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Extrapolation procedure for low-temperature series for the square lattice spin-1 Ising model

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Abstract. The finite-lattice method of series expansions has been combined with a new extrapolation procedure to extend the low-temperature series for the specific heat, spontaneous magnetization, and susceptibility of the spin-1 Ising model on the square lattice. The extended series were derived by directly calculating the series to order 99 (in the variable $u = \exp[-J/k_B T]$) and using the new extrapolation procedure to calculate an additional 13–14 terms.

1. Introduction

In a recent paper [1], we reported on the calculation and analysis of low-temperature series for the square lattice spin-1 Ising model. The series was derived to 79th order (in the variable $u = \exp[-J/k_B T]$) using the finite-lattice method [2] and employed a new algorithm which removed much of the memory-size restrictions of previous implementations. In this paper we report on a further extension of these series to order 113 for the specific heat and spontaneous magnetization and order 112 for the susceptibility. The extension is obtained by direct calculation of the series to order 99 and use of a new extrapolation procedure to extend the series by an additional 13 or 14 terms. The improvement in the direct series derivation is due to a more efficient implementation of the algorithm and the use of parallel computation. The extrapolation procedure is similar to and inspired by work on directed percolation [3].

2. The series expansion technique

The Hamiltonian defining the spin-1 Ising model in a magnetic field h can be written

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

where the spin variable $\sigma_i = 0, \pm 1$. The first sum is over nearest-neighbour pairs and the second sum is over sites. The constants are chosen so the ground state ($\sigma_i = +1\ \forall i$) has zero energy. The low-temperature expansion is based on perturbations from the fully aligned ground state. The expansion is expressed in terms of the temperature variable

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$u = \exp(-\beta J)$ and the field variable $\mu = \exp(-\beta h)$, where $\beta = 1/k_B T$. The expansion of the partition function in powers of u may be expressed as

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

where $\Psi_n(\mu)$ are polynomials in μ. It is more convenient to express the field dependence in terms of the variable $x = 1 - \mu$ and truncate the expansion at x^2

$$Z = Z_0(u) + x Z_1(u) + x^2 Z_2(u) + \cdots \tag{3}$$

where $Z_n(u)$ is a series in u formed by collecting all terms in the expansion of Z containing factors of x^n. Standard definitions yield the spontaneous magnetization

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

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

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

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

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

So in order to obtain the series expansion of the specific heat, spontaneous magnetization and susceptibility it suffices to calculate the three quantities Z_0, Z_1 and Z_2.

On the square lattice the infinite lattice partition function Z can be approximated by a product of partition functions Z_{mn} on *finite* ($m \times n$) lattices,

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

where r is a cut-off which limits the size of the rectangles considered. The weights a_{mn} are small integers and are known explicitly [4] for the square lattice,

$$a_{mn} = \begin{cases} 1 & \text{if } m+n = r \\ -3 & \text{if } m+n = r-1 \\ 3 & \text{if } m+n = r-2 \\ -1 & \text{if } m+n = r-3 \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

Due to the symmetry of the square lattice one obviously has that $Z_{mn} = Z_{nm}$, so one need only consider the case $m \leqslant n$ and change the weights a_{mn} appropriately, i.e. multiply by 2 if $m < n$.

For the low-temperature expansion of the Ising model, Z_{mn} is calculated as the sum over all spin configurations on the finite lattice. All spins outside the $m \times n$ range are fixed at $+1$. The number of terms derived correctly with the finite-lattice method is given by the power of the lowest-order connected graph not contained in any of the rectangles considered, which in this case are chains of sites all in the '0' state. From the Ising Hamiltonian we see that such chains give rise to terms of order $3r + 1$. For a given value of r the series expansion is thus correct to order $3r$.

The efficient way of calculating Z_{mn} is by transfer matrix techniques. We refer to [1] for a detailed description of the algorithm. For this work we used a more efficient implementation of the algorithm and a parallel computer, and we were able to derive the series directly up to a maximal cut-off $r_m = 33$.

3. Extrapolation of series

The series can be extended significantly via an extrapolation method similar to that of [3]. Consider the series for $Z_n(u)$. For each $r \leqslant r_m$ we use the finite-lattice method to calculate the polynomials $Z_{n,r}(u) = \sum_{j=0} z_{n,j,r} u^j$ correct to $\mathcal{O}(u^{3r+20})$. As already noted, these polynomials agree with the series for Z_n to $\mathcal{O}(u^{3r})$. Next, we look at the sequences $d_{n,r,s}$ obtained from the difference between successive polynomials

$$Z_{n,r+1}(u) - Z_{n,r}(u) = u^{3r+1} \sum_{s \geqslant 0} (z_{n,3r+s+1,r+1} - z_{n,3r+s+1,r}) u^s = u^{3r+1} \sum_{s \geqslant 0} d_{n,s,r} u^s. \qquad (9)$$

The first of these correction terms $d_{n,0,r}$ is often a simple sequence which one can readily identify. In the case of Z_0, we find the sequence

$$-d_{0,0,r} = 1, 2, 6, 18, 52, 138, 338, 778, 1712, \ldots$$

from which we conjecture

$$d_{0,0,r} = -2^{r+2} + (r^3 + 3r^2 + 2r + 18)/3 \qquad r \geqslant 2. \qquad (10)$$

The formula for $d_{0,0,r}$ holds for all the $r_m - 1$ values that we calculated and we are very confident that it is correct for all values of r. As was the case in [3], the higher-order correction terms $d_{n,s,r}$ can be expressed as rational functions of $d_{n,0,r}$. Due to the form of the first correction term this leads to the general extrapolation formulae

$$d_{n,s,r} = \frac{1}{6s!n!} \sum_{j=0}^{s+n+3} a_{n,s,j} r^j + \frac{1}{s!n!} \sum_{j=0}^{s+n} b_{n,s,j} r^j 2^r \qquad r \geqslant s + 2. \qquad (11)$$

The factors in front of the sums have been chosen so as to make the leading coefficients particularly simple. We were able to find formulae for all correction terms up to $s = 13$ for Z_0 and Z_1, and up to $s = 12$ for Z_2. The coefficients in the extrapolation formulae are listed in tables 1–3.

It is clear from equation (11) that the $r_m - s - 2$ terms available from the various sequences for the correction terms are not sufficient to determine all the $2(s + n + 2) + 1$ unknown coefficients in the extrapolation formulae for large s. However, from tables 1–3 we immediately see that the leading coeffients, $a_{n,s,s+n+3}$ and $b_{n,s,s+n}$, in the extrapolation formulae are alternating in sign but otherwise constant, for example, $a_{n,s,s+n+3} = (-1)^{s+n} 2$ and $b_{n,s,s+n} = -(-1)^{s+n} 4$. In general we have found that the leading coeffients are expressible as polynomials in s,

$$a_{n,s,s+n+3-k} = \frac{(-1)^{s+n}}{(2s)!} \sum_{j=0}^{2k+l} \alpha_{n,k,j} s^j \qquad (12)$$

and

$$b_{n,s,s+n-k} = \frac{(-1)^{s+n}}{(s+1)!4^{s-1}} \sum_{j=0}^{2k} \beta_{n,k,j} s^j \qquad (13)$$

where $l = \max(k - 3, 0)$. The coefficients of these polynomials are listed in table 4 and table 5.

Table 1. Coefficients $a_{0,s,j}$ and $b_{0,s,j}$ in the extrapolation formula (11) for Z_0.

	j									
s	0	1	2	3	4	5	6	7	8	9
$a_{0,s,j}$										
0	36	540	22872	1107432	63379296	4055122080	288647444160	22547966414400	1918636884702720	176562491228282880
1	4	−388	−15300	−659892	−33706248	−1962612264	−128643760656	−9349955599536	−746245210622400	−64847088398958912
2	6	98	3708	148480	6885452	372299004	22859538096	1569303632880	119023740391728	9880468953163920
3	2	−8	−350	−15378	−692008	−35838744	−2117794652	−140423589580	−10308461906400	−830282122344096
4		−2	12	850	39698	2015962	117161232	7676696540	556423820364	44185336926052
5			2	−18	−1690	−78876	−4420926	−287670222	−20887171580	−1654723702956
6				−2	26	2956	132144	7963662	583444134	46791584450
7					2	−36	−4728	−195000	−12264582	−1033287048
8						−2	48	7080	258576	16303470
9							2	−62	−10080	−309132
10								−2	78	13790
11									2	−96
12										−2
13										
14										
15										
16										

Table 1. (Continued)

	j			
s	10	11	12	13
$a_{0,s,j}$				
0	17472051515349043200	18499530593915255808 00	20868045222778090444800 0	249841335378900619081728 00
1	−6093544542023399040	−61558059730268248128 0	−665234786277059208422 40	−76570406703853803682329 60
2	890825375508579936	866712721369235532 48	904980040816347572428 8	100930371648038257843123 2
3	−72794312849256336	−690142583383674504 0	−703518910546232023200	−69673033843735084198812 8
4	3818076291712376	356800848438240648	3586304651592159067 2	38585173865522055866 40
5	−14221175621228	−13202390656569708	−1317402227058041720	−140668642000137358744
6	4033976898388	373970026441792	37214095717203636	3959799742297856756
7	−91299422789	−8506311905850	−846366898168088	−89980514374296832
8	1658091108	161206833194	16060785342426	1705608425121458
9	−18208734	−2480840274	−265232878130	−27784108335412
10	327676	15045162	3551877714	416896760852
11	−18266	−289710	−2605714	−4993549652
12	116	23558	165102	−24785696
13	2	−138	−29710	81916
14		−2	162	36760
15			2	−188
16				−2

Table 1. (Continued)

s	j = 0	1	2	3	4	5	6	7	8	9	10	11	12	13
$b_{0,s,j}$														
0	−4	−8	−26	−174	−1794	−29040	−621855	−16476705	−470890980	−14775299910	−502882151625	−18429217173675	−734477218900425	−31757793382715400
1		4	10	−70	−863	−13364	$-218665\frac{1}{2}$	$-3099628\frac{1}{2}$	$-50245171\frac{1}{2}$	−1002068919	$-25366148178\frac{3}{4}$	$-911394577226\frac{1}{4}$	$-40664486659736\frac{1}{4}$	$-1919833204276777\frac{1}{2}$
2			−4	−6	409	4105	43289	618625	$-275468\frac{3}{4}$	−186136038	$-6579087314\frac{5}{8}$	$-231588134427\frac{3}{8}$	$-6538249560737\frac{1}{4}$	−170426278459944
3				4	−4	−1085	$-8407\frac{1}{2}$	11116	$819836\frac{1}{2}$	$77789387\frac{3}{4}$	$2571738900\frac{5}{8}$	$58200571408\frac{3}{8}$	$1572709594180\frac{5}{16}$	$32784296682271\frac{7}{8}$
4					−4	20	2165	$8942\frac{1}{2}$	$-429182\frac{1}{4}$	−8136639	$-322113948\frac{1}{8}$	$-8743272683\frac{3}{4}$	$-73717696634\frac{5}{16}$	$687212762691\frac{13}{16}$
5						4	−42	−3689	4144	$1736096\frac{1}{4}$	$23447878\frac{1}{8}$	$610009090\frac{5}{8}$	$12227448244\frac{11}{16}$	$-584353065430\frac{1}{16}$
6							−4	70	5670	−46872	$-4727903\frac{1}{4}$	$-35390845\frac{7}{8}$	$-8870615\frac{3}{16}$	$13285766431\frac{7}{16}$
7								4	−104	−8094	142365	$10435103\frac{1}{4}$	$-3532691\frac{1}{4}$	$-4219620181\frac{9}{16}$
8									−4	144	10920	−321585	$-20006175\frac{3}{4}$	$213929108\frac{1}{4}$
9										4	−190	−14080	623865	$34494495\frac{3}{4}$
10											−4	242	17479	−1097239
11												4	−300	−20995
12													−4	364
13														4

Table 2. Coefficients $a_{1,s,j}$ and $b_{1,s,j}$ in the extrapolation formula (11) for Z_1.

	j									
s	0	1	2	3	4	5	6	7	8	9
$a_{1,s,j}$										
0	−24	−1008	−76272	−5684112	−457173792	−39103403040	−3574330130880	−348267251263680	−36106919860838400	−3973220722801612800
1	−10	242	26776	2132988	169186080	14031817536	1234927394784	115716608013024	11544174716755968	1224242942187936384
2	−13	161	3890	−11104	−10362700	−1228736780	−124161954720	−12398829627432	−1273546890227328	−136597270576055328
3	−5	−76	−2693	−88837	−3049540	−100973728	−1890947308	191723835836	40750032405880	5702911364579304
4	−2	7	312	12959	526035	23570715	1144281164	57449415410	2729697798164	90106090294292
5		2	−11	−793	−35251	−1674878	−88419027	−5114559137	−315077153986	−20142410271322
6			−2	17	1611	71790	3837282	232243641	15355331735	1081711840093
7				2	−25	−2852	−121842	−7085208	−490136073	−36372405428
8					−2	35	4596	180960	11069628	891555753
9						2	−47	−6917	−240352	−14817384
10							−2	61	9883	286375
11								2	−77	−13556
12									−2	95
13										2
14										
15										
16										
17										

Table 2. (Continued)

s	j = 10	11	12	13
$a_{1,s,j}$				
0	−462907224587766067200	−569600923508461684224OO	−738489395006205237964800O	−10065574785987010790083584OO
1	137714989912773327360	163936398645157144435 20	206020420892842843881216O	272692487745604926720576000
2	−153861791108218611 84	−182332612292880438086 4	−227313813910382067927168	−2978610602558157742269888O
3	735898260522888000	943567307178403493 28	1234952103902130310060 8	16690252078864539384543 36
4	−4306747906782568	−16412987365127990 72	−300489154903171705008	−4809400106223286465080O
5	−1282219400735740	−73711506188062096	−2454291894283312912	302424204333008932640
6	80200154284766	6155735350915480	475590666188289368	34934157032467155320
7	−2855093133545	−236164037257269	−20420710128454372	−1819694197681939020
8	73516462976	6324527102839	572875721359139	54403254827920427
9	−1460017005	−132977895083	−12335475680011	−1208966177416998
10	16521220	2223262547	222732548753	21808039004180
11	−300155	−13327961	−3238529375	−355244044168
12	17992	257333	1130371	4637002786
13	−115	−23241	−127937	25630356
14	−2	137	29347	−123620
15		2	−161	−36348
16			−2	187
17				2

Table 2. (Continued)

	j													
s	0	1	2	3	4	5	6	7	8	9	10	11	12	13
$b_{1,s,j}$														
0	0	4	38	669	14274	382185	11367045	374646825	13414424940	521931313260	21950041038975	994043048211675	48323690206458975	$2511969014601108562\frac{1}{2}$
1	4	8	28	294	3154	45380	$659431\frac{1}{2}$	$6912974\frac{1}{4}$	−63875241	−9516059361	$-577638937698\frac{3}{4}$	$-30629467750426\frac{7}{8}$	$-1598349963491021\frac{1}{4}$	$-85844158666522205\frac{5}{8}$
2		−4	−10	52	245	6049	$130525\frac{1}{2}$	$2055016\frac{3}{4}$	$70181556\frac{1}{2}$	$2443225632\frac{3}{4}$	$87983829793\frac{1}{8}$	$3603111185211\frac{3}{16}$	$151803540464029\frac{7}{8}$	$6697300760769555\frac{9}{16}$
3			4	6	−365	−2595	$-32166\frac{1}{2}$	$-703727\frac{1}{2}$	$-4071664\frac{1}{4}$	−104301900	$-4278680737\frac{1}{4}$	−98042635537	$-4951488221400\frac{3}{4}$	$-203120670598106\frac{5}{8}$
4				−4	4	1005	$5647\frac{1}{2}$	$-6373\frac{1}{2}$	$428858\frac{1}{2}$	$-49051827\frac{1}{2}$	−1421306965	$-22978129383\frac{11}{16}$	$-986226770316\frac{9}{16}$	$-22974904327241\frac{3}{4}$
5					4	−20	−2039	$-4700\frac{1}{2}$	$356788\frac{1}{4}$	3508470	$251750258\frac{3}{4}$	6762309950	$33331027784\frac{5}{16}$	$1317242138953\frac{13}{16}$
6						−4	42	3507	−9884	$-1495436\frac{1}{4}$	$-11750983\frac{1}{8}$	$-548505311\frac{3}{4}$	$-13280506010\frac{1}{16}$	$484639075867\frac{3}{8}$
7							4	−70	−5422	53820	$4151708\frac{1}{4}$	$11784625\frac{7}{8}$	$234317647\frac{7}{16}$	$4806055084\frac{3}{16}$
8								−4	104	7770	−149835	$-9271523\frac{1}{4}$	$43741046\frac{1}{4}$	$2899134157\frac{9}{16}$
9									4	−144	−10510	328405	$17901765\frac{3}{4}$	$-272545523\frac{1}{4}$
10										−4	190	13574	−628287	$-30979126\frac{3}{4}$
11											4	−242	−16867	1096849
12												−4	300	20267
13													4	−364
14														−4

Table 3. Coefficients $a_{2,s,j}$ and $b_{2,s,j}$ in the extrapolation formula (11) for Z_2.

	j								
s	0	1	2	3	4	5	6	7	8
$a_{2,s,j}$									
0	0	960	199008	25859664	3105873216	366981638400	43962925841280	5412646450270080	689859653042488320
1	12	724	3872	−3918624	−664081632	−88392730560	−11084244867072	−1384694987443488	−176331199274687232
2	−20	−444	−34224	−1984608	−100703480	−3423052408	152494743744	58829587491792	10515670803566400
3	16	−48	1788	325744	27280764	2042841660	148133624112	10422978961984	671732365773200
4	2	62	2056	49792	547580	−62926964	−9069431144	−924884356296	−87052546757280
5	2	−4	−286	−11426	−409240	−14714408	−466639676	−4246070624	1552859277500
6		−2	8	754	32534	1427150	66602412	3204308732	144793941316
7			2	−14	−1558	−67700	−3405654	−188754426	−11056264376
8				−2	22	2784	116304	6427038	414871986
9					2	−32	−4512	−174028	−10163570
10						−2	44	6816	232224
11							2	−58	−9764
12								−2	74
13									2
14									
15									
16									
17									

Table 3. (Continued)

	j			
s	9	10	11	12
$a_{2,s,j}$				
0	91351020237486105600	12589478624473041715200	1806730592586035116492800	269979775259474769527808000
1	−23140865178023786496	−3146715137132668707840	−444530245545400234049280	−65310818282764528381701120
2	1629900454944139200	243735746832642107520	36500387580624231020736	5565229584050566554128640
3	31014499461745392	−1105330916217243648	−683352705387601823616	−155665991250042317339904
4	−7980855749069280	−715388251788131360	−60821071543388792752	−4414115889872814761376
5	259271668545748	32421044232235536	3730895758411050000	413972960682773319120
6	4584284710972	−173506172385408	−64646756919141120	−10662860072358795800
7	−654356019664	−36883161160012	−1658325705468872	1972409671354252
8	28039294862	1943327703680	135094260867632	8967575039268340
9	−774000120	−58982092862	−4593416253250	−365367972622928
10	13674990	1290331376	109505894322	9324373410550
11	−277408	−15198942	−1993340778	−186906331802
12	13418	290880	11939322	2942846678
13	−92	−17834	−248470	141926
14	−2	112	23062	120410
15		2	−134	−29146
16			−2	158
17				2

Table 3. (Continued)

s \ $b_{2,s,j}$	j = 0	1	2	3	4	5	6	7	8	9	10	11	12
0	0	0	−40	−1848	−72579	−2888655	−118290915	−5121342765	−235010259540	−11456914728105	−592786074379275	−32513880609579600	$-1887019647180154987\frac{1}{2}$
1	4	0	−50	−1176	−26112	−647905	$-16453117\frac{1}{2}$	$-425308222\frac{1}{2}$	$-10281313150\frac{1}{2}$	$-181320757591\frac{1}{2}$	2606202716040	$622231248666307\frac{1}{2}$	$56560097077675104\frac{3}{8}$
2	−4	−12	−40	−344	−3513	−44366	$-486457\frac{1}{2}$	$-878527\frac{1}{2}$	105956879	996828993	−302888778255	$-35962386099941\frac{1}{4}$	$-2973976984644465\frac{15}{16}$
3		4	14	−28	−36	−3009	$-85659\frac{1}{2}$	−1339020	$-70112132\frac{3}{4}$	−2289397563	$-61537586981\frac{5}{8}$	$-1417645036817\frac{1}{2}$	14046475617195
4			−4	−10	325	2170	$29241\frac{1}{2}$	736029	$5619955\frac{3}{4}$	$250213920\frac{1}{4}$	8870308461	$182363269816\frac{3}{4}$	5892713122080
5				4	0	−945	$-5052\frac{1}{2}$	$-5841\frac{1}{2}$	$-1080203\frac{1}{4}$	$34632655\frac{1}{4}$	705890175	1850093234	$713236878450\frac{1}{4}$
6					−4	16	1955	$4147\frac{1}{2}$	$-292766\frac{1}{4}$	$-1058909\frac{1}{4}$	$-217483272\frac{1}{2}$	$-5310678979\frac{3}{8}$	$-1036978067\frac{1}{8}$
7						4	−38	−3395	9954	$1310900\frac{1}{4}$	$5720061\frac{3}{8}$	$539675633\frac{3}{4}$	$13147234615\frac{5}{8}$
8							−4	66	5278	−52674	$-3735338\frac{1}{4}$	$-343039\frac{1}{8}$	$-464689558\frac{7}{16}$
9								4	−100	−7590	146385	$8459448\frac{1}{4}$	$-61062655\frac{1}{2}$
10									−4	140	10290	−321145	$-16469070\frac{3}{4}$
11										4	−186	−13310	615230
12											−4	238	16555
13												4	−296
14													−4

Table 4. The coefficients $a_{n,k,j}$ in the extrapolation formula (12).

	j					
k	0	1	2	3	4	5
$\alpha_{0,k,j}$						
0	2	12	96	25920	0	0
1		2	−1468	510840	1300549152	6977845103040
2		2	−558	−888576	−2703028424	−15961597601040
3			−428	600150	1803808536	12990760770024
4			6	38850	−409368974	−4669644914724
5				−7950	−18927216	667412568090
6				126	5412484	519181770
7					−224616	−5708659068
8					6354	428756328
9					−96	−15678630
10						484770
11						−10656
12						96
$\alpha_{1,k,j}$						
0	2	10	312	7200	967680	0
1		2	−1192	566700	1554817152	8201223021600
2		2	−522	−1082526	−3148467656	−18452430302760
3			−428	592890	2028534576	14630011358544
4			6	39480	−411219494	−5057308922574
5				−7950	−20088936	678397444650
6				126	5432476	1825419990
7					−224616	−5791418388
8					6354	430798878
9					−96	−15704550
10						484770
11						−10656
12						96
$\alpha_{2,k,j}$						
0	2	4	384	−14400	483840	0
1		2	−940	679560	1809266592	9448276380480
2		2	−510	−1261176	−3582329672	−20938915839600
3			−428	598470	2221265016	16212179478024
4			6	39930	−415205294	−5412395679564
5				−7950	−20805456	691017125850
6				126	5445412	2648223930
7					−224616	−5853962268
8					6354	432269568
9					−96	−15721830
10						484770
11						−10656
12						96

This time we note that the two or three leading coefficients are independent of n and, indeed, we find that $\beta_{n,k,2k-j}/3^k$ is a polynomial in k of order $2j+1$. In particular we have

$$\beta_{n,k,2k} = -3^k(k+1)$$
$$\beta_{n,k,2k-1} = 3^k(278k^3 + 99k^2 - 179k)/27$$

Table 5. The coefficients $\beta_{n,k,j}$ in the extrapolation formulae (13).

k	j = 0	1	2	3	4	5	6	7	8
$\beta_{0,k,j}$									
0	−1	0	0	0	0	0	0	0	0
1		22	1658	334656	153601904	109900869120	119835268440320	179701691558215680	358810347942675191808
2		−6	−2385	−649384	$-348301926\frac{2}{3}$	−276393269472	−325054574102944	−517144503241342976	$-1083429067670151410841\frac{3}{5}$
3			754	403500	284418460	266027954552	$350188538012687\frac{1}{9}$	606338380910234368	1357922016436272064896
4			−27	−96524	$-108269551\frac{2}{3}$	−129814389840	−200292896954500	$-388885779063580337\frac{7}{9}$	$-950703086097155610426\frac{2}{3}$
5				7860	20243976	35294435450	$67835150491952\frac{2}{3}$	$153240568087470602\frac{2}{3}$	419124576286737422400
6				−108	$-1748436\frac{2}{3}$	−5461778850	−14237073600841	$-39235294734473786\frac{2}{3}$	$-123701080180932859946\frac{2}{15}$
7					55980	465582548	$1869074318751\frac{1}{3}$	6694588679545816	25258034274069075192
8					−405	−19729020	−150316130097	$-764582679410893\frac{1}{3}$	−3623005587850488121
9						326970	$6996149842\frac{8}{9}$	57616149115192	365799796385163936
10						−1458	−168308595	$-2763401680710\frac{2}{9}$	$-25727820621001866\frac{14}{15}$
11							1688526	$78924402909\frac{1}{3}$	1230228773135952
12							−5103	−1196493480	$-38326543230336\frac{2}{3}$
13								8015112	725790362976
14								−17496	−7483535892
15									35779320
16									−59049

Table 5. (Continued)

	j								
k	0	1	2	3	4	5	6	7	8
$\beta_{1,k,j}$									
0	−1	0	0	0	0	0	0	0	0
1		22	1874	380544	173844464	124703585280	135892573287680	203891746284011520	407060480146447669248
2		−6	−2505	−717448	$-387796806\frac{2}{3}$	−309968480352	−365371396244512	−582626355682555904	$-1221984137726510908569\frac{3}{5}$
3			754	427116	309285900	293508255992	$388934364085487\frac{1}{9}$	676720632830112000	1519953696088914094464
4			−27	−97964	$-114431071\frac{2}{3}$	−140364933360	−219200100776580	$-429068174740539313\frac{7}{9}$	$-1054354166560941235770\frac{2}{3}$
5				7860	20801176	37316508410	$72997883541272\frac{2}{3}$	$166848798285151882\frac{2}{3}$	459887247973724918464
6				−108	$-1759236\frac{2}{3}$	−5648008290	−15047082876273	$-42102339808215418\frac{2}{3}$	$-134133831039985827818\frac{2}{15}$
7					55980	472540628	$1940426816751\frac{1}{3}$	7075210989955416	27042955126506979800
8					−405	−19793820	−153559531937	$-795936397412877\frac{1}{3}$	−3828497810715795865
9						326970	$7058663482\frac{8}{9}$	59143290605752	381544301457679104
10						−1458	−168648795	$-2803243801350\frac{2}{9}$	$-26506146752612586\frac{14}{15}$
11							1688526	$79382817117\frac{1}{3}$	1253639579258096
12							−5103	−1198126440	$-38712986171808\frac{2}{3}$
13								8015112	728717117184
14								−17496	−7490884212
15									35779320
16									−59049

Table 5. (Continued)

	j								
k	0	1	2	3	4	5	6	7	8
$\beta_{2,k,j}$									
0	−1	8	0	0	0	0	0	0	0
1		22	1826	399904	188173424	136763942784	150135943911680	226399980054487040	453481872936027199488
2		−6	−2553	−747352	$-415492486\frac{2}{3}$	−337028036672	−400806757117984	−643091153929042944	$-1354435396148323267737\frac{3}{5}$
3			754	438668	326540300	315331137752	$422565255743151\frac{1}{9}$	$741047725232481564\frac{4}{9}$	1673542368950203659648
4			−27	−98972	$-118710111\frac{2}{3}$	−148615548440	−235371247103300	$-465345164498565169\frac{7}{9}$	$-1151609375547099787322\frac{2}{3}$
5				7860	21201176	38883012026	$77347956643752\frac{2}{3}$	$178970258611925237\frac{1}{3}$	497699046774849639872
6				−108	$-1767876\frac{2}{3}$	−5793139250	−15721316702945	$-44622273568721818\frac{2}{3}$	$-143694733990288250474\frac{2}{15}$
7					55980	478155188	$1999479461647\frac{1}{3}$	$7405891926422253\frac{1}{3}$	28659202377280586328
8					−405	−19848900	−156259593217	$-822961941093677\frac{1}{3}$	−4012551877454570521
9						326970	$7112021962\frac{8}{9}$	$60457289130459\frac{5}{9}$	395524266443898240
10						−1458	−168948171	$-2837772622950\frac{2}{9}$	$-27193733020204138\frac{14}{15}$
11							1688526	$79787198493\frac{1}{3}$	1274324332887664
12							−5103	−1199596104	$-39056845236000\frac{2}{3}$
13								8015112	731355327360
14								−17496	−7497602676
15									35779320
16									−59049

Table 6. New low-temperature series terms for the square lattice spin-1 Ising magnetization, $M(u)$, susceptibility, $\chi(u)$, and specific heat, $C_v(u)$.

n	$M(u)$	$\chi(u)$	$C_v(u)$
80	−54894921926791871723909	1287288269903730631946751	14980548594400026006446720
81	126297750080690225982572	−2932618501022211032818300	−35701518428258787100072584
82	−92489409777625802742528	2052947118516396940212072	27948358015093163176475128
83	−292140800078967381434028	7265393839008482331992336	80787294138478683214133578
84	1131329573810488998686811	−27533569403846138701663365	−328084218297769469375116200
85	−1662612103740713574604884	39920035526199174994626036	500413572618503616248896480
86	−492613608448080934983288	14931369412552677008749932	113883610899578636803467152
87	8211147564410929129324192	−209438337886232625955934292	−2436189367728965310422489418
88	−18878709288285563929234997	476343631011307763277303031	5796339184388631113650158304
89	13785042470417967980505100	−331962548955170787548255312	−4521670273968534171069307750
90	43860793960742590039383898	−1182970662366618284903971030	−13149275656695239669180483520
91	−169598161959998919874255236	4472491833451466220138614096	53268752093378620751877315482
92	249007028837325086293670283	−6471380268030636441237200097	−81105273455462683681912082728
93	74990743692109664334064752	−2453067840623244506560874448	−18811719845845853329570528542
94	−1234426063083531162682558560	34026585140776880977075866240	395621948197278485674431575608
95	2835867624597373150874747480	−77254798018355427358151075836	−939772638538221206856049448380
96	−2064573852622364936737424098	53613918339192473420875219089	730560439047179326970330734464
97	−6616142800429142888692342768	192358286613090067676905433984	2137403950614601807223987280454
98	25541973318840653657077177270	−725486237294161236962098624258	−8637803751685796115480314923276
99	−37462784919716975353690569292	1047757642093298413301695350332	13128860187862258100931770296284
100	−11463726370314369427304114523	402487643299242910269563033131	3102521140136519939724246308400
101	186381597774899493113385553664	−5520950047108379701377201734452	−64169713991043524782724303040306
102	−427804305737711686514509242390	12514441143336335641931499176014	152189962317529977423571879172796
103	310497065688338308368382361752	−8648192214593796849228047528228	−117900563896358034274507714039430
104	1002057377876891572217899261401	−31239827769954401229313918082438	−347042122337706823781434388021392
105	−3862092565977953294672165562608	117548646091803611498084800222172	1399138594951555677686779993658460
106	5658355584526190756409048411218	−169446914107751509953285066975278	−2122963342745826385809572352025484
107	1758697226344654211271247297588	−65942014127753928407511143000684	−510975035983101017637996662363534
108	−28247139203735773793168037850532	894839314320840238617134121410478	10397649426241825241936709101268192
109	64775215576079739888972057107032	−2025063464948777359185732816409016	−24621560654630485557870861813977290
110	−46866364052133130252606723536110	1393635387942882646442005194185966	19008526767153717074391591041349580
111	−152306338289478778693447758360664	5068325152947612595253210347568392	56293290314061858138013078241465190
112	586011194798187595036300267855234	−19027185558928704352441507167871531	−226417646512838638150966074051275808
113	−857572414389308013646509973160724		342972424908794790373332519783688916

$$\beta_{n,k,2k-2} = \begin{cases} 3^k(77284k^5 - 233636k^4 + 145247k^3 + 233636k^2 - 222531k)/1458 & n = 0 \\ 3^k(77284k^5 - 233636k^4 + 148487k^3 + 233636k^2 - 225771k)/1458 & n = 1 \\ 3^k(77284k^5 - 233636k^4 + 151727k^3 + 231692k^2 - 230955k)/1458 & n = 2 \end{cases}$$

and

$$\beta_{n,k,2k-3} = \begin{cases} 3^k(107424760k^7 - 981604100k^6 + 3689847622k^5 - 5987330165k^4 & \\ \quad +1103673490k^3 + 6968934265k^2 - 4900945872k)/590490 & n = 0 \\ 3^k(107424760k^7 - 981604100k^6 + 3703358422k^5 - 6035726045k^4 & \\ \quad +1135273210k^3 + 7017330145k^2 - 4946056392k)/590490 & n = 1 \\ 3^k(107424760k^7 - 981604100k^6 + 3716869222k^5 - 6092228405k^4 & \\ \quad +1180199050k^3 + 7073832505k^2 - 5004493032k)/590490 & n = 2. \end{cases}$$

So when calculating the extrapolation formulae (11) we first used the sequences for the correction terms to predict as many polynomials as possible. When we ran out of terms we then predicted as many of the leading coefficients from (12) and (13) as possible. This in turn allowed us to find more extrapolation formulae, which we could use (together with the formulae for $\beta_{n,k,2k-j}$) to find more of the formulae for the leading coefficients $a_{n,s,s+n+3-k}$ and $b_{n,s,s+n-k}$. We repeated this until the process stopped with the extrapolation formulae listed above.

From $Z_{n,33}(u)$ we extended the series for Z_0 and Z_1 to $\mathcal{O}(u^{113})$, while the series for Z_2 was extended to $\mathcal{O}(u^{112})$. The resulting new low-temperature series terms are listed in table 6. The series terms for $n < 80$ can be found in [1]. The full series is also available by electronic mail or via the worldwide web (see end of article for details).

4. Analysis of the series

We analysed the series using the same methods as in our previous paper [1], to which we refer the reader for details. Here we will give only a short summary of the results including improved estimates for the critical point and amplitudes.

The estimates $u_c = 0.554\,0663(5)$ for the physical singularity and $\beta = 0.125\,07(2)$ for the critical exponent of the spontaneous magnetization were obtained from homogeneous differential approximants (which are equivalent to Dlog Padé approximants) by averaging over $[N, M]$ approximants with $|N - M| \leqslant 1$ using at least 100 series terms. The figure in parenthesis represents the spread among the approximants (basically one standard deviation) and should *not* be viewed as a measure of the true error as they cannot include possible systematic sources of error. From these estimates it is clear that $\beta = \frac{1}{8}$ as expected. However, the estimates converge very slowly towards this value and, even with a series as long as the present 114 terms, the estimates have not yet settled down to their true value and there is a slight downwards drift in the estimates for both u_c and β. Analysis of the susceptibility and specific heat series yield exponent estimates fully in agreement with the expectations that $\gamma' = \frac{7}{4}$ and $\alpha' = 0$. By using our knowledge of the exact values of the critical exponents and assuming that close to u_c the estimates for the exponents depend linearly on the estimates for the critical point (inspection of the various approximants clearly supports this assumption) we are led to the improved estimate for the critical point $u_c = 0.554\,0653(5)$.

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

Table 7. Estimates for the physical critical amplitudes A_M, A_χ, and A_C from the method of Liu and Fisher [6] obtained from inhomogeneous first-order differential approximants. L is the degree of the inhomogeneous polynomial.

L	A_M	A_χ	A_C
5	1.208 284(74)	0.061 712(47)	20.20(26)
6	1.208 270(15)	0.061 73(12)	20.13(22)
7	1.208 256(80)	0.061 70(20)	20.23(23)
8	1.208 266(16)	0.061 64(21)	20.29(20)
9	1.208 24(21)	0.061 70(12)	20.28(32)
10	1.208 269(35)	0.061 866(60)	20.31(26)
15	1.208 272(74)	0.061 65(15)	20.47(32)
20	1.208 24(12)	0.061 67(15)	20.464(75)
25	1.208 250(47)	0.061 72(11)	20.448(46)
30	1.208 236(51)	0.061 74(20)	20.42(12)
35	1.208 228(60)	0.061 792(82)	20.40(20)
40	1.208 263(70)	0.061 59(20)	20.45(12)

$f(u) \sim A(1-u/u_c)^{-\lambda}$, 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) and yields the estimates $A_M = 1.208\,40(5)$ and $A_\chi = 0.061\,72(4)$ where the error bar primarily reflects the uncertainty due to the estimate of u_c. For the specific heat series two different approaches have been used. In the first approach we look at the derivative of the specific heat series for which the above method should work with $\lambda = 1$. This yields the estimate $A_C = 22.3(1)$. 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 quite substantial, though the amplitude estimate is consistent with that listed above. Biasing the estimates at u_c yields $A_C = 22.3(3)$. In the second method, proposed by Liu and Fisher [6], 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 [5]. 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 the amplitude estimates listed in table 7. With the exception of the specific heat amplitude there is excellent agreement between these estimates and those obtained from the first method.

Regarding the value of the confluent exponent Δ_1 we have little to add to our previous results. Even with a series as long as 114 terms we could not obtain accurate estimates for Δ_1. Again the Baker–Hunter [7] transformed series of the magnetization favours a value around 1.05 while estimates from the suceptibility series again fall in two groups around 1.15 and 1.4, respectively. Using the transformation of Adler *et al* [8]

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

where $F(u)$ is the original series and λ the leading critical exponent, yields estimates consistent with $\Delta_1 = 1$ for both the magnetization and susceptibility.

We find a non-physical singularity closer to the origin than u_c at $u_\pm = -0.301\,9395(5) \pm$

0.378 7735(5) with exponents $\beta = -0.1690(2)$, $\gamma' = 1.1692(2)$ and $\alpha' = 1.1693(3)$, and a singularity on the negative u-axis at $u_- = -0.598\,550(5)$ with exponents equal to those at the physical critical point. Note that our estimate for β at $u_\pm$ has changed substantially from that given in our previous paper. This is mainly because we have put greater emphasis on estimates obtained from inhomogeneous first- and second-order differential approximants. We note that we now have firm evidence to show that the scaling law $\alpha' + 2\beta + \gamma' = 2$ holds at both the physical as well as the non-physical singularities.

E-mail or www retrieval of series

The series for the spin-1 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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