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COMMENT

Extended high-temperature series expansions for the spin-*s* Ising model

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Abstract. Extended high-temperature series expansions are presented for the spin-*s* Ising model on the face-centred cubic lattice. Series coefficients for the zero-field internal energy (U_0) and the second moment (μ_2) of the correlation function are derived, for $\frac{1}{2} \leqslant s \leqslant \frac{9}{2}$, to order 14 in the high-temperature expansion variable $K(=J/kT)$. For $s = \frac{1}{2}$, the fourth field derivative of the free energy is calculated to order K^{14} and the magnetisation series is given to order 13 and 27 in the temperature and magnetic field variables respectively. For $s = 1$ to $\frac{9}{2}$, the zero-field susceptibility series are derived to order K^{14}.

1. Introduction

The purpose of this paper is to present new high-temperature series expansion data for the spin-*s* Ising model on the face-centred cubic (FCC) lattice. The use of series expansions in the study of critical behaviour is well established (see Domb 1974a for a review) and extrapolation techniques for estimating critical exponents, amplitudes and other critical parameters are reviewed in Gaunt and Guttmann (1974).

The exponents γ, ν, α and Δ, characterising the high-temperature susceptibility, correlation length, specific heat and successive (even) field derivatives of the free energy, are of interest in establishing the validity of the hyperscaling relations

$$d\nu = 2 - \alpha, \qquad 2\Delta = \gamma + d\nu, \tag{1}$$

where d is the spatial dimensionality of the system. The validity of (1) as assumed by the renormalisation group (RG) theory is still a matter of controversy, as is the observed discrepancy between series estimates and RG calculations of γ, ν, and α (Camp *et al* 1976, Baker 1977, Zinn-Justin 1979). These exponents have been the subject of much recent investigation (Gaunt 1982 and references cited therein), and a difference of opinion exists as to whether the discrepancies can be resolved by invoking 'correction-to-scaling' terms (Nickel 1982, Zinn-Justin 1981, Roskies 1981*a*, *b*), or whether the discrepancies are real, and represent a fundamental difference between the two approaches (Baker 1982, Freedman and Baker 1982).

Longer series expansions are useful for improving the reliability of exponent estimates, especially with the recently developed methods of analysis for confluent

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corrections to scaling (Camp and Van Dyke 1975, McKenzie 1979b, Rehr *et al* 1980, Roskies 1981b). Expansions to order 21 in K for the susceptibility (χ_0) and the second moment (μ_2) of the correlation function on the body-centred cubic (BCC) lattice were derived by Nickel (1982), while the μ_2 series on the simple cubic (SC) lattice was extended to fifteenth order by Roskies (1981a). Earlier work on the $s = \frac{1}{2}$ model is summarised in Gaunt (1982), while that on the general spin model is discussed in Domb (1974a).

In this paper we present new series coefficients for the FCC lattice. It is generally accepted (Baker 1977) that series expansions on this lattice yield the sharpest estimates for critical exponents, while Nickel and Sharpe (1979) conclude that 'the question of the validity of hyperscaling may be resolved by the extension of available series (on this lattice) by a few more terms'.

2. Derivation of series

The data presented here were derived using the linked cluster expansion (Wortis 1974) and the star graph method (Sykes *et al* 1974, Domb 1974b, McKenzie 1980, 1982). Several of the new series coefficients were calculated by both methods, so as to obtain an independent check on the computations.

The vertex renormalised form of the linked cluster expansion was used to derive the magnetisation (M) series to order K^{13}, τ^{27} ($\tau = \tanh mH/kt$ is the usual magnetic field variable) for $s = \frac{1}{2}$ and to order K^{13}, h^5 ($h = mH/kT$), for $1 \leq s \leq \frac{9}{2}$. The renormalised semi-invariants $M_n(K, h = 0)$ were also calculated at this stage. The M_n were then used, together with the necessary graphical data (Wortis 1974, McKenzie 1982) to obtain the spin–spin correlation function $\Gamma(\boldsymbol{r}, K, h = 0)$ to order K^{14} for all lattice sites $\boldsymbol{r}$ accessible in up to 14 steps from the origin. For $s = \frac{1}{2}$, a change of variable yields the corresponding series in $v = \tanh K$, with integer coefficients.

The star graph method was used (for $s = \frac{1}{2}$) to calculate the zero-field free energy ($F_0 = -kT \ln Z_0$, where Z_0 is the zero-field partition function) to order v^{15} and the fourth field derivative of the free energy ($\chi_0^{(2)} = \partial^4 \ln Z/\partial h^4$) to order 14 in v. The susceptibility series to order 15 is available in McKenzie (1975).

The first and third derivatives of M with respect to the field variable h yield χ_0 and $\chi_0^{(2)}$ to order 13 in v ($s = \frac{1}{2}$) or K ($s > \frac{1}{2}$). Thus

$$-F/kT = \ln Z = \ln 2 + \ln \cosh(mH/kT) + 6 \ln(\cosh K) + \sum_n K^n \sum_m t_{nm} h^{2m}, \qquad (2a)$$

$$Z_0 = Z(h = 0), \qquad M/m = \partial \ln Z/\partial h = \sum_n K^n \sum_m b_{nm} h^{2m+1}, \qquad (2b, c)$$

$$kT\chi_0/m_2 = \partial^2 \ln Z/\partial h^2|_{h=0} = \sum_n a_n K^n, \qquad \chi_0^{(2)} = m\partial^4 \ln Z/\partial h^4|_{h=0} = -2 \sum_n d_n K^n. \qquad (2d, e)$$

For $s = \frac{1}{2}$, the expansion variables $v = \tanh K$ and $\tau = \tanh(h)$ were used. Since M is known to order K^{13}, the coefficients in (2c)–(2e) are obtained through $n = 13$. For $s = \frac{1}{2}$, the b_{nm} were calculated for $m \leq 27$, while for $s > \frac{1}{2}$ they were derived only for $m \leq 5$.

The correlation functions yield the zero-field internal energy (U_0), the zero-field susceptibility and the second moment (μ_2) series to order 14 in v or K. Thus, denoting the nearest-neighbour (NN) correlations by $\Gamma(011)$, we obtain

$$-2U_0/J = (2/J)\partial \ln Z_0/\partial\beta = 12\Gamma(011) = \sum_n c_n K^n, \qquad (3a)$$

$$kT\chi_0/m^2 = 1 + \sum_r \Gamma(\boldsymbol{r}) = \sum_n a_n K^n, \qquad \mu_2 = \sum_r |\boldsymbol{r}|^2\Gamma(\boldsymbol{r}) = \sum_n g_n K^n, \qquad (3b, c)$$

where $\boldsymbol{r}$ is measured in units of lattice spacing and $\beta = 1/kT$. For $s=\frac{1}{2}$, the variable v was used instead of K.

3. Series coefficients for $s=\frac{1}{2}$: results and checks

The coefficients c_n, d_n and g_n (equations (2), (3)) are presented in table 1, for $11 \leq n \leq 14$. The c_n were calculated (a) from the star graph expansion for $\ln Z_0$ and (b) from the NN correlations. Exact agreement was obtained. The c_n for $n \leq 13$ can also be obtained from the data in Sykes *et al* (1972). The last coefficient is new. The d_n for $n \leq 10$ agree with those obtained from the data in Katsura *et al* (1977) and McKenzie (1979a). The last four coefficients are new, of which all but d_{14} were calculated by two independent methods. The g_n for $n \leq 11$ are in agreement with Moore *et al* (1969). Their results at the twelfth order are known to contain a systematic error. Since the correlation functions calculated in this work yield the susceptibility coefficients a_n (equation (3b)) which agree with star graph expansion results (McKenzie 1975) to order 14, we are reasonably confident that the g_n are also correct to this order.

Table 1. Spin-$\frac{1}{2}$ Ising model. Series expansion coefficients for the fourth field derivative of free energy, second moment of the correlation function and the zero-field internal energy. See text (equations (2) and (3)) for details. Expansion variable is $v = \tanh(J/kT)$.

n	$d(n)$	$g(n)$	$c(n)$
11	71 478 104 161 584	2 768 965 884 780	2 426 029 920
12	905 771 858 693 612	30 958 968 926 304	20 385 641 184
13	11 275 505 053 670 640	342 680 506 367 244	173 375 661 192
14	138 209 819 523 812 196	3 760 615 283 556 000	1 489 839 525 168

The coefficients b_{nm} of the magnetisation series (equation (2c)) are given in table 2 for $11 \leq n \leq 13$, $m \leq 27$. The earlier terms were found to be in complete agreement with those derived from the data in Katsura *et al* (1977) and McKenzie (1979a).

4. Data for $1 \leq s \leq \frac{9}{2}$

The series coefficients c_n, a_n and g_n of the internal energy (U_0), susceptibility (χ_0) and the second moment of the correlation function (μ_2) for $1 \leq s \leq \frac{9}{2}$, $11 \leq n \leq 14$ are presented in tables 3–5 respectively. The expansion variable is K, not v. All the coefficients to order 11 are in agreement with earlier work (Camp *et al* 1976, Camp and Van Dyke 1975, Saul *et al* 1975). The twelfth-order terms differ slightly from the published ones, but the latter are known to contain a systematic error (Saul *et al* 1975, reference 31). The last two coefficients are new.

Table 2. Coefficients $b(n, m)$ of the magnetisation series for the spin-$\frac{1}{2}$ Ising model. The expansion variables are $v = \tanh(J/kT)$ and $\tau = \tanh(mH/kT)$.

m \ n	11	12	13
1	162 961 837 500	1 634 743 178 420	16 373 484 437 340
3	−23 771 714 108 028	−301 379 038 505 064	−3 753 043 856 411 100
5	679 423 992 056 904	10 633 839 254 218 744	161 207 055 875 954 136
7	−7 785 592 610 770 440	−148 835 296 267 299 336	−2 717 905 704 547 680 600
9	46 684 523 756 745 384	1 088 102 658 184 129 556	23 859 656 665 009 001 184
11	−166 427 520 872 014 248	−4 755 069 400 513 102 400	−125 544 289 447 752 639 072
13	376 498 957 466 012 640	13 356 000 248 106 561 728	428 127 979 493 625 142 944
15	−555 993 772 413 784 416	−25 033 249 777 453 739 200	−988 718 669 065 446 670 368
17	535 336 491 372 858 264	31 708 163 796 312 206 816	1 579 597 613 009 622 561 768
19	−324 400 598 896 549 080	−26 851 090 827 150 877 104	−1 750 522 764 971 515 173 672
21	112 451 334 484 745 472	14 582 382 995 454 822 960	1 322 649 095 505 173 540 928
23	−17 019 637 527 029 952	−4 596 761 931 663 075 312	−650 716 104 810 749 337 600
25		640 023 440 031 480 192	188 072 084 580 154 406 496
27			−24 244 165 639 077 132 384

Table 3. Spin-s Ising model. Coefficients of the internal energy series (3a). The expansion variable is $K = J/kT$.

s \ n	11	12	13	14
1.0	38 220 641.135 876	223 566 184.191 949	1 322 852 889.802 774	7 905 360 519.466 169
1.5	5 350 175.060 976	26 479 837.939 179	132 522 861.464 447	669 639 912.588 496
2.0	1 662 877.567 593	7 458 461.308 557	33 820 591.399 575	154 817 986.148 786
2.5	764 091.837 537	3 210 572.389 300	13 636 891.132 117	58 468 136.874 257
3.0	438 328.177 097	1 757 972.863 055	7 126 766.519 956	29 162 259.813 881
3.5	288 775.271 587	1 118 413.383 102	4 378 182.470 850	17 298 914.515 254
4.0	208 635.210 554	786 361.089 993	2 995 662.931 872	11 518 268.842 479
4.5	160 798.839 897	593 009.933 736	2 210 388.020 245	8 315 552.936 889

Table 4. Spin-s Ising model. Coefficients of the susceptibility series (2d). The expansion variable is $K = J/kT$.

s \ n	11	12	13	14
1.0	1 787 319 915.984	12 428 583 595.406	86 301 184 251.945	598 513 990 397.688
1.5	223 547 197.693	1 311 642 669.304	7 685 298 021.939	44 976 664 698.921
2.0	66 171 918.918	351 330 252.643	1 862 807 383.083	9 865 323 481.933
2.5	29 636 193.932	147 279 452.309	730 935 585.996	3 623 368 321.881
3.0	16 745 024.588	79 387 555.914	375 872 345.928	1 777 575 738.487
3.5	10 924 925.919	49 999 298.115	228 524 782.674	1 043 289 204.303
4.0	7 840 970.927	34 914 268.722	155 260 830.992	689 643 118.857
4.5	6 014 768.061	26 201 220.686	113 985 957.862	495 319 960.265

Table 5. Spin-s Ising model. Series coefficients for the second moment of the correlation function. The expansion variable is $K = J/kT$.

s \ n	11	12	13	14
1.0	27 505 317 890.383	212 457 469 283.931	1 625 420 767 814.491	12 333 782 918 414.818
1.5	3 335 449 160.090	21 711 509 856.038	140 004 046 089.529	895 554 479 535.982
2.0	974 154 748.992	5 734 658 063.513	33 445 456 506.425	193 507 258 378.028
2.5	433 216 160.145	2 386 305 269.158	13 023 160 887.809	70 510 441 213.815
3.0	243 751 368.075	1 280 658 851.091	6 666 537 847.443	34 428 932 166.216
3.5	158 602 597.181	804 308 045.269	4 041 312 628.749	20 145 825 924.397
4.0	113 622 780.496	560 568 785.493	2 740 219 835.286	13 289 504 836.274
4.5	87 045 770.505	420 102 000.503	2 008 900 617.483	9 530 860 923.691

The same graphical data and programs were used in the calculations for all values of spin. Since the $s = \frac{1}{2}$ series could be independently verified in several cases, we can be reasonably confident of the correctness of the data for the other values of s.

5. Conclusions

Extended high-temperature series expansion data are derived for the spin-s Ising model on the FCC lattice. Complete agreement is obtained with all earlier work. Several of the new coefficients are calculated by two independent methods.

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