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1990 J. Phys. A: Math. Gen. 23 4547

(http://iopscience.iop.org/0305-4470/23/20/016)

J. Phys. A: Math. Gen. 23 (1990) 4547-4551. Printed in the UK

High-temperature series expansions for mixed spin-S–spin-S' Ising models

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Received 26 February 1990

Abstract. This paper describes the development of high-temperature series expansions for general mixed spin-S-spin-S' Ising models on simple loose-packed lattices. It extends previous work on the simpler special case $S'=\frac{1}{2}$. Coefficients of the series for the initial susceptibility and specific heat of these models on the square, SC and BCC lattices are presented. A preliminary analysis of the results for the particular case $S=1$, $S'=\frac{3}{2}$ is given, and the critical ratio K_c and the susceptibility exponent γ are estimated.

Ferrimagnetic order is found in many magnetic insulators, notably the ferrites. The majority of these materials contain ionic species with two different spins.

In this paper, we describe the application of the high-temperature cumulant expansion method [1-6] to the initial isothermal susceptibility and zero-field specific heat of a mixed spin-S-spin-S' Ising system, on simple loose-packed lattices, where both S and S' may take arbitrary positive integer or half-integer values. This provides a simple model of a two-sublattice ferrimagnet [7] and generalizes the work of Schofield and Bowers [6] and Yousif and Bowers [8, 9] on the spin-$\frac{1}{2}$-spin-S systems.

The system considered consists of two interpenetrating sublattices of spin S' (A-sublattice) and spin S (B-sublattice) respectively, where each S' has only spin S as nearest neighbours and vice versa. We assume that the Landé g-factor is the same for both species, and we use units such that $g\mu_B = 1$, where μ_B is the Bohr magneton. A uniform nearest-neighbour Ising interaction is assumed, and the Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle i,j\rangle} \sigma_i s_j - H\left(\sum_{i\in A} \sigma_i + \sum_{j\in B} s_j\right)$$

where $\langle i, j\rangle$ denotes that the summation is over all nearest-neighbour pairs of the system, $i\in A$ denotes summation over all the A-sublattice sites, σ_i denotes an A-sublattice spin S', s_j denotes a B-sublattice spin S, J is the exchange constant, and H is the applied magnetic field.

The cumulant expansion technique [1-5] leads naturally to the high-temperature series for the Helmholtz free energy, F, where

$$-\beta F = \ln\langle \exp(-\beta\mathcal{H})\rangle \qquad \beta = 1/kT$$

and thence to the isothermal initial susceptibility

$$\chi_{H=0} = -\left(\frac{\partial^2 F}{\partial H^2}\right)_T\Bigg|_{H=0}$$

and zero-field specific heat

$$C_{H=0} = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_{H=0}$$

By identifying interactions between spins with bonds of topological graphs, part of the problem can be reduced to a combinatorial exercise. We have developed a computer algorithm [10] to generate all the free graphs required in the calculation of the coefficients a_n, b_n, c_n, for any given values of S and S', in the high-temperature series:

$$-\beta F = \sum_{n=2}^{\infty} a_n K^n \qquad (n \text{ even}) \tag{1}$$

$$\chi_{H=0} = \beta \sum_{n=0}^{\infty} b_n K^n \qquad (\text{all } n) \tag{2}$$

$$C_{H=0} = k \sum_{n=2}^{\infty} c_n K^n \qquad (n \text{ even}) \tag{3}$$

where $K = J/kT$. A free graph is defined to be a network of vertices and the bonds connecting them, taking no account of the relative spatial positions of the vertices.

Expressions for the coefficients a_n, b_n in (1) and (2) can be obtained from the results of the analyses of Bowers [4], Schofield [5] and Yousif [11], in the form

$$a_n = \sum E_{[(n,t);G]} P_{(n,t)} M_{(n,t)}$$

$$b_n = \sum E'_{[(n+1,t');G]} P_{(n,t)} \varepsilon M_{(n+1,t')}$$

where the summation for a_n is over all connected graphs of n bonds with all vertices of even degree, and the summation for b_n is over all connected graphs of n bonds, plus one 'dotted bond', such that the underlying graph of n bonds has at most two vertices of odd degree. If the graph (n, t) contains two vertices of odd degree, then the dotted bond in $(n+1, t')$ must join them, otherwise the dotted bond is a simple loop from a vertex back to itself.

In the above, the symbols have the following meaning.

(r, s) denotes a graph of r bonds; s is a distinguishing label;

$1/P_{(n,t)}$ is the product of the factorials of the multiplicities of bonds in (n, t);

ε is equal to the number of vertices (1 or 2) connected by the dotted bond in $(n+1, t')$;

$M_{(u,s)}$ is the cumulant of the graph (u, s). This is zero if (u, s) is disconnected or has any vertices of odd degree;

$E_{[(n,t);G]}$ and $E'_{[(n+1,t');G]}$ are embedding constants given by

$$E_{[(n,t);G]} = \frac{W_{(m,\tau)}}{W_{(n,t)}}((m, \tau); G)$$

$$E'_{[(n+1,t');G]} = \frac{W_{(m,\tau)}}{W_{(n,t)}}((m, \tau); G) f_{(n+1,t')}$$

where $f_{(n+1,t')}$ is the number of ways in which the dotted bond can be repositioned within the graph without changing the latter's topology, $W_{(u,v)}$ is the number of ways that a free graph (u, v) can have its vertices relabelled so that the connectivity of a vertex with any given label remains unchanged, and $((m, \tau); G)$ is the weak embedding constant of the skeleton graph (m, τ) in the lattice graph G. A skeleton graph is defined to be a graph with no simple loops (an edge with coincident ends) and at most one edge between any given pair of vertices.

The values of weak embedding constants for skeletons can be obtained from tables (e.g. Domb [12]).

The f's and the W's are relatively simple combinatorial factors, and (m, τ) is the skeleton graph derived from (n, t) by replacing all multiple bonds by single bonds.

The required cumulants, $M_{(u,v)}$, can be calculated recursively [13].

In summary, only those connected graphs with all vertices even (or, in the case of graphs for the susceptibility series, even once the dotted bond has been included) will give a non-zero contribution. The calculation of the contributions of these graphs involves considerable labour once n becomes large.

The numbers of free graphs making contributions to the coefficients at various orders are shown in tables 1 and 2. It is clear that many more graphs are required at higher orders in this general spin-S-spin-S' case than for the spin-$\frac{1}{2}$-spin-S systems studied by previous authors [6, 9]. These additional graphs, which are articulated at spin S' vertices, give contributions which vanish in the case $S'=\frac{1}{2}$.

The coefficients a_n, b_n, c_n are polynomials symmetric in the variables $X=S(S+1)$, $Y=S'(S'+1)$. a_n and c_n are related by

$$c_n = n(n-1)a_n.$$

The coefficients b_n, c_n for the susceptibility and the specific heat, as defined by equations (2) and (3), are given in tables 3 and 4 below. In the special case $S'=\frac{1}{2}$, these reduce to the results of Yousif and Bowers [8, 9].

Preliminary results have been obtained using one form of the ratio method [12, 14, 15] in the case $S=1$, $S'=\frac{3}{2}$ on the square lattice. A direct Monte Carlo computer simulation for the same system on a periodic 64×64 lattice yielded an estimate of $K_c \approx 0.424$, confirming the trend shown by the ratio method (see figure 1). Use of this estimate as the $1/n=0$ point on the ratio plot gives an estimate of the susceptibility exponent $\gamma \approx 1.79$, in fair agreement with the generally accepted value $\gamma=\frac{7}{4}$ for two-dimensional Ising models with short-range interactions.

Table 1. Numbers of graphs making contributions to a_n, c_n.

Lattice \ n	2	4	6	8
Square	1	4	10	41
SC	1	4	10	41
BCC	1	4	10	45

Table 2. Numbers of graphs making contributions to b_n.

Lattice \ n	0	1	2	3	4	5	6	7
Square	2	1	4	4	16	21	76	118
SC	2	1	4	4	16	21	76	118
BCC	2	1	4	4	16	21	78	122

Table 3. Coefficients, b_n, for the initial susceptibility on square, SC and BCC lattices.

Square
$b_0 = (1/6)(X+Y)$
$b_1 = (4/9)XY$
$b_2 = (2/135)XY[17(X+Y)-3]$
$b_3 = (2/2025)XY[572XY-54(X+Y)+3]$
$b_4 = (1/85\,050)XY[25\,372(X^2Y+XY^2)-2304(X^2+Y^2)-11\,628XY+903(X+Y)-45]$
$b_5 = (1/1786\,050)XY[1117\,904X^2Y^2-256\,008(X^2Y+XY^2)+18\,360(X^2+Y^2)+58\,356XY$ $-3240(X+Y)+135]$
SC
$b_0 = (1/6)(X+Y)$
$b_1 = (2/3)XY$
$b_2 = (1/15)XY[9(X+Y)-1]$
$b_3 = (1/225)XY[484XY-28(X+Y)+1]$
$b_4 = (1/113\,400)XY[212\,856(X^2Y+XY^2)-11\,832(X^2+Y^2)-55\,944XY+2844(X+Y)-90]$
$b_5 = (1/238\,140)XY[1558\,128X^2Y^2-202\,032(X^2Y+XY^2)+9216(X^2+Y^2)+28\,404XY$ $-1026(X+Y)+27]$
BCC
$b_0 = (1/6)(X+Y)$
$b_1 = (8/9)XY$
$b_2 = (4/135)XY[37(X+Y)-3]$
$b_3 = (4/2025)XY[2732XY-114(X+Y)+3]$
$b_4 = (1/42\,525)XY[275\,684(X^2Y+XY^2)-11\,208(X^2+Y^2)-53\,556XY+1941(X+Y)-45]$
$b_5 = (1/893\,025)XY[27\,795\,632X^2Y^2-2680\,584(X^2Y+XY^2)+86\,400(X^2+Y^2)+271\,548XY$ $-7020(X+Y)+135]$

Table 4. Coefficients, c_n, for the zero-field specific heat on the square, SC and BCC lattices.

Square
$c_2 = (2/9)XY$
$c_4 = (1/225)XY[74XY-18(X+Y)+1]$
$c_6 = (1/714\,420)XY[273\,536X^2Y^2-172\,512(X^2Y+XY^2)+18\,360(X^2+Y^2)+88\,344XY$ $-3240(X+Y)+135]$
SC
$c_2 = (1/3)XY$
$c_4 = (1/150)XY[134XY-28(X+Y)+1]$
$c_6 = (1/476\,280)XY[1394\,768X^2Y^2-682\,056(X^2Y+XY^2)+46\,080(X^2+Y^2)+358\,992XY$ $-5130(X+Y)+135]$
BCC
$c_2 = (4/9)XY$
$c_4 = (2/225)XY[294XY-38(X+Y)+1]$
$c_6 = (1/357\,210)XY[5482\,208X^2Y^2-2065\,536(X^2Y+XY^2)+86\,400(X^2+Y^2)+952\,452XY$ $-7020(X+Y)+135]$

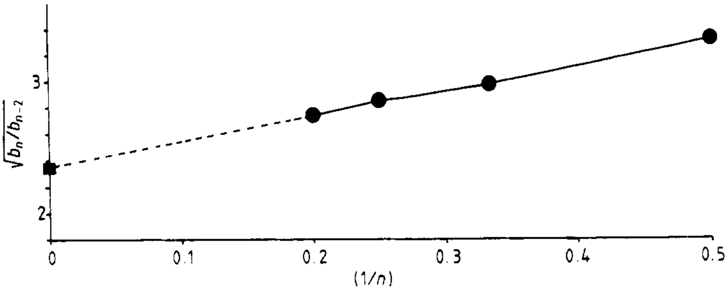

Figure 1. Ratio analysis of susceptibility series for $S=1$, $S'=\frac{3}{2}$ on the square lattice. ■: estimate of $(1/K_c)$ obtained by Monte Carlo computer simulation.

Acknowledgments

This work is supported by the Science and Engineering Research Council of the UK. One of us (GJAH) would like to thank the Governors of Portsmouth Polytechnic for the award of a research assistantship. The calculations were performed on the AMT DAP at Queen Mary and Westfield College, London. We are grateful to the staff of the Centre for Parallel Computing, QMW, particularly John Steel, for advice on the use of this system.

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