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The square-lattice Ising model with first and second neighbour interactions

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Abstract. The critical behaviour of the square-lattice Ising model, with nearest and next-nearest neighbour interactions of either sign, has been investigated by means of high-temperature series. The location of the critical lines in the coupling constant plane has been accurately determined. Along the critical line which corresponds to transitions to the layered or superantiferromagnetic state a breakdown of universality is observed and explicit numerical estimates obtained for the exponent of the ordering susceptibility.

1. Introduction

There has recently been an increase of interest in two-dimensional Ising systems with interactions beyond first neighbours. This is partly due to the discovery and study of real 2D Ising systems, notably gases adsorbed on a crystalline surface, but has also been stimulated by theoretical predictions of more interesting and more complex critical behaviour than had been previously expected.

This paper is devoted to a study of the square-lattice Ising model with first and second neighbour interactions, described by the usual Hamiltonian

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

where the summations are over nearest neighbour pairs and next-nearest neighbour pairs respectively, and J_1 and J_2 are exchange constants which may be either positive or negative. It is usually convenient to incorporate the temperature into the definition of the coupling constants, and to write

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

As is well known, the inclusion of second neighbour interactions makes the model unsolvable by existing techniques. Although no exact results are known, various approximate methods have been used to study the model and our overall knowledge of its properties is good. One of the successful approximate techniques for studying the critical behaviour of cooperative lattice systems is the technique of exact series expansions, and it is this technique which has been used in the present work. However, for completeness, and to motivate the subsequent discussions, we will summarise what is known about the system and give a brief review of previous work by other authors.

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The Hamiltonian (1) has three possible types of ground state, depending on the values of the interaction parameters J_1, J_2. These are the ferromagnetic (F), antiferromagnetic (AF) and 'superantiferromagnetic' (SAF) states, shown in figure 1(*a*). The SAF state is of special interest because of its extra two-fold degeneracy and two-component ($n = 2$) order parameter. For the special case $J_2 = -\frac{1}{2}|J_1|$ the SAF ground state is degenerate with either the F or AF states, and an order parameter with $n = 3$ is appropriate. We shall discuss this in more detail below.

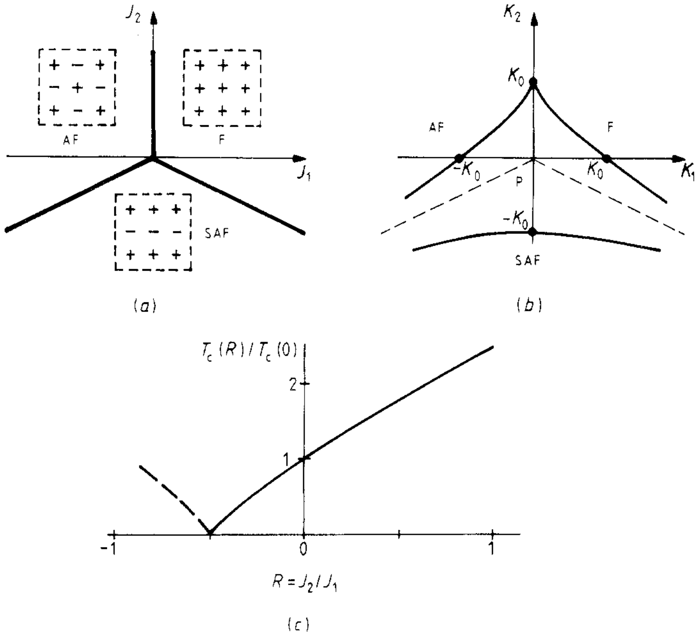

Figure 1. (*a*) Possible ordered states; (*b*) qualitative phase diagram in the (K_1, K_2) plane; (*c*) variation of ferromagnetic critical temperature, for the square-lattice Ising model with nearest and next-nearest neighbour interactions.

The zero-field free energy is given by

$$F(K_1, K_2) \equiv Nf(K_1, K_2) = -(1/\beta) \ln \mathrm{Tr}(e^{-\beta\mathcal{H}}). \tag{3}$$

The function $f(K_1, K_2)$, which is an even function of K_1, will exhibit singularities along critical lines in the (K_1, K_2) plane, the forms of which are depicted in figure 1(*b*). The upper two lines, which represent transitions from the high-temperature paramagnetic phase (P) to either the F or AF phases, intersect the $K_2 = 0$ axis at $K_1 = \pm K_0$ (where $K_0 = \frac{1}{2}\ln(1+\sqrt{2})$ is the Onsager value), and come together in a cusp at the point $K_1 = 0$, $K_2 = K_0$. It is believed that along these lines the system exhibits conventional Ising critical behaviour. The lower line, which represents transitions from the P phase to the SAF phase, intersects the $K_1 = 0$ axis at $K_2 = -K_0$. There is evidence that along this line the system has non-universal exponents, a question which we return to in a later section. This same information is shown in a slightly different way in figure 1(*c*), where we plot the variation of critical temperature T_c as a function of the ratio of interactions $R = J_2/J_1$.

This system has been studied by many authors. Various closed-form approximations have been used (Fan and Wu 1969, Gibberd 1969, Burkhardt 1978). Early renormalisation-group calculations (Nauenberg and Nienhuis 1974, van Leeuwen 1975, Nightingale 1977) have provided qualitative confirmation of the location and shape of the critical lines, and yielded the first suggestion of non-universal critical behaviour along the lower branch of figure 1(*b*). More recent work by Swendsen and Krinsky (1979), using the Monte Carlo renormalisation-group method, has provided confirmation of the violation of universality along the SAF line and has yielded quantitative estimates of critical exponents along this line. Further confirmation of this result was obtained by Barber (1979) by means of a perturbation expansion about the point $K_1 = 0$, $K_2 = -K_0$. The possibility of unusual behaviour in an equivalent model had also been predicted by Jüngling (1976). A more general discussion, emphasising the role of symmetry and dimensionality of the order parameter, has been given by Krinsky and Mukamel (1977).

The model has also been investigated by standard Monte Carlo techniques and by series expansions. The most recent Monte Carlo work (Landau 1980, Binder and Landau 1980) yields estimates of the thermal and magnetic properties for a wide range of values of $R = J_2/J_1$, and the R dependence of the critical temperature. Indications of non-universal behaviour along the SAF line are obtained and the values of critical exponents estimated for the case $J_1 = J_2 < 0$. Dalton and Wood (1969) have derived series expansions for zero-field free energy and the ferromagnetic susceptibility. These series are rather short, and become irregular for $R < 0$, but can be used to obtain the variation of T_c with R for $R > 0$. More recently, Plischke and Oitmaa (1979) derived a high-temperature expansion for the susceptibility which is appropriate to the SAF critical line, but the irregularity of the series prevented conclusive results from being obtained.

The author (Oitmaa 1980) has recently developed a high-temperature expansion for general Ising systems, and it is the aim of the present paper to apply this formalism to the square lattice with first and second neighbour interactions. We obtain a series of order 12 (in the variables $v_1 = \tanh K_1$, $v_2 = \tanh K_2$) for the zero-field free energy, and of order 11 for both the ferromagetic and SAF susceptibilities. These represent an addition of five terms to the series of Dalton and Wood, and an addition of two extra terms to the SAF susceptibility of Plischke and Oitmaa.

In § 2 we present the series and a detailed analysis for the paramagnetic–ferromagnetic transition. The results confirm the expected behaviour and provide rather precise estimates of the critical temperature as a function of the coupling constants.

In § 3 we present a similar discussion for the SAF transition. We find conclusive evidence that the susceptibility exponent is continuous for this transition, confirming the predictions of earlier authors.

Finally in § 4 we summarise our work and present an overall discussion.

2. The ferromagnetic transition

If we expand the exponential in (3), with the Hamiltonian given by (2), and associate the various terms with graphs in the standard way (see for example Domb (1974)), we can obtain a high-temperature expansion for the zero-field free energy. This expansion has the form

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

where $v_1 = \tanh K_1$, $v_2 = \tanh K_2$. We have computed the values of the coefficients a_{mm} for $m + n \leq 12$, and these are given in table 1. The order parameter appropriate to the ferromagnetic–paramagnetic transition is the magnetisation $m = (1/N)\sum_i \sigma_i$. The corresponding susceptibility, which is expected to diverge strongly along the critical line, is

Table 1. Coefficients of high-temperature series.

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

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	2864	8	4	29 369
6	6	$81\,949\frac{1}{3}$	4	8	70 548	2	10	20 046	0	12	$37\frac{1}{3}$

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

1	0	2	0	1	2	2	0	6	1	1	16
0	2	6	3	0	18	2	1	68	1	2	80
0	3	18	4	0	50	3	1	256	2	2	464
1	3	336	0	4	50	5	0	138	4	1	864
3	2	2 152	2	3	2 500	1	4	1 264	0	5	138
6	0	370	5	1	2 784	4	2	8 612	3	3	13 920
2	4	11 696	1	5	4 432	0	6	370	7	0	986
6	1	8 548	5	2	31 896	4	3	64 872	3	4	76 632
2	5	49 668	1	6	14 768	0	7	986	8	0	2 586
7	1	25 584	6	2	110 720	5	3	272 768	4	4	409 552
3	5	377 280	2	6	196 464	1	7	47 376	0	8	2 586
9	0	6 746	8	1	74 560	7	2	368 776	6	3	1 058 876
5	4	1 934 752	4	5	2 284 336	3	6	1 709 400	2	7	735 892
1	8	147 504	0	9	6 746	10	0	17 438	9	1	213 712
8	2	1 183 784	7	3	3 893 040	6	4	8 324 824	5	5	12 017 920
4	6	11 612 780	3	7	7 260 320	2	8	2 639 640	1	9	448 336
0	10	17 438	11	0	44 882	10	1	602 284	9	2	3 702 584
8	3	13 666 056	7	4	33 549 248	6	5	56 899 244	5	6	67 533 752
4	7	54 901 768	3	8	29 274 704	2	9	9 140 372	1	10	1 335 952
0	11	44 882									

(*c*) Coefficients c^{SAF}_{mn} in the expansion of the ordering susceptibility for the superantiferromagnetic transition, equation (7).

0	1	−2	2	0	−2	0	2	6	2	1	4
0	3	−18	4	0	2	2	2	−32	0	4	50
4	1	−16	2	3	52	0	5	−138	6	0	−6
4	2	4	2	4	−336	0	6	370	6	1	−28
4	3	−408	2	5	500	0	7	−986	8	0	−6
6	2	−400	4	4	−432	2	6	−2 976	0	8	2 586
8	1	−192	6	3	−1 828	4	5	−6 368	2	7	4 244
0	9	−6 746	10	0	−42	8	2	−1 816	6	4	−12 744
4	6	−9 908	2	8	−23 944	0	10	17 438	10	1	−852
8	3	−16 040	6	5	−54 868	4	7	−80 376	2	9	33 460
0	11	−44 882									

given by $\chi_F = \Sigma_j \langle \sigma_0 \sigma_j \rangle$ and the high-temperature series for this quantity can be written as

$$\chi_F = 1+2 \sum_{m,n} c^F_{mn} v_1^m v_2^n. \tag{5}$$

The values of the coefficients c_{mn} for $m+n \leq 11$ are also given in table 1. For any choice of the ratio of interactions $R = J_2/J_1$ we can obtain series in a single variable, which can then be analysed in the usual way to determine the critical coupling and exponents. We use the susceptibility series to estimate the value of the critical temperature. Although the series are sufficiently regular for ratio analysis, we have found Padé approximant methods more satisfactory. The first step is to obtain an estimate for $K_c = J_1/kT_c$ from poles of Padé approximants to the series for $d(\lg \chi_F)/dK_1$. In table 2 we show estimates of K_c obtained in this way for the case $R = 0.5$, which is typical. Having obtained an estimate of K_c, we obtain estimates of the critical exponent γ by forming Padé approximants to $(K_c - K)\, d(\lg \chi_F)/dK$ and evaluating these at the estimated $K = K_c$. These results, which are also shown in table 1, provide strong evidence that γ takes the universal value of 1.75. Making this assumption allows us to refine the estimate of K_c, by looking at the poles of Padé approximants to the series for $[\chi_F]^{4/7}$. Typical results, again for the case $R = 0.5$, are shown in table 3. This procedure has been carried out for a

Table 2. Estimates of the ferromagnetic critical 'temperature' $K_C = J_1/kT_C$ from poles of $[N, D]$ PA's to the series $d(\lg \chi_F(K))/dK$ for the case $J_2 = 0.5J_1$. In brackets are shown corresponding estimates of the exponent γ from PA's to $(K_c - K)\, d(\lg \chi_F(K))/dK$ with $K_c = 0.2268$.

D \ N	3	4	5	6	7
3			0.263 31 (1.748 6)	0.262 98 (1.749 1)	0.262 87 (1.749 2)
4		0.263 78 (1.758 2)	0.262 71 (1.749 1)	0.262 78 (1.749 2)	
5	0.263 80 (1.748 9)	0.263 37 (1.749 4)	0.262 78 (1.749 2)		
6	0.262 73 1.749 3)	0.262 82 (1.749 2)			
7	0.262 81 (1.749 2)				

Table 3. Estimates of the ferromagnetic critical 'temperature' $K_c = J_1/kT_c$ obtained from poles of $[N, D]$ Padé approximants to the series $[\chi_F]^{4/7}$ for $J_2 = 0.5J_1$.

D \ N	4	5	6	7
4		0 262 803	0.262 808	0.262 808
5	0.262 789	0.262 807	0.262 808	
6	0.262 809	0.262 808		
7	0.262 807			

sequence of values of R in the range $-0.5 \leqslant R < \infty$. The variation of kT_c/J_1 with R is shown in figure 2. The figure shows the expected behaviour, but we have now obtained much more precise estimates of the critical temperature than had previously been available. For R in the range $-0.5 \leqslant R < -0.4$ the series are irregular and we are unable to conclude whether T_c goes to zero at $R = -\frac{1}{2}$ or whether it approaches a small finite limit. The ferromagnetic critical line in the (K_1, K_2) plane is shown in figure 3.

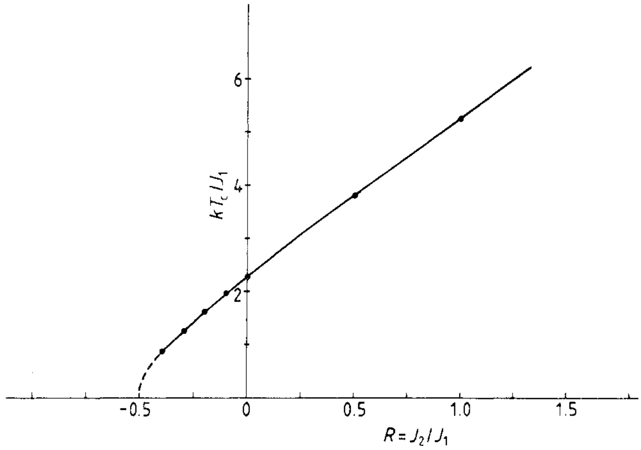

Figure 2. Quantitative variation of the ferromagnetic critical temperature versus the parameter $R = J_2/J_1$, obtained from analysis of the high-temperature susceptibility series. The points represent actual estimates, the error being estimated to be no larger than the size of the points.

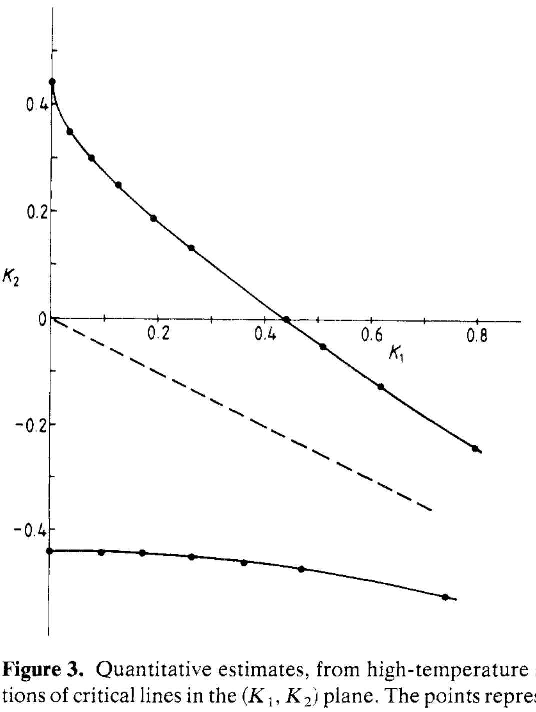

Figure 3. Quantitative estimates, from high-temperature susceptibility series, of the locations of critical lines in the (K_1, K_2) plane. The points represent actual estimates, with errors estimated to be no larger than the points.

3. The SAF transition

In this section we use our high-temperature series to study the critical line which represents the transition to the SAF state. This is the transition which occurs when $J_2 < -0.5\,J_1$, and is depicted as the lower line in figure 1(*b*). It is along this line that non-universal behaviour has been predicted. The most appropriate series to investigate is that for the SAF susceptibility, χ_{SAF}. This quantity is given by

$$\chi_{\mathrm{SAF}} = \sum_j (-1)^{x_j} \langle \sigma_0 \sigma_j \rangle$$

where x_j is the horizontal distance between sites $0, j$. It is this quantity which is expected to exhibit a strong divergence along the SAF line, and hence to provide the most precise estimates of the critical temperature for this transition. The situation is similar to the case of the Ising antiferromagnet, where it is the staggered susceptibility which has a strong divergence. Our high-temperature expansion for χ_{SAF} takes the form

$$\chi_{\mathrm{SAF}} = 1 + 2 \sum_{m,n} c_{mn}^{\mathrm{SAF}} v_1^m v_2^n.$$

The values of the c_{mn} coefficients for $m + n \leqslant 11$ are given in table 1. To obtain series in a form suitable for analysis, we define a parameter $R = -J_1/J_2$ and for a given choice of R obtain series in the single variable $x \equiv -J_2/kT$. For $R = 0$ the series is identical to the usual nearest-neighbour square-lattice ferromagnetic susceptibility, and thus has a singularity at the Onsager value $x_c = K_0$, with exponent $\gamma_{\mathrm{SAF}} = 1.75$. For non-zero R the function χ_{SAF} should have a 'physical singularity' $x_c(R)$, but in addition will have an unphysical singularity on the other critical line at a negative value of x closer to the origin. This unphysical singularity will hinder accurate analysis unless a transformation is first carried out to move it further from the origin than the singularity of interest. We have followed the same procedure as Plischke and Oitmaa (1979), and have used an Euler transformation of the form

$$x = x'/(1 + \lambda x')$$

where we choose $\lambda \simeq 1/x_u$, x_u being the position of the unphysical singularity. The series in x' is much smoother and can be analysed successfully by both ratio and Padé methods. To illustrate these steps we consider explicitly the case $R = 0.4$. In table 4(*b*) we show the results of Padé analysis of the x series. In this case, estimates of the position of the physical singularity are still fairly consistent, but the consistency is greatly improved by the use of an Euler transformation, as shown in table 4(*d*). In table 4(*e*) we show estimates of the critical exponent γ obtained by forming Padé approximants to $(x_c' - x')\,\mathrm{d}(\lg \chi(x'))/\mathrm{d}x'$ and evaluating these at $x' = x_c'$. The uncertainty of x_c' gives a corresponding uncertainty in the estimate of γ, but the most consistent results are for $x_c' = 0.1667$, yielding $\gamma = 1.66 \pm 0.02$. Another way of estimating γ is to look for simple poles in Padé approximants to $[\chi_{\mathrm{SAF}}(x')]^{1/\gamma}$. For a particular choice of γ, Padé's give a spread in the positions of physical poles, as illustrated in figure 4. It is reasonable to take as the best estimate of γ that which gives the smallest spread of x_c' values, and this gives $\gamma \simeq 1.66$ in agreement with the previous estimate.

These techniques have been used to analyse the χ_{SAF} series for a number of R values. Reasonably consistent results are obtained for $R \leqslant 1.2$, and the position of the critical line is shown in figure 3. The location of this line agrees with previous estimates (Nightingale 1977, Swendsen and Krinsky 1979) within the resolution of figure 3. On a

Table 4. Analysis of the χ_{SAF} series for the case $R = 0.4$.

(a) Coefficients of the series in the variable x. 1, 4, 11.36, 33.386 666 67, 81.930 666 67, 225.275 7333, 511.726 5465, 1417.041 650, 2981.887 343, 1592.231 129, 16 445.533 46, 51 592.256 15.

(b) Estimates of physical singularity x_c and unphysical singularity x_u (in brackets) from $[N, D]$ Padé approximants to $d(\lg \chi_{SAF}(x))/dx$. An asterisk denotes no consistent estimate, (cc) denotes complex-conjugate pair near axis.

D \ N	3	4	5	6	7
3			0.4399 (cc)	0.4494 (−0.3011)	0.4459 (−0.2907)
4		0.4385 (−0.2423)	0.4420 (−0.2651)	0.4470 (−0.2888)	
5	0.4407 (cc)	0.4450 (cc)	0.4447 (cc)		
6	0.4413 (−0.2426)	0.4447 (cc)			
7	0.4474 (−0.2826)				

(c) Cofficients of the series in variable x', obtained using the Euler transformation $x' = x/(1+3.75x)$.

1, 4, 26.36, 174.836 6667, 1147.718 167, 7458.501 358, 48 062.127 02, 307 565.9509, 1956 951.020, 12 391 920.24, 78 150 965.49, 491 153 963.0.

(d) Estimates of position of singularity x'_c from $[N, D]$ Padé approximants to $d(\lg \chi_{SAF}(x'))/dx'$.

D \ N	3	4	5	6	7
3			0.1662	0.1665	0.1666
4		0.1661	0.1681	0.1667	
5	0.1661	0.1665	0.1667		
6	0.1660	0.1667			
7	0.1702				

Estimate $x'_c = 0.1667 \pm 0.0003$ gives $x_c = 0.445 \pm 0.002$.

(e) Estimates of critical exponent γ from $[N, D]$ Padé approximants to $(x'_c - x')$ $d(\lg \chi_{SAF}(x'))/dx'$ evaluated at $x' = x'_c$, for three choices of x'_c.

N,D \ x'_c	0.1666	0.1667	0.1668
[3, 7]	1.6435	1.6590	1.6751
[4, 6]	1.6438	1.6593	1.6754
[5, 5]	1.6441	1.6593	1.6757
[6, 4]	1.6438	1.6593	1.6751
[7, 3]	1.6444	1.6594	1.6753
[3, 6]	1.6487	1.6650	1.6817
[4, 5]	1.6447	1.6594	1.6743
[5, 4]	1.6446	1.6592	1.6740
[6, 3]	1.6450	1.6596	1.6743

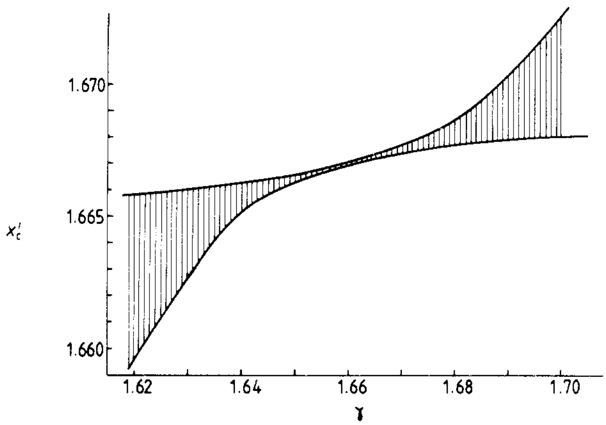

Figure 4. Scatter diagram showing the location of physical poles in high-order Padé approximants to $[\chi_{SAF}]^{1/\gamma}$ for different choices of γ, as explained in the text. The shaded region, being the region occupied by poles, is clearly narrowest for $\gamma \simeq 1.66$.

larger scale there is a small discrepancy between our estimates of x_c and the parametrised result of Swendsen and Krinsky. This is illustrated in figure 5, as are the estimates of the critical exponent γ. The series results for γ show clear evidence for a continuous variation and consequent breakdown of universality. There is again a small disagreement between the series estimates and the earlier Monte Carlo results. The error bars on the series results represent the sort of confidence limits which would have been assumed in the absence of the Monte Carlo results. It may well be that one or both sets of error estimates are too optimistic, and further work will be needed to clarify this.

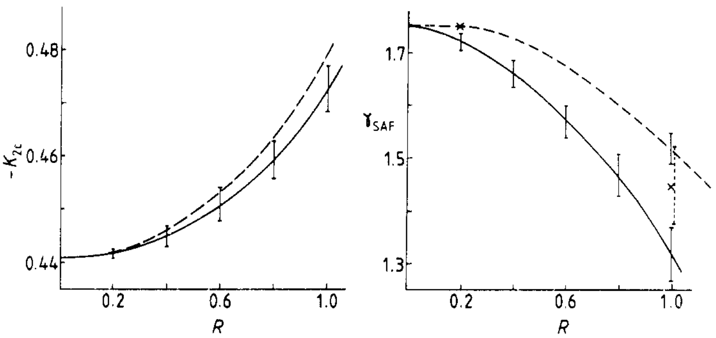

Figure 5. Variation of the critical coupling $-K_{2c}$ and the exponent γ_{SAF} of the ordering susceptibility for the SAF transition, as functions of $R = -J_1/J_2$. For comparison, the Monte Carlo renormalisation-group results of Swendsen and Krinsky (1979) are also shown (as broken lines) and the Monte Carlo results of Binder and Landau (1980) (as crosses).

4. Conclusions

The work reported in this paper has provided, in our view, the most precise information currently available on the critical behaviour of the square-lattice Ising model with nearest and next-nearest neighbour interactions. In particular, the location of the critical lines has been accurately determined, and this information may be useful in interpreting data on suitable experimental systems. Although we have concentrated on the critical behaviour, it would be relatively straightforward to use the series to estimate the magnitude of the susceptibility or specific heat over the whole temperature region $T \geqslant T_c$.

The greatest theoretical interest in this model is in the critical line corresponding to transitions to the SAF state. We have confirmed previous predictions of a continuous non-universal variation of the susceptibility exponent along this line. It has been suggested that along this line the model is in the same universality class as the eight-vertex model. If this is the case, then there should be an explicit mapping between these two models, and it may be possible to discover this by a closer study of the data shown in figure 5.

Another point which requires further study is the behaviour of this model when $J_2 = -\frac{1}{2}J_1$, since in this case the ground state is highly degenerate. Our results tend to suggest that $T_c = 0$ for this ratio of interactions, but a finite transition temperature corresponding to a bicritical point cannot be ruled out. Further study, possibly with the aid of low-temperature series, may be able to clarify this question, and it is hoped to investigate this point in future work.

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