the series the calculations were performed using modular arithmetic (see, for example, Knuth 1969). Utilizing the standard 46-bit integers of the Cray we used the set of primes, $p_i = 2^{23} - x_i$ with $x_i \in \{15, 21, 27, 37, 61, \ldots\}$. We had to use four primes for the spin-1 calculations and five primes for the spin-$\frac{1}{2}$ calculations. Each run with $b_{\max} = 8$ ($b_{\max} = 12$) for the spin-1 (spin-$\frac{1}{2}$) model required approximately 63 (48) CPU hours.

## 3. Expansions

For the spin-1 Ising model in a homogeneous magnetic field $h$ we write the Hamiltonian as

$$\mathcal{H} = \sum_{\langle ij \rangle} J(1 - S_i S_j) + \sum_i h(1 - S_i) \tag{3.1}$$

where the spin variables $S_i = 0, \pm 1$. The first sum is over all nearest-neighbour pairs on the square lattice and the second sum is over all sites. The constants are chosen so that the $S_i = 1$ ground state has zero energy. The low-temperature expansion, as described by Sykes and Gaunt (1973), is based on perturbations from the $S_i = 1$ ground state. The expansions are obtained in terms of the low-temperature variable $u = \exp(-\beta J)$ and the field variable $\mu = \exp(-\beta h)$, where $\beta = 1/kT$. The expansion of the partition function in powers of $u$ may be expressed as

$$Z = \sum_{k=0}^{\infty} u^k \Psi_k(\mu) = 1 + u^4\mu + u^7\mu^2 + \cdots \tag{3.2}$$

where $\Psi_k(\mu)$ are polynomials in $\mu$. We express the field variable as $\mu = 1 - x$ and truncate the field dependence at $x^2$ and thus find

$$Z = Z_0(u) + xZ_1(u) + x^2 Z_2(u) + \cdots . \tag{3.3}$$

According to standard definitions the order parameter, or the spontaneous magnetization, is the derivative of the free energy, $F = -kT \ln Z$, with respect to $h$,

$$M(u) = M(0) + \frac{1}{\beta} \left. \frac{\partial \ln Z}{\partial h} \right|_{h=0} = 1 + Z_1(u)/Z_0(u) \tag{3.4}$$

since $x = 0$ in zero field. For the susceptibility we find

$$\chi(u) = \left. \frac{\partial M(h)}{\partial h} \right|_{h=0} = \frac{\partial}{\partial h} \left. \left( Z^{-1} \frac{\partial Z}{\partial h} \right) \right|_{h=0} = \beta \left[ 2\frac{Z_2(u)}{Z_0(u)} - \frac{Z_1(u)}{Z_0(u)} - \left( \frac{Z_1(u)}{Z_0(u)} \right)^2 \right]. \tag{3.5}$$

The specific-heat series is derived from the zero-field partition function (via the internal energy $U = -(\partial/\partial\beta) \ln Z_0$),

$$C_v(u) = \frac{\partial U}{\partial T} = \beta^2 \frac{\partial^2}{\partial \beta^2} \ln Z_0 = (\beta J)^2 \left( u \frac{d}{du} \right)^2 \ln Z_0(u). \tag{3.6}$$

The resulting series for $M(u)$, $\beta^{-1}\chi(u)$, and $(\beta J)^{-2}C_v(u)$ are given in table 1. The number of terms derived correctly with the finite-lattice method is given by the power of the lowest-order connected graph not contained in any of the rectangles considered. Since we are using the *time-limited* cut-off the simplest such graphs are chains of $3b_{\max}+2=r$ sites all in the '0' state. From the spin-1 Hamiltonian we see that such chains give rise to terms $u^{3r+1}$. The series are thus correct to order $u^{3r}=u^{9b_{\max}+6}$. We have checked this explicitly by calculating the series for $b_{\max}=2,3\ldots,7$ and checking that the terms through $u^{9b_{\max}+6}$ agree with the final 79-term series derived using $b_{\max}=8$. An additional spin-1 coefficient was calculated by a correction procedure explained in the appendix. These new series are significant extensions to the hitherto longest series (45 terms) due to Adler and Enting (1984).

By the same methods *mutatis mutandis*, we calculated, with $b_{\max}=12$, a new 78-term series for the spin-$\frac{1}{2}$ Ising model in the low-temperature expansion variable $u=\exp(-2\beta J)$. Note that the lowest-order graphs not counted are chains of spins flipped with respect to the ground state. But now only *broken* bonds pick up a factor of $u$. With chains of length $r$ there are $2r+2$ broken bonds so the series are correct to order $u^{2r+1}=u^{6b_{\max}+5}$. The

**Table 1.** New low-temperature series for the spin-1 2D Ising magnetization ($M(u)=\sum_n m_n u^n$), susceptibility ($\chi(u)=\sum_n x_n u^n$), and specific heat ($C_v(u)=\sum_n c_n u^n$).

| $n$ | $m_n$ | $x_n$ | $c_n$ |
|---|---|---|---|
| 0 | 1 | 0 | 0 |
| 1 | 0 | 0 | 0 |
| 2 | 0 | 0 | 0 |
| 3 | 0 | 0 | 0 |
| 4 | −1 | 1 | 16 |
| 5 | 0 | 0 | 0 |
| 6 | 0 | 0 | 0 |
| 7 | −4 | 8 | 98 |
| 8 | 3 | −6 | −96 |
| 9 | 0 | 0 | 0 |
| 10 | −30 | 90 | 1000 |
| 11 | 48 | −144 | −1936 |
| 12 | −52 | 192 | 2064 |
| 13 | −120 | 480 | 5070 |
| 14 | 368 | −1372 | −19012 |
| 15 | −612 | 2676 | 31950 |
| 16 | −254 | 1703 | 9024 |
| 17 | 2524 | −11952 | −152014 |
| 18 | −6216 | 33316 | 383616 |
| 19 | 4040 | −18900 | −298186 |
| 20 | 11805 | −64201 | −832320 |
| 21 | −49400 | 304580 | 3575922 |
| 22 | 68268 | −401068 | −5486624 |
| 23 | 14928 | −97928 | −1012506 |
| 24 | −332511 | 2390637 | 27088992 |
| 25 | 734508 | −5130048 | −65115000 |
| 26 | −568038 | 4264858 | 53200524 |
| 27 | −1641320 | 13518716 | 147217176 |
| 28 | 6202774 | −49117798 | −608004040 |
| 29 | −9239676 | 76725752 | 947874280 |
| 30 | −2503162 | 29308994 | 189048900 |

**Table 1.** Continued.

| | | | |
|---|---|---|---|
| 31 | 42749908 | −381566684 | −4568526730 |
| 32 | −99021392 | 915306452 | 11071969920 |
| 33 | 72255812 | −629297848 | −8871938526 |
| 34 | 215763902 | −2149429218 | −24714851124 |
| 35 | −846523304 | 8606730256 | 102572776040 |
| 36 | 1235587854 | −12408220218 | −158562077760 |
| 37 | 315695688 | −3956969996 | −31309254516 |
| 38 | −5897043012 | 65853427044 | 766255508396 |
| 39 | 13498636700 | −149789004280 | −1846277129736 |
| 40 | −10063784956 | 110599540765 | 1479447715520 |
| 41 | −30197995484 | 371951421160 | 4133610817968 |
| 42 | 117108185474 | −1416033283010 | −17054958273276 |
| 43 | −172710840680 | 2102892657652 | 26339112604404 |
| 44 | −46214867144 | 737547145862 | 5331885548880 |
| 45 | 824863285280 | −10822599389744 | −127080932186700 |
| 46 | −1901022089768 | 25078129380684 | 305778947448156 |
| 47 | 1405042568748 | −17797597472844 | −243733007205368 |
| 48 | 4266178550909 | −61005293343300 | −684581856372288 |
| 49 | −16624047456088 | 235876708211784 | 2818178220557042 |
| 50 | 24458757867992 | −344426000745528 | −4339993392475000 |
| 51 | 6610934151948 | −118602900569968 | −894117116934894 |
| 52 | −117973371104457 | 1797119592535141 | 20963370411907352 |
| 53 | 271535984970264 | −4116526192115268 | −50319881932177670 |
| 54 | −200950868428636 | 2947822355097388 | 39972295747477872 |
| 55 | −615007072669600 | 10130142463339880 | 112867555200892470 |
| 56 | 2391435417419895 | −38724154430758393 | −463179370952109840 |
| 57 | −3523264660998628 | 56732375209602912 | 711889569606231690 |
| 58 | −974049037638220 | 20114020125177948 | 149739050620646304 |
| 59 | 17078683955539360 | −294868317310376404 | −3442135262856162448 |
| 60 | −39345145748450867 | 676479764508534719 | 8247102824525820120 |
| 61 | 29026701896553572 | −479158286800083944 | −6525890234473448550 |
| 62 | 89603802847507184 | −1661764311006201920 | −18532244655048816588 |
| 63 | −348363066804818696 | 6354863121022079308 | 75848843620008360720 |
| 64 | 512907395631821606 | −9265243259835533768 | −116335729831253805824 |
| 65 | 144248115519171836 | −3315474781302882096 | −24961184352327362750 |
| 66 | −2500429353847945250 | 48350450407929798098 | 563358836743426377588 |
| 67 | 5757911256695782416 | −110521765873057849552 | −1347235562794556332032 |
| 68 | −4239564000431858236 | 78112180092393615814 | 1062223855357818122632 |
| 69 | −13189936451780437660 | 272577693656067525988 | 3034102236742714342464 |
| 70 | 51212742729615384348 | −1038017985499645393024 | −12384673817861566133360 |
| 71 | −75378650279043338628 | 1511592752767037119280 | 18959244151288425233210 |
| 72 | −21589841096310396846 | 550095300981147667462 | 4149995353996807267776 |
| 73 | 369164127694023873860 | −7896113973546269891772 | −91961341446801674710358 |
| 74 | −849854483657640971250 | 18026239753543948651338 | 219535041878849931107584 |
| 75 | 624038440770346152380 | −12669452007330249289520 | −172468622446186756857750 |
| 76 | 1956508551522393160164 | −44535529209867702398308 | −495562798199277085255224 |
| 77 | −7587615135291641485816 | 169246143976718418368880 | 2017606788248236265104332 |
| 78 | 11159761201704504160824 | −245838982882938309009072 | −3082929124790021245909560 |
| 79 | 32513633241009512417 76 | −906557714700086572256 76 | −6881816798350182004617 74 |

resulting series are listed in table 2. The spin-$\frac{1}{2}$ magnetization and specific-heat series are, of course, known exactly, so only the susceptibility series is new. We nevertheless list the coefficients of all three quantities, partly for completeness and partly for verification of our algorithm.

**Table 2.** New low-temperature series for the spin-$\frac{1}{2}$ 2D Ising magnetization ($M(u) = \sum_n m_n u^n$), susceptibility ($\chi(u) = \sum_n x_n u^n$), and specific heat ($C_v(u) = \sum_n c_n u^n$). All terms with odd $n$ are zero.

| $n$ | $m_n$ | $x_n$ | $c_n$ |
|---|---|---|---|
| 0 | 1 | 0 | 0 |
| 2 | 0 | 0 | 0 |
| 4 | −2 | 1 | 16 |
| 6 | −8 | 8 | 72 |
| 8 | −34 | 60 | 288 |
| 10 | −152 | 416 | 1200 |
| 12 | −714 | 2791 | 5376 |
| 14 | −3472 | 18296 | 25480 |
| 16 | −17318 | 118016 | 125504 |
| 18 | −88048 | 752008 | 634608 |
| 20 | −454378 | 4746341 | 3269680 |
| 22 | −2373048 | 29727472 | 17086168 |
| 24 | −12515634 | 185016612 | 90282240 |
| 26 | −66551016 | 1145415208 | 481347152 |
| 28 | −356345666 | 7059265827 | 2585485504 |
| 30 | −1919453984 | 43338407712 | 13974825960 |
| 32 | −10392792766 | 265168691392 | 75941188736 |
| 34 | −56527200992 | 1617656173824 | 414593263952 |
| 36 | −308691183938 | 9842665771649 | 2272626444528 |
| 38 | −1691769619240 | 59748291677832 | 12502223573304 |
| 40 | −9301374102034 | 361933688520940 | 68996534259040 |
| 42 | −51286672777080 | 2188328005246304 | 381858968527680 |
| 44 | −283527726282794 | 13208464812265559 | 2118806030647328 |
| 46 | −1571151822119216 | 79600379336505560 | 11783826597027256 |
| 48 | −8725364469143718 | 479025509574159232 | 65674579024955904 |
| 50 | −48552769461088336 | 2878946431929191656 | 366728645195006000 |
| 52 | −270670485377401738 | 17281629934637476365 | 2051443799934043632 |
| 54 | −1511484024051198680 | 103621922312364296112 | 11494250259278105304 |
| 56 | −8453722260102884930 | 620682823263814178484 | 64499139095733378176 |
| 58 | −47350642314439048648 | 3714244852389988540072 | 362436080938852037648 |
| 60 | −265579129813183372802 | 22206617664989885664363 | 2039249170926323834880 |
| 62 | −1491465339550559632448 | 132657236460768679560864 | 11487673072269872540904 |
| 64 | −8385872784303807639294 | 791843294876287279547520 | 64786142191741932873984 |
| 66 | −47202746620874986470336 | 4723112509660327575046688 | 365754067103461706996304 |
| 68 | −265975151780412455885826 | 28152514246598001579534217 | 2066925549185792626090544 |
| 70 | −1500179080790296495333960 | 167696255471026758161692328 | 11691314122170272566638200 |
| 72 | −8469330846027919131108866 | 998303936498277539688401212 | 66188283453887221177721568 |
| 74 | −47856040705247407564621400 | 5939502715888619728011515904 | 375021938737150106426702208 |
| 76 | −270636033194089067428986890 | 35318214476286590871820680287 | 2126523853550658555941372768 |

## 4. Analysis of the spin-1 series

The series for the spontaneous magnetization, the susceptibility and the specific heat of the spin-1 Ising model are expected to exhibit critical behaviour of the forms

$$M(u) \sim A_{\mathrm{M}}(u_c - u)^{\beta}[1 + a_{M,1}(u_c - u)^{\Delta_1} + b_{M,1}(u_c - u) + \cdots] \qquad (4.1)$$

$$\chi(u) \sim A_{\chi}(u_c - u)^{-\gamma}[1 + a_{\chi,1}(u_c - u)^{\Delta_1} + b_{\chi,1}(u_c - u) + \ldots] \qquad (4.2)$$

$$C_v(u) \sim A_c(u_c - u)^{-\alpha}[1 + a_{C,1}(u_c - u)^{\Delta_1} + b_{C,1}(u_c - u) + \ldots]. \qquad (4.3)$$

By universality it is expected that the leading critical exponents equal those of the spin-$\frac{1}{2}$ Ising model, i.e. $\beta = \frac{1}{8}$, $\gamma = \frac{7}{4}$ and $\alpha = 0$ (logarithmic divergence). One of the major differences between the two models appears to be that the non-analytic confluent terms are not present in the spin-$\frac{1}{2}$ model (the $a_1$'s equal zero).

### 4.1. $u_c$ and the leading critical exponents

The low-temperature spin-1 series is ill-behaved because there are non-physical singularities closer to the origin than the physical singularity, thus rendering ratio methods useless. The series may still be analysed using differential approximants (Guttmann 1989), which provides an effective analytic continuation beyond the radius of convergence, thus allowing accurate estimation of critical parameters even when the dominant singularity is non-physical. It is also often useful to change the series variable by a transformation leading to a new series in which the singularity closest to the origin is the physical one. However, such 'singularity-moving' transformations may introduce long-period oscillations (Guttmann 1989) seriously impairing the accuracy of ratio methods.

It turns out that ordinary Dlog Padé approximants, equivalent to first-order homogeneous differential approximants, work best for the magnetization series. By averaging over several $[N/M]$ approximants with $|N-M| \leqslant 4$ using at least 65 terms of the series ($N+M > 64$) we find the following estimates for the critical point $u_c = 0.554\,075(15)$ and exponent $\beta = 0.1253(3)$. The number in parentheses is the error in the last digit(s) given as three standard deviations. We find that approximants using fewer than $\simeq 60$ terms deviate systematically from these averages. In figure 2 we have plotted the estimates for $\beta$ versus the number of terms ($N+M+1$) from the series utilized in the Dlog Padé approximants. We see clearly how the $\beta$-estimates settle down to a plateau around $\beta \simeq 0.1253$ when more than 60 terms are used. The estimate for $\beta$ is slightly higher than the expected exact value $\beta = \frac{1}{8}$. In addition to the physical singularity at $u_c$, we find that the magnetization series has a singularity on the negative $u$-axis at $u_- = -0.598\,53(4)$ with exponent $\beta_1 = 0.1247(6)$ and a pair of complex roots at $u_\pm = -0.301\,83(5) \pm 0.378\,70(4)\mathrm{i}$ with exponent $\beta_\pm = -0.127(3)$. Note that the non-physical singularity $u_\pm$ is closer to the origin than the physical singularity $u_c$. First-order *inhomogeneous* and second-order differential approximants do not work very

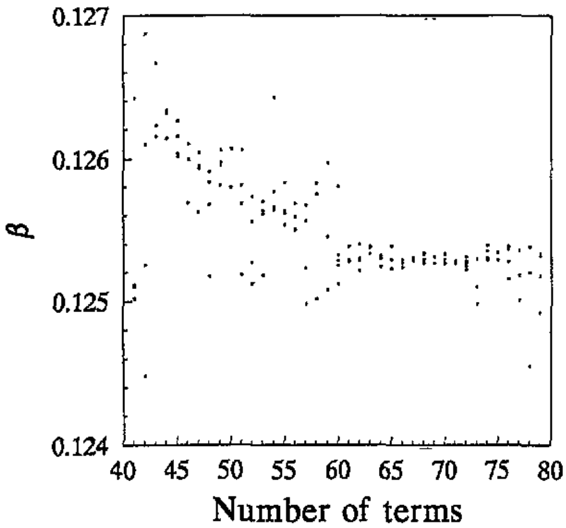


**Figure 2.** Estimates for the leading critical exponent $\beta$ of the spin-1 spontaneous magnetization versus the number of terms used by the Dlog Padé approximants.

well for the magnetization series, as evidenced by error estimates which are generally at least an order of magnitude larger than in the simple Dlog Padé case. If we assume that the exact value of $\beta = \frac{1}{8}$ we have to change our estimate of $u_c$. We find basically a linear relationship between the estimates for $\beta$ and $u_c$, and for $\beta = \frac{1}{8}$ we find $u_c = 0.554\,065(5)$. We have obtained a very similar result by analysing the series for $M^8(u)$ using ordinary (*not* Dlog) Padé approximants. Raising the magnetization series to the eighth power and looking for simple zeros and poles of the resulting series obviously corresponds to biasing the magnetization series to have a leading critical exponent of $\frac{1}{8}$. We find that the function given by this series has zeros at $u_c = 0.554\,063(10)$ and $u_- = -0.598\,555(10)$ plus a conjugate pair of simple poles at $u_\pm = -0.301\,98(3) \pm 0.378\,57(5)\mathrm{i}$. For comparison we note that the spontaneous magnetization of the quadratic spin-$\frac{1}{2}$ Ising model is given by the formula (Onsager 1944, Yang 1952)

$$I(u) = \left[\frac{1+u^2}{(1-u^2)^2}(1-6u^2+u^4)^{1/2}\right]^{1/4}$$

from which we see that the magnetization has singularities with exponent $\frac{1}{8}$ at $\pm(\sqrt{2}-1)$ and $\pm(\sqrt{2}+1)$, with exponent $\frac{1}{4}$ at $\pm\mathrm{i}$ and finally with exponent $-\frac{1}{2}$ at $\pm 1$.

The success of ordinary Dlog Padé approximants in analysing the magnetization series stems from the absence of analytic background terms. In the susceptibility and specific-heat series such background terms are indeed present and obscure the leading critical behaviour. However, inhomogeneous differential approximants are generally successful in dealing with such terms. In table 3 we have listed the estimates for $\gamma$ and $u_c$ obtained by averaging many different approximants to the susceptibility series. We find that ordinary Dlog Padé approximants (the first-order approximants with $L = 0$) yield quite stable estimates but that the estimate for $u_c$ is quite a bit larger than for the magnetization, and that $\gamma$ is markedly larger than the expected exact value $\gamma = \frac{7}{4}$. However, once the order of the inhomogeneous polynomial is larger than 2, the estimates for $\gamma$ becomes fully consistent with the expected behaviour; indeed, we see that the first-order approximants favour a value a little larger than $\frac{7}{4}$ whereas the second-order approximants favour a value slightly below $\frac{7}{4}$. Taken together there seems little doubt the exact value indeed is $\gamma = \frac{7}{4}$. Again assuming a linear relationship between $\gamma$ and $u_c$, we find that $u_c \simeq 0.554\,065$. The estimates for the critical exponent $\gamma$ exhibit the same trend as those for $\beta$, i.e. when fewer than $\simeq 60$ terms are used the estimates are generally clearly $> \frac{7}{4}$ with larger deviations when fewer terms is involved in estimating $\gamma$. When more than 60 terms are used, the estimates reach a plateau around a value $\simeq 1.755$, but with a spread that clearly includes the expected exact value $\gamma = \frac{7}{4}$. In this case we find additional singularities at $u_- = -0.5984(1)$ with exponent $-1.725(15)$ and $u_\pm = -0.301\,94(2) \pm 0.378\,77(2)\mathrm{i}$ with an exponent of $-1.175(10)$. A closer examination of the various approximants revealed that as the estimates of $u_-$ approach the value found from the magnetization series, $u_- \sim -0.598\,555$, the exponent approaches $-1.75$. It is thus very likely that the exponents at $u_c$ and $u_-$ are equal.

The analytic background term is stronger in the specific-heat series, as can be seen in table 4 where we have listed the estimates for $\alpha$ and $u_c$. The first-order approximants yield no useful results with $L = 0, 1$. Once the order of the inhomogeneous polynomial becomes larger than 3 the first-order approximants clearly yield an estimate consistent with $\alpha = 0$. This time a linear relationship between $\alpha$ and $u_c$ indicates $u_c \simeq 0.554\,070$ when $\alpha = 0$. In addition we find a pair of complex roots at $u_\pm = -0.301945(15) \pm 0.378776(10)$ with an exponent (divergence) of $-1.172(10)$. These conclusions are fully confirmed by the results of the analysis using second-order differential approximants. There is also evidence for a

**Table 3.** Estimates of $u_c$ and $\gamma$ from first- and second-order differential approximants. $L$ is the order of the inhomogeneous polynomial.

| | First-order approximants | | Second-order approximants | |
|---|---|---|---|---|
| $L$ | $u_c$ | $\gamma$ | $u_c$ | $\gamma$ |
| 0 | 0.554 111(24) | 1.769(6) | 0.554 033(19) | 1.734(9) |
| 1 | 0.554 105(27) | 1.768(11) | 0.554 053(27) | 1.744(11) |
| 2 | 0.554 076(22) | 1.756(8) | 0.554 057(16) | 1.746(8) |
| 3 | 0.554 081(13) | 1.756(5) | 0.554 082(28) | 1.757(11) |
| 4 | 0.554 083(11) | 1.756(5) | 0.554 085(31) | 1.758(12) |
| 5 | 0.554 078(16) | 1.756(7) | 0.554 071(20) | 1.752(9) |
| 6 | 0.554 082(8) | 1.757(3) | 0.554 061(10) | 1.747(5) |
| 7 | 0.554 079(12) | 1.756(5) | 0.554 061(16) | 1.747(8) |
| 8 | 0.554 085(19) | 1.759(8) | 0.554 058(15) | 1.745(8) |

**Table 4.** Estimates of $u_c$ and $\alpha$ from first and second-order differential approximants. $L$ is the order of the inhomogeneous polynomial.

| | First-order approximants | | Second-order approximants | |
|---|---|---|---|---|
| $L$ | $u_c$ | $\alpha$ | $u_c$ | $\alpha$ |
| 0 | — | — | 0.554 069(41) | 0.001(13) |
| 1 | — | — | 0.554 019(33) | 0.019(12) |
| 2 | 0.554 016(31) | 0.018(11) | 0.554 017(30) | 0.018(12) |
| 3 | 0.554 045(31) | 0.009(10) | 0.554 030(33) | 0.015(15) |
| 4 | 0.554 058(20) | 0.0040(69) | 0.554 044(26) | 0.0074(69) |
| 5 | 0.554 068(25) | 0.0008(88) | 0.554 055(32) | 0.0049(98) |
| 6 | 0.554 053(13) | 0.0062(46) | 0.554 061(25) | 0.0030(77) |
| 7 | 0.554 059(13) | 0.0042(50) | 0.554 058(28) | 0.0039(79) |
| 8 | 0.554 058(14) | 0.0041(48) | 0.554 064(24) | 0.0026(72) |

singularity at $u_- = -0.598(6)$, but as can be seen from the size of the error esimate it is not well defined. This is also reflected in the estimates of the associated exponent, ranging from 0.5 to $-0.5$, with values close to zero when $u_- \sim -0.5985$. This could indicate a logarithmic singularity at $u_-$, though the evidence is very weak. A stronger case can be made by looking at the series for the derivative of the specific heat, $\mathrm{d}C_v(u)/\mathrm{d}u$, which should have simple poles at $u_c$ and $u_-$ if $C_v(u)$ has logarithmic singularities at these points. A Dlog Padé analysis of the series revealed singularities at $u_c = 0.5540(5)$ with exponent $-1.00(4)$, at $u_- = -0.5975(10)$ with exponent $-0.95(5)$, and at $u_\pm = -0.301\,95(1) \pm 0.378\,78(1)\mathrm{i}$ with exponent $-2.177(15)$. These results thus confirm the results from the analysis of the specific-heat series itself.

The scaling law, $\alpha + 2\beta + \gamma = 2$, is seen to hold at both the critical point $u_c$ and at the non-physical singularity $u_-$. Likewise, for the spin-$\frac{1}{2}$ Ising model this scaling law holds at the sigularities $\pm(\sqrt{2} - 1)$ since $\alpha = 0$, $\beta = \frac{1}{8}$, and $\gamma = \frac{7}{4}$ in both cases. At the other non-physical singularity $u_\pm$ we find $\alpha + 2\beta + \gamma = 2.09(3)$ for the spin-1 model. From the exact solutions for the zero-field partition function and spontaneous magnetization of the spin-$\frac{1}{2}$ Ising model it follows that $\alpha = 0$ and $\beta = \frac{1}{4}$ at $u_\pm = \pm\mathrm{i}$. A differential approximant analysis of the susceptibility series yields the estimate $\gamma = 1.555(10)$ at $u_\pm$. So for the spin-$\frac{1}{2}$ we find, at $u_\pm$, that $\alpha + 2\beta + \gamma = 2.055(10)$. It seems highly likely that $\alpha + 2\beta + \gamma = 2$ holds at all the non-physical singularities. This would mean that the exponent corresponding to $\gamma$ at $u = u_{\pm} = \pm i$ for the spin-$\frac{1}{2}$ Ising model would be $\frac{3}{2}$ exactly. For the spin-1 Ising model the situation is less clear. At $u = u_{\pm}$, the analogue of $\alpha$ is 1.172, and the analogue of $\gamma$ is 1.175. It is possible that they are both $\frac{9}{8}$ exactly, or that one is 1 and the other is $\frac{5}{4}$. We have not been able to make these results more precise.

As mentioned above, ratio methods are of use only if one can find a transformation that maps the non-physical singularity outside the transformed physical disc. One such transformation is given by $u = x/(2-x)$, which leads to a new (high-temperature-like) expansion variable, $x = 1 - \tanh(\beta J/2)$. Among the various extrapolation methods (Guttmann 1989) we find that the best overall convergence is obtained from the Neville–Aitkin table. From the magnetization and susceptibility series we obtain the estimates $1/x_c = 1.4024(3)$, $\beta = 0.12(1)$ and $\gamma = 1.75(1)$. The exponent estimates are from biased approximants using the accurate value $x_c = 0.713\,05(1)$ obtained from the differential approximant analysis. While this type of analysis yields estimates of lesser accuracy than the analysis based on differential approximants it is nevertheless reassuring that the two methods are in agreement. Other extrapolation methods generally yield similar though less accurate estimates. The major source of error in all the methods is the presence of long-period oscillations in the extrapolations.

### *4.2. The critical amplitudes*

We have calculated the critical amplitudes using two different methods, both of which are very simple and easy to implement. In the first method, we note that if $f \sim A(1-u/u_c)^{-\lambda}$, then it follows that $(u_c - u)f^{1/\lambda}|_{u=u_c} \sim A^{1/\lambda}u_c$. So we simply form the series for $g(u) = (u_c - u)f^{1/\lambda}$ and evaluate Padé approximants to this series at $u_c$. The result is just $A^{1/\lambda}u_c$. This procedure works well for the magnetization and susceptibility series (it obviously cannot be used to analyse the specific-heat series). For the magnetization we find that the spread of various approximants is minimal at $u_c = 0.554\,063$ where $A_M = 1.208\,496(4)$. Allowing for a value of $u_c$ between 0.554 06 and 0.554 07 we find $A_M = 1.2084(2)$. A similar analysis for the susceptibility yields the closest agreement at $u_c = 0.554\,065$ with $A_\chi = 0.061\,64(1)$. Again allowing for a wider choice in $u_c$ we find $A_\chi = 0.0616(2)$.

In the second method, proposed by Liu and Fisher (1989), one starts from $f(u) \sim A(u)(1-u/u_c)^{-\lambda} + B(u)$ and then forms the auxiliary function $g(u) = (1-u/u_c)^{\lambda} f(u) \sim A(u) + B(u)(1-u/u_c)^{\lambda}$. Thus the required amplitude is now the *background* term in $g(u)$, which can be obtained from inhomogeneous differential approximants (Guttmann 1989, p 89). In table 5 we have listed the estimates obtained by averaging over various first-order differential approximants using at least 65 terms of the series with $u_c = 0.554\,065$. The results for the magnetization $A_M = 1.2090(20)$ and the susceptibility $A_\chi = 0.0625(10)$ agree with those obtained above, though the error estimates are much larger. These results are not seriously affected by allowing for a wider choice of $u_c$. This method can also be used to study the specific-heat series. One now starts from $f(u) \sim A(u)\ln(1-u/u_c) + B(u)$ and then looks at the auxiliary function $g(u) = f(u)/\ln(1-u/u_c)$. As before the amplitude can be obtained as the background term in $g(u)$. The results of the analysis are listed in table 5 from which we get the final estimate $A_C = 19.75(50)$.

Judging from the error estimates it would seem that the first method for calculating the amplitudes is superior to the second. This apparent superiority, however, does not hold

**Table 5.** Estimates for the critical amplitudes of the magnetization $A_M$, the susceptibility $A_\chi$ and the specific heat $A_c$ as obtained from inhomogeneous first-order differential approximants. $L$ is the order of the inhomogeneous polynomial.

| $L$ | $A_M$ | $A_\chi$ | $A_c$ |
|---|---|---|---|
| 4 | 1.2088(18) | 0.0646(58) | 18.98(33) |
| 5 | 1.2095(26) | 0.0617(30) | 19.86(69) |
| 6 | 1.2090(13) | 0.0629(26) | 20.25(61) |
| 7 | 1.2092(12) | 0.0617(20) | 19.95(55) |
| 8 | 1.2090(31) | 0.0598(46) | 19.98(65) |
| 9 | 1.2093(15) | 0.0599(42) | 19.80(33) |
| 10 | 1.2091(5) | 0.0628(15) | 19.93(31) |
| 11 | 1.2089(9) | 0.0627(14) | 19.78(26) |
| 12 | 1.2091(13) | 0.0626(9) | 19.54(29) |
| 13 | 1.2091(5) | 0.0626(12) | 19.50(44) |
| 14 | 1.2089(5) | 0.0627(11) | 19.56(40) |
| 15 | 1.2090(4) | 0.0625(8) | 19.54(40) |
| 16 | 1.2089(18) | 0.0632(22) | 19.42(44) |

up under further scrutiny. We checked the two methods on the spin-$\frac{1}{2}$ susceptibility series where the leading amplitude has been calculated to high accuracy (Wu *et al* 1976). In the widely accepted standard notation (Fisher 1967), $T\chi = C_0|1 - T/T_c|^{-7/4}$, one has, to 10 decimal places, $C_0 = 0.025\,536\,971\,9\ldots$. In our analysis we assumed a singularity, $\chi(u) \sim A_\chi|1 - u/u_c|^{-7/4}$. With $u = \exp(-2\beta J)$ it follows that $C_0 = 4u_c^4(-\ln u_c)^{-7/4}A_\chi$, where the factor $u_c^4$ arises because we analyse the series for $\chi(u)/u^4$, the factor $(-\ln u_c)^{-7/4}$ is caused by the change of variable and the factor 4 is a matter of definition. Since, $u_c = \sqrt{2} - 1$, we find that $A_\chi = 0.584\,850\,251\ldots$. Using the two methods to calculate $A_\chi$ we get the estimates $A_\chi = 0.584\,88(1)$ from the first method and $A_\chi = 0.584\,90(5)$ from the second method. This clearly shows that the smaller error estimate from the first method cannot be taken too seriously as both estimates are only marginally consistent with the exact result.

We thus conclude that $A_M = 1.208(4)$, $A_\chi = 0.0615(2)$ and $A_c = 19.8(1.0)$. Note that these amplitudes are obtained by analysing the series for $M(u)$, $\beta^{-1}u^{-4}\chi(u)$, and $(\beta J)^{-2}u^{-4}C_v(u)$, respectively, assuming in each case a singularity $\propto |1 - u/u_c|^\lambda$. Changing to the standard notation (Fisher 1967) and getting rid of the various prefactors we find: the amplitude of $M(T)$ is $B = (-\ln u_c)^{1/8}A_M = 1.131(4)$, the amplitude of $T\chi(T)$ is $C_- = (-\ln u_c)^{-7/4}u_c^4A_\chi = 0.0146(5)$ and finally the amplitude of $C_v(T)$ is $A_- = (-\ln u_c)^2u_c^4A_c = 0.65(3)$. From this we find the Watson invariant (Watson 1969)

$$A_-B^{-2}C_- = 0.0074(6)$$

which should be independent of the choice of lattice.

### 4.3. The confluent exponent

We have studied the series using three different methods in order to estimate the value of the confluent exponent. In the first method, due to Baker and Hunter (1973), one transforms the function $F$,

$$F(u) = \sum_{i=1}^{N} A_i \left(1 - \frac{u}{u_c}\right)^{-\lambda_i} = \sum_{n=0}^{\infty} a_n u^n \tag{4.4}$$

into an auxiliary function with simple poles at $1/\lambda_i$. We first make the substitution $u = u_c(1 - e^{-\zeta})$ and find

$$F(u(\zeta)) = \sum_{i=1}^{N} A_i \exp\left[-\lambda_i \ln\left(1 - \frac{u}{u_c}\right)\right] = \sum_{i=1}^{N} A_i e^{\lambda_i \zeta} = \sum_{i=1}^{N}\sum_{k=0}^{\infty} \frac{A_i \lambda_i^k \zeta^k}{k!}. \qquad (4.5)$$

By multiplying the coefficient of $\zeta^k$ by $k!$ we get the required auxiliary function

$$\mathcal{F}(\zeta) = \sum_{i=1}^{N}\sum_{k=0}^{\infty} A_i(\lambda_i\zeta)^k = \sum_{i=1}^{N} \frac{A_i}{1 - \lambda_i\zeta} \qquad (4.6)$$

which has poles at $\zeta = 1/\lambda_i$, with residues at the poles of $-A_i/\lambda_i$. In table 6 we have listed the estimates for the leading critical exponent $\beta$ and the confluent exponent $\Delta_1$ and their corresponding amplitudes as obtained from an analysis of the Baker–Hunter transformed spontaneous magnetization series with $u_c = 0.554\,065$. Only the $[N/N+1]$ approximants yield useful information. The $[N+1/N]$ approximants does not even find a pole close to $-8 = -1/\beta$, whereas some of the $[N/N]$ approximants find a pole at $-8.4(2)$ but no corresponding estimate for the confluent exponent. The results of the $[N/N+1]$ approximants certainly confirm that the leading critical exponent is $\frac{1}{8}$, and the corresponding estimates of the critical amplitudes $A_M$ are also in excellent agreement with the results obtained in the previous section. The estimates for $\Delta_1$ are less stable, but the approximants with $N \geqslant 34$ are consistent with an estimate $\Delta_1 = 1.06(2)$. These conclusions are unaltered by looking at $u_c = 0.554\,060$ and $0.554\,070$, although we note that by far the best agreement between different approximants is for $u_c = 0.554\,065$. The results for the susceptibility series are listed in table 7 for $u_c = 0.554\,065$. In this case we again confirm the values of the leading critical exponent and critical amplitudes. The results for the confluent singularity is much more confusing as the $[N/N+1]$ approximants yields the estimate $\Delta_1 = 1.155(5)$, very different from the estimate $\Delta_1 = 1.4(1)$ obtained from the $[N+1/N]$ approximants. The $[N/N]$ approximants generally yield no estimates for this value of $u_c$. However, at slightly higher values of $u_c$, the $[N/N]$ approximants also become useful, though they favour neither one nor the other of the $\Delta_1$-estimates cited above. This is clearly seen in figure 3 where we have plotted the estimate for $\Delta_1$ versus the parameter $u_c$ used in the Baker–Hunter transformation for various approximants with $N \geqslant 36$. The different approximants $[N/N+1]$, $[N/N]$, and $[N+1/N]$ clearly bunch together in three distinct classes. The $[N/N+1]$ approximants exhibit a narrow crossing at $\Delta_1 = 1.13(2)$

**Table 6.** Estimates for the leading critical exponent $\beta$ and the confluent exponent $\Delta_1$ plus the associated amplitudes from $[N/N+1]$ Padé approximants to the Baker–Hunter transformed series for the magnetization with $u_c = 0.554\,065$.

| $N$ | $\beta$ | $A_M$ | $\Delta_1$ | $A_M a_{M,1}$ |
|---|---|---|---|---|
| 30 | 0.124 80 | 1.2070 | 1.147 | −0.375 |
| 31 | 0.124 74 | 1.2066 | 1.180 | −0.424 |
| 32 | 0.124 52 | 1.2052 | — | — |
| 33 | 0.124 86 | 1.2074 | 1.120 | −0.343 |
| 34 | 0.124 96 | 1.2080 | 1.072 | −0.297 |
| 35 | 0.124 95 | 1.2080 | 1.076 | −0.300 |
| 36 | 0.125 00 | 1.2084 | 1.050 | −0.280 |
| 37 | 0.125 00 | 1.2084 | 1.050 | −0.280 |
| 38 | 0.124 98 | 1.2083 | 1.058 | −0.286 |
| 39 | 0.124 98 | 1.2082 | 1.063 | −0.290 |

**Table 7.** Estimates for the leading critical exponent $\gamma$ and the confluent exponent $\Delta_1$ plus the associated amplitudes from $[N/N+1]$ and $[N+1/N]$ Padé approximants to the Baker–Hunter transformed series for the susceptibility with $u_c = 0.554\,065$.

| | $[N/N+1]$ | | | | $[N+1/N]$ | | | |
|---|---|---|---|---|---|---|---|---|
| $N$ | $\gamma$ | $A_\chi$ | $\Delta_l$ | $A_\chi a_{\chi,l}$ | $\gamma$ | $A_\chi$ | $\Delta_l$ | $A_\chi a_{\chi,l}$ |
| 28 | 1.7407 | 0.064 75 | 1.235 | 0.5851 | 1.7372 | 0.066 05 | — | — |
| 29 | 1.7564 | 0.059 91 | 1.110 | 0.4221 | 1.7481 | 0.062 65 | 1.338 | 1.5032 |
| 30 | 1.7529 | 0.060 92 | 1.129 | 0.4429 | 1.7461 | 0.063 24 | 1.369 | 1.8334 |
| 31 | 1.7429 | 0.064 11 | 1.233 | 0.5908 | 1.7405 | 0.065 02 | — | — |
| 32 | 1.7494 | 0.062 01 | 1.155 | 0.4733 | 1.7443 | 0.063 79 | 1.406 | 2.3719 |
| 33 | 1.7492 | 0.062 06 | 1.156 | 0.4750 | 1.7441 | 0.063 87 | 1.413 | 2.4897 |
| 34 | 1.7498 | 0.061 87 | 1.151 | 0.4686 | 1.7448 | 0.063 63 | 1.394 | 2.1671 |
| 35 | 1.7498 | 0.061 87 | 1.151 | 0.4684 | 1.7448 | 0.063 62 | 1.393 | 2.1561 |
| 36 | 1.7494 | 0.061 99 | 1.155 | 0.4727 | 1.7448 | 0.063 62 | 1.394 | 2.1575 |
| 37 | 1.7490 | 0.062 10 | 1.158 | 0.4773 | 1.7448 | 0.063 62 | 1.394 | 2.1633 |

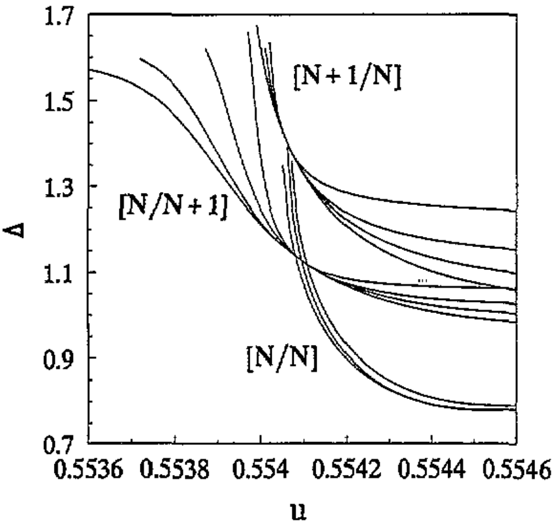


**Figure 3.** Estimates for the confluent exponent $\Delta$ versus the parameter $u_c$ of the Baker–Hunter transformation. All Padé approximants with $36 \leqslant N \leqslant 39$ are shown.

and $u_c = 0.554\,10(5)$, whereas the $[N+1/N]$ approximants cross at $\Delta_1 = 1.40(5)$ and $u_c = 0.554\,06(2)$ and the $[N/N]$ approximants, though not intersecting mutually, do seem to cross through both the above regions. Note that the $[N/N]$ approximant does not yield any estimates below $u_c \simeq 0.554\,06(2)$. From these results it is not possible to infer a final estimate for $\Delta_1$ and we are unable to explain the very different behaviour exhibited by the various sets of approximants.

The second method, due to Adler *et al* (1981), involves studying Dlog Padé approximants to the function $G(u)$, where

$$G(u) = \lambda F(u) + (u_c - u)\mathrm{d}F(u)/\mathrm{d}u\,.$$

The logarithmic derivative to $G(u)$ has a pole at $u_c$ with residue $\lambda + \Delta_1$, where $\lambda$ is the leading critical exponent. We evaluate the Dlog Padé approximants for a range of guesses for $u_c$ and $\lambda$. For each such guess we thus find an estimate for $\Delta_1$; for the correct value of $u_c$ and $\lambda$ we should see a convergence region in the $(u_c, \lambda, \Delta_1)$-space. In practice we always froze $\lambda$ at its expected exact value and plotted $\Delta_1$ as a function of $u_c$. Figure 4 shows $\Delta_1$ as

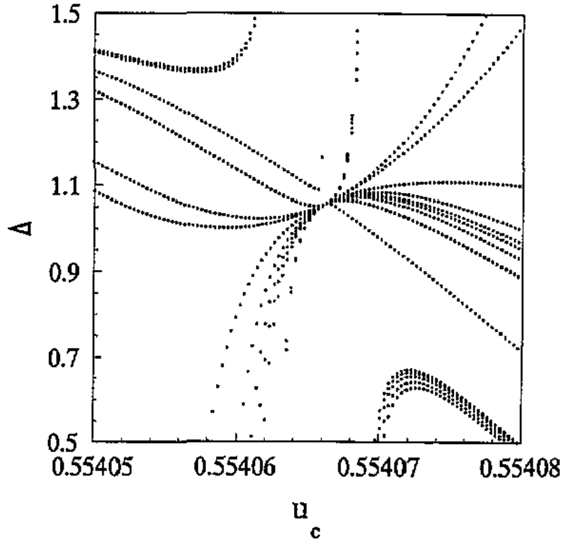


**Figure 4.** The confluent exponent $\Delta$ versus $u_c$ as obtained from the method of Adler *et al* (1981) applied to the spontaneous magnetization series.

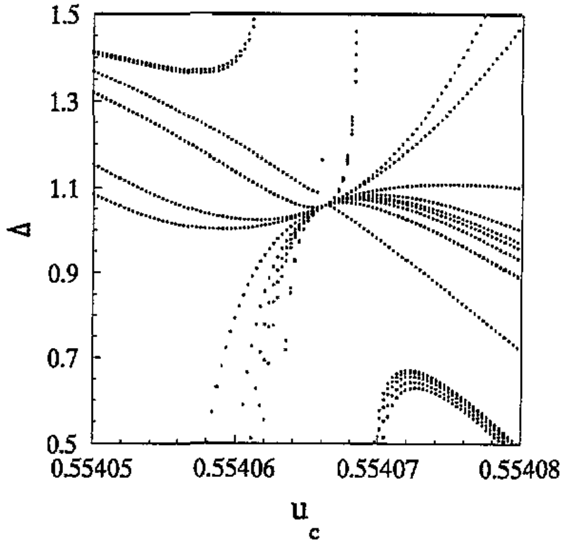


**Figure 5.** Same as in figure 4, but for the susceptibility series.

a function of $u_c$ with $\beta = \frac{1}{8}$ using the spontaneous magnetization series. In this figure we see a very narrow convergence region at $u_c = 0.544066(1)$ and $\Delta_1 = 1.06(2)$. In figure 5 we have plotted similar results from an analysis of the susceptibility series with $\gamma = \frac{7}{4}$. In this case we find a narrow crossing region at $u_c = 0.5540695(15)$ and $\Delta_1 = 1.15(2)$.

The last method, also due to Adler *et al* (1983), is a generalization of an approach devised by Roskies (1981) to study the high-temperature susceptibility of the three-dimensional spin-$\frac{1}{2}$ Ising model. The first step is to transform the series $F(u)$ to ones in

$$y = 1 - (1 - u/u_c)^{\Delta}$$

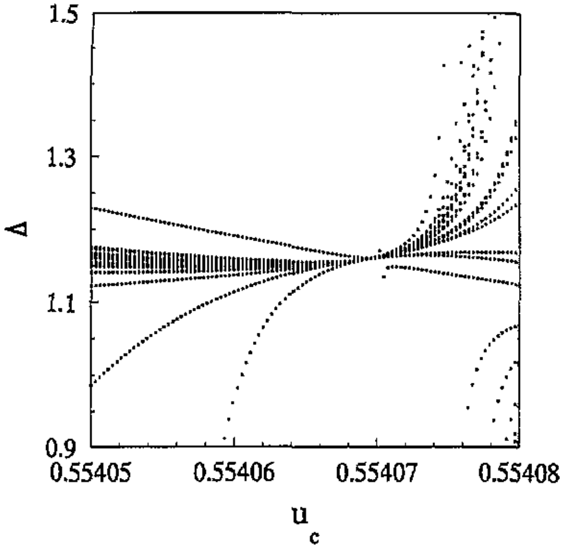


**Figure 6.** The exponent $\beta$ as a function of the parameter $\Delta$ used in the generalized Roskie transformation of Adler *et al* (1983) applied to the spontaneous magnetization series. The inset shows the details of the crossing region.

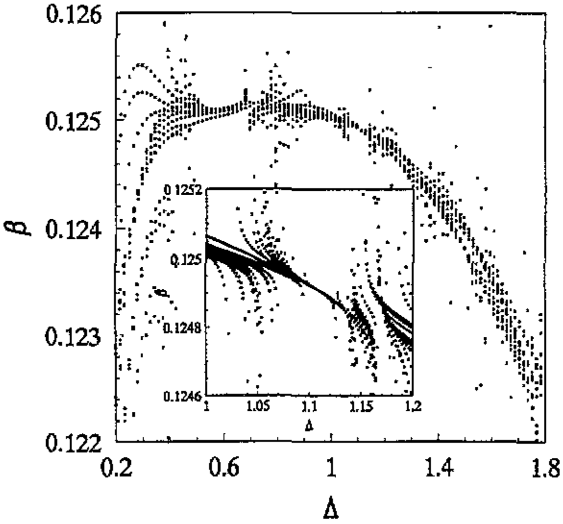


**Figure 7.** Same as in figure 6, but for the susceptibility series.

where $u_c$ is assumed known but $\Delta$ is a variable parameter. Next one looks at different Padé approximants to the function

$$\mathcal{G}_\Delta = \Delta(y-1)\frac{\mathrm{d}}{\mathrm{d}y}\ln F(y,\Delta) \sim \lambda + O[(1-y)^{\Delta_1/\Delta}].$$

For the correct guesses for $u_c$ and $\Delta_1$ the various Padé approximants should intersect and give a correct estimate for the leading critical exponent $\lambda$. In figure 6 we have plotted the estimate for $\beta$ as a function of the transformation variable $\Delta$ with $u_c = 0.554\,065$ using the spontaneous magnetization series. A narrow crossing region is found at $\Delta_1 = 1.11(1)$ and $\beta = 0.124\,90(5)$. Figure 7 shows a similar plot but for the susceptibility series; in this case we locate the crossing at $\Delta_1 = 1.16(1)$ and $\gamma = 1.749(1)$.

The value of the correction-to-scaling exponent of two-dimensional Ising systems has been addressed by several authors. Nienhuis (1982) has mapped the $q$-state Potts model in two dimensions onto a model which is in the Ising universality class (when $q$ is set to 2). In that case one obtains a value $\Delta_1 = \frac{4}{3}$. Barma and Fisher (1985) obtained $\Delta_1 = 1.35 \pm 0.25$ at the pure Ising critical point of the Klauder and double Gaussian models. They point out that while this is inconsistent with the expectation of pure logarithmic corrections to scaling, it is possible for these logarithmic terms to have amplitudes that vanish on approach to the pure Ising limit in such a way as to be describable by an apparent correction-to-scaling exponent $\Delta_1 = \frac{4}{3}$.

The various estimates we have obtained for the spin-1 model appear to be entirely consistent with this complex and subtle behaviour.

## 5. Summary and discussion

In this work we have extended substantially the existing low-temperature series for the two-dimensional spin-1 Ising model by introducing a new version of the finite-lattice method which saves considerable space over previous implementations. The usefulness of such extended series is demonstrated by our analysis, in which we find that the correct results are clearly evident only after more than 60 terms in the series!

The analysis of the new spin-1 series provides us with an accurate estimate of the critical point, $u_c = 0.554\,065(5)$, where the error estimate is chosen rather conservatively, and reflects the descripancy between estimates obtained from the three series and using different methods of analysis. Our value is in excellent agreement with a recent estimate $u_c \simeq 0.554\,066$ obtained by Lipowski and Suzuki (1992) from a transfer-matrix version of the double cluster mean-field approximation, and also agrees with the estimate $u_c = 0.554\,071(3)$ of Blöte and Nightingale (1985) obtained by phenomenological renormalization using the correlation length of a $n \times \infty$ systems calculated with transfer-matrix techniques. However, our results and those mentioned above, clearly rule out a recent conjecture $u_c = 0.553\,887\ldots$ by Urumov (1988) for the *exact* value of the critical point obtained from a generalization of a method proposed by Švrakić (1980) to calculate the exactly known equations for the critical temperature of the spin-$\frac{1}{2}$ Ising model on a chequerboard lattice.

The evidence for the leading critical exponents clearly show that the spin-1 Ising model belongs to the usual Ising universality class, a point also supported strongly by the results of Blöte and Nightingale (1985), i.e. the critical exponents take the values $\beta = \frac{1}{8}$, $\gamma = \frac{7}{4}$, and $\alpha = 0$, exactly. In addition we find a non-analytic confluent correction with an exponent $\Delta_1 > 1$. Generally the magnetization series favours a value of $\sim 1.05$, whereas the susceptibility series yields estimates $\sim 1.15$. One notable exception is the $[N + 1/N]$ approximants to the Baker–Hunter-transformed susceptibility series which leads to estimates $\sim 1.4$. From field-theoretic arguments it is expected that the value of $\Delta_1$ should be the same for both series. This leads us to the final estimate $\Delta_1 = 1.1(1)$, in good agreement with the result $1 < \Delta_1 < 1.3$ of Adler and Enting (1984), but clearly smaller than the field-theoretic prediction $\Delta_1 = 1.4$ (Le Guillou and Zinn-Justin 1980), and the 'exact' value $\Delta_1 = \frac{4}{3}$ found by Nienhuis (1982).

The new finite-lattice method is also directly generalizable to higher-spin Ising models, as well as to other two-dimensional systems. The extended series for the low-temperature susceptibility of the quadratic spin-$\frac{1}{2}$ Ising model is in excellent agreement with the numerical predictions of Gartenhaus and McCullough (1988). Our exact coefficients agree to all seven predicted significant digits.

## Acknowledgments

We would like to thank Michael E Fisher for helpful discussions on the question of correction-to-scaling exponents. Financial support from the Australian Research Council is gratefully acknowledged by AJG and IJ.

## Appendix. First correction term

In section 2 we described how to obtain series expansions from the finite-lattice method. We ran the program up to $b_{\max} = 8$, yielding a series correct through order $u^{78}$. When running the program one may actually calculate the truncated series in $u$ to orders beyond that to which the series coefficients are correct. One would expect at least the first incorrect coefficient derived in this fashion to deviate only a little from the correct one. In this appendix we describe a correction procedure whereby we were able to obtain one additional correct term and thus extend the series to order $u^{79}$. At first we just looked at the first correction term for $b_{\max} = 2$–7, i.e. the difference between the correct series coefficients and the first incorrect ones for a given value of $b_{\max}$, but were unable to find a pattern allowing us to 'guess' the correction term for $b_{\max} = 8$. Next we re-ran the program deriving a series using $q = 2$ hoping that the correction terms for the $q = 2$ case were the same as those for the spin-1 model ($q = 3$). It turns out that the correction terms is the two cases are almost identical. In table A1 we have listed the amount by which the $q = 2$ correction terms fail to predict the spin-1 correction terms. One could thus obtain almost correct spin-1 correction terms for $b_{\max} = 8$ using just the $q = 2$ correction term. However, we found that the numbers in table A1 obey recursive relations. Let $\Delta_x^b = \delta_x^b / b_{\max}$; then we find the following recurrence relations for the $\Delta$'s, in the case of the partition function:

$$\Delta_{Z_0}^{b+2} - 2\Delta_{Z_0}^{b+1} + \Delta_{Z_0}^{b} = -9$$

the magnetization

$$\Delta_{M}^{b+3} - 3\Delta_{M}^{b+2} + 3\Delta_{M}^{b+1} - \Delta_{M}^{b} = 81 \qquad \text{(A.1)}$$

and the susceptibility

$$\Delta_{\chi}^{b+4} - 4\Delta_{\chi}^{b+3} + 6\Delta_{\chi}^{b+2} - 4\Delta_{\chi}^{b+1} + \Delta_{\chi}^{b} = -972\,. \qquad \text{(A.2)}$$

Using these recurrence relations we find $\Delta_\chi^8$ and thus using the $q = 2$ correction terms for $b_{\max} = 8$ we can finally find the correction terms for the spin-1 model and thus the correct coefficient to $u^{79}$.

Though the correction procedure is rather cumbersome it should be noted that the CPU time required to calculate the truncated series with $b_{\max} = 2$–7 for $q = 3$ and $b_{\max} = 2$–9

**Table A1.** The difference between the first correction terms with $q = 2$ and 3 for the partition function ($\delta_{Z_0}$), magnetization ($\delta_{M}$), and susceptibility ($\delta_\chi$).

| $b_{\max}$ | $\delta_{Z_0}$ | $\delta_{M}$ | $\delta_\chi$ |
|---|---|---|---|
| 2 | −20 | 180 | −1 620 |
| 3 | −84 | 1 008 | −12 096 |
| 4 | −220 | 3 300 | −49 500 |
| 5 | −455 | 8 190 | −147 420 |
| 6 | −816 | 17 136 | −359 856 |
| 7 | −1330 | 31 920 | −766 080 |

for $q = 2$ is insignificant compared to the time it takes to run the program with $b_{\max} = 8$ and $q = 3$.

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