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COMMENT

High-temperature series expansion studies of mixed spin-$\frac{1}{2}$–spin-S Ising models

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Abstract. Mixed spin Ising models have less translational symmetry than their 'single spin' counterparts and are well adapted for the study of a certain type of ferrimagnetism. In this article the high–temperature series expansion work of Schofield and Bowers—who studied mixed spin-$\frac{1}{2}$-spin-1 Ising models—is generalised by replacing the spin-1 objects by arbitrary spin-S ones. The new series are used to investigate the spin dependence or independence of critical parameters in a novel setting. There is no evidence to suggest that the exponents studied are spin dependent.

1. Introduction

The purpose of this comment is to present extensions of the work of Schofield and Bowers (1981) on mixed spin-$\frac{1}{2}$-spin-1 Ising models‡. We have generalised their calculations replacing the spin-1 objects by arbitrary spin-S ones. This has allowed us to investigate the spin dependence or independence of parameters describing critical behaviour in a new setting. Mixed spin Ising models have less translational symmetry than their 'single spin' counterparts and are well adapted for the study of a certain type of ferrimagnetism (Néel 1948).

The reduced Hamiltonian of our model takes the form

$$\mathscr{H} = K \sum_{\langle ij \rangle} \sigma_i s_j + L_A \sum_i \sigma_i + L_B \sum_j s_j. \tag{1}$$

The underlying lattice is loose packed and the sites of the A sublattice are occupied by 'spins' σ_i of magnitude $\frac{1}{2}$ whilst those of the alternate B sublattice are occupied by 'spins' s_j of magnitude S. The σ_i take the values $\pm\frac{1}{2}$ and the s_j the values $-S$, $-S+1, \ldots, S$ where S has one of the usual integral or odd half-integral values. The first summation in (1) involves all pairs of nearest-neighbour sites in the lattice. The second and third summations involve all sites of A and B respectively. The quantities K, L_A, L_B—measured in units of kT—are, respectively, an interaction constant and the magnetic fields on the A and B sublattices. If $K > 0$, the situation is potentially ferromagnetic whilst, if $K < 0$, the situation is potentially ferrimagnetic. The symmetry (Schofield and Bowers 1981) between ferromagnet in a uniform field and ferrimagnet

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‡ The mixtures discussed here are of a *non-random* two sublattice type and not of the random type which is of much current interest.

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in a staggered field still applies. Uniform field ferromagnetic critical behaviour is thus studied. It is easy to interpret this ferrimagnetically if required.

2. The Brout expansion

In order to generalise the series expansions of Schofield and Bowers (1981) using Brout's (1959, 1960) technique, it is necessary to recalculate the graph cumulants. This is a laborious but straightforward procedure (Yousif 1983). The diagrams which enter the new calculations remain as before; no other aspects of the calculations are altered. (Many new diagrams do appear if the spin-$\frac{1}{2}$ sublattice is replaced by a general spin-S' sublattice—diagrams articulated at a spin-$\frac{1}{2}$ vertex have zero cumulant. Thus (1) allows us to reach maximum order with the given diagrams.)

The series expansions for the (reduced) initial susceptibility χ and the zero-field specific heat C may be written in the forms

$$\chi = (11/24) \sum b_n(S) K^n, \tag{2}$$

and

$$C = \sum c_n(S) K^n \qquad (n \text{ even}). \tag{3}$$

Table 1. Zero-field susceptibility coefficients for the SQ, SC and BCC lattices with $X = S(S+1)$.

SQ
$b_0(S) = (1/11)(4X+3)$
$b_1(S) = 8X/11$
$b_2(S) = (X/165)(68X+39)$
$b_3(S) = (2X/33)(10X-1)$
$b_4(S) = (X/13\,860)(4460X^2+1721X-177)$
$b_5(S) = (X/6930)(2890X^2-657X+51)$
$b_6(S) = (X/831\,600)(179\,168X^3+39\,268X^2-10\,871X+726)$
$b_7(S) = (X/207\,900)(54\,726X^3-19\,414X^2+2964X-195)$
SC
$b_0(S) = (1/11)(4X+3)$
$b_1(S) = 12X/11$
$b_2(S) = (3X/110)(36X+23)$
$b_3(S) = (2X/55)(67X-4)$
$b_4(S) = (X/9240)(19\,708X^2+10\,749X-615)$
$b_5(S) = (X/4620)(23\,306X^2-2964X+141)$
$b_6(S) = (X/1663\,200)(7266\,168X^3+3372\,858X^2-438\,192X+18\,153)$
$b_7(S) = (X/207\,900)(2102\,787X^3-412\,533X^2+36\,126X-1521)$
BCC
$b_0(S) = (1/11)(4X+3)$
$b_1(S) = 16X/11$
$b_2(S) = (2X/165)(148X+99)$
$b_3(S) = (2X/165)(516X-22)$
$b_4(S) = (X/6930)(52\,148X^2+31\,159X-1305)$
$b_5(S) = (X/1155)(29\,018X^2-2775X+92)$
$b_6(S) = (X/415\,800)(12\,482\,576X^3+6589\,456X^2-645\,199X+19\,971)$
$b_7(S) = (X/207\,900)(20\,370\,104X^3-3075\,616X^2+202\,329X-5871)$

In table 1, coefficients $b_0(S), b_1(S), \ldots, b_7(S)$ are given for the SQ, SC, and BCC lattices. In table 2, coefficients $c_2(S), c_4(S), \ldots, c_{10}(S)$ are given for the same three lattices.

Table 2. Zero-field specific heat coefficients for the SQ, SC and BCC lattices with $X = S(S+1)$.

SQ
$c_2(S) = X/6$
$c_4(S) = (X/24)(3X-1)$
$c_6(S) = (X/6048)(272X^2 - 216X + 51)$
$c_8(S) = (X/259\,200)(3857X^3 - 4038X^2 + 2043X - 390)$
$c_{10}(S) = (X/5322\,240)(28\,568X^4 - 31\,544X^3 + 20\,099X^2 - 7815X + 1285)$
SC
$c_2(S) = X/4$
$c_4(S) = (X/80)(29X-8)$
$c_6(S) = (X/4032)(2026X^2 - 759X + 141)$
$c_8(S) = (X/172\,800)(126\,783X^3 - 58\,532X^2 + 13\,896X - 2028)$
$c_{10}(S) = (X/3548\,160)(3959\,274X^4 - 2127\,059X^3 + 595\,155X^2 - 109\,120X + 13\,585)$
BCC
$c_2(S) = X/3$
$c_4(S) = (X/60)(73X-11)$
$c_6(S) = (X/1512)(5146X^2 - 1443X + 138)$
$c_8(S) = (X/129\,600)(1272\,475X^3 - 469\,350X^2 + 80\,028X - 5871)$
$c_{10}(S) = (X/2661\,120)(78\,680\,700X^4 - 34\,400\,282X^3 + 7566\,392X^2 - 974\,540X + 13\,585)$

Certain checks have been applied to our results. For $S=\frac{1}{2}$, all the results given here reduce to those known for the standard spin-$\frac{1}{2}$ Ising model (Domb and Sykes 1957, Domb 1960). For $S=1$ nearly all our results agree with those of Schofield and Bowers (1981). Where there is disagreement, we feel that the present results are correct. Our calculations correct small errors in $c_{10}(1)$ for the SQ and BCC lattices. (On the BCC lattice there are two free-energy diagrams (Yousif 1983) missing from the list given by Schofield (1980).) The coefficients $b_4(1)$ and $b_6(1)$ given by Schofield and Bowers are also slightly wrong for all three lattices. We have traced the origin of the error to a failure to include all correlation lines in a few highly symmetric graphs.

3. Analysis of the series

We have used the methods of series analysis employed by Schofield and Bowers (1981). To fix attention we have studied the cases $S=\frac{1}{2}, 1, \frac{3}{2}, 5, 10, 100$. For $S=\frac{1}{2}$, which is the standard Ising model, our results can be compared with others which use much longer series (e.g. Domb 1974). For $S=1$ our results can be compared with those obtained, using some slightly different coefficients, by Schofield and Bowers (1981). For the other spin values our results are the first available. We give details of the analysis only for $S=5$ and the BCC lattice. All other cases are dealt with very briefly to save space.

In table 3 we give roots and residues of Padé approximants to the logarithmitic derivative of the susceptibility χ (for $S=5$ and the BCC lattice). These lead us to make

Table 3. Estimates of K_C and γ (in parenthesis) from Padé approximants to $D \ln \chi$ for the BCC lattice and $S=5$.

D \ N	1	2	3	4
2	0.104 88 (1.611)	0.093 11 (1.133)	0.096 13 (1.288)	0.096 48 (1.311)
3	0.095 14 (1.231)	0.095 48 (1.246)	0.096 53 (1.315)	
4	0.095 49 (1.247)	0.094 85 (1.224)		
5	0.096 29 (1.298)			

the preliminary estimates

$$K_C = 0.0957 \pm 0.0008, \qquad \gamma = 1.270 \pm 0.045. \tag{4}$$

We have formed Padé approximants to $\chi^{1/\gamma}$ and $(K_C - K)D \ln \chi$ in the usual way for various values of γ and K_C in the ranges (4). Results for typical values are shown in tables 4 and 5. Overall these calculations lead us to sharpen our estimates somewhat. Our final Padé estimates are

$$K_C = 0.0958 \pm 0.0004, \qquad \gamma = 1.26 \pm 0.02. \tag{5}$$

Table 4. Estimates of K_C for the BCC lattice and $S=5$ from Padé approximants to $\chi^{1/\gamma}$ with $\gamma = 1.26$.

D \ N	1	2	3	4	5	6
1	0.026 72	0.378 04	0.023 91	0.394 14	0.023 18	0.401 53
2	0.094 40	0.096 22	0.095 47	0.095 87	0.095 74	
3	0.096 54	0.095 69	0.095 73	0.095 78		
4	0.094 42	0.095 73	0.096 16			
5	0.095 46	0.095 77				
6	0.095 85					

Table 5. Estimates of γ for the BCC lattice and $S=5$ from Padé approximants to $(K_C - K)D \ln \chi$ evaluated at $K = K_C = 0.0957$.

D \ N	1	2	3	4	5
1	1.354	1.230	1.265	1.259	1.249
2	1.250	1.257	1.260	1.272	
3	1.257	1.262	1.258		
4	1.260	1.258			
5	1.252				

We now turn our attention to the ratio method using the quantities $s_n = (b_n / b_{n-2})^{1/2}$ and alternate pairs of points in the fashion of Schofield and Bowers (1981). We compute sequences

$$l_n = \tfrac{1}{2}[(n+2)s_{n+2} - ns_n], \tag{6}$$

$$g_n = n(K_C s_n - 1), \tag{7}$$

and the extrapolants l'_n and g'_n obtained by replacing s_n in (6) by l_n and g_n respectively. The sequences l_n and l'_n, which provide estimates for K_C^{-1}, are given (for $S=5$ and the BCC lattice) in table 6. These lead us to estimate

$$K_C = 0.0957 \pm 0.0003 \tag{8}$$

Table 6. The sequences l_n and l'_n for the susceptibility χ of the BCC lattice with $S=5$.

n	l_n	l'_n
2	10.260	10.486
3	10.395	10.416
4	10.373	
5	10.403	

Table 7. The sequences g_n and g'_n for the susceptibility χ of the BCC lattice with $S=5$ using $K_C = 0.0957$.

n	g_n	g'_n
2	0.325	0.253
3	0.259	0.233
4	0.289	0.245
5	0.248	0.217
6	0.275	
7	0.239	

in good agreement with the Padé result in (5). In table 7 we use the central value of K_C from (8) to obtain sequences g_n and g'_n which provide estimates for $\gamma - 1$. We have investigated such sequences for other values of K_C and are inclined to feel that

$$\gamma = 1.24 \pm 0.03 \tag{9}$$

represents these results fairly well. The agreement with the Padé result in (5) is really quite good.

Our final estimates of K_C and γ reflect both the Padé and the ratio results already presented. They also reflect a search for consistency between the two methods. In

Table 8. Final estimation of K_C, γ and α for the BCC, SQ, and SC lattices with $S=\frac{1}{2}$, 1, $\frac{3}{2}$, 5, 10, and 100.

	S	K_C	γ	α
BCC	$\frac{1}{2}$	0.628 ± 0.002	1.22 ± 0.03	0.10 ± 0.03
	1	0.376 ± 0.001	1.23 ± 0.02	0.13 ± 0.03
	$\frac{3}{2}$	0.273 ± 0.001	1.24 ± 0.01	0.14 ± 0.04
	5	0.0957 ± 0.0001	1.24 ± 0.02	0.14 ± 0.03
	10	0.04997 ± 0.00012	1.24 ± 0.02	0.14 ± 0.04
	100	0.00522 ± 0.00003	1.24 ± 0.04	0.16 ± 0.06
SC	$\frac{1}{2}$	0.885 ± 0.017	1.23 ± 0.12	0.06 ± 0.20
	1	0.527 ± 0.006	1.24 ± 0.12	0.08 ± 0.10
	$\frac{3}{2}$	0.381 ± 0.003	1.24 ± 0.09	0.08 ± 0.08
	5	0.1336 ± 0.0007	1.22 ± 0.05	0.09 ± 0.06
	10	0.0698 ± 0.0004	1.23 ± 0.06	0.09 ± 0.07
	100	0.00729 ± 0.00005	1.24 ± 0.06	0.10 ± 0.08
SQ	$\frac{1}{2}$	1.764 ± 0.070	1.75 ± 0.45	0.1 ± 0.6
	1	1.025 ± 0.007	1.75 ± 0.07	-0.2 ± 0.3
	$\frac{3}{2}$	0.736 ± 0.015	1.74 ± 0.22	-0.2 ± 0.4
	5	0.2564 ± 0.0080	1.76 ± 0.34	-0.2 ± 0.4
	10	0.1336 ± 0.0044	1.77 ± 0.34	-0.2 ± 0.4
	100	0.0140 ± 0.0006	1.80 ± 0.43	-0.1 ± 0.6

this search estimates obtained from one method are used as input to the other. Our final results are given in table 8. This table contains estimates of K_C and γ for all the spin values and lattices mentioned previously. In each case, the estimates have been obtained by a procedure very similar to that described above.

We now turn to the specific heat. For this series we estimate the critical exponent α using the final estimate of K_C obtained from the susceptibility. Since only even powers of K appear, the series is rather short. Padé analysis is not practical and we have to be content with applying (7) taking K^2 as the variable and replacing s_n by r_n—the ratio of successive terms. Results obtained, using the central and extreme values of K_C given in table 8 for $S=5$ and the BCC lattice, are presented in table 9.

Table 9. Sequences $\alpha_n = 1+g_n$ for the specific heat C of the BCC lattice with $S=5$.

K_C	0.0956	0.0957	0.0958
α_2	0.991	0.996	1.000
α_3	0.291	0.296	0.301
α_4	0.155	0.161	0.168
α_5	0.119	0.128	0.136

These suggest that in this case, $\alpha = 0.14 \pm 0.03$ and this is entered in table 8. Values of α for other spin values and lattices, obtained by the same technique, also appear in this table. (These values must be treated very cautiously. They merely summarise the ranges of α_4 and α_5 which result from the given ranges for K_C.)

4. Conclusion

From table 8 it is clear that, as expected, whilst K_C varies with lattice and spin there is no evidence that the critical exponents vary once the lattice dimension is fixed. The mixed spin models seem to share the same exponent values as their 'single spin' counterparts in agreement with the principle of extended spin independence.

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