Low-temperature series for the square lattice Ising model with first- and second-neighbour interactions

1987 J. Phys. A: Math. Gen. 20 1269

(http://iopscience.iop.org/0305-4470/20/5/035)

J. Phys. A: Math. Gen. **20** (1987) 1269-1276. Printed in the UK

Low-temperature series for the square lattice Ising model with first- and second-neighbour interactions

J Oitmaa and M J Velgakis

School of Physics, The University of New South Wales, Kensington, NSW 2033, Australia

Received 9 July 1986

Abstract. We have derived a low-temperature expansion appropriate to the 'superantiferromagnetic' or (2×1) ordered phase of the Ising model with first- and second-neighbour interactions on a square lattice. The critical exponent β shows a non-universal variation along the critical line, which is in reasonable agreement with the variation expected on the basis of scaling.

1. Introduction

The inclusion of second-neighbour interactions in the square lattice Ising model leads to a new type of ordered phase, the 'superantiferromagnetic' or (2×1) phase. There is by now considerable evidence that the transition from this phase to the high-temperature paramagnetic phase is characterised by continuously varying critical exponents, and thus a violation of universality. This makes the model extremely interesting from a theoretical viewpoint.

The system is described by the Hamiltonian

$$\mathscr{H} = -J_1 \sum_{\langle ij\rangle} \sigma_i\sigma_j - J_2 \sum_{[ij]} \sigma_i\sigma_j \tag{1}$$

where the exchange constants J_1, J_2 can have either sign and the summations are over nearest-neighbour pairs and next-nearest-neighbour pairs respectively. It is often convenient to incorporate the temperature into the definition of coupling constants and to write

$$-\beta\mathscr{H} = K_1 \sum_{\langle ij\rangle} \sigma_i\sigma_j + K_2 \sum_{[ij]} \sigma_i\sigma_j. \tag{2}$$

The nature of the ground states is shown in figure 1(*a*). For sufficiently strong antiferromagnetic next-nearest-neighbour interactions, in particular for $J_2 < -\frac{1}{2}|J_1|$, the ground state consists of alternating rows (or columns) of up and down spins. This phase has been variously referred to as the superantiferromagnetic (SAF) phase, the AF_2 phase or the (2×1) phase.

The free energy per spin $f(K_1, K_2)$ will exhibit singularities along critical lines in the (K_1, K_2) plane, as shown in figure 1(*b*). The upper two lines, which represent transitions from the ferromagnetic (F) or antiferromagnetic (AF) phases to the high-temperature paramagnetic phase (P), are expected to show the usual universal two-dimensional Ising critical behaviour. However, along the lower branch the critical exponents have been found to vary continuously with the coupling constants. The

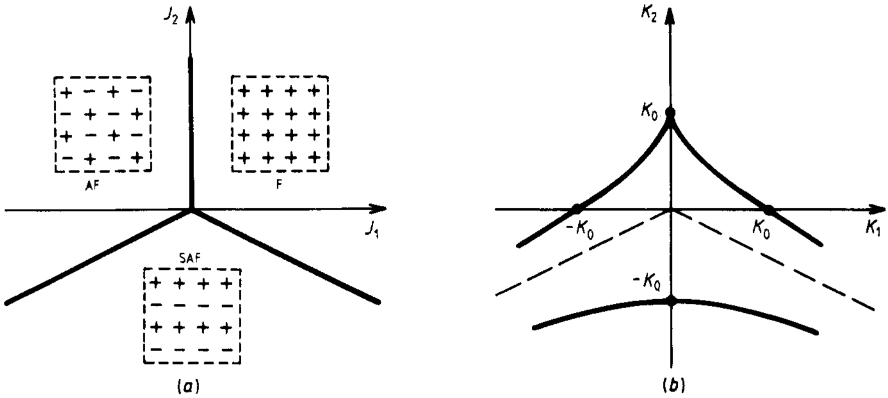

Figure 1. (*a*) The possible ground states of the system. (*b*) Critical lines in the (K_1, K_2) plane, the intercepts on the axes being at $(0, \pm K_0)$ and $(\pm K_0, 0)$ with $K_0 = \frac{1}{2}\ln(1+\sqrt{2})$.

first indication of this was by van Leeuwen (1975) from real space renormalisation group studies. Subsequent work using transfer matrix methods (Nightingale 1977, 1979), Monte Carlo renormalisation group methods (Swendsen and Krinsky 1979), conventional Monte Carlo methods (Landau 1980, Binder and Landau 1980), and high temperature series (Oitmaa 1981) have not only confirmed this non-universal behaviour but provided quantitative estimates of the values of the exponents ν, α, γ along the critical line.

In none of the papers referred to above has a direct estimate been made of the critical exponent β which characterises the vanishing of the appropriate order parameter at T_c. The assumption of scaling, which implies

$$\alpha + 2\beta + \gamma = 2 \tag{3}$$

allows β to be determined from the estimated values of α, γ. In the work reported here we derive low-temperature series for this model in order to obtain an independent estimate of the value of β along the critical line, and hence to check the validity of scaling for this transition.

2. Derivation of the series

Low-temperature series for Ising systems are derived by enumerating configurations which involve successively more and more spin deviations from the appropriate ordered state. We can thus write the partition function as

$$Z = \exp(-\beta E_0)\left(1 + \sum_{\{c\}} \exp(-\beta \Delta E_c)\right) \tag{4}$$

where E_0 is the ground-state energy, ΔE_c is the energy increase for a configuration (c) and the summation is over all configurations.

For systems with nearest-neighbour ferromagnetic interactions, or nearest-neighbour antiferromagnetic interactions for bipartite lattices, there are powerful methods for extracting maximum information for a given amount of effort (Sykes *et al* 1965, 1973a, b, c). These methods, based on the ideas of 'partial generating functions' and 'codes', have been generalised to models with further-neighbour interactions (Plischke and Chan 1976, Velgakis 1980, Velgakis and Ferer 1983). However, for such systems, the need to consider four or more sublattices makes this approach rather complicated and a more primitive approach based on (4) is in our view preferable.

The order parameter for the SAF phase of the system is given by

$$M_s = \frac{1}{N} \sum_i \eta_i \sigma_i \tag{5}$$

where the summation is taken over all N sites of the lattice and $\eta_i = +1, -1$ on successive rows. To stabilise this ground state with respect to the equivalent ground states we introduce a staggered field $h_i = \eta_i h$, which points up on even rows and down on odd rows. Thus the full Hamiltonian is

$$\mathscr{H} = -J_1 \sum_{\langle ij \rangle} \sigma_i \sigma_j - J_2 \sum_{[ij]} \sigma_i \sigma_j - h \sum_i \eta_i \sigma_i. \tag{6}$$

Note that we do not include a uniform external field.

The ground-state energy, for the SAF phase, is given by $E_0 = -2N|J_2| - Nh$. For a configuration of r spins overturned from the ground state, the energy increase can easily be obtained as

$$\Delta E_c = (2h)r + 4J_1(s_v - s_h) + 4|J_2|(2r - t) \tag{7}$$

where s_v, s_h represent the number of vertical and horizontal nearest-neighbour bonds in the configuration and t is the number of second-neighbour bonds. We define variables

$$u = \exp(-4K_1) \qquad v = \exp(-4|K_2|) \qquad \mu = \exp(-2\beta h) \tag{8}$$

in terms of which

$$\exp(-\beta \Delta E_c) = u^{s_v - s_h} v^{2r-t} \mu^r. \tag{9}$$

The free energy per spin can then be obtained from (4) as

$$-\beta f = 2|K_2| + \beta h + \sum_{\{G\}} X_G(u, v)\mu^r \tag{10}$$

where the sum is over all graphs with one or more spins overturned from the ground state, $X_G(u, v)$ is obtained from the embeddings of G in the lattice, and r is the number of vertices in G. Some simple examples are given in figure 2. By grouping the terms in (10) we obtain a low-temperature expansion for the free energy in the form of a 'field grouping'

$$-\beta f = 2|K_2| + \beta h + \sum_{r=1}^{\infty} L_r(u, v)\mu^r. \tag{11}$$

Enumeration of the graphs which contribute to (10) is a well known problem in graph theory (see, e.g., Domb 1974). The number of graphs increases rapidly with the number of vertices r, the numbers at successive orders being 1, 2, 4, 11, 34, 156, 1044, 12 346, ... We have generated all graphs up to eight order by computer. The evaluation of the quantity $X_G(u, v)$ for a given graph has also been carried out largely by computer, using a counting program for 'strong embeddings'.

While we have obtained the complete expressions for $L_r(u, v)$ for $r \leqslant 5$, for $r > 5$ we have only considered contributions up to order v^8. Many of the graphs with $r = 6$, 7, 8 do not contribute to this order. However it is necessary to include a partial set

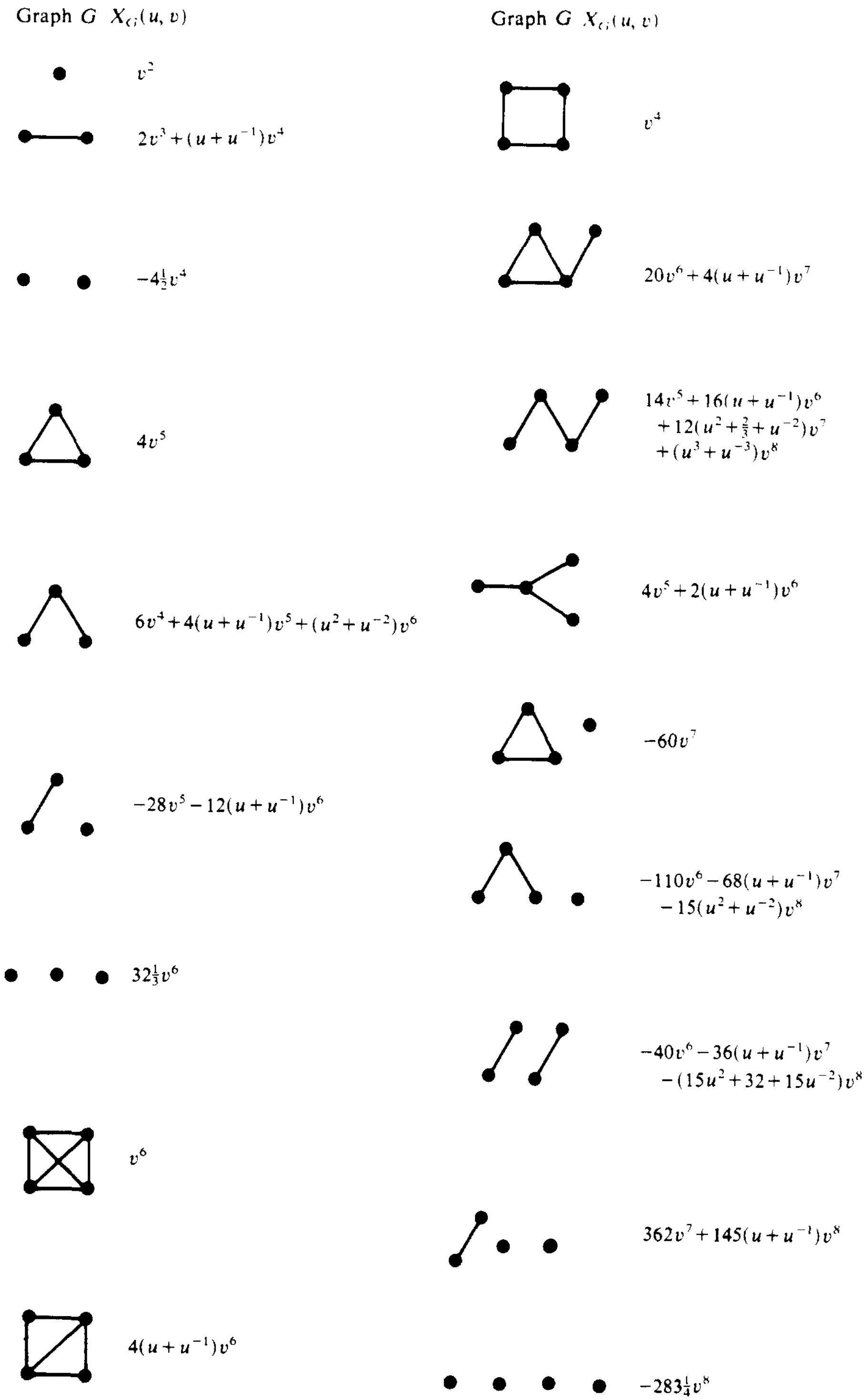

Figure 2. Graphs with up to four overturned spins and the associated factors $X_G(u, v)$.

of graphs with up to 16 vertices. The 173 such graphs with $9 < r \leq 16$ were obtained by hand. The complete expressions for L_1–L_5 and the leading terms for L_6–L_{16} are given in the appendix. By setting $u = 1$, i.e. $J_1 = 0$, the model decouples into two nearest-neighbour Ising models. This provides a valuable check on our results, since in this limit the $L_r(v)$ reduce to the ferromagnetic polynomials given by Sykes *et al* (1965, 1973b).

The order parameter is obtainable from (11) through

$$M_s = \frac{1}{\beta} \lim_{h\to 0} \frac{\partial}{\partial h}(-\beta f) = 1 - 2\sum_{r=1}^{\infty} rL_r(u, v). \tag{12}$$

Using the data from the appendix we then obtain a low-temperature expansion for M_s in powers of v:

$$M_s = 1 - 2v^2 - 8v^3 - (4\theta_1 + 26)v^4 - (24\theta_1 + 104)v^5 - (6\theta_2 + 124\theta_1 + 454)v^6 - (48\theta_2 + 680\theta_1 + 2016)v^7 - (8\theta_3 + 356\theta_2 + 3656\theta_1 + 9278)v^8 - \ldots \tag{13}$$

where we introduce the notation $\theta_n = u^n + u^{-n}$. In a similar way the low-temperature susceptibility can be obtained as

$$\chi_s = \frac{1}{\beta} \lim_{h\to 0} \frac{\partial^2}{\partial h^2}(-\beta f) = 4\beta \sum_{r=1}^{\infty} r^2 L_r(u, v) \tag{14}$$

which gives

$$kT\chi_s = 4v^2 + 32v^3 + (16\theta_1 + 208)v^4 + (144\theta_1 + 1376)v^5 + (36\theta_2 + 1176\theta_1 + 8740)v^6 + (384\theta_2 + 9392\theta_1 + 53\,632)v^7 + (64\theta_3 + 4112\theta_2 + 69\,408\theta_1 + 324\,896)v^8 + \ldots. \tag{15}$$

3. Analysis of the series

Having obtained the low-temperature series for the order parameter M_s (13), we then seek to estimate the critical 'temperature' v_c and exponent β defined by

$$M_s \sim (v_c - v)^{\beta}. \tag{16}$$

It is convenient to analyse the series for fixed values of K, and hence u, as the series then becomes a single variable series in v.

The quantities v_c and β are most simply estimated as the pole and residue of Padé approximants to the logarithmic derivative series $(\mathrm{d}/\mathrm{d}v) \ln M_s$. In fact, for $K = 0$, where the critical point singularity is exactly factorisable, the Dlog Padé approximants give v_c and β exactly. In table 1 we show results obtained in this way for two cases, $K = 0.1$ and $K = 0.3$. As is apparent from the tables, for $K = 0.1$ the results are very consistent and allow both v_c and β to be estimated, with confidence, to higher than 1% accuracy. As K increases the estimates become more erratic, but for $K \leq 0.6$ quite confident estimates can be made for both v_c and β.

It is important to compare the estimates of v_c obtained in this way with other estimates. The most reliable results would appear to be from the transfer matrix

Table 1. Estimates of v_c and β (lower line) from $[N, D]$ Padé approximants to $(d/dv)\ \ln M_s$. For $K = 0.1$, estimates of $v_c = 0.1704 \pm 0.0001$, $\beta = 0.1235 \pm 0.0005$; for $K = 0.3$, estimates of $v_c = 0.161 \pm 0.001$, $\beta = 0.112 \pm 0.002$.

K	$D \backslash N$	2	3	4	5
0.1	2		0.170 13	0.170 29	0.170 35
			0.122 51	0.123 15	0.123 44
	3	0.170 39	0.170 39	0.170 35	
		0.123 65	0.123 66	0.123 46	
	4	0.170 39	0.170 39		
		0.123 66	0.123 65		
	5	0.170 37			
		0.123 56			
0.3	2		0.159 87	0.160 76	0.160 89
			0.108 59	0.111 94	0.112 53
	3	0.161 94	0.161 21	0.160 91	
		0.117 35	0.114 06	0.112 59	
	4	0.160 17	0.160 37		
		0.108 04	0.109 35		
	5	0.160 37			
		0.109 34			

calculations (Nightingale 1979). For $K = 0.1$ and 0.3 these are

$$K = 0.1 \rightarrow K' = -0.4425 \pm 0.0001 \qquad v_c = 0.1703 \pm 0.0001$$

$$K = 0.3 \rightarrow K' = -0.4567 \pm 0.0001 \qquad v_c = 0.1609 \pm 0.0001$$

both consistent with our estimates. It is interesting to note that the estimates of v_c from high-temperature series (Oitmaa 1981) appear to be less accurate, particularly for larger values of K.

If v_c is assumed to be known then refined estimates of β can be obtained in at least two ways:

(i) by forming Padé approximants to the series for $(v_c - v)(d/dv)\ \ln M_s$ and evaluating these at $v = v_c$, and

(ii) by forming Padé approximates to the series for $M_s^{-1/\beta}$ for a range of β values and choosing the value of β for which the approximants have a pole at v_c.

In table 2 we give estimates of β obtained by both of these methods. The two estimates are fully consistent although those obtained by method (ii) have smaller

Table 2. Estimates of the critical exponent β from low-temperature series and from the scaling relation $\alpha + 2\beta + \gamma = 2$.

K	Padé approximants to $(v_c - v)(d/dv)\ \ln M_s$	Padé approximants to $M_s^{-1/\beta}$	Transfer matrix plus scaling
0.1	0.123 ± 0.005	0.1233 ± 0.0001	0.123 ± 0.002
0.2	0.118 ± 0.001	0.1183 ± 0.0002	0.120 ± 0.005
0.3	0.113 ± 0.001	0.1125 ± 0.0004	0.115 ± 0.005
0.4	0.107 ± 0.001	0.1068 ± 0.0008	0.110 ± 0.008
0.5	0.101 ± 0.0015	0.101 ± 0.001	0.104 ± 0.008
0.6	0.094 ± 0.002	0.095 ± 0.001	0.098 ± 0.008

error estimates. There is a clear continuous variation of β along the critical line, confirming the non-universal nature of the SAF transition in this model.

To test the validity of the scaling relation $\alpha+2\beta+\gamma=2$ we proceed as follows. We take the values of α and γ obtained from the transfer matrix results of Nightingale as the best estimates of these quantities, and from these determine a value of β. These values are also shown in table 2. The error estimates are rather large since β is given as the difference of two quantities of comparable magnitude. However, it is clear from table 2 that our estimates of β lie well within the range obtained from scaling. Hence we concluded that, although α, β, γ all vary along the SAF line, the relation $\alpha+2\beta+\gamma=2$ remains valid.

Finally we remark that analysis of the low-temperature series for the susceptibility χ_s, while considerably less precise, yields estimates of γ' consistent with the scaling result $\gamma'=\gamma$.

4. Conclusions

We have derived low-temperature series for the superantiferromagnetic or (2×1) ordered phase of the square lattice Ising model with first- and second-neighbour interactions. Our experience in the actual series derivation has been that the primitive approach, based on direct enumeration of spin configurations, is simpler than the partial generating function approach.

The low-temperature series for the order parameter of this phase has been derived up to eighth order in the appropriate temperature variable and has been analysed to obtain the first direct estimates of the critical exponent β. β is found to vary continously along the SAF critical line, in accordance with expectations. Our estimates of β confirm the validity of the scaling relation $\alpha+2\beta+\gamma=2$ along this line, but provide more precise estimates of β than obtainable indirectly from the scaling relation.

It is an intriguing yet unanswered question whether the SAF transition for this model is in fact related to the non-universal transition of the eight-vertex model.

Acknowledgments

This work forms part of a project which is being funded under the Australian Research Grants Scheme (ARGS).

Appendix

Complete and partial expressions for the quantities $L_r(u, v)$ as defined by (11). The abbreviation $\theta_n=u^n+u^{-n}$ is used to simplify the expressions

$$L_1=v^2$$

$$L_2=2v^3+(\theta_1-4\tfrac{1}{2})v^4$$

$$L_3=6v^4+(4\theta_1-24)v^5+(\theta_2-12\theta_1+32\tfrac{1}{3})v^6$$

$$L_4=v^4+18v^5+(22\theta_1-129)v^6+(6\theta_2-100\theta_1+306)v^7+(\theta_3-22\tfrac{1}{2}\theta_2+145\theta_1-299\tfrac{1}{4})v^8$$

$$L_5 = 8v^5 + (2\theta_1 + 39)v^6 + (104\theta_1 - 608)v^7 + (44\theta_2 - 748\theta_1 + 2334)v^8$$
$$+ (8\theta_3 - 244\theta_2 + 1860\theta_1 - 4120)v^9$$
$$+ (\theta_4 - 36\theta_3 + 405\theta_2 - 1822\theta_1 + 3199\tfrac{1}{5})v^{10}$$

$$L_6 = 2v^5 + 40v^6 + (32\theta_1 - 34)v^7 + (8\theta_2 + 378\theta_1 - 2423)v^8 + \ldots$$

$$L_7 = 22v^6 + (4\theta_1 + 128)v^7 + (260\theta_1 - 1006)v^8 + \ldots$$

$$L_8 = 6v^6 + 134v^7 + (92\theta_1 + 10\tfrac{1}{2})v^8 + \ldots$$

$$L_9 = v^6 + 72v^7 + (16\theta_1 + 508)v^8 + \ldots$$

$$L_{10} = 30v^7 + (2\theta_1 + 457)v^8 + \ldots$$

$$L_{11} = 8v^7 + 310v^8 + \ldots$$

$$L_{12} = 2v^7 + 151v^8 + \ldots$$

$$L_{13} = 68v^8 + \ldots$$

$$L_{14} = 22v^8 + \ldots$$

$$L_{15} = 6v^8 + \ldots$$

$$L_{16} = v^8 + \ldots.$$

References

Binder K and Landau D P 1980 *Phys. Rev.* B **21** 1941-62
Domb C 1974 *Phase Transitions and Critical Phenomena* vol 3, ed C Domb and M S Green (New York: Academic) pp 357-80
Landau D P 1980 *Phys. Rev.* B **21** 1285-97
Nightingale M P 1977 *Phys. Lett.* **58A** 486-8
—— 1979 *Proc. Konink. Nederl. Akad. Wetenschappen* B **82** 235-91
Oitmaa J 1981 *J. Phys. A: Math. Gen.* **14** 1159-68
Plischke M and Chan C F S 1976 *Can. J. Phys.* **54** 1646-50
Swendsen R H and Krinsky S 1979 *Phys. Rev. Lett.* **43** 177-80
Sykes M F, Essam J W and Gaunt D S 1965 *J. Math. Phys.* **6** 283-98
Sykes M F, Gaunt D S, Essam J W and Hunter D L 1973a *J. Math. Phys.* **14** 1060-5
Sykes M F, Gaunt D S, Martin J L, Mattingly S R and Essam J W 1973b *J. Math. Phys.* **14** 1071-4
Sykes M F, Gaunt D S, Mattingly S R, Essam J W and Elliott C J 1973c *J. Math. Phys.* **14** 1066-70
van Leeuwen J M J 1975 *Phys. Rev. Lett.* **34** 1056-8
Velgakis M J 1980 *MS Thesis* West Virginia University
Velgakis M J and Ferer M 1983 *Phys. Rev.* B **27** 401-12