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LETTER TO THE EDITOR

Extension of the high temperature free energy expansion for general Ising systems

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Abstract. We have obtained the diagrams and weights for the thirteenth and fourteenth terms of the high temperature multigraph expansion for the free energy of general Ising systems. As an application we have computed the coefficients through fourteenth order for the square lattice with nearest- and next-nearest-neighbour interactions.

The method of exact series expansions continues to be a valuable approach to the study of critical phenomena and phase transitions in model lattice systems. There are two basic techniques for deriving the series coefficients: the direct combinatorial approach, originally developed by the King's College group, and the algebraic renormalised linked-cluster expansion of Wortis and co-workers (see the articles by Domb (1974) and Wortis (1974)). The easiest series to derive are for systems with a single type of interaction, and consequently most effort in this field has been devoted to the spin-$\frac{1}{2}$ Ising model with isotropic nearest-neighbour interactions. There are, however, many interesting problems in which there is more than one type of interaction; for example, systems with further-neighbour interactions, lattice anisotropy or even random couplings. Particularly interesting are systems with competing interactions.

Some years ago we derived (Oitmaa 1981) a high temperature multigraph expansion for general Ising systems. This is a variant of the direct combinatorial approach, in which disconnected diagrams are eliminated in favour of diagrams with multiple lines (multigraphs). For the zero-field free energy per spin the expansion takes the form

$$-\beta f = \ln 2 + \tfrac{1}{2}\sum_{\alpha} q_\alpha \ln\cosh(\beta J_\alpha) + \sum_{\{G\}} W_G X_G(L, \{v_\alpha\}) \qquad (1)$$

where $\{J_\alpha\}$ is the set of interactions, q_α is the partial coordination number, $\{G\}$ is the set of all connected multigraphs with every vertex of even degree, W_G is a graph weight and X_G is a multinomial in $v_\alpha = \tanh \beta J_\alpha$ which specifies the number of embeddings of the particular graph on the lattice L. The graph weights $\{W_G\}$ are simple rational numbers which are the same for any Ising problem which, once determined, are available for any specific future application.

The free energy expansion was previously derived through twelfth order (Oitmaa 1981), to which order a total of 508 diagrams contribute. We have recently extended this through fourteenth order, involving an additional 3554 diagrams. While it is clearly impossible to tabulate the diagrams and their weights here, a list can be supplied. In table 1 we list, for interest, the number of diagrams which contribute to each order. Factors which limit the number of terms achievable are the rapid increase in the number of diagrams and the computer time needed to determine the weights.

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Table 1. Number of diagrams in the free energy expansion.

Order	Number of diagrams	Total
3	1	1
4	1	2
5	1	3
6	3	6
7	4	10
8	10	20
9	19	39
10	47	86
11	107	193
12	315	508
13	849	1357
14	2705	4062

In order to check our expansion we have computed the free energy series for the face-centred cubic lattice, using available lists of lattice constants. We obtain complete agreement with the coefficients given by Domb (1974). This test is not completely exhaustive as a small number of the diagrams do not contribute to the FCC lattice, but it is a strong check.

We have applied these general results to extend the free energy series for the square lattice with nearest- and next-nearest-neighbour interactions. The expansion can be written as

$$-\beta f = \ln 2 + 2 \ln \cosh \beta J_1 + 2 \ln \cosh \beta J_2 + \sum_{m,n} a_{m,n} v_1^m v_2^n. \tag{2}$$

The coefficients $a_{m,n}$ for $m+n \leqslant 12$ were obtained previously (Oitmaa 1981) and in table 2 we give the values of these as well as the new coefficients.

Table 2. Coefficients $a_{m,n}$ in the expansion (2) for the square lattice with nearest- and next-nearest-neighbour interactions.

m	n	$a_{m,n}$	m	n	$a_{m,n}$	m	n	$a_{m,n}$
2	1	4	4	0	1	2	2	10
0	4	1	4	1	8	2	3	28
6	0	2	4	2	34	2	4	72
0	6	2	6	1	20	4	3	136
2	5	188	8	0	$4\frac{1}{2}$	6	2	132
4	4	509	2	6	482	0	8	$4\frac{1}{2}$
8	1	64	6	3	$753\frac{1}{3}$	4	5	1 832
2	7	1 236	10	0	12	8	2	596
6	4	3 872	4	6	6 358	2	8	3 140
0	10	12	10	1	236	8	3	4 496
6	5	18 380	4	7	21 448	2	9	7 956
12	0	$37\frac{1}{3}$	10	2	2 864	8	4	29 369
6	6	$81\,949\frac{1}{3}$	4	8	70 548	2	10	20 046
0	12	$37\frac{1}{3}$	12	1	952	10	3	26 900
8	5	172 560	6	7	347 204	4	9	227 272
2	11	50 396	14	0	130	12	2	14 242
10	4	213 080	8	6	933 952	6	8	1410 260
4	10	718 706	2	12	126 200	0	14	130

Although no analysis of the free energy or of the derived quantities such as internal energy or specific heat is given here, it would be straightforward to evaluate these over the whole disordered region $T > T_c$, using a Padé approximant representation. This could be useful in the interpretation of experimental data on, for example, adsorbed monolayer systems (Selke *et al* 1983). A rather different reason for deriving the free energy expansion for the square lattice with first- and second-neighbour interactions is the hope, perhaps vain, that some insight may be obtained into the algebraic structure of the free energy for this simple but unsolved model. It may be possible, for instance, to discover some kind of inversion relation (Maillard 1985) which holds for this model.

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References

Domb C 1974 *Phase Transitions and Critical Phenomena* vol 3, ed C Domb and M S Green (New York: Academic) p 357

Maillard J M 1985 *J. Physique* **46** 329-41

Oitmaa J 1981 *Can. J. Phys.* **59** 15-21

Selke W, Binder K and Kinzel W 1983 *Surface Sci.* **125** 74-93

Wortis M 1974 *Phase Transitions and Critical Phenomena* vol 3, ed C Domb and M S Green (New York: Academic) p 113