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The triangular lattice Ising model with first and second neighbour interactions

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Abstract. We report studies of the critical behaviour of the Ising model with first and second neighbour interactions J_1, J_2 on the triangular lattice. High-temperature series have been used to determine the locations of the ferromagnetic critical line and the critical line in the region ($J_1<0$, $J_2>0$). On the latter line the ordering susceptibility appears to diverge algebraically with the exponent $\gamma\sim 2.4$. The existence of a sinusoidal phase and an associated Lifshitz point are conjectured.

1. Introduction

This paper reports a continuation of studies of Ising systems with more than one type of interaction. The present author (Oitmaa 1981a) has recently developed a high-temperature expansion formalism for such systems. This method has been used to derive series expansions for the square lattice Ising model with first and second neighbour interactions, and to investigate the critical behaviour of this system (Oitmaa 1981b).

Another system, which is of both theoretical and experimental interest, is the triangular lattice with first and second neighbour interactions, and the present paper is devoted to this topic. The experimental relevance of the model stems from the fact that helium adsorbed on graphite can be modelled by a triangular lattice gas with repulsive nearest neighbour and attractive next nearest neighbour interactions (Dash 1978 and references therein). There is a well known correspondence between a lattice gas and an Ising model in an external field.

Theoretical interest in the model arises from predictions of rather unusual critical behaviour in some regions of the phase diagram. In particular, when the first and second neighbour interactions are antiferromagnetic and ferromagnetic respectively, as in the case of the helium/graphite system, then there are three equivalent ordered states and it has been suggested (Alexander 1975) that the critical behaviour should be the same as for the three-state Potts model, rather than Ising-like. Monte Carlo studies by Mihura and Landau (1977) have been unable to confirm this unequivocally, but have revealed the possibility of a new kind of bicritical point as well as other unusual features.

The Hamiltonian of the system is written as

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

where J_1, J_2, h are respectively the first and second neighbour exchange constants and the external field, and the first two summations are over all first and second neighbour pairs on a triangular lattice of N sites. In the present work we consider only the zero field case, $h = 0$. The first step in understanding the behaviour of this system is to determine the nature of the ground state for different values of J_1, J_2. This has been done by Tanaka and Uryû (1976) (see also Metcalf 1974, Kaburagi and Kanamori 1978), and is illustrated in figure 1. There are four possible ordered states

(i) ferromagnetic (F),
(ii) Potts state (P),
(iii) alternating up down lines (A1) and
(iv) alternating double up down lines (A2).

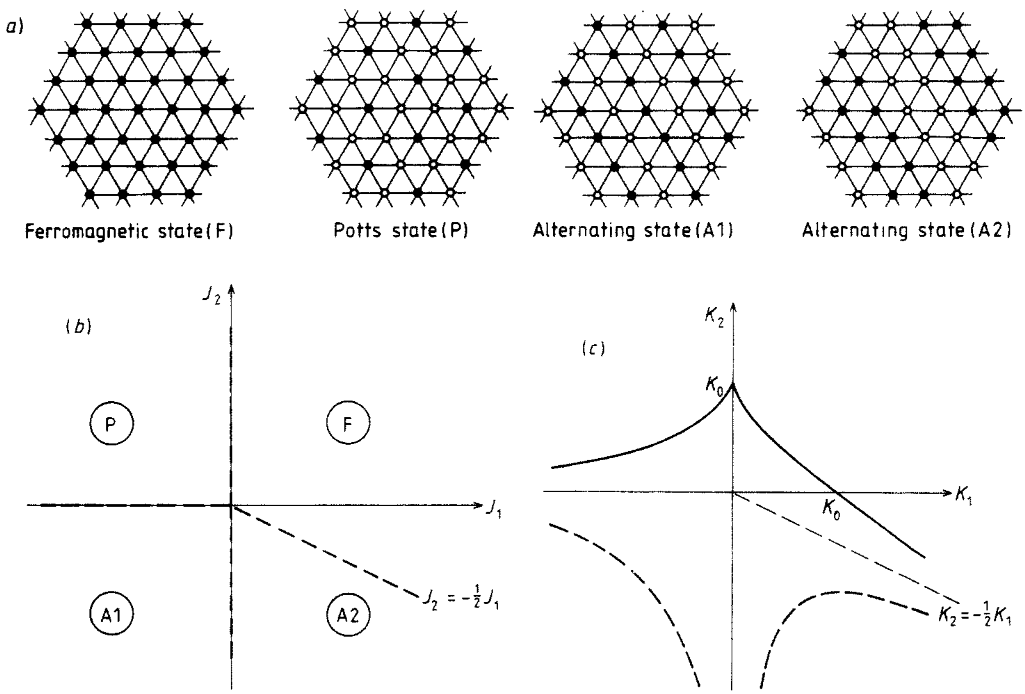

Figure 1. (*a*) The four possible ordered states at $T = 0$, (*b*) phase diagram at $T = 0$ and (*c*) location of critical lines in the (K_1, K_2) plane, for the triangular Ising model with first and second neighbour interactions.

Along the boundary lines P/A1, A1/A2 and F/A2 there are an infinite number of ground states and a non-zero ground-state entropy. We use the terms 'Potts state' and 'Potts transition' for the ordered state (ii) and the transition from this state to the disordered state although, strictly speaking, it is only in the presence of a field that the correspondence to the three-state Potts model is expected to be valid.

For each of the ordered regions one can define an order parameter, which will vanish at some finite temperature $T_c(J_1, J_2)$ corresponding to a transition to the disordered phase. The location of these critical lines can best be discussed in terms of the free energy per site $f(K_1, K_2)$ $(K_i = J_i/k_B T)$. The nearest neighbour Ising problem has been solved exactly (Houtappel 1950) and has a singularity at the critical coupling $K_0 = \frac{1}{4}\ln 3$. Thus $f(K_1, K_2)$ has singularities at the points $(K_0, 0)$ and $(0, K_0)$ with conventional two-dimensional Ising exponents. These two points lie on a critical line separating the ferromagnetic and disordered phases. According to universality one would expect Ising exponents along this entire line. There will be other critical lines in the (K_1, K_2) plane separating the other ordered phases from the disordered phase. These lines are shown schematically in figure 1(c). The main task of the present work is to attempt to locate the positions of these various lines and to determine the nature of the singularities along them.

There have been a number of previous studies of this problem. Campbell and Schick (1972) have studied the model using the Bethe–Peierls approximation but the work of Mihura and Landau (1977) has shown that this approximation does not even give qualitatively correct results. Some real space renormalisation group calculations have been reported for the nearest neighbour model in a field (Mahan and Claro 1977, Schick *et al* 1977). These calculations include three-spin interactions in the Hamiltonian, but not second neighbour interactions. There is clearly need for more work in this direction.

The most extensive series work on the model is that of Dalton and Wood (1969), who have obtained both high- and low-temperature expansions. High-temperature series for the ferromagnetic susceptibility are used to estimate the variation of critical temperature with the ratio $R = J_2/J_1$ $(J_1, J_2 > 0)$. The series are too short to extend the analysis to $R < 0$. The other transitions have not been investigated.

We have extended the high-temperature series for the ferromagnetic susceptibility to 10 terms, and have also obtained the series for the Potts susceptibility to the same order. The zero-field free energy series has been obtained to order 11. In § 2 of the paper we discuss the method of derivation of the series and present the coefficient data. In § 3 we describe the analysis of the series and present results for the locations of the ferromagnetic and Potts critical lines. Some evidence is found for the possible occurrence of a Lifshitz point. Finally in § 4 we present our conclusions and indicate areas in which further work is required.

2. Derivation of series

The techniques for deriving high-temperature series for the Ising model have been described in many articles (see for example Domb 1974). The zero-field free energy and susceptibility expansions for the simple Ising model take the form

$$-\beta f(K) = \ln 2 + \tfrac{1}{2}q \ln \cosh K + \sum_{n=1}^{\infty} a_n v^n \qquad (2)$$

$$\chi = 1 + 2 \sum_{n=1}^{\infty} c_n v^n \qquad (3)$$

where q is the coordination number of the lattice and v is the high-temperature variable $v = \tanh K$, with $K = J/k_B T$. The coefficients a_n, c_n are given as sums of 'lattice constants' of graphs with n edges and zero and two vertices of odd degree, respectively. The lattice constant of a graph is the coefficient of N in the number of embeddings of the graph on the lattice of interest. The graphs which contribute include those with more than one component.

For systems with more than one type of interaction these expansions take a more general form. In particular, for the triangular lattice with nearest and next nearest neighbour coupling constants K_1 and K_2 we can write

$$-\beta f(K_1, K_2) = \ln 2 + 3 \ln \cosh K_1 + 3 \ln \cosh K_2 + \sum_{m,n} a_{mn} v_1^m v_2^n \tag{4}$$

where $v_1 = \tanh K_1$, $v_2 = \tanh K_2$. We have computed the values of the coefficients a_{mn} for $m + n \leqslant 11$ and these are given in table 1. The method used was developed by the

Table 1. Coefficients of high-temperature series.

(*a*) Coefficients a_{mn} in the zero-field free energy expansion, equation (4).

3	0	2	2	1	6	0	3	2
4	0	3	3	1	18	2	2	27
0	4	3	5	0	6	4	1	48
3	2	120	2	3	114	0	5	6
6	0	11	5	1	114	4	2	432
3	3	714	2	4	465	0	6	11
7	0	24	6	1	270	5	2	1 350
4	3	3 252	3	4	3 912	2	5	1 878
0	7	24	8	0	$55\frac{1}{2}$	7	1	678
6	2	3 942	5	3	12 654	4	4	$21\,997\frac{1}{2}$
3	5	20 214	2	6	7 521	0	8	$55\frac{1}{2}$
9	0	$138\frac{2}{3}$	8	1	1 824	7	2	11 610
6	3	44 490	5	4	102 696	4	5	137 508
3	6	100 152	2	7	29 874	0	9	$138\frac{2}{3}$
10	0	363	9	1	5 202	8	2	35 541
7	3	151 938	6	4	424 857	5	5	753 882
4	6	808 992	3	7	480 510	2	8	117 837
0	10	363	11	0	990	10	1	15 474
9	2	113 646	8	3	524 712	7	4	1 663 200
6	5	3 603 726	5	6	5 130 894	4	7	4 537 368
3	8	2 247 144	2	9	462 186	0	11	990

(*b*) Coefficients c^{F}_{mn} in the zero-field ferromagnetic susceptibility expansion, equation (5).

1	0	3	0	1	3	2	0	15
1	1	36	0	2	15	3	0	69
2	1	270	1	2	288	0	3	69
4	0	303	3	1	1 644	2	2	2 964
1	3	1 908	0	4	303	5	0	1 293
4	1	8 952	3	2	22 872	2	3	25 566
1	4	11 304	0	5	1 293	6	0	5 409
5	1	45 444	4	2	150 516	3	3	242 388
2	4	190 146	1	5	62 172	0	6	5 409
7	0	22 287	6	1	220 074	5	2	894 042
4	3	1 888 668	3	4	2 164 140	2	5	1 277 394
1	6	324 216	0	7	22 287	8	0	90 771
7	1	1 029 708	6	2	4 950 336	5	3	12 942 876
4	4	19 645 452	3	5	17 138 316	2	6	7 963 932
1	7	1 624 140	0	8	90 771	9	0	366 339
8	1	4 692 780	7	2	26 039 922	6	3	81 097 746
5	4	153 511 212	4	5	178 887 024	3	6	124 108 764
2	7	46 884 042	1	8	7 884 072	0	9	366 339
10	0	1 467 609	9	1	20 947 356	8	2	131 708 610
7	3	475 711 284	6	4	1 078 937 334	5	5	1 578 261 444
4	6	1 473 394 656	3	7	838 301 940	2	8	263 726 322
1	9	37 314 900	0	10	1 467 609			

Table 1. (continued).

(*c*) Coefficients c^{P}_{mn} in the zero-field Potts susceptibility expansion, equation (6).

1	0	−1	0	1	3	2	0	1
1	1	−18	0	2	15	3	0	−3
2	1	27	1	2	−144	0	3	69
4	0	1	3	1	−66	2	2	291
1	3	−954	0	4	303	5	0	−7
4	1	33	3	2	−834	2	3	2 481
1	4	−5 652	0	5	1 293	6	0	−9
5	1	−204	4	2	513	3	3	−8 154
2	4	18 345	1	5	−31 086	0	6	5 409
7	0	−37	6	1	−246	5	2	−3 240
4	3	6 327	3	4	−68 508	2	5	122 901
1	6	−162 108	0	7	22 287	8	0	−88
7	1	−1 224	6	2	−4 218	5	3	−40 524
4	4	64 161	3	5	−518 694	2	6	765 057
1	7	−812 070	0	8	90 771	9	0	−267
8	1	−3 447	7	2	−24 852	6	3	−60 114
5	4	−436 290	4	5	561 735	3	6	−3 632 430
2	7	4 499 739	1	8	−3 942 036	0	9	366 339
10	0	−772	9	1	−12 186	8	2	−81 981
7	3	−397 248	6	4	−748 458	5	5	−4 193 796
4	6	4 421 739	3	7	−23 921 406	2	8	25 296 909
1	9	−18 657 450	0	10	1 467 609			

present author and is described in a recent paper (Oitmaa 1981a). There are 508 graphs which contribute to this order.

In the ferromagnetic regime ($J_1>0, J_2>-\frac{1}{2}J_1$) the susceptibility which will diverge at the transition is the ordinary ferromagnetic susceptibility $\chi_{\mathrm{F}}=\Sigma_j\langle\sigma_0\sigma_j\rangle$. The high-temperature series for this quantity can be written as

$$\chi_{\mathrm{F}}=1+2\sum_{m,n}c^{\mathrm{F}}_{mn}v_1^m v_2^n. \tag{5}$$

We have evaluated the c_{mn} coefficients for $m+n\leq 10$ (1055 graphs) and the values are given in table 1.

In the Potts regime the susceptibility χ_{F} is not the ordering susceptibility, and is not expected to show a strong divergence. In the ordered phase the order parameter is

$$\eta=\sum_{i=1}^{3}\lambda_i\sigma_i$$

where $\lambda_i=1, -\frac{1}{2}, -\frac{1}{2}$ for sublattices *A*, *B*, *C* respectively. The appropriate ordering susceptibility is then

$$\chi_{\mathrm{P}}=\langle\eta^2\rangle=\sum_j\lambda_j\langle\sigma_0\sigma_j\rangle$$

(where site 0 is taken on sublattice *A*), and this can be expanded as

$$\chi_{\mathrm{P}}=1+2\sum_{m,n}c^{\mathrm{P}}_{mn}v_1^m v_2^n. \tag{6}$$

These coefficients are also given in table 1.

In a similar way one can define ordering susceptibilities for the other two transition lines and obtain series expansions for these. In the present work we have not attempted to do this.

3. Analysis of series

3.1. The ferromagnetic transition

In the ferromagnetic regime ($J_1 > 0, J_2 > -\frac{1}{2}J_1$), as the temperature is lowered, the system will undergo a transition from a disordered to a ferromagnetic phase. The critical behaviour is expected to be of the normal Ising form. The critical temperature is known exactly for $J_2 = 0$ and increases monotonically with increasing J_2. It seems reasonable to suppose that when $J_2 = -\frac{1}{2}J_1$, at which point the ferromagnetic state is no longer the unique ground state, T_c is zero.

Analysis of the series for the ferromagnetic susceptibility χ_F should provide an estimate of the variation of T_c with J_2. To obtain series in a form suitable for analysis we define a parameter $R = J_2/J_1$ and, for a given choice of R, obtain series in the single variable $x = J_1/k_B T$

$$\chi_F = 1 + \sum_{n=1}^{\infty} c_n x^n.$$

These series can be analysed by standard techniques (Gaunt and Guttmann 1974) to determine the critical coupling x_c and exponent γ. We have generally used Padé approximants supplemented where appropriate by ratio methods. A typical example is the series for $R = 1$. In figure 2 we show two ratio plots, a direct plot of the ratios $\mu_n = c_n/c_{n-1}$ against $1/n$ and a plot of the modified ratios $\mu_n^* = n\mu_n/(n + 0.75)$. These plots show some residual curvature, indicating that the coefficients have not yet settled down to their asymptotic behaviour. However the results are certainly consistent with a value of 1.75 for the exponent, as expected from universality, and yield the estimate $x_c = 0.1140 \pm 0.0005$. In table 2 we show the Padé analysis of the same series. The first column gives estimates of x_c from poles of Padé approximants (PA) to d ln $\chi_F/\mathrm{d}x$ while remaining columns give estimates of γ obtained by evaluating PA to $(x_c - x)$ d ln $\chi_F/\mathrm{d}x$ at $x = x_c$ for three different choices of x_c. As can be seen the estimates of γ are quite

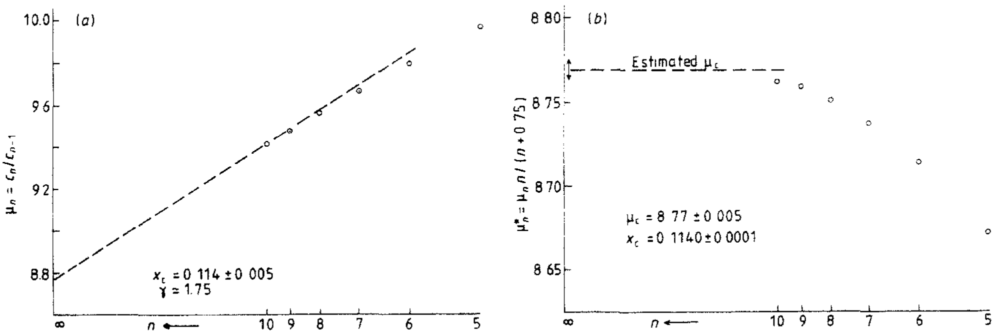

Figure 2. Ratio plots of the ferromagnetic susceptibility series for $J_2 = J_1$. (*a*) plot of the direct ratios $\mu_n = c_n/c_{n-1}$ which should approach x_c^{-1} linearly with slope γ and (*b*) plot of the modified ratios μ_n^* which should approach x_c^{-1} with zero slope.

Table 2. Padé approximant analysis of the ferromagnetic susceptibility series for $J_2 = J_1$. The first column shows estimates of x_c, the other columns estimates of γ for three choices of x_c. An asterisk indicates a defect in the PA.

		Estimates of γ		
$[N, D]$	Estimate of x_c	$x_c = 0.1140$	$x_c = 0.1145$	$x_c = 0.1150$
[3, 6]	0.115 93*	1.725	1.864	1.958
[4, 5]	0.114 53	1.723	1.863	1.957
[5, 4]	0.115 10*	1.722	1.862	1.957
[6, 3]	0.114 57	1.726	1.864	1.957
[3, 5]	0.115 00*	1.695	1.850	1.957
[4, 4]	0.114 97*	1.740	1.863	1.957
[5, 3]	0.114 98*	1.609	1.827	1.957
[3, 4]	0.114 92	1.588	1.822	1.957
[4, 3]	0.114 87	1.510	1.801	1.957
[3, 3]	0.114 96	1.803	1.877	1.958

sensitive to the choice of x_c. The value $x_c = 0.114$, favoured by the ratio plot, yields $\gamma \simeq 1.72$. Making the assumption that $\gamma = 1.75$ permits a refinement in the estimate of x_c, obtained by looking for poles in PA to the series for $[\chi_F]^{4/7}$. These results, again for the case $R = 1$, are shown in table 3, and, while there is still some scatter, the PA of highest order are consistent with $x_c \simeq 0.114$. This procedure has been used to obtain the variation of $k_B T_c/J_1$ with R shown in figure 3. The general behaviour for $R > 0$ is as expected but we have obtained much more precise estimates of T_c than had previously been available.

Table 3. Estimates of the ferromagnetic critical 'temperature' $x_c = J_1/k_B T_c$ obtained from poles of $[N, D]$ Padé approximants to the series $[\chi_F]^{4/7}$ for $J_2 = J_1$. An asterisk denotes a defect in the PA.

D \ N	3	4	5	6	7
3		0.116 66	0.114 43	0.114 03	0.114 12
4	0.116 22	0.114 70	0.113 57	0.114 10	
5	CC	0.113 40	0.114 19		
6	0.113 41	0.115 77*			
7	0.114 11				

For $R < 0$ the series are more irregular. This is due, at least in part, to the presence of a singularity on the negative real axis. The singularity lies on the Potts transition line (see figure 1). Consistent estimates of x_c can still be obtained from PA to $[\chi_F]^{4/7}$ for $-0.3 < R < 0$ and the plot of $k_B T_c/J_1$ against R appears to be moving smoothly towards $T_c = 0$ at $R = -0.5$. For $R < -0.3$ the Potts singularity begins to lie nearer the origin than the ferromagnetic singularity, and the Padé results become rather inconsistent. The use of an Euler transformation to move the Potts singularity further from the origin than the physical one results in a marked improvement. We illustrate the analysis for the case $R = -0.4$ in table 4. The series $\chi_F(x)$ is very irregular and direct Padé analysis

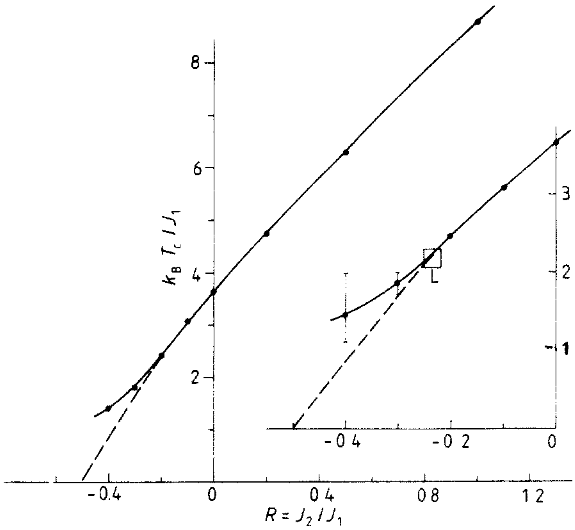

Figure 3. Variation of ferromagnetic critical temperature $k_B T_c/J_1$ with ratio $R = J_2/J_1$. The small square in the inset is the location of the conjectured Lifshitz point.

does not provide any consistent results at all. The transformed series is much more regular and Padé analysis of both d ln $\chi_F(x')/dx'$ and $[\chi_F(x')]^{4/7}$ yields a consistent pole on the real axis at $x' \simeq 0.26 \pm 0.03$. From figure 3 we see that for $R < -0.25$ the values of T_c begin to deviate appreciably from the previous trend towards zero at $R = -0.5$. This may, of course, be an artifact due to the series being too short to reflect the true singularity behaviour of χ in this region. We believe rather that these results may indicate the presence of a spatially modulated or 'sinusoidal' phase, which separates the ferromagnetic and A2 phases at finite temperatures. Such a phase has been predicted in simple cubic and square Ising lattices with competing axial next nearest neighbour interactions (the so-called ANNNI models, see e.g. Selke and Fisher (1980)). This model has a very similar ground-state degeneracy at $R = -0.5$. We conjecture therefore that there exists a Lifshitz point in this model with approximate position $R_L \simeq -0.23 \pm 0.02$. For $R < -0.4$ the series are too irregular to allow any conclusions to be drawn.

3.2. The Potts transition

In the regime $J_1 < 0$, $J_2 > 0$ the ordered state is the 'Potts state', with the spins on one sublattice up and those on the other two down, or vice versa. The ordered phase is terminated by a critical line which is expected to have the general form shown in figure 1(*c*). The susceptibility χ_P is expected to diverge along this line. Our series for χ_P is in terms of two variables v_1, v_2 and in order to carry out the analysis we define a parameter $R = -J_1/J_2$ and, for a given choice of R, obtain series in the single variable $x = J_2/k_B T$. These series are quite regular and can be analysed by both ratio and Padé methods. As an example we consider the series for $R = 1$. Ratio plots, shown in figure 4, yield the estimates $x_c \simeq 0.197 \pm 0.003$, $\gamma \simeq 2.25$. In table 5 we show Padé analysis of the same series. These results are consistent with the ratio results and our overall estimates are $x_c = 0.198 \pm 0.002$, $\gamma = 2.4 \pm 0.02$. The high value of γ is rather surprising, although there is no reason to expect that along this line the critical behaviour would be Ising-like.

Table 4. Padé analysis of the ferromagnetic susceptibility series for $R = -0.4$.

(a) Coefficients of direct series $\chi_F(x)$ for $R = -0.4$.

1, 3.6, 6, 3.456, 1.1936, 2.450 688, 76.715 690 6667, 28.680 194 9257, −134.324 931 389, −307.648 470 123, 1003.644 698 90

(b) Coefficients of transformed series $\chi_F(x')$ obtained using the Euler transformation $x' = x/(1+2.4x)$.

1, 3.6, 14.64, 52.992, 179.5232, 584.563 968, 1934.615 210 67, 6949.574 249 33, 27.655 209 284 8, 116 612.174 764, 490 271.461 651

(c) Estimates of position of singularity x'_c from poles of $[N, D]$ Padé approximants to $\mathrm{d}\ln \chi_F(x')/\mathrm{d}x'$. An asterisk denotes a defect in the PA.

D \ N	3	4	5	6
3		0.2715	0.2395	0.2450
4	0.2721	0.2935*	0.2440	
5	0.2442	0.2458		
6	0.2461			

(d) Estimates of position of singularity x'_c from poles of $[N, D]$ Padé approximants to $[\chi_F(x')]^{4/7}$.

D \ N	3	4	5	6	7
3			0.3081	0.2836	0.2765
4		0.3114	0.2392	0.2736	
5	0.3106	—	0.2754		
6	0.2555	0.2660			
7	0.2666				

Estimate $x'_c = 0.26 \pm 0.03$ gives $x_c = 0.7 \pm 0.2$

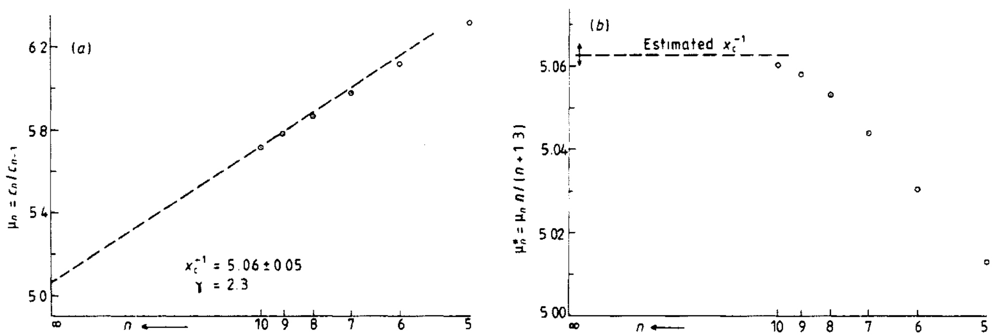

Figure 4. Ratio plots for the Potts susceptibility series for $J_1 = -J_2$. (a) plot of the direct ratios μ_n and (b) plot of the modified ratios $\mu_n^* = n\mu_n/(n+\gamma-1)$ with $\gamma = 2.3$.

It is of relevance to discuss the general features of the phase diagram in the temperature–field plane, as revealed by the Monte Carlo work of Mihura and Landau (1977). We sketch this in figure 5 for the case $R > 0$. The line $H = 0$, $T < T_M$ is a

Table 5. Padé approximant analysis of the Potts susceptibility series for $J_1 = -J_2$. The first column shows estimates of x_c, the other columns estimates of the exponent γ for three choices of x_c.

$[N, D]$	Estimate of x_c	Estimate of γ		
		$x_c = 0.197$	$x_c = 0.198$	$x_c = 0.199$
[3, 6]	0.198 72	2.338	2.412	2.509
[4, 5]	0.198 72	3.356	2.546	2.529
[5, 4]	0.198 49	2.391	2.421	2.511
[6, 3]	0.199 17	2.361	2.418	2.507
[3, 5]	0.198 67	2.304	2.411	2.504
[4, 4]	0.198 36	2.312	2.413	2.504
[5, 3]	0.198 34	2.210	2.405	2.479
[3, 4]	0.199 73	2.364	2.426	2.502
[4, 3]	0.198 53	2.344	2.418	2.500
[3, 3]	0.195 75	2.355	2.430	2.514

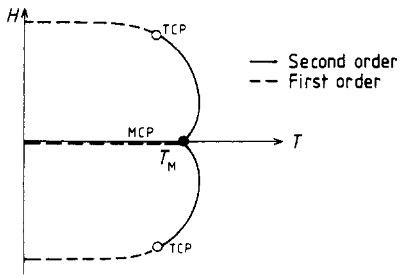

Figure 5. Phase diagram in the (T, H) plane for the Potts regime $(J_1 < 0, J_2 > 0)$. Along the second-order lines the critical behaviour is expected to be Potts-like.

first-order line separating Potts phases with net magnetisation up or down. For $H \neq 0$ there are second-order lines separating ordered and disordered phases which become first order at two symmetrically located tricritical points (TCP). The point ($H = 0$, $T = T_M$) is a multicritical point (MCP). It has been argued that for $H \neq 0$ the critical behaviour should be three-state Potts-like (Alexander 1975) with the susceptibility exponent presumably taking the value $\gamma = \frac{13}{9}$. Our series cannot probe the $H \neq 0$ region but only the behaviour at the multicritical point, and there is no reason to expect the behaviour at this point to be Potts-like. It can be argued on the basis of symmetry, using the approach of Domany *et al* (1978), that the critical behaviour should be like the Z_6 model with the susceptibility having an essential singularity of the type $\chi \sim \exp[c(1 - x/x_c)^{-\gamma}]$. Guttmann (1978) has proposed a method of series analysis which should be capable of distinguishing between an essential singularity and an algebraic singularity of the usual form $\chi \sim (1 - x/x_c)^{-\gamma}$. The second logarithmic derivation of χ is expected to have the form

$$D_L^2 \chi \equiv \frac{d}{dx} \ln\left(\frac{d}{dx} \ln \chi\right) = \begin{cases} 1/(x_c - x) & \text{algebraic} \\ (\gamma + 1)/(x_c - x) & \text{essential.} \end{cases}$$

Thus Padé approximants to $D_L^2 \chi$ should exhibit a pole at $x = x_c$. Evaluating PA to $(x_c - x) D_L^2 \chi$ should yield values either near unity if the singularity is algebraic or near

$\gamma+1$ if the singularity is of the exponential form. In table 6 we show the location of the pole and the values of $(x_c - x)D_L^2\chi$. The results clearly indicate that the singularity is algebraic. We have also looked for the presence of confluent singularities, which might mask the true behaviour, using the inhomogeneous differential approximant technique of Rehr *et al* (1980). No evidence is found for confluent singularities.

The same type of analysis has been carried out for other values of R and the line of singularities, or rather the multicritical line, is shown in figure 6. The singularity appears to be algebraic with an exponent of $\gamma \simeq 2.4$ along the entire line.

Table 6. Padé approximant analysis of the second logarithmic derivation of χ_P for $J_1 = -J_2$. The first column shows the value of the physical pole, the other columns the values of $(x_c - x)D_L^2\chi_P$ at $x = x_c$ for three choices of x_c. An asterisk denotes a defect in the PA.

		Values of $(x_c - x)D_L^2\chi_P$		
$[N, D]$	Estimate of x_c	$x_c = 0.198$	$x_c = 0.1985$	$x_c = 0.199$
[2, 6]	0.2031	0.967	0.983	1.001
[3, 5]	0.1992	0.985	0.999	1.013
[4, 4]	0.1985	0.982	0.998	1.013
[5, 3]	9.2065	0.983	0.998	1.013
[6, 2]	0.2246	0.953	0.971	0.989
[2, 5]	0.1969	0.990	1.005	1.020
[3, 4]	0.1673*	0.988	1.001	1.014
[4, 3]	0.1943	0.985	0.998	1.010
[5, 2]	—	0.995	1.011	1.028

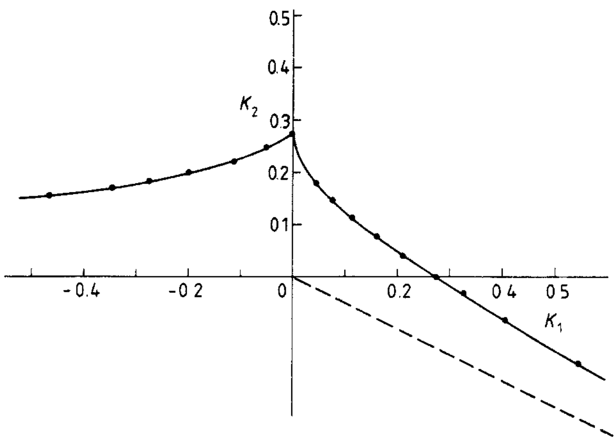

Figure 6. Location of the ferromagnetic critical line and the Potts multicritical line, as determined from high-temperature series. The points represent actual estimates, with errors estimated to be no larger than the points.

4. Conclusions

The main results of the work reported in this paper are the accurate determination of the location of the ferromagnetic and Potts critical lines. These results will hopefully prove to be of value in interpreting data on suitable experimental systems as well as being useful for further theoretical work.

We have conjectured that there may exist in this model a spatially modulated phase, similar to that which is believed to occur in the ANNNI model. Our evidence for this is two-fold — the behaviour of T_c as a function of $R = J_2/J_1$ in the region $R \simeq -0.3$ is suggestive of such a phase as is the type of ground-state degeneracy at $R = -0.5$. This conjecture could be tested in various ways. High-T series for the wavevector dependent susceptibility $\chi(q)$ could be used to locate the high-temperature boundary (see for example Redner and Stanley 1977), while the boundary between the ferromagnetic and sinusoidal phases could presumably be located by low-temperature series.

In the region of antiferromagnetic first neighbour and ferromagnetic second neighbour interactions symmetry arguments suggest that, in non-zero field, the model should be in the universality class of the Z_3 (three-state Potts) model and, in zero field, that of the Z_6 model. To test the first of these predictions requires series in a field and these cannot be simply obtained using our expansion formalism. As far as the zero field behaviour is concerned our series support the existence of a conventional algebraic singularity rather than an essential singularity of the Kosterlitz–Thouless form which is expected for the Z_6 model. The value of the exponent is surprisingly large (~2.4), and while this is fairly strong evidence that the behaviour along this line is not Ising-like, the true asymptotic form of the singularity remains uncertain.

Finally it is to be hoped that the present study will stimulate work on this system by other complementary methods, such as the Monte Carlo renormalisation group technique (Swendsen 1979).

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References

Alexander S 1975 *Phys. Lett.* **54A** 353–4
Campbell C E and Schick M 1972 *Phys. Rev.* A **5** 1919–25
Dalton N W and Wood D W 1969 *J. Math. Phys.* **10** 1271–302
Dash J G 1978 *Phys. Rep.* **38** 177–226
Domany E, Schick M, Walker J S and Griffiths R B 1978 *Phys. Rev.* B **18** 2209–17
Domb C 1974 in *Phase Transitions and Critical Phenomena* vol 4 ed C Domb and M S Green (New York: Academic) pp 357–484
Gaunt D S and Guttmann A J 1974 in *Phase Transitions and Critical Phenomena* vol 4 ed C Domb and M S Green (New York: Academic) pp 181–243
Guttmann A J 1978 *J. Phys. A: Math. Gen.* **11** 545–53
Houtappel R M F 1950 *Physica* **16** 425–55
Kaburagi M and Kanamori J 1978 *J. Phys. Soc. Japan* **44** 718–27
Mahan G D and Claro F H 1977 *Phys. Rev.* B **16** 1168–76
Metcalf B D 1974 *Phys. Lett.* **46A** 325–6
Mihura B and Landau D P 1977 *Phys. Rev. Lett.* **38** 977–80

Oitmaa J 1981a *Can. J. Phys.* **59** 15–21
—— 1981b *J. Phys. A: Math. Gen.* **14** 1159–68
Redner S and Stanley H E 1977 *Phys. Rev.* B **16** 4901–6
Rehr J J, Joyce G S and Guttmann A J 1980 *J. Phys. A: Math. Gen.* **13** 1587–602
Schick M, Walker J S and Wortis M 1977 *Phys. Rev.* B **16** 2205–19
Selke W and Fisher M E 1980 *J. Mag. Mag. Mat.* **15–18** 403–4
Swendsen R H 1979 *Phys. Rev.* B **20** 2080–7
Tanaka Y and Uryû N 1976 *Prog. Theor. Phys.* **55** 1356–72