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Abstract. A high-temperature series expansion in the cumulant form of Brout is applied to mixed-spin Ising models on simple quadratic, simple cubic and body-centred cubic lattices. Motivation is provided primarily by an investigation of critical phenomena in Ising models with less than the usual translational symmetry and of relevance to the study of ferrimagnetism. Secondary motivation, appropriate to the simple quadratic lattice, is derived from a desire to obtain results that can be compared with those of renormalisation-group calculations performed elsewhere by the authors. Series expansions of the susceptibility and specific heat are obtained to seventh and tenth order, respectively. The derived expansion coefficients are analysed through both ratio and Padé approximant methods, and exponent values are found to be in good agreement with those suggested by the universality hypothesis.

1. Introduction

With regard to analyses of Ising models employing techniques based on the high-temperature series expansion, interest has been largely focused on those model systems suited to a simulation of the critical properties of ferro- and antiferromagnets (Domb 1960, 1970). Essentially all calculations have so far dealt with systems in which all lattice sites are equivalent in the sense that only a single kind of spin is present, and it is this restriction that has limited the analyses to ferro- and antiferromagnetism. It appears desirable to extend the scope of investigation in a manner such that a study of ferrimagnetism (Néel 1948) is facilitated. The present paper achieves this objective by means of high-temperature series expansion analyses of a particularly simple model capable of uniaxial ferrimagnetism.

Of the various methods of high-temperature series expansion (Domb 1960, 1970), the form based on the cumulant expansion of Brout (1959, 1960) is employed in this paper. The basic system considered is an Ising model consisting of both spin-$\frac{1}{2}$ and spin-1 objects, and is analysed on several different loose-packed lattices, namely the two-dimensional simple quadratic (SQ) and three-dimensional simple cubic (SC) and body-centred cubic (BCC). Treatment of such loose-packed lattices facilitates the consideration of the system as consisting of two inter-penetrating sublattices of spin-$\frac{1}{2}$ and spin-1 objects, where each spin-1 has only spin-$\frac{1}{2}$'s as nearest neighbours, and vice versa. This procedure is readily seen to be conducive to the study of a particular form of uniaxial ferrimagnetism.

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Considering only nearest-neighbour interactions between the spin-$\frac{1}{2}$ and spin-1 objects, the reduced Hamiltonian of the system in the presence of an applied magnetic field is given by

$$\mathscr{H} = K \sum_{\langle ij \rangle} \sigma_i s_j + H\Big(\sum_i \sigma_i + \sum_j s_j\Big) \tag{1}$$

where $\sigma = -\frac{1}{2}, \frac{1}{2}$ and $s = -1, 0, 1$ are the allowed spin values, and K and H are expressed in units of kT. Schofield (1980) has employed a sublattice spin reversal (e.g. $s_j \rightarrow -s_j, \forall j$) to derive an exact result showing that the properties of the nearest-neighbour ferromagnet (characterised by $K > 0$) in a uniform magnetic field (H, H) are identical to those of the corresponding anti-aligning ferrimagnet (characterised by $K < 0$) in a staggered field $(H, -H)$ where the notation indicates the fields acting on the individual sublattices of the mixed-spin Ising model under consideration. Series expansion analyses are carried out for the uniform field case by Schofield (1980) and in the present paper. Singularities $K_c > 0$ are studied, but—because of the above symmetry—derived critical exponents are appropriate either to ferromagnetism in a uniform field or to ferrimagnetism in a staggered field.

The above models, appropriate to the SQ, SC and BCC lattices, are expected to belong to the same respective universality classes (Wilson 1971) as more simple Ising models (such as spin-$\frac{1}{2}$) on the given lattices. Such a property is reflected in the results of the present paper, providing evidence in support of the expected similarities between critical phenomena associated with ferro- and antiferromagnetism on the one hand and ferrimagnetism on the other. With particular regard to the SQ lattice appropriate to two dimensions, direct comparison can be made with the results of the renormalisation-group analyses of Schofield and Bowers (1980). Such comparison is of considerable importance with respect to the quantity $K_c = J/kT_c$ (where T_c and J denote, respectively, the critical temperature and nearest-neighbour exchange energy, and k denotes Boltzmann's constant) which cannot be estimated from arguments based purely on the principle of universality (Wilson 1971).

2. Brout cumulant expansion applied to mixed-spin system

The Brout expansion formalism (Brout 1959, 1960) is readily applied to the system described by (1), and is given by Schofield (1980). The results of this analysis are summarised immediately below:

If F and χ denote, respectively, the zero-field free energy and susceptibility of the system, then we have (Brout 1959, 1960, Schofield 1980), employing $\beta = 1/kT$,

$$-\beta F = \sum_{m,\tau} ((m, \tau); G) \sum_{n,t} K^n M_{n,t} P_{n,t} (W_{m,\tau} W_{n,t}^{-1}) \tag{2}$$

$$\chi = \sum_{m,\tau} ((m, \tau); G) \sum_{n,t} K^n P_{n,t} (W_{m,\tau} W_{n,t}^{-1}) \sum_{n+1,t'} \varepsilon M_{n+1,t'} \tag{3}$$

where (2) and (3) represent the Brout form of the high-temperature series expansions of F and χ. The notation employed is described as follows:

(i) $\Sigma_{m,\tau}$ is a sum over all connected diagrams (m, τ) containing no multiple bonds (Brout 1959, 1960), where m denotes the number of bonds and τ is an arbitrary label for distinguishing diagrams with the same number of bonds;

(ii) $((m, \tau); G)$ is the weak embedding constant of the diagram (m, τ);

(iii) $\Sigma_{n,t}$ is a sum over all diagrams (n, t) possessing the same underlying (single-bonded) diagram (m, τ), where n denotes the total number of bonds and t is a label whose purpose is analogous to that of τ;

(iv) $M_{n,t}$ is the cumulant (Brout 1959, 1960, Schofield 1980) of the diagram (n, t);

(v) $P_{n,t}$ is given by the product $\Pi_{s=1}^{m} 1/p_s!$ where p_s denotes the multiplicity of the edge s of diagram (n, t);

(vi) $W_{m,\tau}$ and $W_{n,t}$ are, respectively, the number of ways of labelling the vertices of diagrams (m, τ) and (n, t) in such a way that the connectivity of the labels is unchanged;

(vii) $\Sigma_{n+1,t'}\, \varepsilon M_{n+1,t'}$ is a sum over all connected diagrams $(n+1, t')$ which may be derived from (n, t) through the addition of one bond. If this bond is incident twice on one vertex, $\varepsilon = 1$; otherwise, $\varepsilon = 2$. The sums in (2) and (3) are taken over connected diagrams, since it can be shown (Brout 1959, 1960, Schofield 1980) that the cumulants $M_{n,t} = 0$ for all separated diagrams.

The expansions of (2) and (3) have been described using diagrams whose vertices show no distinction between spin-$\frac{1}{2}$ and spin-1 sites. In calculating cumulants, however, we must consider vertex-decorated diagrams which are furnished with spins in the obvious way. Because of the loose-packed structure, these occur in pairs—one diagram being obtained from the other by the transposition of the spin-$\frac{1}{2}$ and spin-1 sites. The cumulant of any undecorated diagram is then equal to the average of the cumulants of its two vertex-decorated derivatives (Schofield 1980). In the case of diagrams with an articulation point, only the derivative in which this vertex has spin-1 can contribute to the average. The other contribution can be shown to vanish (Schofield 1980). Vanishing cumulants are also appropriate in (2) for free energy diagrams possessing odd vertices (those from which an odd number of bonds emanate) and in (3) for diagrams with this property consequent upon the addition of the extra bond of (vii). Those diagrams not possessing the above properties, and thereby providing non-vanishing contributions to (2) and (3), are listed in Schofield (1980). Here, diagrams appropriate to (2) involve only even values of n (because of the vanishing of odd-vertex diagrams) and those diagrams are given for $n = 2, 4, 6, 8$ and 10. In the case of the susceptibility, all values of n are appropriate, and those diagrams for $n = 0, 1, 2, \ldots, 7$ have been considered. By way of summary, it is necessary to consider only those (vertex-decorated) diagrams which are (a) connected, (b) not articulated at a spin-$\frac{1}{2}$ vertex, and (c) possessive only of even degree vertices, in the case of the free energy; in the case of the susceptibility we consider diagrams which can be put into the form of (a), (b) and (c) through the addition of one bond. The entries of table 1 give, for each lattice, the numbers of free energy and susceptibility diagrams of the above type appropriate to the given values of n. It is seen that the numbers increase significantly for the highest values.

Table 1. Numbers of free energy and susceptibility diagrams for each lattice for different values of n.

	Free energy					Susceptibility							
Lattice \ n	2	4	6	8	10	0	1	2	3	4	5	6	7
SQ	1	3	6	20	54	2	1	3	3	9	12	35	55
SC	1	3	6	20	60	2	1	3	3	9	12	35	55
BCC	1	3	6	24	74	2	1	3	3	9	12	37	59

Explicit evaluation of terms of (2) and (3) appropriate to the values of n given above can be found in Schofield (1980). Let us write the corresponding (truncated) series in the forms

$$-\beta F = \sum_{n=2}^{10} a_n K^n, \qquad n \text{ even} \tag{4}$$

and

$$\chi = \sum_{n=0}^{7} b_n K^n. \tag{5}$$

A series expansion form for the zero-field specific heat C is readily found from (4) and the relation $C = -T(\partial^2 F/\partial T^2)_{H=0}$, and is given by

$$C = \sum_{n=2}^{10} c_n K^n, \qquad n \text{ even} \tag{6}$$

where the coefficients c_n are given in terms of a_n by $c_2 = 2a_2$, $c_4 = 12a_4$, $c_6 = 30a_6$, $c_8 = 56a_8$ and $c_{10} = 90a_{10}$. The coefficients for each lattice were calculated to six significant figures; subsequent analysis in § 3 is with regard to the specific heat and susceptibility coefficients, and these are presented in table 2.

Table 2. Series expansion coefficients for the specific heat and susceptibility.

	SQ	SC	BCC
c_2	1.000 00	1.000 00	1.000 00
c_4	1.250 00	2.500 00	6.750 00
c_6	0.701 388	6.673 60	35.388 9
c_8	0.425 923	18.655 1	195.754
c_{10}	0.302 556	54.685 0	1156.52
b_0	1.000 00	1.000 00	1.000 00
b_1	1.454 55	2.181 82	2.909 09
b_2	2.121 21	5.181 81	9.575 76
b_3	2.303 03	9.454 55	24.484 9
b_4	3.025 25	21.522 7	77.565 6
b_5	2.971 71	37.851 5	191.539
b_6	3.760 92	84.943 9	599.006
b_7	3.519 81	146.637	1453.17

3. Analysis of series coefficients

Both the ratio and Padé approximant methods (Stanley 1971, Domb 1960, 1970) have been employed in an analysis of the expansion coefficients of table 2, and the relevant details are presented by Schofield (1980). For a series given generally in the form

$$f(K) = \sum_{n=0}^{\infty} \alpha_n K^n \tag{7}$$

the analysis assumes that

$$f(K) \sim A_i(1-K/K_i)^{-\lambda_i}+B_i \qquad \text{as } K \to K_i^- \tag{8}$$

and attempts to determine K_i and λ_i for the physically interesting singularities (Stanley 1971) of the function $f(K)$. No explicit details are given of the ratio and Padé analyses in this paper—instead, we briefly describe the procedures involved and the manner in which the results of the respective analyses are combined to yield, for each lattice, a singularity K_c and associated critical exponents α and γ.

3.1. *Ratio method*

The coefficients b_n of the susceptibility series (5) are analysed through the employment of $a(1/n)$ plot (Domb 1960, 1970) involving ratios of alternate coefficients defined by $s_n = (b_n/b_{n-2})^{1/2}$. By this means, estimates are obtained of K_c and γ. In the case of the specific heat series (6), ratios of successive coefficients, defined by $r_n = c_n/c_{n-1}$, are employed. Here, K^2 is regarded as the appropriate expansion variable, since the series (6) is given in even powers of K. The number of terms present in (6) is too small to yield sufficiently precise estimates of K_c and the associated specific heat exponent α using only the ratios r_n. The value of K_c obtained from the susceptibility series (which contains more terms than (6)) is therefore employed in a specific heat $(1/n)$ plot, to yield an estimate of α. By means of this strategy, we obtain from the ratio method estimates of K_c, γ and α appropriate to each lattice.

3.2. *Padé approximant method*

This method is applied only to the susceptibility series (5), for reasons which become apparent below. The general procedure is such that all Padé approximants $P_D^N(K)$ (Stanley 1971) to the logarithmic derivative series (obtained from (5)) are formed with $N+D=1, \ldots, 6$ (except those with N or D zero). The derived singular points K_i and associated residues λ_i are displayed in triangular arrays with N labelling the columns and D the rows. Convergence of this Padé table is then searched for, and initial estimates of K_c and γ are obtained. These estimates are then employed to construct the functions

$$\{f(K)\}^{1/\gamma} \sim A^{1/\gamma}K_c(K_c-K)^{-1} \qquad \text{as } K \to K_c^- \tag{9}$$

and

$$(K_c-K)(\partial/\partial K)\ln f(K) \sim \gamma \qquad \text{as } K \to K_c^-. \tag{10}$$

Padé approximants to (9) and (10) now yield improved estimates for K_c and γ, respectively, where now $N+D=1, \ldots, 7$ and $N+D=1, \ldots, 6$. As expected, the triangular Padé arrays obtained from (9) and (10) display improved convergence over the arrays appropriate to the initial estimates of K_c and γ. For comparison purposes, values of γ suggested by the universality hypothesis (1.75 for SQ and 1.25 for SC and BCC) are employed in (9) to obtain corresponding Padé estimates of K_c; these are found to be in good agreement with the previously derived values.

With regard to the specific heat series (6) it is found that Padé analyses yield rather poor convergence. Consequently, results relating to such analyses are not employed, and the regime of investigation of (6) is restricted to that of the ratio test.

Final estimates of K_c and γ are obtained through a search for consistency between the ratio and Padé results. These estimates are given in table 3, together with those of α obtained from employment in the ratio test of 'final estimate' values of K_c. The results for the exponent γ are seen to be in good agreement with the predictions $\gamma = 1.75$ (SQ) and $\gamma = 1.25$ (SC and BCC) obtained from the universality hypothesis. The same remark applies to the exponent α for the SC and BCC lattices, where universality suggests the value 0.125. In the case of the SQ lattice, the negative value of α appearing in table 3 is inconsistent with singular behaviour of the form (8); this is somewhat consistent, however, with a (universality-suggested) logarithmic divergence in specific heat (Stanley 1971) which presents difficulties for the analysis employed in this paper.

With regard to K_c, the lower estimates appropriate to the SC and BCC lattices in comparison with that for the SQ lattice is consistent with analogous results obtained for other models, as is the lower estimate for the BCC lattice compared with that for the SC case (Domb 1960, 1970). The estimate of K_c appropriate to the SQ lattice is seen to lie fairly close to the values 1.186 and 1.374 obtained from respective renormalisation group analyses of Schofield and Bowers (1980); such agreement is seen to be satisfactory considering the questionable nature of the method employed to obtain K_c in the latter analyses (Schofield 1980).

Table 3. Final estimates of K_c, γ and α.

	SQ	SC	BCC
K_c	1.02 ± 0.01	0.52 ± 0.01	0.375 ± 0.002
γ	1.74 ± 0.10	1.23 ± 0.17	1.23 ± 0.05
α	-0.3 ± 0.1	0.15 ± 0.08	0.15 ± 0.03

4. Summary

The results obtained for the critical exponents are seen to provide good evidence—relevant to the case of ferrimagnetism—supporting the usual form of the universality hypothesis. Overall results are consistent with those obtained from previous calculations on other models, and in particular with renormalisation group analyses of Schofield and Bowers (1980) appropriate to the (two-dimensional) SQ lattice.

It is to be expected that improved agreement with the predictions of universality would be obtained in extended series expansion analyses employing more terms than are present in (5) and (6). It may be mentioned here that such an exercise would involve a considerable number of diagrams appropriate to the higher orders, arising partly from the presence of those diagrams articulated at spin-1 vertices (which possess non-vanishing cumulants, in general (Schofield 1980)). Indeed it is seen from the entries of table 1 that significant numbers of diagrams are required for the analyses of this paper.

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