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Series studies of the Potts model: I. the simple cubic Ising model

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Abstract. The finite-lattice method of series expansion is generalized to the q-state Potts model on the simple cubic lattice. It is found that the computational effort grows exponentially with the square of the number of series terms obtained, unlike two-dimensional lattices where the computational requirements grow exponentially with the number of terms. For the Ising ($q = 2$) case we have extended the low-temperature series for the partition functions, magnetization and zero-field susceptibility to u^{26} from u^{20}. The high-temperature series for the zero-field partition function is extended from v^{18} to v^{22}. Subsequent analysis gives critical exponents in agreement with those from field theory.

1. Introduction

This is the first of a series of papers describing the application of the finite-lattice method of series expansion to various cases of the q-state Potts model. A major objective in this work is the study of the $q = 3$ case in three dimensions because of its relevance to quantum chromodynamics. However, in the course of this project we have developed extremely powerful techniques for series expansion. This has made it possible to obtain considerable extensions to many Potts model series and so we have been able to investigate a large range of lattice statistics problems.

In this paper we describe the application of the finite-lattice method of series expansions to the derivation of high- and low-temperature expansions for the free energy of the Potts model on the simple cubic lattice. We present series for the Ising model which is the $q = 2$ case of the Potts model. We have been able to extend the low-temperature series for the zero-field partition function, magnetization and susceptibilty from order u^{20} (Sykes *et al* 1973) or u^{24} (M F Sykes, unpublished) to u^{26}. The zero-field high-temperature series for the partition function has been extended from v^{18} (Sykes *et al* 1972) to v^{22}. The variables $u = \exp(-4J/kT)$ and $v = \tanh(J/kT)$ are the usual low- and high-temperature model expansion variables for the Ising model. (A recent paper by Bhanot *et al* (1992) calculates low-temperature series for the simple cubic Ising model using a variant of the finite-lattice method that is apparently less efficient than ours. They obtain series for the magnetization to u^{20} and the internal energy to order u^{24}, thus duplicating the work of Sykes *et al* (1973) and Sykes (unpublished) respectively.)

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The extension of these series is particularly pertinent as their behaviour is quite difficult to determine. While the high-temperature series are well behaved, with uncertainty as to critical exponents being confined to the fourth, or at the worst third, decimal place, the situation at low temperatures is far less satisfactory. For many years there was considerable controversy as to the symmetry or otherwise of the critical exponents above and below the critical temperature. That this is now less controversial is not based on good numerical evidence however, but rather on a strengthening belief in universality based on a better understanding of the connection between field theory and critical phenomena. Nickel (1991) has also recently argued for the extension of perturbation series, in order to remove any lingering doubts about the equivalence of the ϕ^4 field theory, and the lattice models.

The new low-temperature series we have obtained here permits an improved analysis, though the quality of the numerical estimates is still inferior to that of the high-temperature series. Nevertheless, by biasing our analysis with the value of the critical temperature, obtained from the high-temperature series, and by assuming a confluent exponent around $\frac{1}{2}$ (the exact value is unimportant), exponent estimates are obtained that are consistent with the best field-theory estimates. We have also extended the high-temperature zero-field free energy series, which allows us to estimate α considerably more accurately than has been possible previously.

The finite-lattice method of series expansions for lattice statistics problems has been applied to a number of different systems on a range of two-dimensional lattices. The initial application was in calculating the high-temperature expansion of the three-state Potts model (de Neef 1975, de Neef and Enting 1977). The expansion of the limit of chromatic polynomials (Kim and Enting 1979) was formally a high-temperature expansion and the enumeration of self-avoiding polygons (Enting 1980a, Enting and Guttmann 1985, Guttmann and Enting 1988a) is closely related to high-temperature expansions. However most of the subsequent applications of the method (based on the work of Enting (1978a)) have been in the derivation of low-temperature or high-field expansions, generally on the square lattice (e.g. Enting 1980b, Adler *et al* 1983). Series for triangular lattice systems have been obtained by regarding them as square lattices with additional interactions (Enting 1980c, Enting and Wu 1982). Specific combinatorial expressions for triangular lattice systems are known (Enting 1980d, 1987a). However these involve the additional complication of calculating the partition functions of hexagonal finite lattices. The only application using full triangular symmetry has been in the enumeration of polygons on the triangular lattice (Enting and Guttmann 1992). The finite-lattice method has also been applied to Potts models on the chequerboard lattice (Enting 1987b) and polygons on the honeycomb lattice (Enting and Guttmann 1989). These last two cases were treated as modifications of the square lattice.

Enting (1978b) quoted some of the combinatorial results required for the finite-lattice method on the simple cubic lattice but until now these results have not been applied. In this paper we describe the formalism for obtaining either high-temperature or low-temperature expansions for the Potts model on the simple cubic lattice. We present and analyse specific results for the Ising model case.

The outline of the remainder of the paper is as follows. Section 2 analyses the combinatorial aspects of applying the finite-lattice method on the simple cubic lattice. Section 3 describes the expansions that we have calculated. Section 4 describes an analysis of these series.

2. Finite-lattice expansions on the simple cubic lattice

We begin by defining the notation that we shall use throughout this series of papers. The Potts model is defined on a lattice in terms of a 'spin' variable, s_j at each site, j, taking integer values from 0 to $q-1$. There is an energy difference, ΔE, between aligned and non-aligned states that interact. Generally we consider interactions confined to pairs of nearest-neighbour sites, i.e. those joined by the bonds of the lattice. Sites aligned in the '0' direction differ by a field energy H from sites with other alignments. Thus with $\delta(m,n)=1$ of $m=n$ and 0 otherwise, the Hamiltonian is written

$$\hat{H} = \sum_{(i,j)} \Delta E(1-\delta(s_i,s_j)) + \sum_i H(1-\delta(s_i,0)) \tag{1}$$

where the first sum is over all pairs of interacting sites and the second sum is over all sites.

The low-temperature expansion variable is $z=\exp(-\beta\Delta E)$ where $\beta = 1/kT$. For the field dependence, we use the expansion variables $\mu = \exp(-\beta H)$ and $x = 1-\mu$. The general Potts model high-temperature expansion variable is $v=(1-z)/(1+(q-1)z)$.

For the Ising model (i.e. $q=2$), only even powers of z occur and the natural low-temperature expansion variable is $u=z^2=\exp(-4\beta J)$ and the high-temperature expansion variable can be written as $v=\tanh(\beta J)$ with $2J=\Delta E$. For zero-field on bi-partite lattices, only even powers of v have non-zero coefficients in the high-temperature Ising model expansion.

The basic formulation of the finite-lattice method approximates the partition function per site, Z, as

$$Z = \lim_{|\Gamma|\to\infty} Z_\Gamma^{1/|\Gamma|} \approx \prod_{\alpha\in A} Z_\alpha^{W(\alpha)} \tag{2a}$$

where Γ denotes a lattice that becomes arbitrarily large in all directions and $|\Gamma|$ denotes the number of sites in Γ. Here A is a set of finite lattices, α, with A closed under the operation of intersection of finite lattices. For the simple cubic lattice, this general relation has the specific form:

$$Z = \lim_{N\to\infty} Z_{NNN}^{1/N^3} \approx \prod_{[p,q,r]\in A} Z_{pqr}^{W(p,q,r)} \tag{2b}$$

where Z_{pqr} is the partition function of a cuboid of dimensions $p\times q\times r$ sites. For low-temperature expansions, the Z_{pqr} are to be evaluated with a surrounding layer of fully ordered sites. For high-temperature expansions, the Z_{pqr} are to be evaluated with free boundary conditions. (It is also convenient to remove common factors as described below.) The weights $W(p,q,r)$ depend on the set, A, over which the product is taken. In approximations (2*a*, 2*b*) an appropriate choice of weights will give Z as a series correct up to, but not including, the order of the first connected graph that will not fit into any of the cuboids of set A (Enting 1978a).

The method of Bhanot *et al* (1992) uses generalized helical boundary conditions imposed in a sequence of configurations so that they can ultimately remove the effect of unwanted graphs that occur under helical or periodic boundary conditions.

Inspection of the low-temperature expansion of the Potts model shows that the limiting graphs are trees that do not double back in any direction: all planes drawn perpendicular to bonds of the lattice intersect such trees at most once. Such a tree can span a cuboid of size $p \times q \times r$ with $p+q+r-2$ sites and $p+q+r-3$ bonds in the tree and will give powers of $4(p+q+r)-6$ or more in the Potts model low-temperature variable, z.

Therefore it is appropriate to take A as the set of cuboids whose spans, σ, satisfy

$$\sigma = p+q+r \leqslant s.$$

For this choice of A, the first incorrect low-temperature term is of order $4(s+1)-6$, i.e. the series is correct to order $4s-3$. We use the notation $A(s) = \{[p,q,r] : p+q+r \leqslant s\}$ to denote the set of cuboids used.

Inspection of the high-temperature expansion shows that, for general fields, the same tree graphs are limiting. However, for zero field, the limiting graphs are maximally extended polygons. These are polygons that have at most two intersections with any plane perpendicular to the lattice bonds. These are the three-dimensional generalization of the convex polygons (Guttmann and Enting 1988b) that were used to obtain corrections in the polygon enumeration by Guttmann and Enting (1988a). For cuboids of span $s+1$ the maximally extended polygons will have $2(s+1)-6$ steps so that cuboids of span $\leqslant s$ will give the zero-field high-temperature series correct to $2s-5$. The combinatorial factors from Enting (1978b) give

$$W(d,w,\ell) = \sum_{[p,q,r]\in A(s)} \eta(p-d)\,\eta(q-w)\,\eta(r-\ell) \qquad \text{for } [d,w,L] \in A(s) \quad (3)$$

where

$$\eta(0) = 1 \tag{4a}$$

$$\eta(1) = -2 \tag{4b}$$

$$\eta(2) = 1 \tag{4c}$$

$$\eta(k) = 0 \qquad \text{otherwise.} \tag{4d}$$

This implies

$$W(d,w,\ell) = 1 \qquad \text{for } d+w+\ell = s \tag{5a}$$

$$= -5 \qquad \text{for } d+w+\ell = s-1 \tag{5b}$$

$$= 10 \qquad \text{for } d+w+\ell = s-2 \tag{5c}$$

$$= -10 \qquad \text{for } d+w+\ell = s-3 \tag{5d}$$

$$= 5 \qquad \text{for } d+w+\ell = s-4 \tag{5e}$$

$$= -1 \qquad \text{for } d+w+\ell = s-5 \tag{5f}$$

$$= 0 \qquad \text{otherwise.} \tag{5g}$$

In actual computation it is convenient to exploit the cubic symmetry and consider only $d \leqslant w \leqslant \ell$. We define $B(s) = \{[p,q,r] : p+q+r \leqslant s, p \leqslant q \leqslant r\}$. The expansion becomes

$$Z \approx \prod_{[p,q,r] \in B(s)} Z_{pqr}^{V(p,q,r)} \tag{6a}$$

with

$$V(p,q,r) = \sum_{\pi(p,q,r)} W(\pi(p,q,r)) \qquad \text{for } p \leqslant q \leqslant r \tag{6b}$$

where the sum is over all *distinct* permutations, $\pi(p,q,r)$ of the indices.

The partition functions are constructed by using a transfer-matrix formalism to build up ℓ layers of size $d \times w$. As in all of the most recent applications of the finite-lattice method, we used the approach of building up the finite lattices one site at a time. The computational complexity of the calculation is determined by the value of $d \times w$ that is required and this is determined by the limiting span s. Exploiting the cubic symmetry allows the series to be generated using cuboids whose size is subject to

$$1 \leqslant d \leqslant d_{\max} \qquad \text{and } d \leqslant w \leqslant \lfloor (s-d)/2 \rfloor \qquad \text{and } w \leqslant \ell \leqslant s-d-w.$$

If $s = 3m+1$ then $d_{\max} = m$ and the maximum size of $d \times w$ is $m \times m$. If $s = 3m-1$ then $d_{\max} = m-1$ and the largest size of $d \times w$ is $(m-1) \times m$. (The case of $s = 3m$ has $d \times w = m \times m$ but this is of little interest because the transfer matrices will be the same size as is required for the case $s = 3m+1$ which gives four extra low-temperature series terms and two extra high-temperature terms.)

The limiting factor in the finite-lattice series computations is the size of the vector required to store the site configurations at the end of a partly built lattice. In a departure from the earlier high-temperature calculations noted in the introduction, it has been desirable to use a site representation rather than a bond representation when calculating the Z_{pqr} required for high-temperature expansions. Thus size considerations are the same for both high- and low-temperature expansions. For the expansions of q-state models on the simple cubic lattice the number of site configurations required is q^k with $k = d \times w$. For the q-state Potts model ($q \geqslant 3$) the symmetry between the states can be used to remove redundant elements. There will be approximately $q^k/(q-1)!$ distinct vector elements. The precise number can be calculated using a recurrence relation. Since the present paper only considers $q = 2$ for which exactly 2^k states are required, the general recurrence relation will be described in the second paper. For zero-field high-temperature expansions, there is no need to distinguish the '0' state and so for a cross section of k sites, approximately $q^k/q!$ vector elements are needed.

Thus vectors of approximately $q^{m^2}/(q-1)!$ elements give Potts series correct to z^{12m+1} while vectors of $q^{m(m-1)}/(q-1)!$ elements give Potts series to z^{12m-7}. Vectors of size 2^{m^2} elements give Ising series correct to u^{6m} while vectors of size $2^{m(m-1)}$ elements give Ising series correct to u^{6m-4}. For zero-field high-temperature expansions, vectors of approximately $q^{m^2}/q!$ elements give Potts series correct to v^{6m-3} while vectors of $q^{m(m-1)}/q!$ elements give Potts series to v^{6m-7}. Vectors of

size 2^{m^2-1} elements give Ising series correct to v^{6m-4} while vectors of size 2^{m^2-m-1} elements give Ising series correct to v^{6m-8}.

In contrast, for the square lattice, the cross section, k, corresponds to the width of the lattice (expressed as a number of sites) and so vectors of size $\approx q^k/(q-1)!$, will give Potts model low-temperature series correct to $4k+3$. Duality gives the high-temperature series to the same order. Table 1 lists the low-order values of m together with the number of series terms obtainable for models on the simple cubic lattice and the size of vector required for the Ising model.

Table 1. Combinatorial factors determining the computational complexity of finite-lattice series expansions on the simple cubic lattice. Column 1 gives the various possible cutoff points as specified by the largest cross-section that need be considered after making optimal use of cubic symmetry. The second column is s, the largest value of the sum of length plus width plus depth for any of the cuboids used in the expansion. The low-temperature series for the Potts model can be obtained to order z^{4s-3} and the high-temperature series to v^{2s-5}. Ising model series can be obtained to u^{2s-2} and v^{2s-6}. The final column, $R(.,2)$, gives the number of vector elements required for the low-temperature Ising expansion.

		Order of Potts (Ising) series		
Cross section	s	Low-T	High-T	$R(d \times w, 2)$
1 × 1	4	13 (6)	3 (2)	2
1 × 2	5	17 (8)	5 (4)	4
2 × 2	7	25 (12)	9 (8)	16
2 × 3	8	29 (14)	11 (10)	64
3 × 3	10	37 (18)	15 (14)	512
3 × 4	11	41 (20)	17 (16)	4096
4 × 4	13	49 (24)	21 (20)	65 536
4 × 5	14	53 (26)	23 (22)	1 048 576
5 × 5	16	61 (30)	27 (26)	33 554 432

While Bhanot *et al* (1992) compared the combinatorial complexity of their technique with the finite-lattice method with periodic boundary conditions, they made no comparisons with our formalism (see Enting 1987a, Guttmann and Enting 1990b) using fixed boundary conditions. Their note gives too few details of the characterstics of their cancellation procedure for us to make a general comparison. However from the specific example, it appears that they need 24 spins (i.e. 2^{24} configurations) to reach u^{24}, while, as shown in table 1, we require only 16 spins.

In principle, it is possible to consider extending the series by determining correction terms to the finite-lattice expansion. Previous studies (Enting and Wu 1982, Guttmann and Enting 1988b) have obtained explicit expressions for the leading-order correction terms for various models. For the minimal spanning trees direct enumeration seems difficult. However, examination of the series shows that M such trees will give a correction of

$$(q-1)M\mu^{s-1}[z^{4s-2} + \tfrac{1}{2}(q-2)(s-2)z^{4s-1}]$$

to the low-temperature series for the q-state Potts model. For $q \geqslant 3$ the number M can be determined by noting the correction required at the corresponding s value for the less complex $q = 2$ (Ising model) case. For the high-temperature series, the

zero-field correction from maximally extended polygons is of the form $K(q-1)v^{2s-4}$. Again the Ising case can be used to determine the correction for higher q. Since the smaller the q the larger the lattice that can be used, our highest-order Ising cases can be used to provide the correction terms for future $q = 3$ studies, as used in paper III of this series (Enting and Guttmann 1993).

3. Expansions

The finite-lattice method obtains the high- and low-temperature expansions for the partition function, Z. For actual calculations, specific normalizations must be chosen. For low-temperature expansions, the appropriate choice is to define the partition function such that the fully aligned (all sites '0') state is taken as having zero energy, since the low-temperature series is a perturbation expansion about this state. This is the normalization that we have chosen for equation (1), defining the Hamiltonian. In this normalization, the partition function is often denoted Λ. On the simple cubic lattice, the Ising model expansion begins

$$\Lambda = 1 + u^3\mu + 3u^5\mu^2 + \cdots. \tag{7}$$

As noted above, we express the field variable as $\mu = 1 - x$ and, in order to reduce the memory required by the computer program, truncate the field dependence at x^2 so that

$$\Lambda = \Lambda_0(u) + x\Lambda_1(u) + x^2\Lambda_2(u) + \cdots. \tag{8}$$

We express Λ_0 as

$$\Lambda_0 = \sum_{n=0}^{\infty} \lambda_n u^n \tag{9}$$

and define an order parameter

$$M = 1 + \frac{q}{q-1}\frac{\Lambda_1}{\Lambda_0} = \sum_{n=0}^{\infty} m_n u^n \tag{10}$$

and susceptibility

$$\chi = 2\frac{\Lambda_2}{\Lambda_0} - \frac{\Lambda_1}{\Lambda_0} - \left(\frac{\Lambda_1}{\Lambda_0}\right)^2. \tag{11}$$

We have determined the low-temperature expansion using cross-sections up to 4×5, giving Λ_0, M and χ correct to u^{26}. The coefficients λ_n, m_n, c_n are listed in table 2.

The calculations build up the finite lattice one site at a time, running through all q states of the site and applying a weight of 1 for state '0' and μ (expressed as $1 - x$) for all other states. The bonds linking each new site to the partly constructed lattice are given weight 1 if the sites at each end are in the same state and weight z otherwise. For low-temperature expansions, the set of bonds considered includes

Table 2. Coefficients in low-temperature expansions for Λ_0, M and χ and high-temperature expansion for Φ, defined by equations (9), (10), (11) and (17). The incomplete coefficient, a_{24}, was not derived using the finite-lattice method, but represents an extrapolation obtained using differential approximants.

n	λ_n	m_n	c_n	a_n
0	1	1	0	1
3	1	−2	1	0
4	0	0	0	3
5	3	−12	12	0
6	−3	14	−14	22
7	15	−90	135	0
8	−30	192	−276	192
9	101	−792	1520	0
10	−261	2148	−4056	2046
11	807	−7716	17 778	0
12	−2308	23 262	−54 392	24 853
13	7065	−79 512	213 522	0
14	−21 171	252 054	−700 362	329 334
15	65 337	−846 628	2 601 674	0
16	−200 934	2 753 520	−8 836 812	4 649 601
17	627 249	−9 205 800	31 925 046	0
18	−1 962 034	30 371 124	−110 323 056	68 884 356
19	6 192 066	−101 585 544	393 008 712	0
20	−19 610 346	338 095 596	−1 369 533 048	1 059 830 112
21	62 482 527	−1 133 491 188	4 844 047 090	0
22	−199 807 110	3 794 908 752	−16 947 396 000	16 809 862 992
23	641 837 193	−12 758 932 158	59 723 296 431	0
24	−2 068 695 927	42 903 505 030	−209 328 634 116	27 337xxxxxx
25	6 691 611 633	−144 655 483 440	736 260 986 208	0
26	−21 710 041 944	488 092 130 664	−2 582 605 180 212	

bonds connecting the finite lattice to an outer boundary of sites taken as being in state '0'.

The high-temperature expansions have been obtained using cross-sections up to 4×5, giving Z to order v^{22}. While table 1 indicates that the vector size increases by a factor of 16 (or more generally q^4) on going from 4×4 to 4×5, for high-temperature expansions, the memory requirements are reduced by a factor of 2 (or more generally a factor of q) by making full use of the symmetry and by a further factor of 3 since the high-temperature field dependence is truncated at zeroth order compared with the x^2 truncation of the low-temperature series. In principle it is possible to further reduce the memory requirements for the high-temperature Ising free energy calculation by making use of the ferromagnetic/antiferromagnetic symmetry of the zero-field Ising model to reduce the vector sizes by a further factor of 2. Since we have been using programs designed for general q, we have not exploited this possibility.

For the high-temperature expansions, the field weighting is not included and the set of bonds does not include any bonds extending beyond the finite lattice. However the main difference from the low-temperature expansion arises from the relation $z=(1-v)/(1+(q-1)v)$. For a finite lattice α, rather than expand Λ_α we expand

$$\Phi_\alpha = q^{-s(\alpha)}(1+(q-1)v)^{b(\alpha)}\,\Lambda_\alpha \tag{12}$$

whence

$$\Lambda_\alpha = q^{s(\alpha)-b(\alpha)}(1+(q-1)z)^{b(\alpha)}\,\Phi_\alpha \tag{13}$$

where $b(\alpha)$ and $s(\alpha)$ are the number of bonds and sites respectively in lattice α. The expansion of Φ_α is obtained by giving bonds a weight of $1+(q-1)v$ for pairs of sites in the same state and weight $1-v$ otherwise. An additional weight of q^{-1} is applied at each site.

For the infinite lattice limit, we have

$$q^{1-\nu/2}(1+(q-1)z)^{\nu/2}\Phi(v) = q(1+(q-1)v)^{-\nu/2}\Phi(v) = \Lambda \approx \prod_{\alpha\in B(s)} \Lambda_\alpha^{V(\alpha)} \tag{14}$$

where ν is the lattice coordination number so that $\nu/2$ is the number of bonds per site, which is 3 on the simple cubic lattice. By using the facts that $\sum_{\alpha\in B(s)} b(\alpha)V(\alpha) = \nu/2$ and $\sum_{\alpha\in B(s)} s(\alpha)V(\alpha) = 1$ we obtain the relation

$$\Phi(v) \approx \prod_{\alpha\in B(s)} \Phi_\alpha(v)^{V(\alpha)}. \tag{15}$$

It is this last expression that we use in our high-temperature calculations.

For the Ising model, it is usual to shift the zero of energy so that parallel and antiparallel pairs have energies $\pm J$ with $J = \frac{1}{2}\Delta E$. This leads to the more familiar form of the Ising model expansion:

$$Z = \exp(+J/kT)^{\nu/2}\Lambda = 2[\cosh(J/kT)]^{\nu/2}\Phi(v). \tag{16}$$

The high-temperature expansion for the free energy is written as

$$\Phi(v) = \sum_n a_n v^n = 1 + 3v^4 + \cdots \tag{17}$$

(or more generally $1+3(q-1)v^4\ldots$). The coefficients a_n for $n \leqslant 22$ are listed in table 2.

The internal energy, U, is derived from the free energy, F, or the partition function Λ by

$$U = \frac{\partial}{\partial\beta}\beta F = -\frac{\partial}{\partial\beta}\ln\Lambda.$$

For low temperatures we use

$$\frac{\mathrm{d}}{\mathrm{d}\beta} = \frac{\mathrm{d}z}{\mathrm{d}\beta}\frac{\mathrm{d}}{\mathrm{d}z} = -\Delta E z\frac{\mathrm{d}}{\mathrm{d}z}$$

to give

$$U = \Delta E\, z\frac{\mathrm{d}\Lambda}{\mathrm{d}z}\Lambda^{-1}.$$

For high temperatures we use $z = (1-v)/(1+(q-1)v)$ and $\mathrm{d}z/\mathrm{d}v = -q/(1+(q-1)v)^2$ to give

$$\frac{\mathrm{d}}{\mathrm{d}\beta} = \Delta E\frac{(1-v)(1+(q-1)v)}{q}\frac{\mathrm{d}}{\mathrm{d}v}$$

whence

$$U = \Delta E \frac{\nu}{2} \frac{q-1}{q}(1-v) - \Delta E \frac{(1-v)(1+(q-1)v)}{q} \frac{\mathrm{d}}{\mathrm{d}v} \ln \Phi(v).$$

The high- and low-temperature expansions were computed using two very similar Fortran programs written for general (integer) q. Our programs work in terms of the general variables z or v, even in those special cases where only even powers occur. Most of the other technical aspects are similar to our previous calculations using the finite-lattice method. The calculations were performed using arithmetic modulo various primes, p, slightly below 2^{15}. Calculations were performed using 32-bit integers and the large vectors of residues stored as 16-bit integers. The factor $(q-1)^{-1}$ required in the general form of M is calculated as $(q-1)^{p-2}$ modulo p by virtue of Fermat's theorem. Similarly the factors q^{-1} required in evaluating the Φ_α were expressed as q^{p-2} modulo p. Since all of the Φ_α and Λ_α are of the form $1+kv^4+\cdots$ and $1+(q-1)\mu z^\nu+\cdots$ respectively, the expansions for negative powers of the Φ_α and Λ_α can readily be calculated. The programs were run on an IBM 3090/400J with $\frac{1}{2}$ Gbyte of main memory and 2 Gbyte of extended storage.

4. Analysis

Before presenting the analysis of our new series, we note a number of relevant prior studies. Gaunt and Sykes (1973) extended the diamond and FCC low-temperature series, and obtained $0.307 \leqslant \beta \leqslant 0.317$ and a value for γ around 1.27–1.30. They noted that the sequences of exponent estimates were converging rather slowly. A range of previous work was consistent with these estimates. At high temperatures, Sykes *et al* (1972) and Camp *et al* (1976) found estimates for α consistent with 0.125, in accordance with the belief at the time that α was a simple fraction, probably $\frac{1}{8}$.

The field-theory estimates of Le Guillou and Zinn-Justin (1980), in which scaling and high/low-temperature exponent symmetry are implicit, are $\gamma = 1.241(2)$, $\alpha = 0.110(5)$, $\beta = 0.325(2)$. Recently Oitmaa *et al* (1991) obtained extended low-temperature series for the (2+1)-dimensional Ising model, equivalent to a Z_2 gauge model in 2+1 dimensions, which is in the three-dimensional Ising universality class. They also derived and analysed series on the triangular and honeycomb lattices. Unbiased exponent estimates were given as $\gamma = 1.28(2)$, $\beta = 0.311(4)$ and $\alpha = 0.11(4)$, while biased estimates were given as $\gamma = 1.25(2)$, $\beta = 0.318(4)$ and $\alpha = 0.096(6)$.

Nickel (1991) recently re-examined the ϕ^4 field theory exponents, and showed that, by permitting a second confluent exponent, critical exponent estimates were obtained that agreed rather well with those obtained from high-temperature series expansions. Nickel's preferred values are $\gamma = 1.238$, $\nu = 0.630$, $\eta = 0.0355$. Hence $\alpha = 0.110$ and $\beta = 0.326$. The critical exponent $\Delta_1 = \omega_1 \nu = 0.53$.

Recently Mojumder (1991) has developed a theory based on partial non-renormalization of superconformal dimensions of matter fields on a (2,0) supersymmetric string world sheet. A consequence of this theory is the predicition of critical exponents which are supposed to be exact. These are $\alpha = \frac{1}{8}$, $\beta = \frac{3}{8}$, from which follows $\gamma = \frac{9}{8}$ and $\nu = \frac{5}{8}$.

Before analysing the newly obtained series, we remark that the analysis of the low-temperature series is made more difficult than the analysis of their high-temperature

counterparts by the presence of non-physical singularities closer to the origin than the physical singularity. While differential approximants effectively afford analytic continuation beyond the nearest singularity, the series coefficients are nevertheless dominated by the non-physical singularity. Another approach to this difficulty is to apply a transformation, to move the physical singularity closer to the origin than the non-physical singularity. However, such 'singularity-moving' transformations introduce long-period oscillations (Hunter 1987, Guttmann 1989) thus rendering suspect extrapolations based on such transformed series as in the analysis by Bhanot *et al* (1992).

Another problem with the analysis of the three-dimensional Ising series is the presence of confluent singularities (which are extremely weak or non-existent in the two-dimensional model). Both field-theory and high-temperature series analysis suggests a value for the confluent exponent not very different from 0.5. Roskies (1981) introduced an effective transformation for analysing such series, in which one replaces the original expansion variable z by a new variable y, defined by $1-y = (1-z/z_c)^{1/2}$. If the original series had square root correction terms, the transformed series has analytic correction terms. If there were no square root correction terms, then nothing is lost by applying this transformation. One problem is that the critical temperature must be accurately known, but for the three-dimensional Ising model this is the case. The consensus of extensive high-temperature series and Monte Carlo work is $\tanh(J/kT_c) = 0.218\,093$, or $u_c = \exp(-4J/kT_c) = 0.412\,0494$, with errors being a few parts in the sixth decimal place (Guttmann 1987b).

Our initial analysis of the three low-temperature series (specific heat, magnetization and susceptibility) by Padé approximants and differential approximants was not particularly illuminating. Exponent estimates were $\alpha' = -0.1$ to 0.2, $\beta = 0.30$ to 0.32 and $\gamma' = 1.2$ to 1.3. Biased estimates (with the critical point specified) were $\alpha' \approx 0.20, \beta \approx 0.32$ and $\gamma' \approx 1.25$.

Table 3. Estimates of β using Dlog Padé approximants to Roskies-transformed series.

N	$[N-2/N]$	$[N-1/N]$	$[N/N]$	$[N+1/N]$	$[N+2/N]$
5	0.4192	0.3590	0.2290	0.5032	0.3240
6	0.3261	0.3346	0.3431	0.3437	0.3325
7	0.4559	0.3437	0.3431	0.3332	0.3326
8	0.3027	0.3388	0.3258	0.3342	0.3322
9	0.3358	0.3419	0.3731	0.2900	0.3279
10	0.3275	0.3186	0.3580	0.3215	0.3230
11	0.3270	0.3318	0.3233	0.3210	0.3391
12	0.3290	0.3274	0.2624	0.2113	0.3286
13	0.3286	0.2154			

Analysing the Roskies-transformed series by evaluating Dlog Padé approximants at $y = 1$ gave the results shown in tables 3 to 5. The approximants are fairly consistent, a few wildly deviant ones being due to defective approximants. For all three exponents we have taken the mean of the last few values (from 14 to 16 approximants), and ignored the wildly different outlying ones. The mean of these approximants, with error given as one standard deviation, is $\alpha' = 0.124 \pm 0.006$, $\beta = 0.329 \pm 0.009$, $\gamma' = 1.251 \pm 0.028$.

The effect of allowing for the correction-to-scaling shows that its neglect in the

Table 4. Estimates of γ' using Dlog Padé approximants to Roskies-transformed series.

N	$[N-2/N]$	$[N-1/N]$	$[N/N]$	$[N+1/N]$	$[N+2/N]$
5	1.1962	1.2342	1.2997	1.3836	1.1646
6	1.4124	1.4975	1.3363	1.2835	1.1892
7	1.4200	1.3068	1.3431	2.5047	1.1088
8	1.7242	1.2416	1.2809	1.2551	1.2049
9	1.2981	1.2655	1.2940	1.2087	1.2047
10	2.7628	1.2466	1.2493	1.2767	1.2511
11	1.2494	1.2461	1.2605		
12	1.2643				

Table 5. Estimates of α' using Dlog Padé approximants to Roskies-transformed series.

N	$[N-2/N]$	$[N-1/N]$	$[N/N]$	$[N+1/N]$	$[N+2/N]$
5	0.1850	0.1197	0.1102	0.1410	0.0829
6	0.1078	0.1173	0.1236	0.1319	0.1265
7	0.1224	0.1131	0.1284	0.1329	0.1109
8	0.1260	0.1207	0.1239	0.1261	0.1364
9	0.1234	0.1686	0.1226	0.1208	0.1658
10	0.1221	0.1214	0.1227	-0.686	0.2232
11	0.1221	0.1182	0.1743		
12	0.1375				

analysis by Bhanot *et al* (1992) is an even more serious problem for their analysis than the use of the Euler transformation.

It can be seen that, with the exception of the estimate of α', the exponent estimates above are consistent with the field-theory estimates. The value for α' just fails to overlap the range of the field-theory estimate, but we believe that the high-temperature series result (see below) must also be taken into account.

We have also tested the sensitivity of our estimates to changes in both the critical-point estimate, and the exponent estimate used in the Roskies transformation. Changing the estimate of the critical point by two parts in the fifth significant digit produced a change in the exponent estimate of one-tenth of the error estimates quoted above. That change in the critical point is far greater than the uncertainty in the critical point, so that we can safely assert that the results quoted include errors due to the uncertainty in the critical point. Changing the exponent estimate to 0.53 from the value 0.5 used in the Roskies transformation produced an error that was less than one-fifth of the errors quoted above, so that the uncertainty in the correction-to-scaling exponent is also negligible in this analysis.

We have also looked carefully at the non-physical singularity that is closer to the origin than the physical singularity. We find its position to be at $u = -0.2853 \pm 0.0003$, and the exponents of the susceptibilty, magnetization and specific heat to be ≈ 1.03, -0.01 and 1.01 respectively. It is difficult not to suggest that these are 1, 0 and 1 respectively, with presumably logarithmic corrections. These values also satisfy the same scaling relation $\alpha' + 2\beta + \gamma' = 2$ that the exponents at the critical point satisfy, though the thermodynamic argument that leads to this result at the critical point is not obviously applicable in this non-physical region.

For the high-temperature series, the critical temperature is the radius of convergence of the series. It follows that the ratio method and its variants can be

used. Unbiased differential approximants, using the method of analysis described in Guttmann (1987a) give $v_c^2 = 0.0475185$, $\alpha = 0.126$. Utilizing the linear dependence between the estimates of v_c and α gives a biased estimate of 0.11 for α at the correct $v_c^2 = 0.047565$.

With a 'correction-to-scaling' exponent close to 0.5, the ratio of successive terms in the specific heat expansion is expected to behave as $r_n = \mu[1 + (\alpha - 1)/n + c/n^{3/2} + O(1/n^2)]$ so estimators of α are given by the sequence $(r_n/\mu - 1)n + 1 = \alpha_1 + c/n^{1/2} + O(1/n)$ where $\mu = v_c^{-2}$. In figure 1 we show the plot of this sequence against $1/n^{1/2}$. The series we have used is the expansion of C_H/R in powers of v^2, just as was used by Sykes (1972), but with three further terms. Linear regression to the data gives $\alpha = 0.113 - 0.0637/n^{1/2} + 0.389/n$. As we have shown in previous work, the method of differential approximants can accurately predict the most significant digits of the next term in the series (see e.g. Guttmann and Enting 1988a). In this way we have estimated the coefficient of v^{24} in the zero-field high-temperature partition function to be $2.733\,76 \times 10^{11}$, where only the last quoted digit is uncertain. Using the additional term in the analysis just described, we obtain an estimate for α of 0.111, with the correction terms given by $-0.0511/n^{1/2} + 0.364/n$. This estimate of α is impervious to the uncertainty in the estimated coefficient. We conclude from this analysis that $\alpha = 0.110 \pm 0.005$. The comparatively small amplitude of the term proportional to $1/n^{1/2}$ helps us to understand why the series is so well behaved.

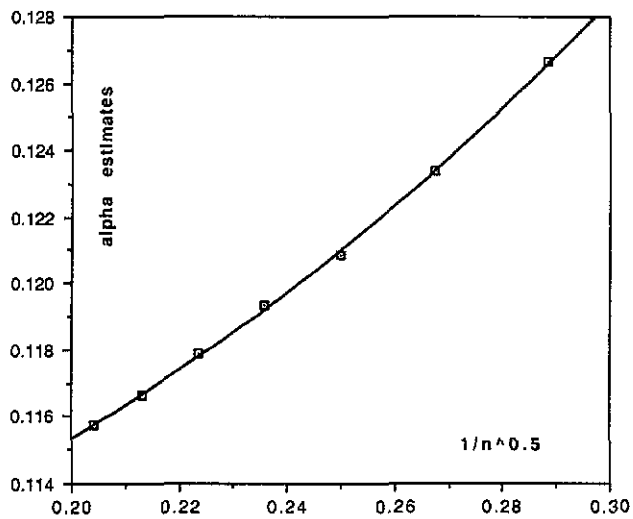

Figure 1. Ratio method estimates of α, plotted against $n^{1/2}$. The series used was C_H/R, expanded in powers of v^2. The slope gives the amplitude of the 'correction-to-scaling' term and the intercept gives the estimated value of α after taking the correction-to-scaling into account.

Recently, Liu and Fisher (1990) studied the correction-to-scaling amplitudes of the three-dimensional Ising model and argued that the amplitudes of the correction-to-scaling term should be negative. Writing $C \approx A|t|^{-\alpha}[1 + a_\theta|t|^\theta + a_1 t + \cdots]$ where $t = (T - T_c)/T_c$ and $\theta = \frac{1}{2}$ our result transforms to $a_\theta \approx -0.040$, which has the predicted sign.

Biased first-order differential approximants give $\alpha = 0.104 \pm 0.018$, where the analysis is precisely that described in Guttmann (1987a). The error bars correspond to two standard deviations. A Roskies-transformed Padé analysis was also performed for the high-temperature series, paralleling the low-temperature investigation. The short series meant that very few approximants were obtained, and so the results are not particularly helpful (exponent estimates in the range 0.08 to 0.3 were obtained).

5. Concluding remarks

The calculations presented here have shown that on the simple cubic lattice the finite-lattice method of series expansion compares favourably with conventional expansion methods. However, there is not the dramatic difference that occurs for many two-dimensional problems. Nevertheless, significant extensions of both high- and low-temperature series have been obtained.

Our exponent estimates are all consistent with field-theory exponent estimates. The two best behaved series give $\beta = 0.329 \pm 0.009$ and $\alpha = 0.110 \pm 0.005$. The estimates of α' and γ', while consistent with field-theory estimates, had rather wide error bars, and so the agreement with field theory was less convincing. Our estimates of α and β are not consistent with the conjectured exact values of Mojumder.

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Note added in proof. After acceptance of this paper, we received a preprint from Vohwinkel (1992), as well as some additional series. Vohwinkel has used a version of the shadow-lattice method of Sykes, and has obtained six further low-temperature series coefficients. Analysis of these longer series by the methods used in this work do not significantly change our exponent estimates.

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