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Susceptibility amplitudes for the three- and four-state Potts models

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Abstract

The finite lattice method of series expansions is used to calculate a number of extended series for susceptibilities of the three- and four-state Potts models on the square lattice. We analyse all these series and estimate their critical amplitudes. We resolve an uncertainty in amplitude ratios for high- to low-temperature susceptibilities, and thus provide confirmation of field-theoretic predictions.

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1. Introduction

Over the last three decades, the Potts models [1] have provided a number of challenges to the understanding of cooperative phase transitions. Many characteristics of the models are described in the review by Wu [2]. The capability of the finite lattice method (FLM) to generate long series expansions [3] has been important in studying the Potts models [4–10]. The FLM techniques used in the present study build on a series of papers in which we studied the critical behaviour of the q-state Potts model in both two and three dimensions [11–13]. In particular, Guttmann and Enting [11] gave the general expressions used to derive high- and low-temperature expansions for the q-state Potts model. These techniques were applied to the $q=2$ (Ising) case on the simple cubic lattice. The analysis confirmed estimates of critical exponents obtained by field theoretical techniques. In a subsequent paper [12] we presented and analysed

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series for the bulk thermodynamic properties for Potts model on the square lattice for integer q ranging from 2 to 10. These were used to test series analysis techniques that could distinguish between first-order and continuous transitions. These techniques were applied [13] to the three-state model on the simple cubic lattice. We found the transition to be first order, and estimated the latent heat, the discontinuity in the order parameter, and a number of other properties.

The present study addresses the susceptibilities of the Potts models. For $q > 2$ there are three naturally occurring susceptibilities. They are the high-temperature susceptibility, χ, and for low-temperatures, the longitudinal susceptibility, χ_L and the transverse susceptibility, χ_T, defined in terms of a transverse field H_T that is independent of the symmetry-breaking field H. We follow the notation of Delfino et al. [14] and write these, in the critical region, as

$$\chi \sim \Gamma t^{-\gamma}, \quad \chi_L \sim \Gamma_L t^{-\gamma'}, \quad \chi_T \sim \Gamma_T t^{-\gamma_T'} ,$$

respectively, where $t = |T - T_c|/T_c$. The critical amplitudes Γ, Γ_L and Γ_T are defined using normalisations given below.

In 1998 Delfino and Cardy [15] using the exact scattering theory of Chim and Zamolodchikov [16] considered the scaling limit of the two-dimensional q-state Potts model for $q \leqslant 4$. They then computed correlation functions and combinations of critical amplitudes expected to be universal within the two-kink approximation of the form factor approach. In particular, they calculated the amplitude ratio Γ/Γ_L. That work was extended by Delfino, Barkema and Cardy in 2000 [14] to the consideration of the low-temperature susceptibility amplitude ratio Γ_T/Γ_L. They tested their results against Monte Carlo data, and found the comparison inconclusive for $q = 4$ because of the large uncertainties due to logarithmic correction-to-scaling terms, while for $q = 3$ they found agreement with their prediction for Γ_T/Γ_L, but not for Γ/Γ_L.

A more extensive Monte Carlo analysis by Shchur et al. [17] found agreement with the Γ/Γ_L prediction for the $q = 3$ case. More precisely, in Ref. [14], for $q = 3$ the ratio Γ/Γ_L was estimated to be 13.848 in the two-kink approximation, but around 10 or slightly less by Monte Carlo methods. However in Ref. [17] both series and Monte Carlo estimates of this ratio were found consistent with the two-kink approximation results. For the other ratio Γ_T/Γ_L the two-kink estimate of 0.327 was just consistent with the Monte Carlo estimates of around 0.333 or a little lower.

For q=4 the ratio Γ/Γ_L was estimated [14] to be 4.013 in the two-particle approximation, but around 2 by Monte Carlo analysis. For the ratio Γ_T/Γ_L the two-kink estimate of 0.129 was rather lower than the Monte Carlo estimate of around 0.155. The authors argued that the complexities introduced by confluent logarithmic corrections-to-scaling which arise at $q = 4$ rendered their Monte Carlo comparison inconclusive.

However, a more comprehensive Monte Carlo analysis was carried out by Caselle et al. [18], in which they allowed for the expected logarithmic corrections to the power-law singularity. They estimated $\Gamma = 0.0223(40)$ and $\Gamma_L = 0.0071(30)$, so that $\Gamma/\Gamma_L = 3.14(70)$, in rough agreement with the two-kink estimates.

Another ratio, R_ξ, which involves the specific heat amplitude and the exponential correlation length (inverse mass) has recently been calculated exactly by Seaton [19]. That result is also contained implicitly in Ref. [15]. Seaton's results follow from the connection between the Potts model and the dilute A model in regime 1. In Ref. [15] a similar ratio, but involving the second moment correlation length (which cannot be calculated exactly) was also given. The two amplitude ratios, while unequal, are found to be within 1% of each other for $q = 1, 2, 3, 4$. Unfortunately, it does not yet seem possible to extend Seaton's methods to extract the various amplitude ratios approximated in Ref. [15].

Caselle et al. [18] also estimated R_ξ by Monte Carlo methods and found $R_\xi = 0.220(20)$. This last estimate is consistent both with the two-kink result of Ref. [15] and the exact result of Ref. [19], $R_\xi = 2^{1/2}3^{-7/4} = 0.20680\ldots$

Thus while more recent Monte Carlo calculations provide support for all the susceptibility amplitude ratio predictions from the two-kink approximation, it would seem worthwhile to independently study these questions by series analysis techniques. In the present paper we have derived extensive new series in order to address the above discrepancies, and to provide independent tests of the two-kink predictions. Our analysis also provides estimates of the individual amplitudes, not just amplitude ratios, which should be useful in other contexts, and for other amplitude ratios.

Our ratio estimates for $q = 3$ have largely resolved an uncertainty in the high–low-temperature normalisation of the field theory calculations, and thus imply their essential correctness for $q = 4$ also [20].

The contents of the remainder of this paper are as follows: Section 2 reviews the series expansions for the Potts model and describes how transverse fields are introduced, leading to expansions for χ_T. Section 3 considers the application of the FLM to calculating these series. Section 4 describes the series analysis, while Section 5 provides a brief conclusion.

2. Series expansions for the Potts model

In analysing Potts model series, our definitions and notation generally follow our previous usage [11–13]. The standard q-state Potts model is defined on a lattice with each site having a 'spin' variable s_i at each site i that takes on q possible integer values from 0 to $q-1$. An energy ΔE is associated with each pair of interacting sites that are in different spin states, and an energy of 0 applies to pairs of interacting sites in the same state. We consider only the square lattice, with each site interacting only with its four nearest neighbours. Each site not in state '0' has an additional field energy H. When the transverse field, H_T is zero, this normalisation is such that the state with all sites in state '0' has zero energy.

In this normalisation, the partition function, Z, is commonly denoted Λ and is termed the reduced partition function. In this paper, our definition of Λ includes a contribution from the transverse field in the 'all-zero' state.

We use the same expansion variables as previously [11–13] and put $z = \exp(-\Delta E/kT)$, $\mu = \exp(-H/kT)$ and the high-temperature variable $v = (1-z)/(1+(q-1)z)$.

The new feature that we introduce in the present paper is a transverse field, H_T and a corresponding expansion variable $v = \exp(-H_T/kT)$. If we define fields that give an energy $-h_j$ to each site in state j, we can construct composite fields, h_j

denoted by energy q-plets $[-h_0, -h_1, \ldots, -h_{q-1}]$. It is clear that only $q-1$ of these fields are independent, since apart from the definition of the zero-point energy, the thermodynamics is invariant under the transformation $[-h_0, -h_1, \ldots, -h_{q-1}] \to [-h_0 - a, -h_1 - a, \ldots, -h_{q-1} - a]$. In these terms the ordering field for $q=3$ corresponds to energies $[-H, 0, 0] \equiv [0, H, H]$. The transverse susceptibility defined by Delfino et al. [14] corresponds to a field $H_T \equiv [0, H_T, 0]$. Straley and Fisher [21] introduced a transverse field in the form $H_\tau \equiv [0, H_\tau, -H_\tau]$, but as noted below, there are only two independent susceptibilities and so we do not need to consider this case explicitly.

The Hamiltonian that we consider is

$$\hat{H} = \sum_{\langle r,r' \rangle} \Delta E(1 - \delta(s_r, s_{r'})) + \sum_r H(1 - \delta(s_r, 0)) + \sum_r H_T \delta(s_r, 1) , \tag{2.1}$$

where the first sum is over all nearest-neighbour pairs of sites and the second and third sums are over all sites. The term $\delta(m,n) = 1$ if $m = n$ and 0 otherwise.

When the fields H and H_T are zero, there is a q-fold degeneracy. Nevertheless, at sufficiently low temperatures (for $\Delta E > 0$) this symmetry is spontaneously broken and the system adopts one of q possible states with one of the spin-states favoured. In actual calculations, a particular choice of the ‘favoured’ state is made by treating the spontaneous symmetry breaking as the limit of an explicit symmetry breaking. Two common choices are: (i) taking the limit $H \to 0^+$, or (ii) fixing boundary spins to the zero spin state while going to the infinite size thermodynamic limit. Results for bulk properties will be equivalent regardless of whether we break the symmetry by using $N \to \infty$ with fixed boundaries or $H \to 0^+$ or use both of these in either order. However, when we consider breaking two different symmetries, the order of the limits may become important.

The reduced partition function Λ can be defined by the limit of partition functions, λ_{JK} for finite $J \times K$ lattices as

$$\Lambda = \lim_{J,K \to \infty} (\lambda_{JK})^{1/JK} . \tag{2.2}$$

For a single field, this has the expansion

$$\Lambda = \sum_{m,n} z^m \mu^n = 1 + (q-1) z^4 \mu + \cdots \tag{2.3}$$

which can be regrouped as

$$\Lambda(z, \mu) = \sum_n L'_n(z) \mu^n \tag{2.4a}$$

and

$$\Lambda(z, \mu) = \sum_m \psi'_m(\mu) z^m \tag{2.4b}$$

where the $\psi'_m(\mu)$ are polynomials in μ and (on the square lattice) the $L'_n(\mu)$ are polynomials of order z^{4n} in z. (We use the notation $L'(.)$, $\psi'(.)$ since $L(.)$ and $\psi(.)$ have traditionally been used for the corresponding coefficients in expansions of $\ln \Lambda$.)

For $q = 3$ the introduction of separate fields h_1 and h_2, i.e., energies $[0, -h_1, -h_2]$, generalises (2.3) to

$$\Lambda(z, \mu_1, \mu_2) = \sum_{mn} L'_{mn}(z) \mu_1^m \mu_2^n \;, \tag{2.5}$$

where

$$\mu_j = \exp(-h_j/KT) \quad j = 1, 2 \;. \tag{2.6}$$

The site expectations are defined in terms of variables $n_j(r)$ that equal 1 if the spin at site r is in state j and equal zero otherwise. Using $\langle \cdot \rangle$ to denote expectations, we have

$$\langle n_j \rangle = \mu_j \frac{\partial}{\mu_j} \ln \Lambda \quad \text{for } j = 1, 2 \;, \tag{2.7}$$

while $\langle n_0 \rangle$ can be obtained directly from (2.7) by using the relation

$$\sum_{j=0,1,2} n_j = \sum_{j=0,1,2} \langle n_j \rangle \equiv 1 \;. \tag{2.8}$$

Note that the order parameter or magnetisation, M, is conventionally defined to span the range $[0, 1]$ and so

$$M = \tfrac{3}{2}[\langle n_0 \rangle - \tfrac{1}{3}] = 1 - \tfrac{3}{2}[\langle n_1 \rangle + \langle n_2 \rangle] \;. \tag{2.9}$$

We consider susceptibilities defined as the $H \to 0^+$ limit of

$$C_{ij} = \sum_r [\langle n_i(r) n_j(0) \rangle - \langle n_i \rangle \langle n_j \rangle] \;, \tag{2.10}$$

where the sum is over all lattice sites.

The $H \to 0^+$ limit breaks the three-fold symmetry, but (2.5) still has the symmetry relations $C_{ij} = C_{ji}$, $C_{01} = C_{02}$ and $C_{11} = C_{22}$ and using (2.8)

$$\sum_{j=0,1,2} C_{ij} = 0 \quad \text{for } q = 3 \text{ and all } i \;. \tag{2.11}$$

The two independent fields define only two independent susceptibilities because of these symmetry relations.

For the longitudinal susceptibility χ_L, (denoted by χ in our previous papers) we put

$$kT\chi_L = C_{00} = C_{11} + C_{22} + 2C_{12} = \mu \frac{\partial}{\partial \mu} \mu \frac{\partial}{\partial \mu} \ln \Lambda \tag{2.12}$$

and, following Delfino et al. [14], define the transverse susceptibility as

$$kT\chi_T = C_{11} = C_{22} = \mu_j \frac{\partial}{\partial \mu_j} \mu_j \frac{\partial}{\partial \mu_j} \ln \Lambda \quad \text{for } j = 1, 2 \;. \tag{2.13}$$

However, Straley and Fisher [21] defined the transverse susceptibility as

$$kT\chi^\tau = C_{11} + C_{22} - 2C_{12} = kT(4\chi_T - \chi_L) \tag{2.14}$$

and suggested that, as an independent susceptibility, χ^τ could have a distinct exponent which they estimated as $\gamma^\tau \approx 1.1$. However, since $\chi_t = \frac{1}{4}(\chi_L + \chi^\tau)$, the existence of a distinct exponent $\gamma^\tau < \gamma'$ would imply $\Gamma_T/\Gamma_L = \frac{1}{4}$, in disagreement with field theory, Monte Carlo and our series analysis.

For general q, (2.11) generalises to

$$\sum_{j=0}^{q-1} C_{ij} = 0 \quad \text{for all } i\ . \tag{2.15}$$

Together with the symmetries, this implies that only two of the C_{ij} are independent, and so there are still only two independent susceptibilities for all $q > 2$. They can be chosen to be

$$kT\chi = C_{00} = \sum_{i=1}^{q-1}\sum_{j=1}^{q-1} C_{ij} = \mu \frac{\partial}{\partial \mu} \mu \frac{\partial}{\partial \mu} \ln \Lambda \tag{2.16}$$

and

$$kT\chi_T = C_{jj} = \mu_j \frac{\partial}{\partial \mu_j} \mu_j \frac{\partial}{\partial \mu_j} \ln \Lambda \quad \text{for } j > 0\ . \tag{2.17}$$

For high temperatures and zero field we have full permutation symmetry for the spin states and so

$$C_{ij} = \frac{-1}{q-1} C_{kk} \quad \text{for all } k \text{ and } i \neq j \tag{2.18}$$

and so there is only one independent susceptibility.

3. Series expansions from the FLM

3.1. The FLM

The FLM has provided an extremely powerful technique for deriving a range of series expansions for problems in lattice statistics. Since its original development [4,22] it has been applied to a range of lattice models, including self-avoiding polygons [23]. A series of refinements to the method as well as the increase in available computing capacity over the last two decades has made it possible to greatly extend a number of series expansions for lattice statistics problems. In Ref. [3] Enting has reviewed the development of the FLM. In addition to the Potts model studies (mostly referenced in this paper) the FLM has been a powerful tool for analysing self-avoiding walks and rings. The power of the FLM comes from its convenience and the fact that, for two-dimensional systems, it is exponentially faster than direct enumeration. In three dimensions it is asymptotically less efficient than direct graph counting [24]. In two dimensions the FLM is asymptotically less efficient than the corner transfer matrix method described by Baxter and Enting [25], at least for $q=2$, but the FLM scales much more readily to large problems. It is the computational convenience of the FLM that has made it extremely successful in two dimensions and led to a useful niche role in three dimensions.

For the q-state Potts model, Arisue and Tabata [9,10] have refined the techniques by combining series for Potts models with $2 \leqslant q' \leqslant q$. This method is a generalisation of the techniques, used in some of our earlier studies, of using Ising (i.e., $q=2$) series to derive 'correction terms' to extend FLM calculations for $q > 2$. The refined technique has proved very effective for larger q, but has not been used in the present calculations (though we do manage to extend the high-temperature series by one term by making use of the $q = 2$ results).

In his review of the FLM, Enting [3] identified three key aspects that characterised the calculations:

- the way in which the finite lattices are evaluated;
- the expansion variable(s);
- the type of boundary condition.

In evaluating the partition functions of the finite lattices we follow the approach developed for the spin-1 Ising model [26]. Two different techniques are used in a combination designed to minimise the requirements for computer memory. Lattices with a high aspect ratio are evaluated using the same technique as in most of our earlier work: the rectangle is built up by adding one column at a time and these columns are built up one site at a time. Rectangles that are more nearly square are built up starting from a specified line near the centre and adding one site at a time to build up an expanding sector with the initial line as one boundary and the other boundary pivoting around the centre as the lattice is built up. The choices of expansion variable and boundary conditions differ for different expansions and are considered on a case-by-case basis in the following subsections.

3.2. Low-temperature series and the transverse susceptibility

The basis of the finite lattice method is the approximation of the reduced partition function by a mutliplicative combination of reduced partition functions for finite lattices:

$$\Lambda(z,\mu) \approx \prod_{(J,K)\in B} \lambda_{JK}^{w(J,K)} , \tag{3.1}$$

where the product is over rectangular $J \times K$ lattices, whose reduced partition function is λ_{JK} and the weights $w(J,K)$ are integers given by Enting [27]. The set B is all rectangles up to some chosen maximum perimeter.

As noted in our previous studies, the low-temperature series for the limit $H \to 0^+$ can be obtained by re-expressing the low-temperature polynomials $\psi'(\mu)$ as functions of $x = 1 - \mu$ and keeping only the coefficients of x^0, x^1 and x^2. Thus to order x^2 we have

$$\Lambda(z,\mu = 1 - x) = \Lambda_0(z) + x\Lambda_1(z) + x^2\Lambda_2(z) + \cdots \tag{3.2}$$

from which we obtain the zero-field (reduced) partition function directly as Λ_0, the order parameter as

$$M = 1 - \frac{q}{q-1}\frac{\Lambda_1}{\Lambda_0} \tag{3.3}$$

and the susceptibility as

$$kT\chi_L = \frac{\Lambda_2}{\Lambda_0} - \frac{\Lambda_1}{\Lambda_0} - \frac{\Lambda_1^2}{\Lambda_0^2} . \tag{3.4}$$

We have previously published [12] series for $\Lambda_0(z)$, $M(z)$ and $\chi_L(z)$ to order z^{47} for $q = 3$, to order z^{43} for $q = 4$, and shorter series for $q = 5, 6, \ldots, 10$.

In order to determine the transverse susceptibility we can truncate the expansion at $x = 0$ but keep terms to second order in $x' = 1 - v$ to give

$$\Lambda = \Lambda_{[0]} + x'\Lambda_{[1]} + x'^2\Lambda_{[2]} + \cdots , \tag{3.5}$$

$$kT\chi_T = \frac{\Lambda_{[2]}}{\Lambda_0} - \frac{\Lambda_{[1]}}{\Lambda_0} - \frac{\Lambda_{[1]}^2}{\Lambda_0^2} . \tag{3.6}$$

The expansions for $q = 3$ are

$$kT\chi_L = C_{00} = 2z^4 + 16z^6 + 16z^7 + 100z^8 + \cdots , \tag{3.7a}$$

$$C_{10} = C_{20} = -C_{00}/2 = -z^4 - 8z^6 - 8z^7 - \cdots , \tag{3.7b}$$

$$kT\chi_T = C_{11} = C_{22} = z^4 + 8z^6 + 4z^7 + 55z^8 + \cdots , \tag{3.7c}$$

$$C_{12} = C_{21} = -C_{11} - C_{10} = C_{00}/2 - 2C_{11} = -z^4 - 8z^6 - 40z^8 + \cdots , \tag{3.7d}$$

whence

$$kT\chi^\tau = 4C_{11} - C_{00} = 2z^4 + 16z^6 + 120z^8 + \cdots \tag{3.7e}$$

as given by Straley and Fisher [21].

For the longitudinal susceptibility, we have extended our earlier series [11] to z^{71} for $q = 3$ and to z^{59} for $q = 4$ by using rectangles of widths up to 17 and 14, respectively. For the transverse susceptibility, the lower symmetry restricts us to shorter series and χ_T has been extended to z^{53} and z^{47} for $q = 3$ and 4. The full low-temperature series for χ_L and χ_T for $q = 3$ and 4 are given in Tables 1 and 2, respectively.

3.3. High-temperature series

In our derivation of high-temperature expansions on the simple cubic lattice [11], we noted that the high-temperature form of the reduced partition functions for a $J \times K$ rectangle could be written in terms of the dual variable $v = (1 - z)/(1 + (q - 1)z)$. On the square lattice, this takes the form

$$\phi_{JK} = q^{-s(J,K)}(1 + (q - 1)v)^{b(J,K)}\lambda_{JK} , \tag{3.8}$$

where the number of sites and bonds in a $J \times K$ rectangle are denoted, respectively, $s(J, K) = J \times K$ and $b(J, K) = 2JK - J - K$. Thus, the finite lattice expansion is

$$\prod_{J,K} \phi_{JK}^{w(J,K)} = q^{-1}(1 + (q - 1)v)^2 \prod_{J,K} \lambda_{JK}^{w(J,K)} \tag{3.9}$$

Table 1
Low-temperature expansions for longitudinal and transverse suspectibilities for $q=3$

n	$\chi_{L:3,n}$	$\chi_{T:3,n}$
4	2	1
5	0	0
6	16	8
7	16	4
8	100	55
9	216	60
10	844	422
11	1552	488
12	7844	3442
13	12 112	4140
14	60 268	25 538
15	118 944	40 708
16	424 072	179 468
17	1 081 392	372 788
18	3 201 728	1 315 260
19	8 670 688	3 067 168
20	25 713 154	10 094 945
21	67 206 560	24 283 072
22	203 077 760	77 421 180
23	532 881 432	193 348 736
24	1 558 159 918	585 993 433
25	4 250 639 632	1 537 063 688
26	11 956 293 152	4 449 320 504
27	33 296 697 848	12 023 427 848
28	92 820 406 096	34 131 573 090
29	257 249 275 776	92 891 336 824
30	721 023 458 656	262 469 036 732
31	1 986 080 278 600	715 813 170 684
32	5 561 045 323 298	2 011 024 319 429
33	15 359 165 767 512	5 515 400 326 388
34	42 717 426 328 784	15 374 322 504 080
35	118 457 421 095 792	42 384 238 200 312
36	328 170 466 563 836	117 579 714 452 884
37	909 829 346 983 664	324 587 464 251 848
38	2 520 622 606 225 868	899 267 595 353 422
39	6 973 368 153 491 880	2 480 979 415 435 896
40	19 322 697 243 220 158	6 868 920 754 575 604
41	53 409 977 638 363 032	18 947 896 082 014 752
42	147 820 297 067 842 856	52 390 674 496 684 820
43	408 655 295 665 071 080	144 572 880 155 009 760
44	1 129 521 213 462 962 520	399 239 230 835 459 300
45	3 122 011 116 123 891 464	1 101 717 549 846 319 108
46	8 624 059 746 484 047 468	3 040 426 186 261 928 118
47	23 820 051 913 808 354 000	8 386 522 076 202 610 820
48	65 781 549 551 603 584 820	23 136 477 796 219 902 695
49	181 574 426 737 144 694 888	63 789 890 298 643 383 796
50	501 221 619 866 663 098 644	175 909 195 824 990 626 762
51	1 382 992 929 006 302 617 408	484 867 468 799 586 765 288
52	3 815 565 409 174 634 122 462	1 336 459 982 170 836 797 329

Table 1. Continued

n	$\chi_{L:3,n}$	$\chi_{T:3,n}$
53	10 524 878 842 654 526 569 848	3 682 860 710 265 693 605 928
54	29 024 398 721 218 107 686 556	—
55	80 030 932 690 952 491 499 224	—
56	220 628 552 950 671 705 158 938	—
57	608 117 853 500 544 719 343 880	—
58	1 675 936 326 492 393 722 337 944	—
59	4 617 862 345 765 106 089 694 856	—
60	12 722 441 083 845 010 673 495 788	—
61	35 045 424 395 956 284 235 051 760	—
62	96 522 386 339 584 747 363 002 768	—
63	265 809 374 651 559 045 594 453 456	—
64	731 896 605 822 361 878 096 090 984	—
65	2 015 002 285 596 660 573 863 374 648	—
66	5 546 865 453 218 790 278 395 156 868	—
67	15 267 395 388 739 048 317 780 983 504	—
68	42 017 866 370 437 457 482 465 144 594	—
69	115 625 057 273 677 603 164 078 168 112	—
70	318 143 187 191 549 908 959 681 336 668	—
71	875 280 734 613 897 956 571 923 101 480	—

using

$$\sum_{J,K} s(J,K)\, w(J,K) = 1 \tag{3.10a}$$

and

$$\sum_{J,K} b(J,K)\, w(J,K) = p/2 \tag{3.10b}$$

where p is the coordination number. As in our derivation of series for the simple cubic Ising model [11], the evaluation of the ϕ_{JK} is performed as for the low-temperature expansion of Λ, but with free boundary conditions, a site weight of $1/q$ and all bond weights multiplied by $(1+(q-1)v)$ so that like neighbours have a weight of $(1+(q-1)v)$ and unlike neighbours have a weight of $z\times(1+(q-1)v)=1-v$. The field weight remains $\mu=1-x$, with expansions truncated at x^2 as in low-temperature calculations. Eq. (2.18) remains valid, but can be re-expressed as

$$C_{00} = \sum_{i=1}^{q-1}\sum_{j=1}^{q-1} C_{ij} = \mu\frac{\partial}{\partial\mu}\,\mu\frac{\partial}{\partial\mu}\ln\Lambda = \mu\frac{\partial}{\partial\mu}\,\mu\frac{\partial}{\partial\mu}\ln\Phi \tag{3.11}$$

since the prefactor is independent of μ. As for low-temperature expansions, if we express Φ in powers of x as

$$\Phi(v,\mu=1-x) = \Phi_0(v) + x\Phi_1(v) + x^2\Phi_2(v) + \cdots \tag{3.12}$$

Table 2
Low-temperature expansions for longitudinal and transverse suspectibilities for $q = 4$

n	$\chi_{L:4,n}$	$\chi_{T:4,n}$
4	3	1
5	0	0
6	24	8
7	48	8
8	120	50
9	648	120
10	1608	464
11	4176	928
12	21 093	4827
13	38 064	8664
14	175 608	39 912
15	494 616	101 248
16	1 365 726	315 664
17	5 077 200	1 018 592
18	13 549 704	2 915 440
19	43 359 768	8 938 768
20	140 590 629	28 354 415
21	389 348 688	80 082 328
22	1 296 882 504	258 319 368
23	3 834 279 072	760 724 872
24	11 499 126 642	2 292 134 168
25	36 680 416 368	7 120 276 352
26	107 193 301 920	21 000 696 720
27	333 178 056 720	64 423 941 216
28	1 019 415 082 779	195 440 775 461
29	3 037 827 148 632	583 592 203 080
30	9 438 120 599 520	1 790 312 889 088
31	28 340 399 493 144	5 367 859 627 024
32	86 034 549 347 280	16 231 677 410 270
33	263 586 587 279 472	49 328 875 238 208
34	791 349 060 376 776	148 017 337 779 264
35	2 417 035 981 737 624	449 263 248 220 168
36	7 324 176 466 760 445	1 356 012 064 511 831
37	22 116 375 075 991 056	4 085 501 316 468 536
38	67 378 910 515 598 736	12 379 046 552 684 504
39	203 361 542 589 030 720	37 278 028 157 261 192
40	616 448 061 791 922 708	112 607 706 225 695 046
41	1 869 466 917 535 240 656	340 196 982 546 434 040
42	5 644 507 206 242 675 400	1 024 944 022 015 475 456
43	17 116 665 818 567 515 608	3 096 907 377 690 777 728
44	51 753 556 619 100 749 007	9 338 791 347 840 313 497
45	156 457 717 377 195 712 344	28 162 243 379 840 734 608
46	473 752 203 624 837 787 560	85 013 412 955 096 179 888
47	1 430 961 995 874 582 295 344	256 216 624 977 034 974 472
48	4 327 940 385 869 521 592 382	—
49	13 084 162 308 258 168 292 728	—
50	39 518 759 852 443 173 359 784	—
51	119 473 899 852 730 151 402 736	—
52	360 838 308 137 136 612 755 433	—

Table 2. Continued

n	$\chi_{L:4,n}$	$\chi_{T:4,n}$
53	1 089 899 345 148 336 599 592 432	—
54	3 292 517 731 377 439 401 644 088	—
55	9 939 757 951 162 682 068 137 120	—
56	30 016 345 311 144 609 620 362 422	—
57	90 617 252 419 865 912 767 571 472	—
58	273 502 986 597 190 549 918 225 488	—
59	825 601 891 969 581 003 968 678 544	—

we have

$$C_{00} = \frac{\Phi_2}{\Phi_0} - \frac{\Phi_1}{\Phi_0} - \frac{\Phi_1^2}{\Phi_0^2} . \tag{3.13}$$

Note that the conventional definition of the Ising (i.e., $q=2$) susceptibility is in terms of a field H with energies $[-H, H]$ and so (using 2.18) it corresponds to

$$kT\chi_{Ising}(v) = C_{00} + C_{11} - C_{10} - C_{01} = 4C_{00} . \tag{3.14}$$

Since as $T \to \infty$, $C_{jj} \to (q-1)/q^2$, we calculate and tabulate $C_{00} \times q^2/(q-1)$.

If we use rectangles with perimeter $p \leqslant 2k+1$, then the zero-field free energy series will be correct to order $4k+3$. However the susceptibility series will only be correct to order $2k+1$. Comparison with the FLM expansion of the Ising model gives a correction term. When the series are normalised to $C_{00} \times q^2/(q-1)$, the correction terms are independent of q. This enabled us to extend the series by a further term, so that our series are to order v^{28} and v^{24} for $q=3$ and $q=4$. The series are listed in Table 3. This represents a dramatic increase in the available series, which were previously known only to order v^{10} for general q, [28].

4. Analysis of series

For both the three-state and four-state Potts model we have derived three series: the usual high-temperature susceptibility, χ, the usual low-temperature susceptibility, χ_L and the low-temperature transverse susceptibility, χ_T. As already discussed, we write these, in the critical region, as

$$\chi \sim \Gamma t^{-\gamma}, \quad \chi_L \sim \Gamma_L t^{-\gamma'}, \quad \chi_T \sim \Gamma_T t^{-\gamma'_T} ,$$

respectively, where $t = |T - T_c|/T_c$.

The critical exponents for $q \leqslant 4$ can all be derived from the thermal exponent, given by Black and Emery [29], based on a conjecture of den Nijs [30], while the magnetic exponent was first given by den Nijs [31], and the (thermal) correction-to-scaling exponent was obtained by Nienhuis [32]. For the three-state Potts model, the susceptibility exponents are thus known to be $\gamma' = \gamma'_T = \gamma = \frac{13}{9}$ and the critical point in both the usual high- and low-temperature variable is $z_c = v_c = 1/(1+\sqrt{3}) = 0.366025404\ldots$ [1].

Table 3
High-temperature expansions for suspectibilities for $q = 3$ and 4

n	c_n $(q = 3)$	c_n $(q = 4)$
0	1	1
1	4	4
2	12	12
3	36	36
4	112	124
5	316	356
6	952	1164
7	2672	3492
8	7812	10 748
9	22 072	33 348
10	63 048	100 844
11	178 244	309 252
12	504 560	946 748
13	1 418 980	2 863 204
14	4 001 528	8 769 388
15	11 207 800	26 581 284
16	31 477 096	80 733 564
17	87 997 608	245 668 836
18	246 167 940	743 479 660
19	687 191 100	2 257 886 532
20	1 917 063 612	6 842 299 132
21	5 342 096 000	20 710 012 996
22	14 876 259 128	62 780 824 620
23	41 382 022 480	189 886 902 628
24	115 069 223 208	574 659 610 940
25	319 652 907 064	—
26	887 627 725 088	—
27	2 463 052 247 532	—
28	6 831 350 077 080	—

For the four-state Potts model, the susceptibility exponents are similarly known to be $\gamma' = \gamma'_T = \gamma = \frac{7}{6}$ and the critical point in both the usual high- and low-temperature variable is $z_c = v_c = \frac{1}{3}$ [1]. Additionally, we assume the predicted confluent logarithmic term of the form $|\log|t||^{3/4}$ is associated with all susceptibilities. This and further correction terms are discussed in [33].

As discussed in the previous section, we now have 28 terms in the high-temperature series for χ for the 3-state Potts model, and 24 terms for χ for the four-state Potts model. The low-temperature series for χ_L are known to z^{71} for $q = 3$ and to z^{59} for $q = 4$. Our new series for χ_T extend to z^{53} for $q = 3$ and to z^{47} for $q = 4$.

When analysing these series, certain normalisations must be included. Note that low-temperature susceptibility series begin with the coefficient of z^4 as their first non-zero coefficient. This must be taken into account when calculating amplitudes, by inclusion of a factor z_c^4. The high-temperature series start at v^0, but we have calculated and tabulated series for $C_{00} \times q^2/(q-1)$ and so the normalisation factor of $(q-1)/q^2$ needs to be restored before comparing amplitudes.

4.1. Three-state Potts model susceptibilities

For all three series, we first carried out a simple Padé analysis to estimate the amplitudes, by generating Padé approximants to $(y_c - y)\chi(y)^{1/\gamma}$ and evaluating these at y_c. These gave well-converged results, from which we estimate $\Gamma = 0.176(1), \Gamma_L = 0.01266(6)$ and $\Gamma_T = 0.004168(9)$. Combining these results, we find $\Gamma_T/\Gamma_L = 0.329(2)$ and $\Gamma/\Gamma_L = 13.90(15)$.

We also analysed all series by a second method, taking into account the confluent correction-to-scaling term, the exponent of which is expected to be [32] $\Delta = \frac{2}{3}$. By fitting successive pairs of coefficients to the sequence $a_0 n^{4/9} + a_1 n^{-2/9}$, we estimated $a_0 = 0.890(2)$, and $a_1 = 0.40(1)$ for the high-temperature susceptibility. This converts to $\Gamma = 0.1751(6)$. An identical analysis of the low-temperature susceptibility gave $a_0 = 0.2915(1)$ and $a_1 = -0.20(1)$, which gives $\Gamma_L = 0.01266(4)$, in excellent agreement with the Padé estimate above. The same analysis applied to the transverse susceptibilty gave $a_0 = 0.0946(3)$, and $a_1 = 0.03(1)$, which gives $\Gamma_T = 0.00411(2)$. The amplitude ratios are thus $\Gamma/\Gamma_L = 13.83(9)$ and $\Gamma_T/\Gamma_L = 0.325(2)$.

A third method of analysis we used was to analyse the series formed by the coefficient-by-coefficient quotient of the terms in the two low-temperature series, in order to estimate the amplitude Γ_T/Γ_L. We then extrapolated the resulting sequence of estimates of the ratio of amplitudes by a variety of standard sequence extrapolation algorithms. It was necessary to extrapolate the odd and even terms separately, due to an odd–even oscillation caused by a singularity on the negative axis. Neither sequence extrapolated particularly smoothly, and the most elementary method, that of Neville table extrapolation, produced the best-converged results. From both odd and even sub-sequences we estimate $\Gamma_T/\Gamma_L = 0.33 \pm 0.01$. This is entirely consistent with, but less accurate than, the results from the two analyses given above.

As we have 28 terms in the high-temperature series and more than twice this number in the low-temperature series, this quotient method wastes a lot of low temperature information, so is not an efficient way to estimate Γ/Γ_L. The best we can do is to note that the ratio sequence is rapidly declining, and that the last entry, combined with the decreasing trend, permits us only to say that $\Gamma/\Gamma_L < 15$.

All these results are mutually consistent, and are also consistent with the analytic results, in a two-particle approximation, of Delfino et al. of $\Gamma_T/\Gamma_L = 0.327$ and $\Gamma/\Gamma_L = 13.848$. They are also in agreement with, and more precise than, the Monte Carlo and series estimates of Ref. [17].

4.2. Four-state Potts model susceptibilities

Because of the presence of the confluent logarithmic term mentioned above, standard extrapolation techniques such as the Padé method, are known to be misleading when $q = 4$. In order to quantify this belief, we generated 30 terms in the expansion of

$$f(y) = (1 - 3y)^{-7/6} \left(-\frac{1}{3y} [\log(1 - 3y)]^{3/4} \right) ,$$

which we expect to mimic the high-temperature susceptibility of the 4-state Potts model, to leading order. The amplitude is of course precisely 1. Using the Padé method described above, one obtains a seemingly well-behaved sequence of approximants to the amplitude, steadily increasing as we include more and more series coefficients. Unfortunately, these estimates are steadily increasing *away from* 1, the last few estimates being greater than 3.0 and rising! This is not surprising, as the asymptotic behaviour of the coefficients of the above function is

$$[y^n]f(y) \sim 3^n n^{1/6}(\log(n))^{3/4}/\Gamma\left(\frac{7}{6}\right).$$

The factor $(\log(n))^{3/4}$ takes the value $2.504\ldots$, which is approximately equal to the error factor in the amplitude estimate. We therefore did not use this method of analysis, but restricted ourselves to the two other methods discussed above.

We first analysed the series formed by the coefficient-by-coefficient quotient of the terms in the two low-temperature series, in order to estimate the amplitude Γ_T/Γ_L. We then extrapolated the resulting sequence of estimates of the amplitude ratio by a variety of standard sequence extrapolation algorithms. There is a tacit assumption here that the confluent logarithmic term will essentially cancel in the ratio. While this is likely to be true at leading order, the sub-dominant terms (discussed below), cannot be expected to cancel. We therefore expect convergence to be slower than was observed for the three-state model, and that was indeed the case.

It was again necessary to extrapolate the odd and even terms separately, due to an odd–even oscillation caused by a singularity on the negative axis. Neither sequence extrapolated particularly smoothly, and the most elementary method, that of Neville table extrapolation, again produced the best-converged results. From both sequences we estimate $\Gamma_T/\Gamma_L = 0.15 \pm 0.02$. This is just consistent with the estimate of Delfino et al. of 0.129.

Finally, as a direct measure of the individual amplitudes, we again used the asymptotic form of the coefficients. That is to say, if

$$f(y) = A(1 - y/y_c)^{-\alpha-1}\left(-\frac{y_c}{y}[\log(1 - y/y_c)]^{3/4}\right),$$

then

$$[y^n]f(y) = \frac{An^{\alpha}}{\Gamma(1+\alpha)y_c^n}(\log n)^{3/4}\left[1 + \frac{c}{\log n} + \mathrm{O}(1/\log^2 n)\right].$$

So dividing out by the n-dependent terms and the gamma function gives a direct sequence of estimates of the amplitude A, with corrections of order $1/\ln n$. We extrapolated alternate terms against $1/\ln n$. and obtained sequences that were stable enough to allow us to estimate their limits. In this way we made the preliminary estimates $\Gamma = 0.031 \pm 0.005, \Gamma_L = 0.0088 \pm 0.0004$ and $\Gamma_T = 0.0010 \pm 0.0003$. In fact, there are other non-analytic correction-to-scaling terms present as well. Salas and Sokal [33] showed that near the critical temperature the high- and low-temperature susceptibilities behave as

$$\chi_{\pm} \sim \Gamma_{\pm}|t|^{-7/6}(-\log|t|)^{3/4}\left[1+\frac{9\log(-\log|t|)}{-8\log|t|}+\mathrm{O}(1/\log|t|)\right], \quad t \to 0.$$

We have crudely, and hence somewhat hesitantly, included the effect of this additional logarithmic term into our asymptotic analysis. By standard transfer theorems, it follows that the sub-dominant term makes a contribution to the asymptotic form of the coefficients of $9\log\log n/(8\log n)$. Thus, the amplitudes estimated without this term need to be corrected by dividing by the factor $1+9\log\log n/(8\log n)$. For $n=24$, the maximal value we have for the high-temperature series, this is 1.41. For the low temperature and transverse susceptibilities, $n_{\max}=59$ and 47, respectively, producing a correction factor of 1.39 in both cases. Applying these corrections, we arrive at our final estimates of the amplitudes, $\Gamma=0.022\pm0.004, \Gamma_L=0.0063\pm0.0003$ and $\Gamma_T=0.0007\pm0.0002$.

Caselle et al. [18] obtained, from Monte Carlo analysis, based on the same asymptotic scaling assumptions, $\Gamma=0.0223\pm0.0040$ and $\Gamma_L=0.00711\pm0.00030$. They did not attempt to analyse the transverse susceptibility. The high-temperature amplitude estimates agree well within error bars, while the low-temperature estimates are just outside overlapping error estimate range.

We emphasise that these estimates depend *critically* on the assumed form of the sub-dominant terms, and on the further assumption that the other sub-dominant terms, which include powers of logarithms, powers of logarithms of logarithms etc, can all be neglected. We doubt that this is true. Rather, the best we can say is that if we make the same assumptions as Caselle et al., our series work is consistent with their Monte Carlo work.

In neither case should the error bars be considered strict. In the analysis of Ref. [18] they are only systematic errors, and in our analysis they are confidence limits based on the behaviour of sequences subject to the assumptions we have made. No attempt has been made to include the effect of additional, neglected, terms.

Our direct amplitude estimates then give for the amplitude ratios $\Gamma_T/\Gamma_L=0.11\pm0.04$ and $\Gamma/\Gamma_L=3.5\pm0.4$. Notice that these same ratios are obtained from our preliminary amplitude estimates also, which is reassuring as we do not feel terribly confident about the manner in which we have attempted to include the additional logarithmic terms into the analysis.

These can be compared to the analytic results, obtained in the two-particle approximation of Delfino et al., of $\Gamma_T/\Gamma_L=0.129$ and $\Gamma/\Gamma_L=4.013$. The two results are consistent, though our numerical results are less precise than we would have liked. This is no doubt a consequence of the notoriously slow convergence of series with logarithmic corrections.

In Ref. [14] Delfino et al. argue that their earlier results [15] for the ratio Γ/Γ_L may be incorrect. Delfino [20] reminded us that they were led to this hypothesis when looking for a reason for their disagreement with their Monte Carlo analysis. They identified this as a possible problem in the way they fixed the relative normalization between the high- and low-temperature results. The good agreement we obtain in the $q=3$ case rules out this hypothesis, and so there is no reason to doubt their results for $q=4$.

5. Conclusions

Our results are entirely consistent with the field-theoretical results in the two-kink approximation, both for $q = 3$ and 4. For $q = 3$ our amplitude ratio estimates agree to better than 1% with the field theory results, while for $q = 4$ the agreement is much weaker, being not much better than 20%. The amplitude estimates for $q = 4$ obtained by Monte Carlo analysis [18] agree within the rather large combined error bars. As discussed above, the agreement for the $q = 4$ case may well be of limited value.

Both for the three- and four-state models, our results appear to be considerably more accurate than those obtained by the Monte Carlo analysis of Delfino et al., though it is likely that their field-theoretical amplitude ratios in the two-kink approximation are more accurate than either our series work, or the Monte Carlo work of Ref. [18], particularly for $q = 4$ where reliable numerical work is extremely difficult by any known technique.

The agreement between our estimate of the ratio Γ/Γ_L at $q = 3$ and that of Delfino et al. [15] effectively eliminates the one element of uncertainty in their calculations, the high–low-temperature normalisation. This confirmation then means that their results for $q = 4$ are not in doubt.

We have also substantially extended known series expansions for the three- and four-state Potts models, and estimated individual amplitudes, as well as amplitude ratios. The individual amplitudes are of course non-universal, that is to say lattice dependent, and inaccessible to field theory calculations. The four-state data will hopefully be of use in subsequent analyses when the nature of the logarithmic corrections near the critical point are better known.

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