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Low-temperature series expansions for the square lattice Ising model with spin $S > 1$

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Abstract. We derive low-temperature series (in the variable $u = \exp[-\beta J/S^2]$) for the spontaneous magnetization, susceptibility, and specific heat of the spin-S Ising model on the square lattice for $S = \frac{3}{2}$, 2, $\frac{5}{2}$, and 3. We determine the location of the physical critical point and non-physical singularities. The number of non-physical singularities closer to the origin than the physical critical point grows quite rapidly with S. The critical exponents at the singularities which are closest to the origin and for which we have reasonably accurate estimates are independent of S. Due to the many non-physical singularities, the estimates for the physical critical point and exponents are poor for higher values of S, though consistent with universality.

1. Introduction

In an earlier paper [1] we presented low-temperature series for the spontaneous magnetization, susceptibility and specific heat of the spin-1 Ising model on the square lattice. In this paper we extend this work to higher spin values ($S = \frac{3}{2}$, 2, $\frac{5}{2}$, and 3). From general theoretical considerations, in particular renormalization group theory, it is expected that the critical exponents (at the physical singularity) depend only upon the dimensionality of the lattice and on the symmetry of the ordered state, and thus do not vary with spin magnitude. Numerical work on the Ising model with $S > 1$ is quite sparse and little has been published since the mid 1970's. Low-temperature expansions were obtained by Fox and Guttmann [2] for $S = 1$ and $S = \frac{3}{2}$ for various two- and three-dimensional lattices. High-temperature expansions have been reported by a number of authors [3–5] who mainly focused on three-dimensional lattices. Generally the numerical work has confirmed spin independence. Recently, Matveev and Shrock [6] studied the distribution of zeros of the partition function of the square lattice Ising model for $S = 1, \frac{3}{2}$, and 2. While the physical critical behaviour of the spin-S Ising model is fairly well understood, little is known about the non-physical singularities. One major reason for seeking more knowledge about the complex-temperature behaviour is the hope that this will help in the search for exact expressions for thermodynamic quantities which have not yet been calculated exactly.

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2. Low-temperature series expansions

The Hamiltonian defining the spin-S Ising model in a homogeneous magnetic field h may be written

$$\mathcal{H} = \frac{J}{S^2}\sum_{\langle ij\rangle}(S^2 - \sigma_i\sigma_j) + \frac{h}{S}\sum_i (S - \sigma_i) \tag{1}$$

where the spin variables σ_i may take the $(2S+1)$ values $\sigma_i = S, S-1, \ldots, -S$. The first sum runs over all nearest-neighbour pairs and the second sum over all sites. The constants are chosen so the ground state ($\sigma_i = S\ \forall i$) has zero energy. The low-temperature expansion, as described by Sykes and Gaunt [7], is based on perturbations from the ground state. The expansion is expressed in terms of the low-temperature variable $u = \exp(-\beta J/S^2)$ and the field variable $\mu = \exp(-\beta h/S)$, where $\beta = 1/kT$. The expansion of the partition function in powers of u may be expressed as

$$Z = \sum_{k=0}^{\infty} u^k \Psi_k(\mu) \tag{2}$$

where $\Psi_k(\mu)$ are polynomials in μ. It is more convenient to express the field dependence in terms of the variable $x = 1 - \mu$

$$Z = \sum_{k=0}^{\infty} x^k Z_k(u). \tag{3}$$

Using the standard definitions, we find the spontaneous magnetization

$$M(u) = M(0) + \frac{1}{\beta}\left.\frac{\partial \ln Z}{\partial h}\right|_{h=0} = S + Z_1(u)/Z_0(u) \tag{4}$$

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

$$\chi(u) = \left.\frac{\partial M}{\partial h}\right|_{h=0} = \frac{\partial}{\partial h}\left.\left(Z^{-1}\frac{\partial Z}{\partial h}\right)\right|_{h=0} = \beta/S^2\left[2\frac{Z_2(u)}{Z_0(u)} - \frac{Z_1(u)}{Z_0(u)} - \left(\frac{Z_1(u)}{Z_0(u)}\right)^2\right]. \tag{5}$$

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

$$C_v(u) = \frac{\partial U}{\partial T} = \beta^2\frac{\partial^2}{\partial\beta^2}\ln Z_0 = (\beta J/S^2)^2\left(u\frac{\mathrm{d}}{\mathrm{d}u}\right)^2 \ln Z_0(u). \tag{6}$$

Thus in order to calculate the specific heat, spontaneous magnetization, and susceptibility one need only calculate the first three moments (with respect to x), $Z_k(u)$ for $k \leqslant 2$, of the partition function. These moments are most efficiently evaluated using the finite lattice method. The algorithm was described in an earlier paper [1]. For our present purpose it suffices to note that the infinite lattice partition function Z can be approximated by a product of partition functions Z_{mn} on *finite* $(m \times n)$ lattices,

$$Z \approx \prod_{m,n} Z_{mn}^{a_{mn}} \qquad \text{with } m \leqslant n \text{ and } m+n \leqslant r. \tag{7}$$

The weights a_{mn} were derived by Enting [8], and are modified in the present algorithm to utilize the rotational symmetry of the square lattice. 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. We use the *time-limited* version of the algorithm [1] in which the largest rectangles are determined by a cut-off parameter $b_{\max}$, $m + n \leqslant r = 3b_{\max} + 2$. The simplest connected graphs not contained in such rectangles are chains of r sites all in the '$S-1$' state. From (1) we see that such chains give rise to terms of order $2(r+1)[S^2 - S(S-1)] + (r-1)[S^2 - (S-1)^2] = r(4S-1)+1$, from the $2(r+1)$ interactions between spins in states 'S' and '$S-1$' and the $r-1$ interactions between spins both in state '$S-1$'. For a given value of $b_{\max}$ the series expansion is thus correct to order $u^{(3b_{\max}+2)(4S-1)}$. In an earlier paper [1] we reported on the $S=1$ case where we went to $b_{\max}=8$ giving a series correct to u^{78}. We have since extended these series to u^{113} using a more efficient parallel algorithm and a new extrapolation procedure [9]. For the present work we have calculated the series expansions for $S=\frac{3}{2}$, 2, $\frac{5}{2}$ and 3, deriving series correct to u^{100} ($b_{\max}=6$) for $S=\frac{3}{2}$, u^{119} ($b_{\max}=5$) for $S=2$, u^{126} ($b_{\max}=4$) for $S=\frac{5}{2}$, and u^{154} ($b_{\max}=4$) for $S=3$.

3. Analysis of the series

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

$$M(u) \sim \prod_j A_j(u_j-u)^{\beta_j}[1 + a_{j,1}(u_j-u) + a_{j,\Delta}(u_j-u)^{\Delta_j} + \cdots] \tag{8}$$

$$\chi(u) \sim \prod_j B_j(u_j-u)^{-\gamma_j'}[1 + b_{j,1}(u_j-u) + b_{j,\Delta}(u_j-u)^{\Delta_j} + \cdots] \tag{9}$$

$$C_v(u) \sim \prod_j C_j(u_j-u)^{-\alpha_j'}[1 + c_{j,1}(u_j-u) + c_{j,\Delta}(u_j-u)^{\Delta_j} + \cdots] \tag{10}$$

where the terms involving Δ_j represent the leading non-analytic confluent singularity and the dots $\cdots$ represent higher-order analytic and non-analytic confluent terms. By universality, it is expected that the leading critical exponents at the physical singularity, u_c, 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).

We analysed the series using differential approximants (see [10] for a comprehensive review), which allows one to locate the singularities and estimate the associated critical exponents fairly accurately, even in cases such as these where there are many singularities. We find that ordinary Dlog Padé approximants (first-order homogeneous differential approximants) yield the most accurate estimates for the physical singularity of the magnetization series, whereas first- and second-order inhomogeneous approximants are required in order to analyse the susceptibility and specific heat series. Here it suffices to say that a Kth-order differential approximant to a function f is formed by matching the first series coefficients to an inhomogeneous differential equation of the form (see [10] for details)

$$\sum_{i=0}^{K} Q_i(x)\left(x\frac{\mathrm{d}}{\mathrm{d}x}\right)^i f(x) = P(x) \tag{11}$$

where Q_i and P are polynomials of order N_i and L, respectively. First- and second-order approximants are denoted by $[L/N_0; N_1]$ and $[L/N_0; N_1; N_2]$, respectively.

3.1. The physical singularity

In this section we focus on the behaviour at the physical critical point. First we give a somewhat detailed summary of the analysis of the spin-$\frac{3}{2}$ series so as to introduce the various techniques and approximation procedures that we have applied in the analysis. Generally the estimates for the critical parameters at the physical singularity are quite poor because the series have many non-physical singularities closer to the origin and even for the spin-1 series [1, 9] the convergence of the estimates to the true values of the critical parameters is very slow. We see no evidence that the critical exponents of spin-S Ising model are not in agreement with the universality hypothesis. Under this assumption, we have derived improved estimates for the location of the physical critical point and the critical amplitudes.

In table 1 we have listed the estimates for the physical singularity and critical exponent for the spontaneous magnetization of the spin-$\frac{3}{2}$ Ising model. The estimates were obtained from homogeneous differential approximants (which are equivalent to Dlog Padé approximants). There is a quite substantial spread among the various approximants with most approximants yielding estimates around $u_c \simeq 0.7380$ and $\beta \simeq 0.130$. The estimates of β, while generally on the large side, are consistent with expectations of universality which would indicate that $\beta = \frac{1}{8}$. If we assume this value to be exact, we see that the approximants (assuming a linear dependence of β on u_c) would lead to $u_c \simeq 0.737\,75$.

Table 1. Estimates for u_c and β for the spin-$\frac{3}{2}$ Ising model as obtained from $[N, M]$ homogeneous first-order differential approximants.

	$[N-1, N]$		$[N, N]$		$[N+1, N]$	
N	u_c	β	u_c	β	u_c	β
40	0.738 148	0.1306	0.738 167	0.1308	0.738 049	0.1295
41	0.738 124	0.1303	0.738 020	0.1291	0.738 081	0.1298
42	0.737 908	0.1275	0.737 948	0.1281	0.737 125	0.1085
43	0.737 918	0.1277	0.738 046	0.1294	0.738 099	0.1300
44	0.738 128	0.1303	0.738 105	0.1301	0.738 098	0.1300
45	0.738 123	0.1303	0.738 059	0.1296	0.740 267	0.1038
46	0.737 958	0.1283	0.738 135	0.1304	0.738 140	0.1304
47	0.738 140	0.1304	0.738 135	0.1304	0.738 331	0.1317
48	0.736 928	0.1047	0.737 705	0.1242	0.737 673	0.1236
49	0.737 676	0.1236	0.737 700	0.1241	0.737 867	0.1271
50	0.738 187	0.1313	0.737 810	0.1261		

In tables 2 and 3 we have listed estimates for the position of the physical singularities and critical exponents of the series for susceptibility and specific heat of the spin-$\frac{3}{2}$ model. Since the first non-zero term in these series is u^6, the estimates were obtained by analysing the series $\chi(u)/u^6$ and $C_v(u)/u^6$. The estimates were obtained by averaging first-order $[L/N; M]$ and second-order $[L/N; M; M]$ inhomogeneous differential approximants with $|N - M| \leqslant 1$. For each order L of the inhomogeneous polynomial we averaged over most approximants to the series, which as a minimum used all the series terms up to the last 15 or so. Some approximants were excluded from the averages because the estimates were obviously spurious. Examples include the [47, 48] and [46, 45] approximants in table 1. The error quoted for these estimates reflects the spread (basically one standard deviation) among the approximants. Note that these error bounds should *not* be viewed as a measure of the true error as they cannot include possible systematic sources of error. While the estimates are not very good, we see that the estimates for u_c are consistent with the value $u_c \simeq 0.737\,75$ obtained from the magnetization series by demanding $\beta = \frac{1}{8}$ and that the exponent estimates are consistent with universality expectations of $\gamma' = \frac{7}{4}$ and $\alpha' = 0$.

As for the critical exponents, it is obvious that the behaviour at u_c (except for $S = \frac{1}{2}$ and 1) is not represented very well by the series. This discrepancy, which becomes more

Table 2. Estimates for u_c and γ' for the spin-$\frac{3}{2}$ Ising model as obtained from inhomogeneous first- and second-order differential approximants (DA).

	First-order DA		Second-order DA	
L	u_c	γ'	u_c	γ'
0	0.737 87(40)	1.848(63)	0.738 02(37)	1.864(58)
1	0.738 08(31)	1.882(52)	0.738 10(26)	1.868(49)
2	0.738 00(19)	1.864(34)	0.738 18(20)	1.882(39)
3	0.738 04(23)	1.874(43)	0.738 04(33)	1.848(72)
4	0.737 92(48)	1.82(10)	0.738 05(38)	1.863(69)
5	0.738 03(46)	1.895(65)	0.738 08(25)	1.852(69)
6	0.737 87(53)	1.839(99)	0.738 03(53)	1.82(18)
7	0.738 23(18)	1.50(98)	0.737 92(51)	1.80(12)
8	0.737 74(64)	1.76(20)	0.738 08(31)	1.861(62)

Table 3. Estimates for u_c and α' for the spin-$\frac{3}{2}$ Ising model as obtained from inhomogeneous first- and second-order differential approximants (DA).

	First-order DA		Second-order DA	
L	u_c	α'	u_c	α'
0	0.740 62(88)	0.343(16)	0.7393(18)	0.17(25)
1	0.740 30(88)	0.320(80)	0.7382(15)	0.20(80)
2	0.7397(20)	0.24(32)	0.7389(18)	0.12(20)
3	0.7401(10)	0.32(10)	0.7384(16)	0.07(23)
4	0.7370(28)	0.06(71)	0.7381(17)	0.03(31)
5	0.7381(21)	0.04(38)	0.7378(21)	0.05(48)
6	0.7373(25)	0.24(61)	0.7388(29)	0.07(53)
7	0.7357(24)	0.21(64)	0.7381(28)	0.33(90)
8	0.7356(24)	0.25(68)	0.7386(25)	0.02(66)

pronounced as S increases, is hardly surprising given that the number of non-physical singularities within the physical disc increases rapidly with spin magnitude (see the following section for details). The quite complicated singularity structure of the series simply tends to obscure the behaviour at the physical singularity. This problem is possibly further aggravated by the presence of confluent terms. The only series which yields reasonably accurate estimates is the magnetization from which we estimate $\beta = 0.139(4)$, $0.138(5)$, and $0.132(2)$ for $S = 2$, $\frac{5}{2}$, and 3, respectively. Again, the quoted errors are merely a measure of the spread among the approximants rather than the true error. The differential approximant analysis of the higher S series for the susceptibility and specific heat yields little of value. Estimates for the critical exponent γ' fluctuate wildly and lie somewhere between 0.5 and 2 while generally favouring values below $\frac{7}{4}$. Similarly, estimates for α' lie between -0.5 and 1. So while no sensible estimates can be obtained there is no evidence to suggest that the exponents are not consistent with universality.

While this situation is somewhat disappointing it is hardly surprising in light of the behaviour of the spin-1 series, where our earlier analysis showed a very slow convergence of estimates towards the true values of the critical parameters [1, 9]. Although the order to which the higher spin-S series are correct exceeds that of the spin-1 series, this is really just a consequence of the definition of the expansion variable u. We would expect the accuracy of estimates to depend not so much on the actual order of the series as much as on the maximal cut-off given by b_{max}. In essence, the accuracy is determined by the number of distinct graphs, consisting of spins flipped from the ground state (irrespective of the actual value of the spins), that one has summed over. One should therefore not expect more accurate estimates from the higher spin-S series than those one could have obtained by truncating the spin-1 series at an order determined by the associated value of b_{max}.

One may hope to obtain improved estimates for u_c by raising the relevant series to the power $1/\lambda$, where λ is the expected leading critical exponent, and look for simple zeros and poles of the resulting series. This procedure of biasing works quite well for the magnetization and susceptibility series (it obviously cannot be used for the specific heat series). It is well known that the analysis of series exhibiting a logarithmic divergence, as we expect of the specific heat series, is particularly difficult. A fairly simple way of circumventing these problems is to study the derivative of the specific heat, $\mathrm{d}/\mathrm{d}uC_v(u)$. The series for this quantity should have a simple pole at u_c, a situation much more amenable to analysis by either differential approximants or even just ordinary Padé approximants. This approach does indeed confirm the logarithmic divergence at u_c, though the evidence becomes rather circumstantial for higher values of S. The estimates for u_c derived in this fashion are tabulated in table 4 and were obtained by averaging ordinary $[N + K, N]$ Padé approximants ($K = 0, \pm 1$) with $2N + K + 15$ not less than the order of the series. The error quoted for these estimates again merely reflects the spread among the approximants.

Table 4. Biased estimates for the physical singularity.

S	Magnetization	Susceptibility	Specific heat
$\frac{3}{2}$	0.737 74(2)	0.7372(2)	0.7379(5)
2	0.8293(2)	0.8288(2)	0.833(3)
$\frac{5}{2}$	0.8795(3)	0.881(3)	0.882(2)
3	0.9107(4)	0.914(1)	0.905(4)

It is often possible to find a transformation of variable which will map the non-physical singularities outside the transformed physical disc. One such transformation is given by $u = x/(2 - x)$. Although the series in the transformed variable have radii of convergence determined by the physical singularity, this transformation turns out to be of little use and does not allow us to obtain better estimates for the critical parameters. This is probably because there are still singularities close to the physical disc and because such singularity-moving transformations may introduce long-period oscillations [10].

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 $f(u) \sim A(1-u/u_c)^{-\lambda}$, 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 specific heat series two different approaches have been used. In the first approach we use the 'trick' applied previously and look at the derivative of the specific heat series for which the above method should work with $\lambda = 1$. In table 5 we have listed the estimates for the critical amplitudes obtained in this fashion. As usual, estimates for any given value of u_c were obtained by averaging over many higher-order approximants, and the error estimates in table 5 reflect both the spread among the various approximants as well as the dependence on u_c. In the second approach we start from $f(u) \sim A \ln(1 - u/u_c)$ and form the series $g(u) = \exp(-f(u))$ which has a singularity at u_c with exponent A. One virtue of this approach is that no prior estimate of u_c is needed. However, the spread among estimates from different approximants is very substantial although consistent with table 5. Biasing the estimates at u_c also confirms the value of the amplitude, although generally the spread is larger than for the first approach. For the spin-3 susceptibility and specific heat series we could not obtain reliable amplitude estimates since the spread tended to be larger than the average value and the poor estimate of u_c leads to even greater errors.

Table 5. Estimates for the amplitudes at the physical singularity.

S	Magnetization	Susceptibility	Specific heat
$\frac{3}{2}$	1.875(5)	0.019(3)	52(2)
2	2.57(2)	0.0088(5)	110(5)
$\frac{5}{2}$	3.33(3)	0.006(2)	190(10)
3	4.10(5)	—	—

In the second method, proposed by Liu and Fisher [11], 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 [10]. 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 $g(u)$. This analysis yields amplitude estimates consistent with those in table 5, but with larger error bars.

In table 6 we have listed our final estimates for the physical singularities and the associated exponents and amplitudes. For the estimates of the position of the physical singularities we have placed most weight on the biased analysis of the magnetization series. In the spin-$\frac{1}{2}$ case, u_c and the exponents α' and β and the amplitudes A_C and A_M are known exactly due to the calculation of the free energy by Onsager [12] and the magnetization by Yang [13]. The susceptibility amplitude A_χ is known to very high precision [14]. The spin-1 estimates are from [9].

Table 6. The physical singularities and associated exponents and amplitudes.

S	u_c	β	A_M	γ'	A_χ	α'	A_C
$\frac{1}{2}$	$3-2\sqrt{2}$	$\frac{1}{8}$	1.138 789	$\frac{7}{4}$	0.584 850	0	5.406 58
1	0.554 065 3(5)	0.125 07(3)	1.2083(2)	1.750(1)	0.0617(1)	0.0005(10)	22.3(5)
$\frac{3}{2}$	0.737 75(15)	0.128(3)	1.875(15)	1.85(15)	0.019(5)	0.0(3)	52(4)
2	0.8293(3)	0.139(4)	2.57(4)	—	0.009(1)	—	110(10)
$\frac{5}{2}$	0.8795(5)	0.138(5)	3.33(6)	—	0.006(2)	—	190(20)
3	0.911(1)	0.132(2)	4.1(1)	—	—	—	—

3.2. Non-physical singularities

Except for $S = \frac{1}{2}$, the series have a radius of covergence smaller than u_c due to singularities in the complex u-plane closer to the origin than the physical critical point. Since all the coefficients in the expansion are real, complex singularities always come in pairs. The number of non-physical singularities appears to increase quite dramatically with S, thus making it exceedingly hard to locate them accurately for large S.

Table 7. Non-physical singularities u_s and associated exponents of the spin-S series.

	u_s	$\|u_s\|/u_c$	β	γ'	α'
Spin-1					
1	−0.598 550(5)	1.08	0.1248(3)	1.750(5)	0.005(10)
1	−0.301 939 5(5) ± 0.378 773 5(5)i	0.87	−0.1690(2)	1.1692(2)	1.1693(3)
Spin-$\frac{3}{2}$					
3	0.63(1) ± 0.45(1)i	1.05	−1.8(5)	2.7(5)	2.4(6)
1	0.094 77(2) ± 0.641 17(5)i	0.88	−0.174(5)	1.185(5)	1.185(1)
2	−0.0654(5) ± 0.7113(4)i	0.97	−0.18(3)	1.21(2)	1.22(3)
1	−0.529 24(2) ± 0.337 97(2)i	0.85	−0.177(5)	1.184(5)	1.188(5)
Spin-2					
2	−0.842(5)	1.02	0.130(4)	1.2(5)	0.3(4)
1	0.3767(2) ± 0.6401(1)i	0.90	−0.16(3)	1.19(1)	1.19(3)
2	0.302(6) ± 0.727(8)	0.95	—	1.3(4)	1.2(3)
4	0.215(15) ± 0.805(15)i	1.00	—	—	—
1	−0.225 61(2) ± 0.682 47(4)i	0.87	−0.16(2)	1.194(6)	1.192(6)
2	−0.394(5) ± 0.700(6)i	0.97	—	1.8(6)	1.6(4)
1	−0.648 90(4) ± 0.286 96(4)	0.86	−0.180(5)	1.197(6)	1.194(6)
3	−0.685(15) ± 0.485(15)i	1.01	—	2.3(5)	1.4(3)
Spin-$\frac{5}{2}$					
1	0.5501(3) ± 0.5842(2)i	0.91	−0.4(1)	1.19(2)	1.19(4)
3	0.522(5) ± 0.645(10)i	0.94	−1.2(4)		
1	0.0612(2) ± 0.7759(2)i	0.88	−0.2(1)	1.20(3)	1.19(2)
3	−0.03(1) ± 0.83(1)i	0.94	—	—	—
1	−0.4227(1) ± 0.6400(1)i	0.87	−0.20(5)	1.185(15)	1.21(3)
3	−0.575(5) ± 0.61(2)i	0.95	—	—	—
3	−0.665(15) ± 0.53(1)i	0.97	—	—	—
1	−0.7213(2) ± 0.245 95(15)i	0.87	−0.175(25)	1.20(2)	1.20(2)
4	−0.745(15) ± 0.39(2)i	0.96	—	—	—
Spin-3					
	−0.92(1)	1.01	—	—	—
1	0.6608(4) ± 0.5232(5)i	0.93	—	1.20(3)	1.20(3)
3	0.645(15) ± 0.595(15)i	0.96	−1.4(5)	2.0(5)	2.0(5)
1	0.2729(3) ± 0.7730(4)i	0.90	—	1.20(4)	1.19(4)
4	0.220(15) ± 0.840(15)i	0.95	—	1.6(4)	1.6(4)
1	−0.1686(1) ± 0.7902(1)i	0.89	−0.19(3)	1.20(2)	1.20(2)
2	−0.275(5) ± 0.825(5)i	0.95	—	1.2(3)	1.2(3)
1	−0.549 55(5) ± 0.583 51(3)i	0.88	−0.20(4)	1.196(6)	1.197(5)
2	−0.68(1) ± 0.54(1)i	0.95	—	1.1(4)	1.0(4)
1	−0.769 25(10) ± 0.214 30(5)i	0.88	−0.185(25)	1.205(15)	1.205(15)

In order to locate the non-physical singularities in a systematic fashion we used the following procedure. We calculate all $[L/N; M]$ inhomogeneous first-order differential approximants with $|N - M| \leqslant 1$ using all, or almost all, series terms for $10 \leqslant L \leqslant 16$. (We discard no more than the last 15–20 terms.) Each approximant yields M possible singularities and associated exponents from the M zeros of Q_1 (many of these are, of course, not actual singularities of the series but merely spurious zeros of Q_1). Next we sort these 'singularities' into equivalence classes by the criterion that they lie at most a distance 2^{-k} apart. An equivalence class is accepted as a singularity if it contains more

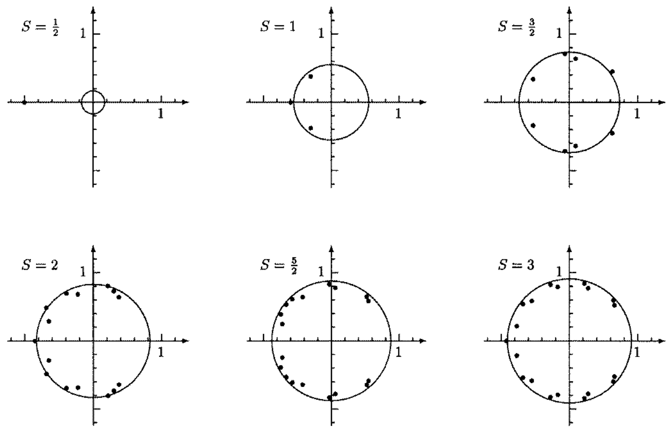

Figure 1. The distribution of singularities in the complex u-plane. In all cases the circle has radius u_c.

than N_a approximants (N_a can be adjusted but we typically use a value around $\frac{2}{3}$ of the total number of approximants), and an estimate for the singularity and exponent is obtained by averaging over the approximants (the spread among the approximants is also calculated). This calculation is then repeated for $k - 1$, $k - 2$, ... until a minimal value of roughly five. To avoid outputting well converged singularities at every level, once an equivalence class has been accepted, the approximants which are members of it are removed, and the subsequent analysis is carried out on the remaining data only. This procedure is applied to each series in turn producing tables of possible singularities. Next we look at these tables in order to identify the true singularities.

In table 7 we have listed the non-physical singularities that we believe to have been identified with some degree of certainty and accuracy. For higher spin values several of these are marred by large error bounds and it is quite possible that we have not been able to locate all non-physical singularities of the series, particularly for $S = \frac{5}{2}$ and 3. First we accepted any singularity which appeared in all the series at a reasonably early level, say $k \geqslant 10$. These singularities are marked 1 in table 7 and all of them are undoubtedly true singularities. Singularities which appear for $k < 10$ are a lot more tricky to deal with. Generally we also expect that a singularity which appears for $k = 8$ or 9 (or higher) in all series and for the majority of values of L is a true singularity of the series (these are marked 2 in table 7). However, we often find that some singularities appear for $k = 8$ or higher in some series but at lower values of k all the way down to 5 in other series, and it is not easy to determine which ones are true singularities and which ones are not. Those marked 3 appear in all series and for all values of L while those marked 4 appear in some series for all L but not neccesarily for all L in other series.

The distribution of singularities is shown in figure 1. A remarkable feature of the singularity distribution is its regularity. As S increases the complex singularities move closer to the perimeter of the physical disc and the distance between the various singularities become more uniform. In the limit $S \to \infty$ it thus seems likely that the singularities will converge onto the unit circle.

We find the very old conjecture by Fox and Guttmann [2] that the number of singularities inside the physical disc equals $qS - 2$, where q is the coordination number of the lattice ($q = 4$ for the square lattice), to be invalid for $S > 1$. Recently, Matveev and Shrock [6] studied the distribution of zeros of the partition function of the square lattice Ising model for $S = 1$, $\frac{3}{2}$, and 2. They conjectured that all divergences of the magnetization occur at endpoints of arcs of zeros protruding into the ferromagnetic phase and that there are $4[S^2] - 2$ such arcs for $S \geqslant 1$, where $[x]$ denotes the integer part of x. Our analysis seems to confirm these conjectures for the magnetization series up to $S = 2$. In particular, we find evidence of singularities close to the endpoints located by Matveev and Shrock [6] for these spin values.

The estimate for γ' at the singularity $u_- = -1$ of the spin-$\frac{1}{2}$ susceptibility and the estimates for the spin-1 series are based on the low-temperature series we published elsewhere [1, 9]. The estimate for γ' of the spin-$\frac{1}{2}$ case is consistent with the exact value $\gamma' = \frac{3}{2}$ also reported by Matveev and Shrock [15].

From table 7 we observe that the exponents at the singularities in the complex plane which are well converged (those marked 1) appear to be independent of S. In the case of integer spin it appears that the exponents associated with the singularity on the negative u-axis equal those at u_c. While the exponents are independent of S, note that they do depend on the lattice structure [15], so a much weaker version of universality holds at the non-physical singularities. In all these cases we observe that the Rushbrooke inequality [16],

$$\alpha' + 2\beta + \gamma' \geqslant 2 \tag{12}$$

is satisfied, and it does indeed seem quite possible that the exponents satisfy the equality in equation (12). At the remaining singularities the errors on the exponent estimates are too large to make any such assertion.

E-mail or www retrieval of series

The low-temperature series for the spin-S Ising model can be obtained via e-mail by sending a request to iwan@maths.mu.oz.au or via the worldwide web on http://www.maths.mu.oz.au/~iwan/ by following the instructions.

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References

[1] Enting I G, Guttmann A J and Jensen I 1994 *J. Phys. A: Math. Gen.* **27** 6987
[2] Fox P F and Guttmann A J 1973 *J. Phys. C: Solid State Phys.* **6** 913
[3] Saul D M, Wortis M and Jasnow D 1975 *Phys. Rev.* B **11** 2571
[4] Camp W J and Van Dyke J P 1975 *Phys. Rev.* B **11** 2579
[5] Nickel B G 1981 *Physica* **106A** 48
[6] Matveev V and Shrock R 1995 *J. Phys. A: Math. Gen.* **28** L533
[7] Sykes M F and Gaunt D S 1973 *J. Phys. A: Math. Gen.* **6** 643
[8] Enting I G 1978 *J. Phys. A: Math. Gen.* **11** 563
[9] Jensen I and Guttmann A J 1996 *J. Phys. A: Math. Gen.* **29** 3817
[10] Guttmann A J 1989 *Phase Transitions and Critical Phenomena* vol 13, ed C Domb and J Lebowitz (New York: Academic) pp 1–234
[11] Liu A J and Fisher M E 1989 *Physica* **156A** 35

[12] Onsager L 1944 *Phys. Rev.* **65** 117
[13] Yang C N 1952 *Phys. Rev.* **85** 808
[14] Barouch E, McCoy B M and Wu T T 1973 *Phys. Rev. Lett.* **31** 1409
[15] Matveev V and Shrock R 1995 *J. Phys. A: Math. Gen.* **28** 1557
[16] Rushbrooke G S 1963 *J. Chem. Phys.* **39** 842