

## LOW-TEMPERATURE SERIES EXPANSIONS FOR SQUARE-LATTICE ISING MODEL WITH FIRST AND SECOND NEIGHBOUR INTERACTIONS

YEE MOU KAO

*Institute of Physics, National Chiao Tung University,  
Hsinchu 300, Taiwan, Republic of China*

MALL CHEN

*Department of Applied Physics, Chung Cheng Institute of Technology,  
National Defence University, Ta-Hsi Tao-Yuan 335, Taiwan, Republic of China*

KEH YING LIN

*Department of Physics, National Tsing Hua University,  
Hsinchu 300, Taiwan, Republic of China*

Received 30 May 2002

Revised 9 September 2002

We have calculated the low-temperature series expansions of the spontaneous magnetization and the zero-field susceptibility of the square-lattice ferromagnetic Ising model with first-neighbour interaction  $J_1$  and second-neighbour interaction  $J_2$  to the 30th and 26th order respectively by computer. Our results extend the previous calculations by Lee and Lin to six more orders. We use the Padé approximants to estimate the critical exponents and the critical temperature for different ratios of  $R = J_2/J_1$ . The estimated critical temperature as a function of  $R$  agrees with the estimation by Oitmaa from high-temperature series expansions.

*Keywords:* Ising model; low temperature series expansions.

The partition function of the square-lattice Ising model with nearest neighbour interactions in the absence of magnetic field was derived by Onsager.<sup>1</sup> The spontaneous magnetization of this model was also obtained by Onsager but he never published his derivation. Yang<sup>2</sup> was the first to publish a detailed derivation of the spontaneous magnetization and the critical exponent  $\beta$  is 0.125. The zero-field susceptibility of the square-lattice Ising model is still unsolved, but the critical exponents  $\gamma(T > T_c)$  and  $\gamma'(T < T_c)$ , where  $T_c$  is the critical temperature of the Ising model, are known<sup>3</sup> to be 1.75. The square-lattice Ising models with interactions beyond first neighbours are unsolvable by existing methods. According to the universality hypothesis, the critical exponents are expected to be the same.

The square-lattice Ising model with first and second neighbour interactions was first studied by Dalton and Wood.<sup>4</sup> They derived the low-temperature series expansions of the spontaneous magnetization and the zero-field susceptibility up to the 17th and 13th orders respectively. They used the Padé approximants to estimate the critical exponents and found that  $0.122 < \beta < 0.134$ . However their series for the susceptibility is too short and no conclusion was obtained for  $\gamma'$ . Lee and Lin<sup>5</sup> calculated the low-temperature series expansions of the spontaneous magnetization and the zero-field susceptibility up to the 24th and 20th order respectively and found that  $0.122 < \beta < 0.128$  and  $1.75 < \gamma' < 1.85$ . In this paper, we further extend the result of Lee and Lin to six more orders and use the Padé approximants to estimate the critical temperature and the critical exponents.

The Hamiltonian of the square-lattice Ising model with first and second neighbour interactions is

$$\mathbf{H} = -J_1 \sum_{nn} \sigma_i \sigma_j - J_2 \sum_{nnn} \sigma_i \sigma_j \quad (1)$$

where the first and second summations are over nearest neighbour ( $nn$ ) pairs and next nearest neighbour ( $nnn$ ) pairs respectively.

The method of low-temperature series expansions is well known.<sup>6</sup> The spontaneous magnetization  $M(x, y)$  and the zero-field susceptibility  $\chi(x, y)$  are expanded in power series of  $x$  and  $y$  where

$$x = \exp\left(\frac{-4J_1}{kT}\right), \quad y = \exp\left(\frac{-4J_2}{kT}\right). \quad (2)$$

We have calculated the low-temperature series expansions of the spontaneous magnetization  $M(x, y)$  and the susceptibility  $\chi(x, y)$  for the square-lattice Ising model with first and second neighbour interactions up to the 30th order and 26th order respectively. The results are

$$M(x, y) = 1 - 2x^2y^2 + \sum_{m,n} a(m, n)x^m y^n \quad (3)$$

$$\chi(x, y) = 1 + \sum_{m,n} b(m, n)x^m y^n \quad (4)$$

where the coefficients  $a(m, n)$  and  $b(m, n)$  are given in Tables 1 and 2 respectively.

In the special case of  $x = y$ , we have

$$\begin{aligned} M(x, x) = & 1 - 2x^4 - 16x^7 + 18x^8 - 24x^9 - 104x^{10} + 248x^{11} - 516x^{12} - 328x^{13} \\ & + 2292x^{14} - 7200x^{15} + 4676x^{16} + 13720x^{17} - 81148x^{18} + 128960x^{19} \\ & - 32368x^{20} - 713056x^{21} + 1945752x^{22} - 2600056x^{23} - 3692616x^{24} \\ & + 21775624x^{25} - 49678052x^{26} + 21759936x^{27} + 173941332x^{28} \\ & - 668655828x^{29} + 971318640x^{30} + \dots \end{aligned} \quad (5)$$

Table 1. Coefficients of the series expansions for spontaneous magnetization.

$m, n$	$a(m, n)$	$m, n$	$a(m, n)$	$m, n$	$a(m, n)$	$m, n$	$a(m, n)$
3,4	-8	4,3	-8	4,4	18	4,5	-24
4,6	-20	5,5	-48	6,4	-36	5,6	80
6,5	168	5,7	-144	6,6	-364	8,4	-8
5,8	-40	6,7	144	7,6	-288	8,5	-144
6,8	-52	7,7	1184	8,6	1160	6,9	-504
7,8	-2704	8,7	-3872	9,6	-40	10,5	-80
6,10	-70	7,9	1440	8,8	5358	9,7	-1712
10,6	-340	7,10	-1648	8,9	-2704	9,8	11464
10,7	6632	12,5	-24	7,11	-1344	8,10	-8064
9,9	-37328	10,8	-33356	11,7	-576	12,6	-480
7,12	-112	8,11	2672	9,10	56368	10,9	76880
11,8	-7664	12,7	816	8,12	-8524	9,11	-57136
10,10	-84864	11,9	88608	12,8	29968	13,7	-112
14,6	-308	8,13	-3024	9,12	-10696	10,11	-45808
11,10	-407200	12,9	-239176	13,8	-5584	14,7	-1568
8,14	-168	9,13	-13168	10,12	167404	11,11	963392
12,10	828616	13,9	-16384	14,8	16156	16,6	-96
9,14	-29512	10,13	-311072	11,12	-1445272	12,11	-1448928
13,10	551920	14,9	87168	15,8	-2216	16,7	-2144
9,15	-6048	10,14	-23220	11,13	956384	12,12	496260
13,11	-3643744	14,10	-1439614	15,9	-34752	16,8	2136
18,6	-18	9,16	-240	10,15	-118792	11,14	-298432
12,13	2618528	13,12	12257544	14,11	7089248	15,10	118184
16,9	111384	17,8	-504	18,7	-1296	9,17	-1497984
10,16	-7901600	11,15	-10183888	12,14	-3557904	13,13	-15541072
14,12	-14323744	15,11	3088944	16,10	272480	17,9	-25024
18,8	-8260	10,17	-11088	11,16	-286264	12,15	5900896
13,14	30843176	14,13	19729328	15,12	-27347504	16,11	-7023008
17,10	-117680	18,9	72760	19,8	-80	20,7	-600
10,18	-330	11,17	-533632	12,16	-5363752	13,15	-20101024
14,14	19749266	15,13	125751456	16,12	52267388	17,11	1747920
18,10	443756	19,9	-10816	20,8	-8900	11,18	-197888
12,17	-3854936	13,16	-11201256	14,15	-119303842	15,14	-351894966
16,13	-185818284	17,12	6993368	18,11	-3204304	19,10	-174528
20,9	984	22,7	-176	11,19	-19008	12,18	-1804944
13,17	17185120	14,16	201958068	15,15	618347936	16,14	329430948
17,13	-170524608	18,12	-24134784	19,11	303408	20,10	587212
21,9	-3888	22,8	-6820				

$$\begin{aligned}
 \chi(x, x) = & 1 + 16x^3 - 18x^4 + 36x^5 + 160x^6 - 340x^7 + 980x^8 + 808x^9 - 3802x^{10} \\
 & + 16464x^{11} - 7175x^{12} - 24432x^{13} + 221346x^{14} - 300192x^{15} \\
 & + 180712x^{16} + 2314428x^{17} - 5521804x^{18} + 9422824x^{19} + 14985996x^{20} \\
 & - 71270104x^{21} + 193417806x^{22} - 54203752x^{23} - 629440122x^{24} \\
 & + 2864059974x^{25} - 3814925920x^{26} + \dots .
 \end{aligned}
 \tag{6}$$

The lattice constant  $c(n, r)$  is the number of connected graphs with  $r$  vertices and  $b = 4r - n$  bonds. The lattice constants for  $n \leq 30$  are given in Tables 3 and 4.

Table 2. Coefficients  $b(m, n)$  of the series expansions for susceptibility.

$m, n$	$b(m, n)$	$m, n$	$b(m, n)$	$m, n$	$b(m, n)$	$m, n$	$b(m, n)$
1,2	8	2,1	8	2,2	-18	2,3	36
2,4	34	3,3	72	4,2	54	3,4	-88
4,3	-252	3,5	328	4,4	636	6,2	16
3,6	104	4,5	-160	5,4	576	6,3	288
4,6	626	5,5	-2128	6,4	-2300	4,7	1628
5,6	6256	6,5	8280	7,4	100	8,3	200
4,8	259	5,7	-1360	6,6	-11300	7,5	4376
8,4	850	4,9	8536	6,7	10416	7,6	-27148
8,5	-16308	10,3	72	5,9	5856	6,8	28452
7,7	97464	8,6	86406	9,5	1728	10,4	1440
5,10	560	6,9	15392	7,8	-137160	8,7	-200648
9,6	24028	10,5	-2364	6,10	50568	7,9	213704
8,8	259222	9,7	-256656	10,6	-87596	11,5	392
12,4	1078	6,11	17112	7,10	128932	8,9	172792
9,8	1240288	10,7	729888	11,6	19928	12,5	5488
6,12	1092	7,11	216152	8,10	-282466	9,9	-2903456
10,8	-2564024	11,7	65680	12,6	-55166	14,4	384
7,12	210468	8,11	1555840	9,10	5026084	10,9	4785740
11,8	-1882952	12,7	-289832	13,6	8900	14,5	8576
7,13	43152	8,12	981880	9,11	-2601680	10,10	-1431332
11,9	12792400	12,8	5065695	13,7	143904	14,6	-8104
16,4	81	7,14	1968	8,13	1404308	9,12	3905488
10,11	-7335936	11,10	-43165120	12,9	-25242080	13,8	-414684
14,7	-432148	15,6	2268	16,5	5832	7,15	7092736
8,14	35470520	9,13	46834296	10,12	12209208	11,11	53215208
12,10	51602088	13,9	-12136984	14,8	-1021124	15,7	114608
16,6	37250	8,15	97416	9,14	7376136	10,13	-12267944
11,12	-114028180	12,11	-72783160	13,10	109160104	14,9	27983744
15,8	574544	16,7	-319812	17,6	400	18,5	3000
8,16	3333	9,15	6466912	10,14	48215780	11,13	106268896
12,12	-65961853	13,11	-504320608	14,10	-210794544	15,9	-7512968
16,8	-1904178	17,7	54608	18,6	44500	9,16	2017056
10,15	52559808	11,14	86278308	12,13	506072141	13,12	1463559527
14,11	768993890	15,10	-30879880	16,9	14560120	17,8	899488
18,7	-1452	20,5	968	9,17	201696	10,16	40996948
11,15	39152672	12,14	-776591430	13,13	-2610404376	14,12	-1374685066
15,11	763348848	16,10	107041820	17,9	-1184072	18,8	-2861950
19,7	21480	20,6	37510				

Oitmaa<sup>7</sup> calculated the high-temperature series expansion of zero-field susceptibility up to 11th order. His result was extended to two more orders by Soehanie and Oitmaa.<sup>8</sup> From analysis of the high-temperature susceptibility series, Oitmaa obtained precise estimates of the ferromagnetic critical temperature as a function of  $R = J_2/J_1$ .

We have applied the method of Oitmaa to analysis the low-temperature series and to estimate the critical temperature and exponents. The special case of  $R = 0.5$  has been discussed in detail by Oitmaa and he obtained  $K_c = J_1/kT_c = 0.2628$ . We shall consider the same case first so that we can compare our results with

Table 3. Lattice constants  $c(n, r)$  for  $n \leq 26$ .

$n, r$	$c(n, r)$	$n, r$	$c(n, r)$	$n, r$	$c(n, r)$	$n, r$	$c(n, r)$
4,1	1	18,11	30	22,12	3386	25,9	119908
7,2	4	18,12	1	22,13	1900	25,10	115816
9,3	4	19,6	1670	22,14	924	25,11	95416
10,3	16	19,7	1884	22,15	390	25,12	72010
10,4	1	19,8	1250	22,16	129	25,13	51096
11,4	8	19,9	752	22,17	14	25,14	34550
12,4	29	19,10	394	23,8	31306	25,15	22660
12,5	9	19,11	152	23,9	27616	25,16	13540
13,4	72	19,12	54	23,10	21152	25,17	7604
13,5	16	19,13	4	23,11	15424	25,18	3814
13,6	6	20,7	4512	23,12	10452	25,19	1732
14,5	80	20,8	2985	23,13	6568	25,20	666
14,6	28	20,9	1820	23,14	3646	25,21	152
14,7	6	20,10	1128	23,15	1916	25,22	16
15,5	192	20,11	634	23,16	816	26,9	211576
15,6	80	20,12	268	23,17	320	26,10	241918
15,7	32	20,13	105	23,18	66	26,11	218188
15,8	6	20,14	14	23,19	4	26,12	177438
16,5	341	21,7	7552	24,8	45969	26,13	135664
16,6	204	21,8	7344	24,9	61946	26,14	97854
16,7	116	21,9	5380	24,10	53700	26,15	67012
16,8	52	21,10	3324	24,11	39172	26,16	43912
16,9	9	21,11	2012	24,12	27285	26,17	27142
17,6	624	21,12	1118	24,13	18248	26,18	15670
17,7	288	21,13	500	24,14	11874	26,19	8340
17,8	132	21,14	210	24,15	6772	26,20	3960
17,9	68	21,15	48	24,16	3738	26,21	1772
17,10	16	21,16	2	24,17	1734	26,22	570
18,6	1220	22,7	8382	24,18	738	26,23	116
18,7	820	22,8	15551	24,19	222	26,24	9
18,8	482	22,9	12538	24,20	30		
18,9	224	22,10	8826	24,21	1		
18,10	94	22,11	5620	25,8	42864		

his result. The case  $R = 0.5$  means  $x = y^2$ . The estimated critical temperature from low-temperature series should be the same as (or very close to) the estimated temperature from high-temperature series. We have

$$\begin{aligned}
 M(y^2, y) = & 1 - 2y^6 - 8y^{10} - 8y^{11} + 18y^{12} - 24y^{13} - 20y^{14} - 48y^{15} + 44y^{16} \\
 & + 24y^{17} - 404y^{18} + 144y^{19} - 348y^{20} + 536y^{21} - 1614y^{22} - 2432y^{23} \\
 & + 3670y^{24} - 5840y^{25} + 2948y^{26} - 28024y^{27} + 14488y^{28} + 16120y^{29} \\
 & - 103872y^{30} + 30448y^{31} - 239340y^{32} + 406984y^{33} + 646008y^{34} \\
 & - 2127272y^{35} - 7135696y^{36} - 11133024y^{37} + 6971120y^{38} \\
 & - 3121456y^{39} + 11078112y^{40} + \dots .
 \end{aligned}
 \tag{7}$$

Table 4. Lattice constants  $c(n, r)$  for connected graphs with  $26 \leq n \leq 30$ .

$r$	$c(26, r)$	$c(27, r)$	$c(28, r)$	$c(29, r)$	$c(30, r)$
9	211576	276724	222421		
10	241918	496890	886380	1402474	1653338
11	218188	499500	1021922	2022792	3843400
12	177438	421536	958600	2092768	4405280
13	135664	332960	812639	1888458	4182618
14	97854	252248	647780	1586980	3655386
15	67012	185140	493114	1266500	2977250
16	43912	129730	364828	968132	2493596
17	27142	86640	259347	719640	1935270
18	15670	55162	176044	517250	1458870
19	8340	32868	114942	356996	1064002
20	3960	18596	70421	237528	750562
21	1772	9252	41676	150452	507712
22	570	4476	22098	91870	330886
23	116	1772	11250	51920	207348
24	9	530	5098	27640	123432
25		92	1926	13784	68576
26		6	536	6014	36560
27			84	2228	17598
28			6	574	7734
29				92	2728
30				6	718
31					116
32					9

Table 5. Estimates of the critical point  $y_c = \exp(-2J_1/kT)$  from poles of the  $[n + j, n]$  Padé approximants to the  $(d/dy) \log M(y^2, y)$  series. In brackets are shown corresponding estimates of the exponent  $\beta$  from Padé approximants to  $(y - y_c)(d/dy) \log M(y^2, y)$  evaluating at  $y = y_c = 0.59146$ .

$n$	$j = -1$	$j = 0$	$j = 1$
15	0.59144 (0.127)	0.59148 (0.127)	0.59147 (0.123)
16	0.59148 (0.127)	0.59148 (0.126)	0.59147 (0.123)
17	0.59147 (0.127)	0.59147 (0.126)	0.59144 (0.125)
18	0.59145 (0.126)	0.59147 (0.126)	0.59143 (0.126)

The first step is to obtain an estimate for  $K_c$  from the pole of Padé approximants to the series  $d(\log M(y^2, y))/dy$  such that  $K_c = -0.5 \log y_c$ . In Table 5, we show estimates of  $y_c$  and find  $y_c = 0.59146$ . Therefore our estimate for  $K_c$  is  $-0.5 \log 0.59146 = 0.2626$  which is very close to 0.2628. The next step is to make biased estimate of the exponent  $\beta$  by forming Padé approximants to  $(y - y_c)d(\log M(y^2, y))/dy$  and evaluating these at  $y = y_c = 0.59146$ . The results are shown in Table 5 and the conclusion is  $\beta = 0.125 \pm 0.002$ .

In Fig. 2 of Ref. 7, quantitative estimates from the high-temperature series of the critical temperature versus the parameter  $R$  are shown. The estimated critical

Table 6. The estimated critical temperature  $kT_c/J_1$  for various values of  $R$ . In brackets are shown corresponding estimates from high-temperature series expansion derived by Oitmaa.

$R$	$kT_c/J_1$	$R$	$kT_c/J_1$	$R$	$kT_c/J_1$
0	2.269 (exact)	1/2	3.808 (3.81)	-0.1	1.944 (1.94)
1	5.256 (5.26)	1/3	3.305 (3.31)	-0.2	1.608 (1.61)
2	8.012 (8.01)	1/4	3.052 (3.05)	-0.3	1.251 (1.25)
3	10.692 (10.7)	1/5	2.912 (2.91)		
4	13.355 (13.4)				
5	15.886 (15.9)				

temperatures  $kT_c/J_1$  from the low-temperature ferromagnetic series for different values of  $R$  are given in Table 6, where the critical temperature for  $R = 0$  is exactly known.<sup>9</sup> The corresponding estimates from high-temperature series expansion derived by Oitmaa are shown in brackets and the agreement is remarkable. Our estimates from low-temperature magnetization series fit his curve very well.

The critical temperature can be estimated also from the low-temperature susceptibility series. However the results are not satisfactory, because the series is relatively short.

### Acknowledgment

This research is supported by the National Science Council of R.O.C. under grant No. NSC89-2112-M007-009. We are grateful to the assistance of the National Center for High-Performance Computing.

### References

1. L. Onsager, *Phys. Rev.* **65**, 117 (1944).
2. C. N. Yang, *Phys. Rev.* **85**, 808 (1952).
3. B. M. McCoy and T. T. Wu, *The Two-Dimensional Ising Model* (Boston, Harvard University Press, 1973)
4. N. W. Dalton and D. W. Wood, *J. Math. Phys.* **10**, 1271 (1969).
5. S. F. Lee and K. Y. Lin, *Chin. J. Phys.* **34**, 1261 (1996).
6. C. Domb, *Adv. Phys.* **9**, 149 (1960).
7. J. Oitmaa, *J. Phys. A: Math. Gen.* **14**, 1159 (1981).
8. A. Soehanie and J. Oitmaa, *Mod. Phys. Lett.* **B11**, 609 (1997).
9. H. A. Kramers and G. H. Wannier, *Phys. Rev.* **60**, 252 (1941).