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1982 J. Phys. A: Math. Gen. 15 3593

(http://iopscience.iop.org/0305-4470/15/11/037)

J. Phys. A: Math. Gen. **15** (1982) 3593–3598. Printed in Great Britain

Phase equilibrium in the three-state antiferromagnetic Potts model

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Received 2 June 1982

Abstract. A phase equilibrium surface for the 2D (square lattice) antiferromagnetic Potts model in the presence of its ordering fields has been constructed using the phenomenological scaling transformation.

1. Introduction

In a recent publication, Baxter (1982) has obtained the exact solution to the q-state antiferromagnetic Potts model at its zero-field critical point. This shows that in terms of a continuous q variable, the critical point decreases to zero at $q=3$ ($q=2$ is the Ising model antiferromagnetic). This result confirms a recent conclusion of Nightingale and Schick (1982) who employed the scaling transformation (Nightingale 1976, 1977, Sneddon 1978, Wood and Goldfinch 1980, Roomany *et al* 1980, Wood and Osbaldestin 1982) to examine the critical behaviour of the three-state antiferromagnetic Potts model in zero field. The present authors have recently demonstrated how the scaling transformation method can be used to yield an accurate view of the *whole phase equilibrium surface*, and in this note we use the method to construct the phase equilibrium surface of the three-state antiferromagnetic Potts model in the presence of its ordering fields.

2. Phase structure in the model

The field dependent Hamiltonian of this model is given by

$$\mathscr{H} = J\sum_{ij}\delta_{\sigma_i\sigma_j} - \sum_{p=1}^{p=3} h_p \sum_i \delta_{\sigma_i p} \qquad (J>0) \tag{1}$$

where the site variables σ_i take the values 1, 2, or 3, and where the nearest-neighbour interactions spanned in the first summation are zero if neighbouring site variables assume different values. The three ordering fields $h_k (k=1, 2, 3)$ in (1) favour the corresponding states $\sigma=k$, and following the treatment by Straley and Fisher (1973) of the corresponding ferromagnetic model, the symmetry condition

$$h_1+h_2+h_3=0 \tag{2}$$

is imposed.

In any of the three limits $h_k \to -\infty$ the model reduces to the two-state Potts model (the antiferromagnetic Ising model in a field) the phase diagram for which is well known (Muller-Hartman and Zittartz 1977, Sneddon 1979, Wood and Osbaldestin 1982). A simple analysis of the ground states of (1) shows where to expect to find phase transitions on the zero-temperature plane. If we consider the line $h_2 = h_3 = -h_1/2$, then at high positive h_1 values the ground state is as depicted in figure 1(a) for the aligned phase, and at small positive h_1 values the ground state is that shown

1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1

(a)

1	$\frac{2}{3}$	1	$\frac{2}{3}$
$\frac{2}{3}$	1	$\frac{2}{3}$	1
1	$\frac{2}{3}$	1	$\frac{2}{3}$
$\frac{2}{3}$	1	$\frac{2}{3}$	1

(b)

1	2	1	2
2	1	2	1
1	2	1	2
2	1	2	1

(c)

Figure 1. Some zero-temperature ground state phases. (a) shows the disordered phase at high values of $h_1 (h_3 < 0)$ from which an order–disorder transition can occur into either of the phases shown in (b) and (c), these are ordered phases and are respectively in the domains $h_2 = h_3 = -h_1/2$ in between $\frac{8}{3} > h_1/J > 0$, and $h_1/J < 4 + h_2/J (h_3 < 0)$ (see equation (5)).

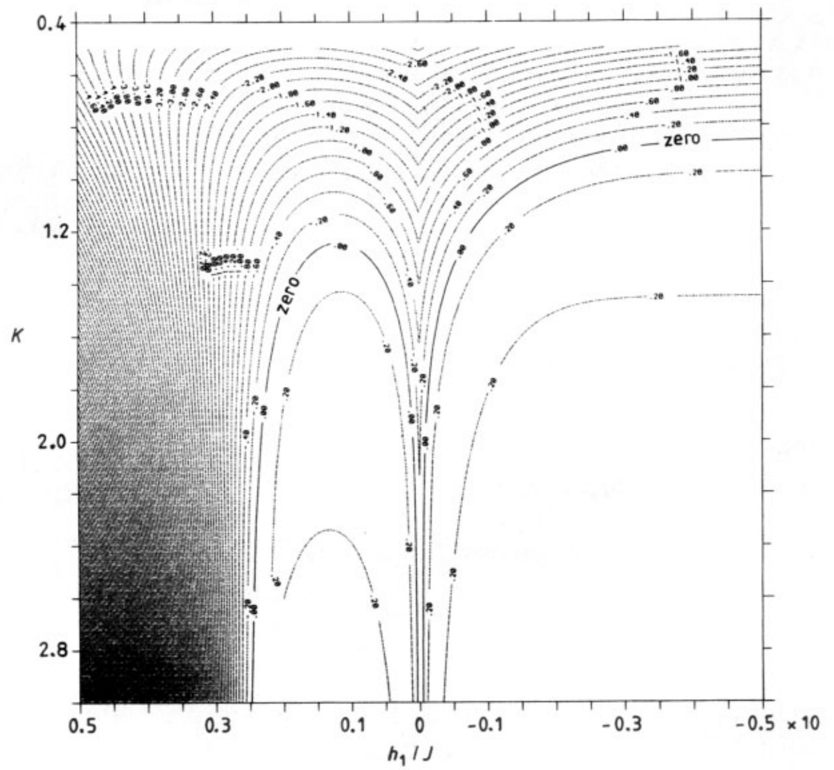

Figure 2. The contours of $\varphi_2(T, \boldsymbol{h})$ for $h_2 = h_3 = -h_1/2$ in the Th_1-plane. The zero contour is the locus of order–disorder transition points, and the two plateau regions represent coexistence sheets in the phases of figure 1(b) ($h_1 > 0$) and figure 1(c) ($h_1 < 0$) in which the spin states shown exchange sublattices across a domain wall. Approximations to the limit points $h_1/J = \frac{8}{3}(T = 0)$ and $K_c = 0.8814\ldots$ ($h_1 = -\infty$) are clearly seen.

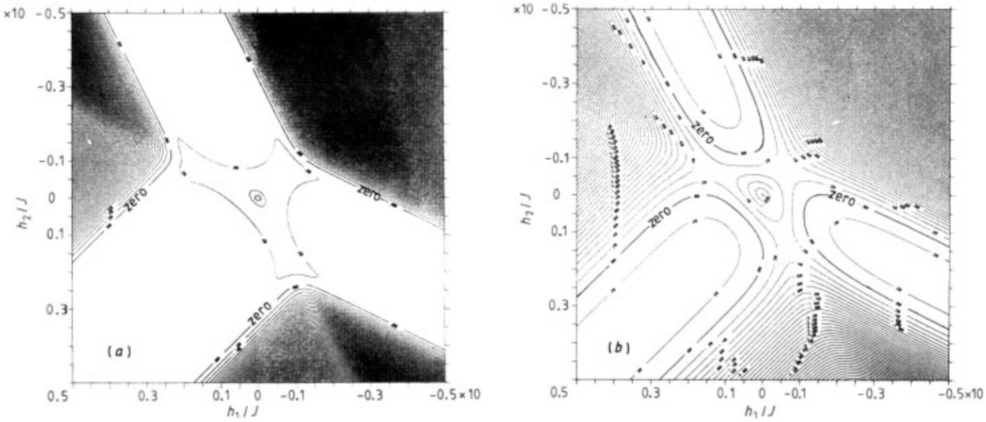

Figure 3. (a) The contours of $\varphi_2(T, \boldsymbol{h})$ at a fixed 'low temperature' in the h_1h_2-plane. The zero contour borders a large region in which $\varphi_2 \sim 0$ containing various types of antiferromagnetic ordering (see figures 4(a) and (b)). The zero contour is quite close to the exact limiting form of (5), and the contours encircling the origin represent the disordered phase in the region of very small fields, the innermost contour is on $\phi_2 = 0$.

(b) The contours of $\varphi_2(T, \boldsymbol{h})$ in the h_1h_2 plane at a fixed temperature chosen between the maximum T_c of figure 2 inside $h_1 > 0$, and the Ising model limit at $h_1 = -\infty$. The three loops of the zero contour enclose regions of typical antiferromagnetic ordering on two sublattices (see figure 4(a))

in figure 1(b) for the 'ordered' phase. These two states have energies

$$E_a = 2NJ - Nh_1 \tag{3a}$$

$$E_b = -Nh_1/2 + Nh_1/4 \tag{3b}$$

respectively, hence a transition between these two zero-temperature phases can be expected at $h_1/J = 8/3$. On moving off the line $h_1 = h_2$ in the domain $h_3 < 0$, h_1, $h_2 > 0$, and $h_1 \gg h_2$ the zero-temperature state will be that shown in figure 1(a) but will suffer a transition into the state of figure 1(c) along the line $E_a = E_c$ where

$$E_c = -Nh_1/2 - Nh_2/2 \tag{3c}$$

yielding second-order transitions along the line

$$h_1/J - h_2/J = 4. \tag{4}$$

Second-order transitions of this type on the zero-temperature plane can be expected along the six line segments

$$h_k/J - h_p/J = \pm 4 \tag{5}$$

and these are shown in figure 4(b) as the boundary lines of the whole phase surface which is illustrated in figure 4(a).

The schematic view of the phase equilibrium surface which is shown in figure 4(a) has been built up using the scaling transformation (Wood and Osbaldestin 1982) in which the functions

$$\varphi_m(T, \boldsymbol{h}) = m\xi_m^{-1}(T, \boldsymbol{h}) - (m+2)\xi_{m+2}^{-1}(T, \boldsymbol{h}) = 0 \tag{6}$$

act as a sequence of rapidly convergent approximants to the phase surface in

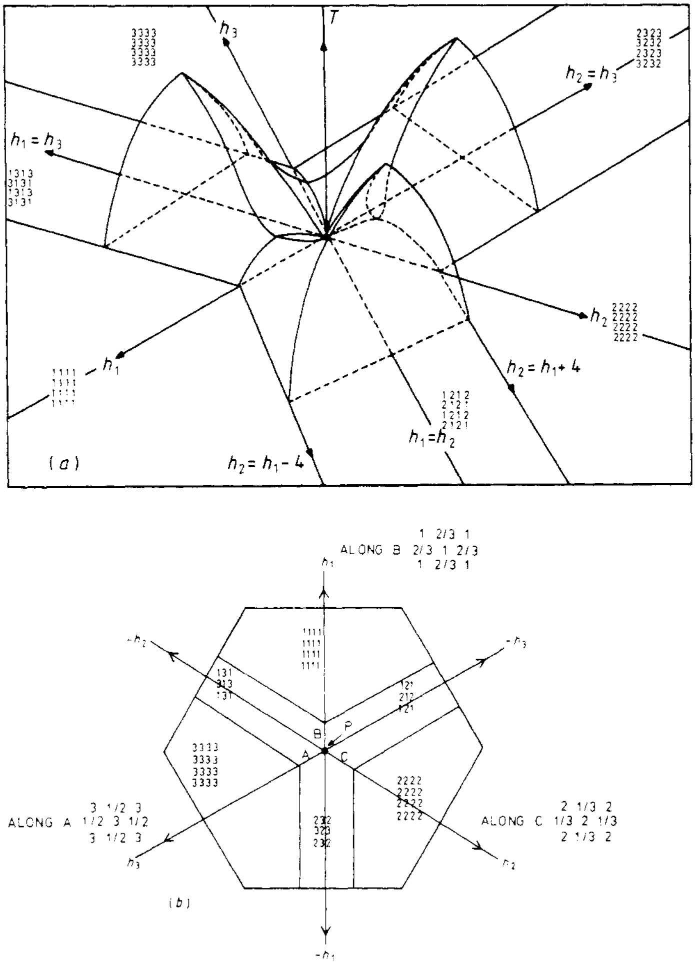

Figure 4. (*a*) The schematic view of the whole phase equilibrium surface, points on the surface itself are all order–disorder transition points. The points in the interior of the volume enclosed between the surface and the zero-temperature plane are points at which phase coexistence can occur. The various types of order and disorder are depicted on the figure.

(*b*) The phase structure of the zero-temperature plane of figure 4(*a*). The three line segments A, B, and C are unique to the structure in that the ordered phase has a disordered occupancy of one sublattice where two of the three species randomly populate one sublattice. The various ordered and disordered state are depicted on the figure, the boundaries between order and disorder are the six line segments of equation (5). The point P is Baxter's zero-field critical point (Baxter 1982) and is the infinitely degenerate ground state given by the three colourings of the square lattice.

$(T, \boldsymbol{h})$-space. In (6) ξ_m is the correlation length of an $m \times \infty$ square lattice. Here we have investigated the surface generated by $\varphi_2(T, \boldsymbol{h}) = 0$. Figure 2 shows the contours of φ_2 on the K, h_1-plane ($K = \beta J$) with the condition $h_2 = h_3 = -h_1/2$ imposed (the values of φ_2 are shown on the contours). The figure clearly shows two large and disjoint plateau regions on each side of the $h_1 = 0$ line, each of these is bounded by the zero contour which appears to be asymptotic to the $h_1 = 0$ line and to connect the two regions at $T=0$. This is Baxter's zero-field critical point (Baxter 1982). Both the expected zero-temperature transition at $h_1/J=8/3$, and the Ising-model limit at $h_1 \to -\infty$ ($K_c = 0.8814\ldots$) are seen to be well approximated by the zero contour.

Phase transitions occur at all points on the zero contour, and the plateaus are regions of coexisting phases. On moving from left to right across figure 2 (at $K=2$ say) we encounter the following phases. First the aligned phase in figure 1(a), then a second-order transition into the ordered phase of figure 1(b) in which we have coexistence between the phases in which the spin state $\sigma=1$, and the mixed states $\sigma=2,3$ exchange sublattices across domain walls made up of 1–1 pairs. When h_1 is close to zero a new transition occurs into a new disordered phase, and as h_1 increases negatively there is a further transition into the ordered antiferromagnetic phases in which spin states $\sigma=2$ and $\sigma=3$ each occupy one sublattice with domain walls of either 2–2 or 3–3 pairs.

Figures 3(a) and 3(b) exhibit the phase equilibrium approximated by φ_2 at a fixed temperature in the h_1h_2-plane. Figure 3(a) is at a low temperature, and in figure 3(b) the temperature is between the approximated Ising model limit at $h_1 \to -\infty$ and the maximum critical temperature inside $h_1>0$ shown in figure 2. In figure 3(a) the zero contour excloses a large coexistence sheet and is close to its limiting form of (5). The zero contour has a branch encircling the origin corresponding to the narrow disordered region about the $h_1=0$ line in figure 2. At the temperature of figure 3(b) the h_1h_2-plane will cut the phase surface on the right-hand plateau of figure 2. The zero contour of figure 3(b) generates three loops which are the cross-sections of the three large ridges shown in figure 4(a) which is our schematic illustration of the nature of the whole surface.

On the surface shown in figure 4(a) are all the second-order transition points, and various forms of phase coexistence exists inside the volume enclosed by the surface and the zero-temperature plane, this coexistence is between various types of antiferromagnetic ordering depending on the location; some of these ordered phases are illustrated on the figure. The three saddle points of the surface correspond to the maximum critical points on the lines such as $h_2=h_3$ ($h_1>0$) shown in figure 2. Figure 4(b) portrays the types of ordered phases on the zero-temperature plane which are mainly the regions determined by the line segments of (5). The short line sections A, B, and C are special and interesting in that the 'ordered' phases are ones in which one sublattice is randomly populated by one of two spin states while the third state occupies one sublattice totally. The meeting point of these three phases is the infinitely degenerate ground state generated by the 'three colourings' of the square lattice (Baxter 1982, Lieb and Wu 1972).

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