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Examples of phase equilibrium in lattice models

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Abstract. The general Z_4 and Z_5 models on the simple quadratic lattice, and the pair triplet Ising model on the triangular lattice are employed to illustrate an extension of the finite size scaling technique which obtains the qualitative structure of the phase equilibrium surface in terms of multiple phase coexistence.

1. Introduction

In an earlier paper Wood and Osbaldestin (1983) argued that the computational method of finite size scaling and phenomenological renormalisation in the treatment of lattice models exhibiting phase transitions can be extended to obtain a breakdown of the phase diagram which identifies regions on the coexistence surface Σ where multiple phase coexistence occurs. In such applications of finite size scaling theory formal expressions for generalised correlation lengths of two semi-infinite lattice systems are compared as a renormalisation under a simple rescaling factor. In this a hierarchy of approximants is created in the form of implicit functions for Σ (Wood and Osbaldestin 1982, Osbaldestin and Wood 1982) and its internal structure in terms of multiple phase coexistence.

A short review of phenomenological renormalisation has been given by Nightingale (1982, see also Burkhardt and van Leeuwen 1982) and a comprehensive review of finite size scaling theory has recently been given by Barber (1983). Detailed examples of such calculations can be found in papers by Nightingale (1976, 1977), Sneddon (1978), Nightingale and Blöte (1980), Blöte *et al* (1981), Sneddon and Stinchcombe (1979), Hamer and Barber (1980), Roomany *et al* (1980), Wood and Goldfinch (1980), Blöte and Nightingale (1982), Goldfinch and Wood (1982), Kinzel and Schick (1982), Turban and Debierre (1984), and Beale (1984). A critical analysis of the factors relating to the convergence of the approximations obtained in phenomenological renormalisation has recently been given by Privman and Fisher (1983).

The present work is in real lattice space in two dimensions; the notation is that introduced by Wood and Osbaldestin (1983) where the implicit functions $\phi_{n,k}(\boldsymbol{K})=0$ define a sequence of approximants on n which will approximate regions in interaction space $\boldsymbol{K}$ where k-fold phase coexistence is possible. In introducing this variant of phenomenological renormalisation we used only the scalar Potts models where some features of Σ are known exactly (Wu 1982). The purpose of the paper is to present further applications of the method in obtaining the qualitative structure of the phase diagram under more challenging conditions.

As examples of very general models we have selected the most general form of the Z_4 and Z_5 models in zero field, where the Hamiltonian is defined purely in terms of

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Z_4 and Z_5 symmetry. Here the objective is to obtain the phase structure of any specific realisations of such models. Z_5 symmetry is of special interest because of its possible similarity to the O(2) models which are thought to have a soft Kosterlitz-Thouless (KT) phase within Σ (Kosterlitz and Thouless 1973). It is known that a KT phase exists in Z_n models when $n \geq 5$ (Cardy 1980). We have also examined the Z_5 five-state vector Potts model in an ordering field to see whether the Σ surface in the field-temperature plane gives any indication that a KT phase exists in zero field. As an interesting example of an Ising type system with competing interactions we have applied the technique to models on a triangular lattice where both three spin triplet terms and the usual pair interactions are present; both ferromagnetic and antiferromagnetic cases are considered. The results and discussion of all these calculations are described in §§ 2, 3 and 4, which are devoted to Z_4, Z_5, and triplet spin models respectively.

2. Z_4 models

In lattice models with Z_p symmetry the configuration space $\{\theta_i\}$ of the lattice sites $i = 1, 2, \ldots, N$ is mapped out by the angular variables θ_i which can take the p discrete values $\theta_i = 2\pi k/p$, $k = 0, 1, \ldots, p-1$. A model with Z_p symmetry on nearest-neighbour interactions has a Hamiltonian in the general form

$$\mathcal{H} = \sum_{ij} V(\theta_i - \theta_j), \tag{1}$$

where $V(\phi)$ is the potential function between nearest-neighbour sites (i, j) and is symmetric. The partition function can be written in terms of the $[p/2]$ variables

$$\omega_r = \exp - \beta[V(2\pi r/p) - V(0)] \leq 1, \qquad r = 1, 2, \ldots, [p/2]. \tag{2}$$

Thus the ground state is p-fold degenerate and 'ferromagnetic' with all the θ_i equal to one of the possible angles. The partition function for the Z_4 model takes the form

$$Z(\omega_1, \omega_2) = \omega_0^{Nq/2} \sum_{\{\theta_i\}} \omega_1^{n_1}\omega_2^{n_2}, \qquad \omega_0 = \exp(-\beta V(0)) \tag{3}$$

where q is the nearest-neighbour coordination and n_1 and n_2 are the numbers of nearest-neighbour pairs with relative angular orientations of $\pi/2$ and π respectively. Here the unit square in the ω_1, ω_2 plane contains the infinite temperature and interaction range. The phase equilibrium surface on this square maps out the possible phase structure of any specific model with Z_4 symmetry over the whole temperature range.

Duality relations and the conjectured outline form of the phase diagrams of Z_p models on the simple quadratic lattice have been considered by several authors (Cardy 1980, Wu 1979, Domany *et al* 1980, Alcaraz and Koberle 1980, Ruján *et al* 1981). The Z_4 model is equivalent to the symmetric Ashkin-Teller (AT) model, and can be written in terms of two coupled Ising models (Fan 1972, Betts 1964). A conjectured form of the phase diagram of the AT model was given by Wu and Lin (1974), the form of the phase diagram for the Z_4 model is shown schematically in figure 1. The line L'E is invariant under the duality relations of the model, which are

$$\omega_1^* = (1-\omega_2)/(1+2\omega_1+\omega_2), \qquad \omega_2^* = (1-2\omega_1+\omega_2)/(1+2\omega_1+\omega_2). \tag{4}$$

The thermodynamic path of a specific model in which $V(\pi/2)$ and $V(\pi)$ are related will be a curve connecting L ($T=0$) and H ($T=\infty$). For example the line $\mathrm{LP_4H}$ is the four state scalar Potts model where $V(\theta_i - \theta_j) = -J\delta_{\theta_i\theta_j}$, and the curve HVL is the

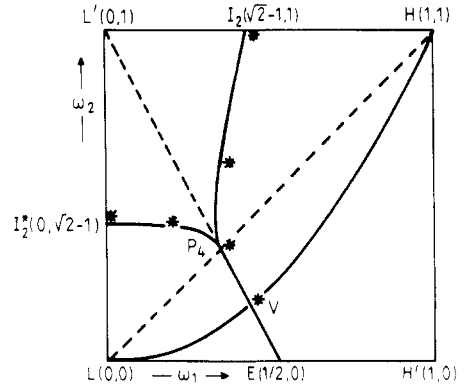


Figure 1. The phase diagram of the Z_4 model. P_4E is an exact critical line and part of the self dual line L'E. The sections P_4I_2 and $P_4I_2^*$ are conjectured to be lines of Ising-like transitions. The phases can be characterised by M_1 and M_2. The points * are those obtained by Ruján *et al* (1981). HVL is the vector Potts model.

vector Potts model where $V(\theta_i - \theta_j) = -J\cos(\theta_i - \theta_j)$. The critical line P_4E is the only part of the phase diagram which is known exactly, it is related by duality to the critical line of the eight-vertex model (Baxter 1972, Fan 1972) and the point V is the point where the model decouples into two non-interacting Ising models (Betts 1964). The construction of Wu and Lin (1974) conjectures both that the dual transition lines P_4I_2 and $P_4I_2^*$ exist, and that they are lines of Ising-like transitions.

A characterisation of the three phases shown in figure 1 can be made in terms of the other parameters

$$M_1 = \langle \exp(\mathrm{i}\theta_j)\rangle, \qquad M_2 = \langle \exp(2\mathrm{i}\theta_j)\rangle, \tag{5}$$

which effectively measure directional expectations at a site, but where M_2 is the expected direction under the operation where each site doubles its angle, hence $(\pi/2, 3\pi/2) \to \pi$ and $(0, \pi) \to 0$. The low-temperature ordered phase inside $EP_4I_2^*$ is characterised as a sheet of four phase coexistence where $M_1 \neq 0$ and $M_2 \neq 0$ arising from the four ground states. When heated up along a direction intersecting $P_4I_2^*$ the model is expected to undergo an Ising transition at which M_1 vanishes, into a phase which has a residual Z_2 symmetry under the operation of M_2. This is the phase enclosed by $I_2^*P_4I_2$ in which $M_1 = 0$ and $M_2 \neq 0$, and the extreme point L' has infinitely many ground states. The high-temperature disordered phase is the region $I_2P_4EH'H$ where $M_1 = M_2 = 0$. The only quantitative attempts known to the authors to calculate the positions of transition points on figure 1 are those of Ruján *et al* (1981) who used the Migdal-Kadanoff renormalisation group method, their calculations are represented by * on the diagram.

The contours of the approximants $\phi_{2,k}(\omega_1, \omega_2)$ and $\phi_{3,k}(\omega_1, \omega_2)$ for $k = 2$, 3 and 4 are shown in the figure sequence 2, 3, and 4. These approximants are based upon calculations with $4\times\infty$, $3\times\infty$, and $2\times\infty$ strips, the whole phase structure of the Z_4 model appears with quite amazing clarity. As expected the zero contour of the approximants $\phi_{2,2}$ and $\phi_{3,2}$ represents the whole of the high-temperature phase boundary EP_4I_2 and is probably very close to the exact curve. The exact transition point along the boundary $\omega_2 = 1$ is marked I_2. The contour map represents a rising valley bottom along the scalar Potts line LH and clearly suggests that the zero contour is the ridge edge of a plateau which covers the whole square on the low-temperature side of

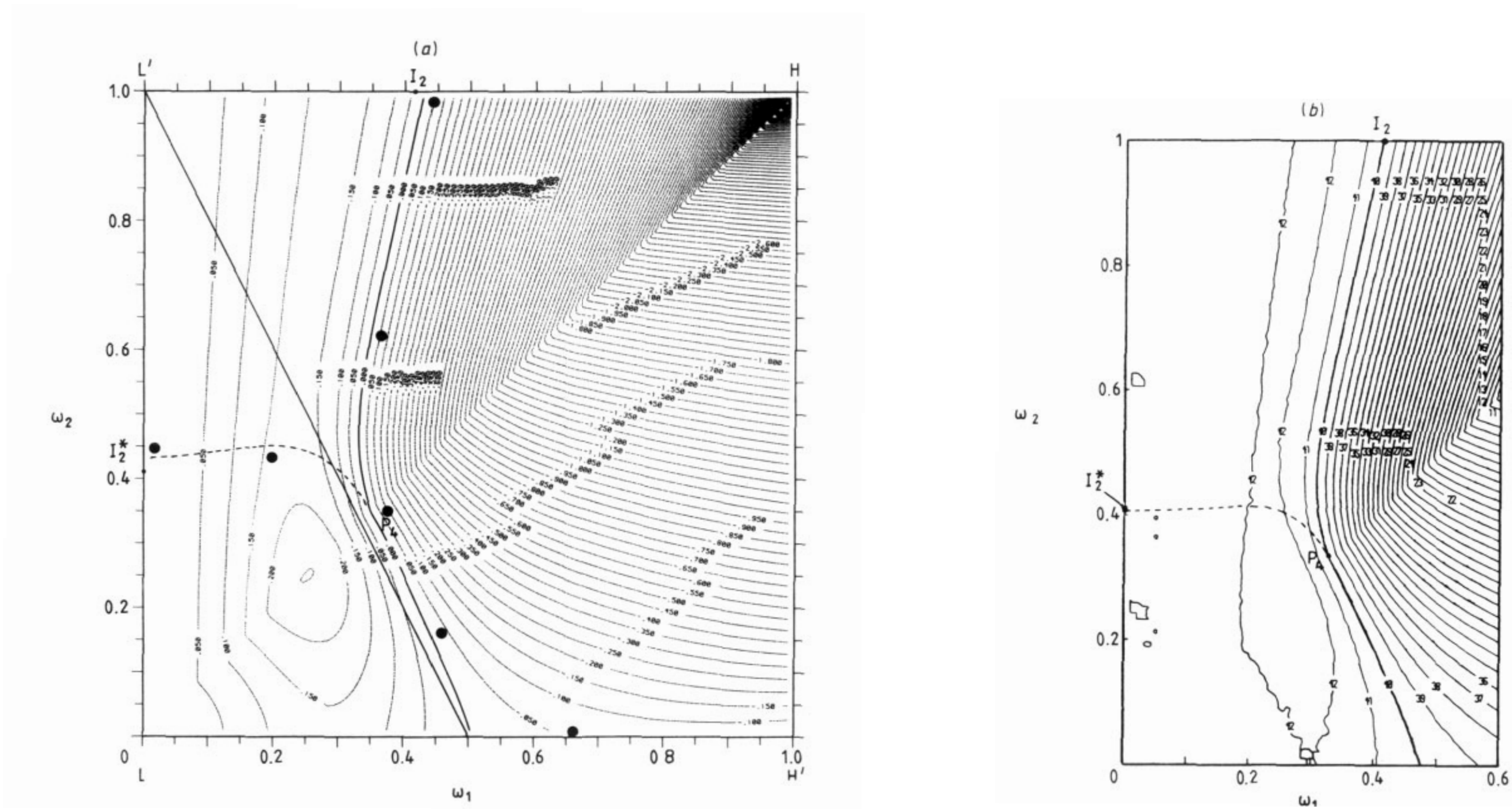


Figure 2. The contours of $\phi_{2,2}(\omega_1, \omega_2)$ (a) and $\phi_{3,2}$ (b) for the Z_4 model. The points marked I_2 and I_2^* are the exact dual pairs on the edges $\omega_1 = 0$ and $\omega_2 = 1$. The zero contour on $\phi_{3,2}$ is labelled 10. The exact scalar Potts critical point lies on the intersection of the dual line and LH, P_4 is the contour's approximation to this point. The broken curve is the zero contour of $\phi_{2,3}$ and $\phi_{2,4}$ (a) and $\phi_{3,3}$, $\phi_{3,4}$ (b) superimposed onto these contours.

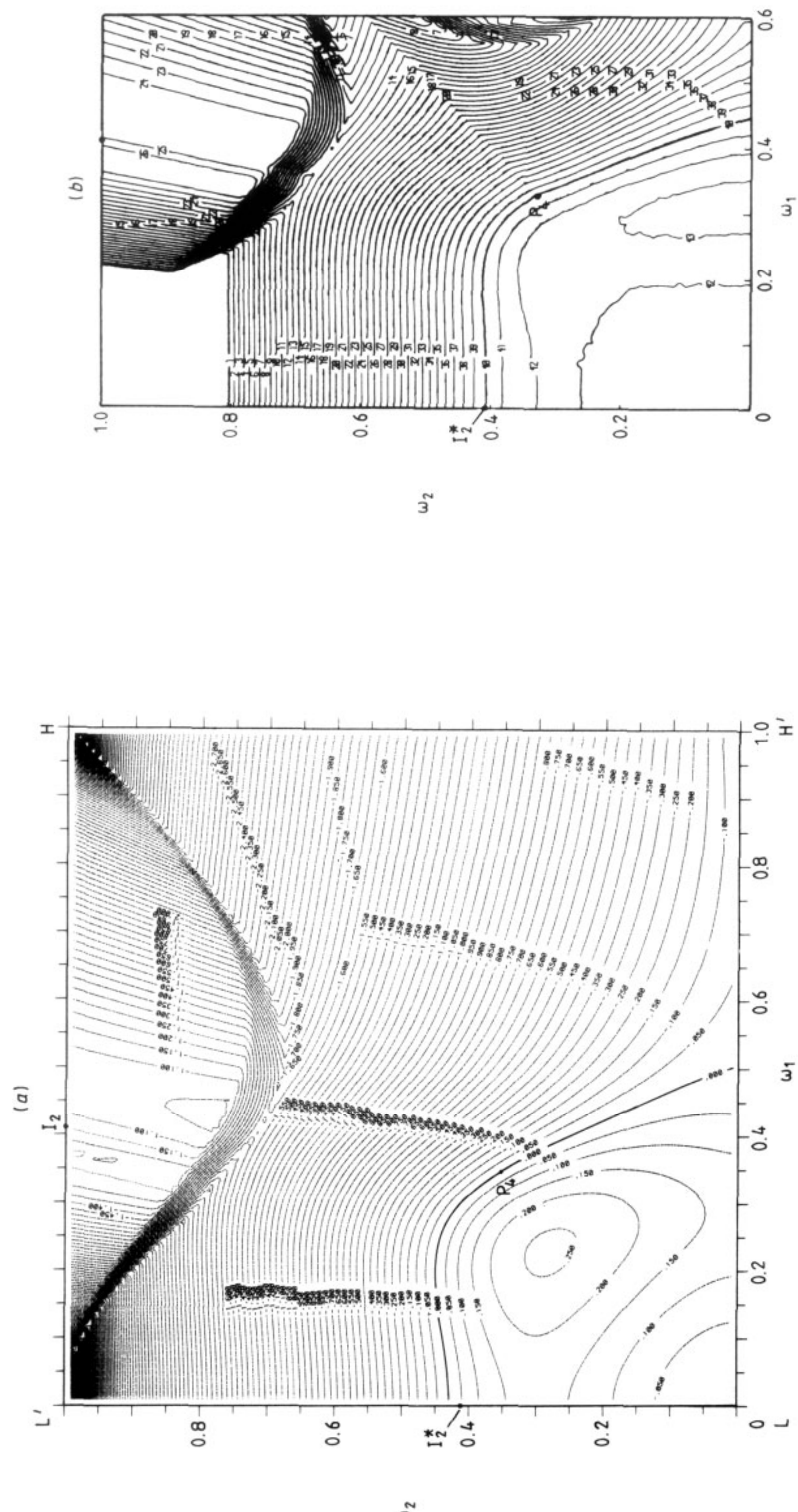


Figure 3. The corresponding cont u·s of $\phi_{2,3}$ and $\phi_{3,3}$ respectively for the Z_4 model The z ro contours approximate the l w temp rature phase boundary.

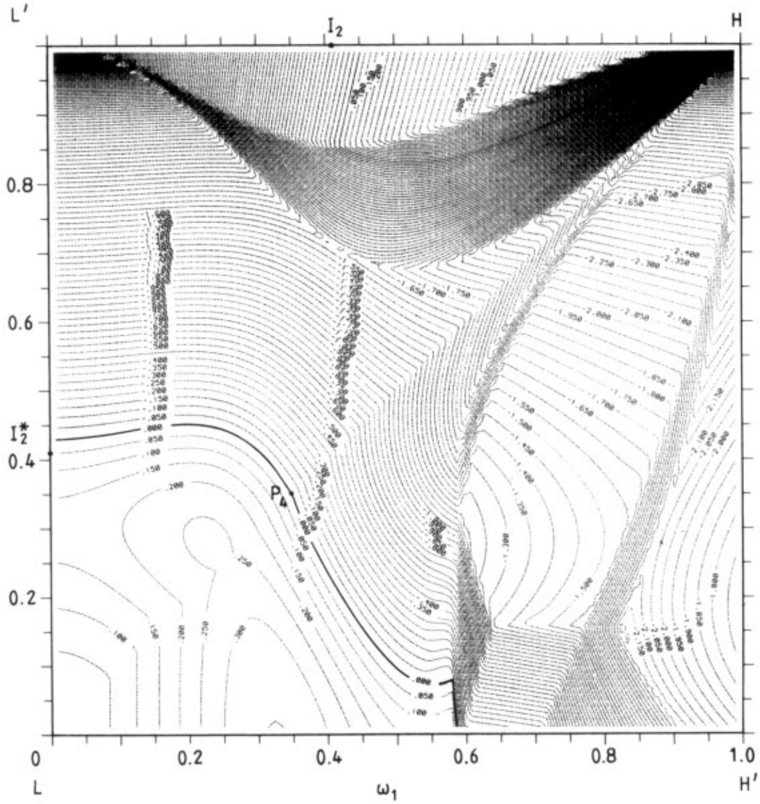


Figure 4. The contours of $\phi_{2,4}$ for the Z_4 model.

the boundary, thus denoting the region where some form of phase coexistence is possible. The contours of the approximants $\phi_{2,3}(\omega_1, \omega_2)$ and $\phi_{3,3}(\omega_1, \omega_2)$ are shown in figure 3 and $\phi_{2,4}(\omega_1, \omega_2)$ in figure 4. These clearly reveal the low-temperature phase boundary, and the low-temperature phase itself (by the broad summit) to be a region of four-fold phase coexistence. Again the contour along the section $P_4I_2^*$ is probably very close to the exact curve, I_2^* marks the exact critical point on the boundary $\omega_1 = 0$. These contours suggest the scalar Potts transition point P_4 to be the bifurcation point of the phase boundary. The zero contours of the approximants with $k = 3$, or 4 are the same along the section $P_4I_2^*$, this is superimposed as a broken line onto figure 2 and the points marked • are the numerical estimates of transition points obtained by Ruján *et al* (1981).

3. Z_5 models

The partition function of the Z_5 model is also in the form of (3), and since the operation $\theta_i \to 2\theta_i$, $i = 1, 2, \ldots, N$ leaves the partition function invariant all properties of the model are invariant to an interchange of ω_1, and ω_2. Consequently the phase diagram will be symmetric about the line $\omega_1 = \omega_2$. The outline form of the phase diagram has been conjectured on the basis of symmetry and generalised duality relations (Wu 1979,

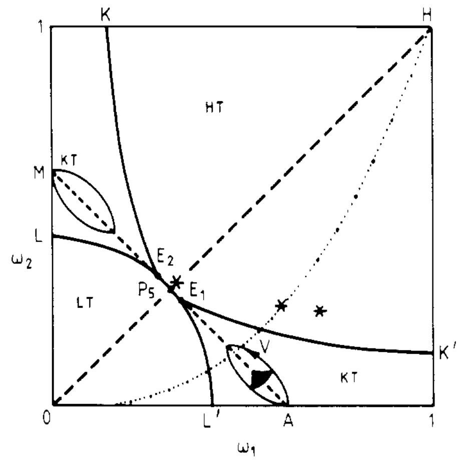


Figure 5. The conjectured form of the phase diagram of the Z_5 model. The scalar Potts model transition at P_5 is the only exactly known point of the diagram. The three phases are marked LT (low temperature), HT (high temperature) and KT phases. AM is the self dual line. HVO is the vector Potts model. The bulb shaped region about the dual line is a possible form of the KT phase suggested by the present work.

Domany *et al* 1980, Cardy 1980, Rujám *et al* 1981) and is summarised in figure 5. The line AM is the self dual line under the relations

$$\omega_1^* = [1 + 2\omega_1 \cos(2\pi/5) + 2\omega_2 \cos(4\pi/5)]/(1 + 2\omega_1 + 2\omega_2) \qquad (6a)$$

$$\omega_2^* = [1 + 2\omega_1 \cos(4\pi/5) + 2\omega_2 \cos(2\pi/5)]/(1 + 2\omega_1 + 2\omega_2) \qquad (6b)$$

where $\cos(2\pi/5) = (\sqrt{5} - 1)/4$, and $\cos(4\pi/5) = -(\sqrt{5} + 1)/4$; these relations map the lower triangle OMA onto the upper triangle HMA. P_5 is the self dual point and is the only exactly known part of the phase surface since it is the first-order transition point in zero field of the five-state scalar Potts model (Baxter 1973). The majority view is that a section of the dual line AM probably forms part of the low-temperature phase boundary between the bifurcation points E_1 and E_2, marking off a line segment of first-order transitions where the ordered and disordered phases can coexist.

The Z_5 model is particularly interesting since it seems likely to be a model where a conventional second-order transition between ordered and disordered phases cannot occur. The third phase of Σ is shown schematically in figure 5 bounded by the low- and high-temperature (LT and HT) phase boundaries L'E$_1$ and K'E$_1$ respectively, and is the KT massless phase where $M_1 = M_2 = 0$, and is distinguished by spatial correlations which decay algebraically, not exponentially. The existence of three phases for Z_p models where $p \geq 5$ has been proved by Cardy (1980) who gave a lower bound to the extension of this phase; in the case of Z_5 this is shown schematically by the shaded region on figure 5. The conjectured boundaries of the KT phase are dual curves along which the transitions are of infinite order, and the whole KT phase maps into itself under the duality relations (6).

The only attempts known to the authors to obtain numerical estimates of points on the phase boundaries in figure 5 are the Migdal–Kadanoff RG calculations of Rujján *et al* (1980) who obtained the points marked * as upper bounds to the KT phase boundary. To test the qualitative outline form of Σ shown in figure 5 Ruján *et al* carried out calculations near to the edge $\omega_1 = 1$ but found *no* evidence of a transition.

They concluded that the KT phase probably did not exist. Our calculations reveal precisely these features along this boundary but point to a different conclusion.

In the present technique we would expect the approximants $\phi_{n,2}$ to converge to the high-temperature phase boundary KP_5K' and the sequence $\phi_{n,5}$ to approximate the low-temperature boundary LP_5L'. In fact the contours of $\phi_{n,5}$ and $\phi_{n,4}$ reveal only minor differences and those of $\phi_{n,2}$ and $\phi_{n,3}$ are identical. The contour maps for $n=2$, and 3 are shown in figures 6 and 7. The close packing of contours in $\phi_{2,2}$ and $\phi_{3,2}$ ends abruptly in the neighbourhood of the contour at -0.01, beyond which the hillside flattens off very rapidly. A new numerical feature appears in these contours, this is the evident instability of the zero contour to small changes in the value of the approximant in the neighbourhood of zero. This effect has tightened up a little between $\phi_{2,2}$ and $\phi_{2,3}$ but in both cases is most pronounced in precisely the region where the KT phase is thought to be. The feature of a single line segment (Domany *et al* 1980) E_1E_2 in figure 5 is clearly supported by these contours; the zeros of $\phi_{3,4}$ and $\phi_{3,2}$ are indistinguishable up to the points marked E_1 and E_2 on figure 6. The contour maps of $\phi_{2,3}$ (and $\phi_{3,3}$) are identical to those of $\phi_{2,2}$ (and $\phi_{3,2}$) in figure 6 which suggests that the sequence $\phi_{n,3}$ will converge onto the HT–KT phase boundary; this is a very interesting feature. The authors had expected that $\phi_{n,3}$, $\phi_{n,4}$ and $\phi_{n,5}$ would all approximate the LT–KT phase boundary (compare Z_4).

The KT phase has been given a spin configurational characterisation by Einhorn *et al* (1980) in the form of vortex-antivortex pair dissociation. The fact that the zero contours of $\phi_{2,3}$ and $\phi_{3,3}$ separate off from the LT phase boundary suggests that the KT phase has a threefold characterisation. Following Einhorn *et al* (1980) excitations in the LT phase are either domains of sites with the same orientation (the boundaries of which are known as strings) or vortex pairs which are tightly bound with energies proportional to the vortex-antivortex separation. The low-temperature transition is a condensation of strings and as such should be represented in the zero contours of $\phi_{2,5}$ and probably $\phi_{2,4}$ characterising the fivefold phase coexistence in the low-temperature phase. The condensation of strings and the dissociation of vortex pairs occur at different temperatures, hence the appearance of the KT phase, the HT boundary of which is characterised by the dissociation of vortex pairs. A typical vortex pair in Z_5 is shown schematically in figure 5 (the angular states are numbered $1, \ldots, 5$). If we fix a characteristic excitation energy of a pair, then there are three configurational types possible in Z_5, these are the five, four, and three line pairs shown in figure 8. The pairs in figure 8(b) and (c) contain islands with angular separations of $4\pi/5$ from their neighbours. We advance the interpretation that the separation of the $\phi_{2,3}$ and $\phi_{3,3}$ zero contours onto the HT–KT phase boundary reflects the threefold degeneracy of vortex pairs in the Z_5 model. In the neighbourhood of the edges $\omega_2=0$ and $\omega_1=0$ a large asymmetry in the potentials $V(2\pi/5)$ and $V(4\pi/5)$ exists, which will progressively distort the vortex pairs of four and three lines until on the boundary lines these pairs cannot form. In addition the pairs in figure 8(a) cannot be formed on a square net when ω_1 or ω_2 is zero. It follows from this that the intersection of the HT phase boundary and the line $\omega_2=0$ is a termination point of this threefold characterisation of the KT phase which cannot exist along this line. Our conjecture based upon these calculations is that the LT, KT, and HT phases all meet in the end point of the dual line, and that along $\omega_2=0$ there is a fivefold coexisting LT phase along OA with a transition into a disordered phase at A. There are only slight differences between the contours for $k=4$ and 5, the former for $n=2$, and 3 are shown in figure 7. The boundary depicted in $\phi_{3,4}$ has been depressed closer to the lines $\omega_1=0$ and $\omega_2=0$.

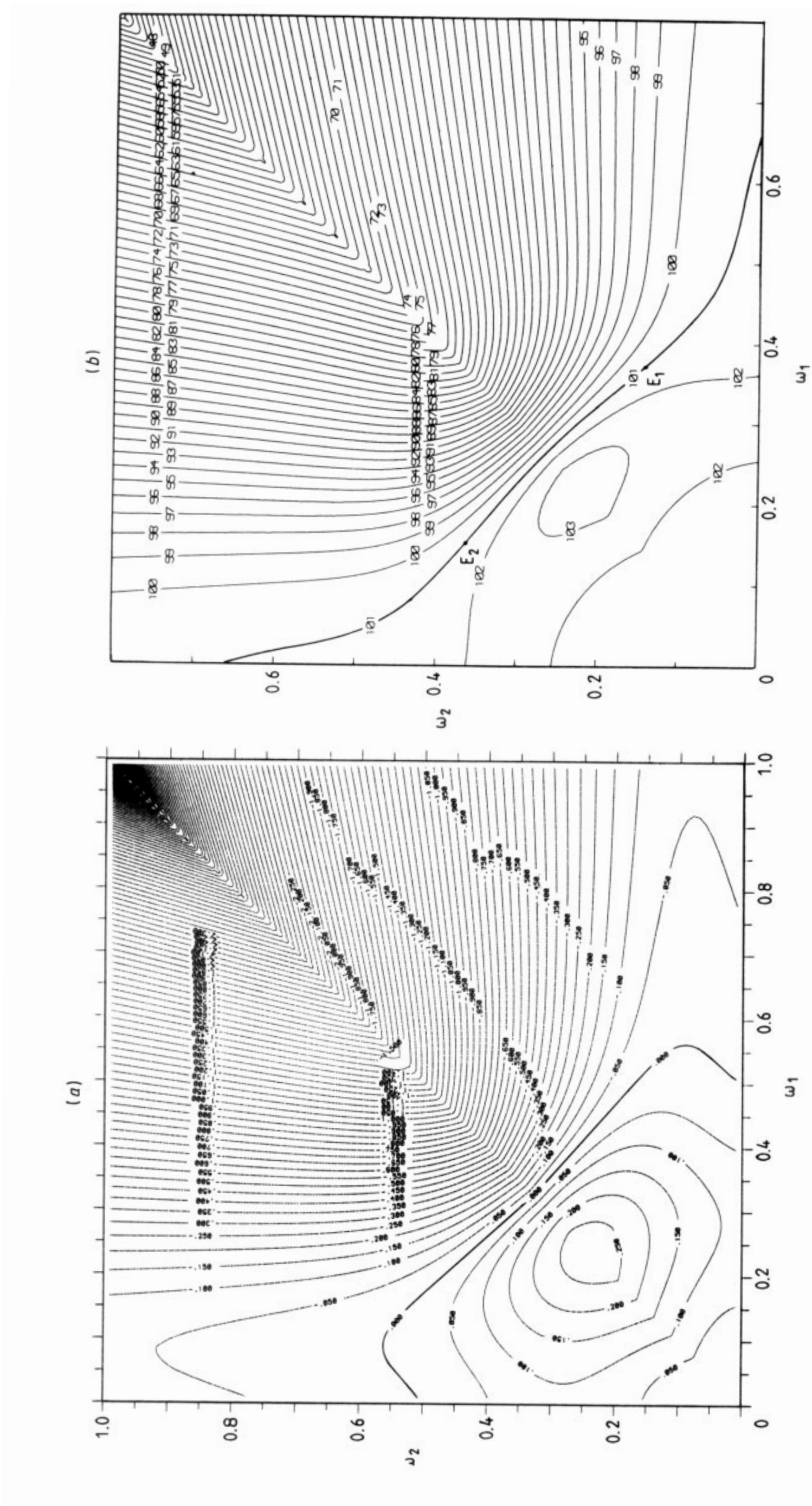


Figure 6. The cont urs f $\phi_{2\,2}$ and $\phi_{3,2}$ for the Z_5 model. The z ro contour of $\phi_{3\,2}$ is labelled 101

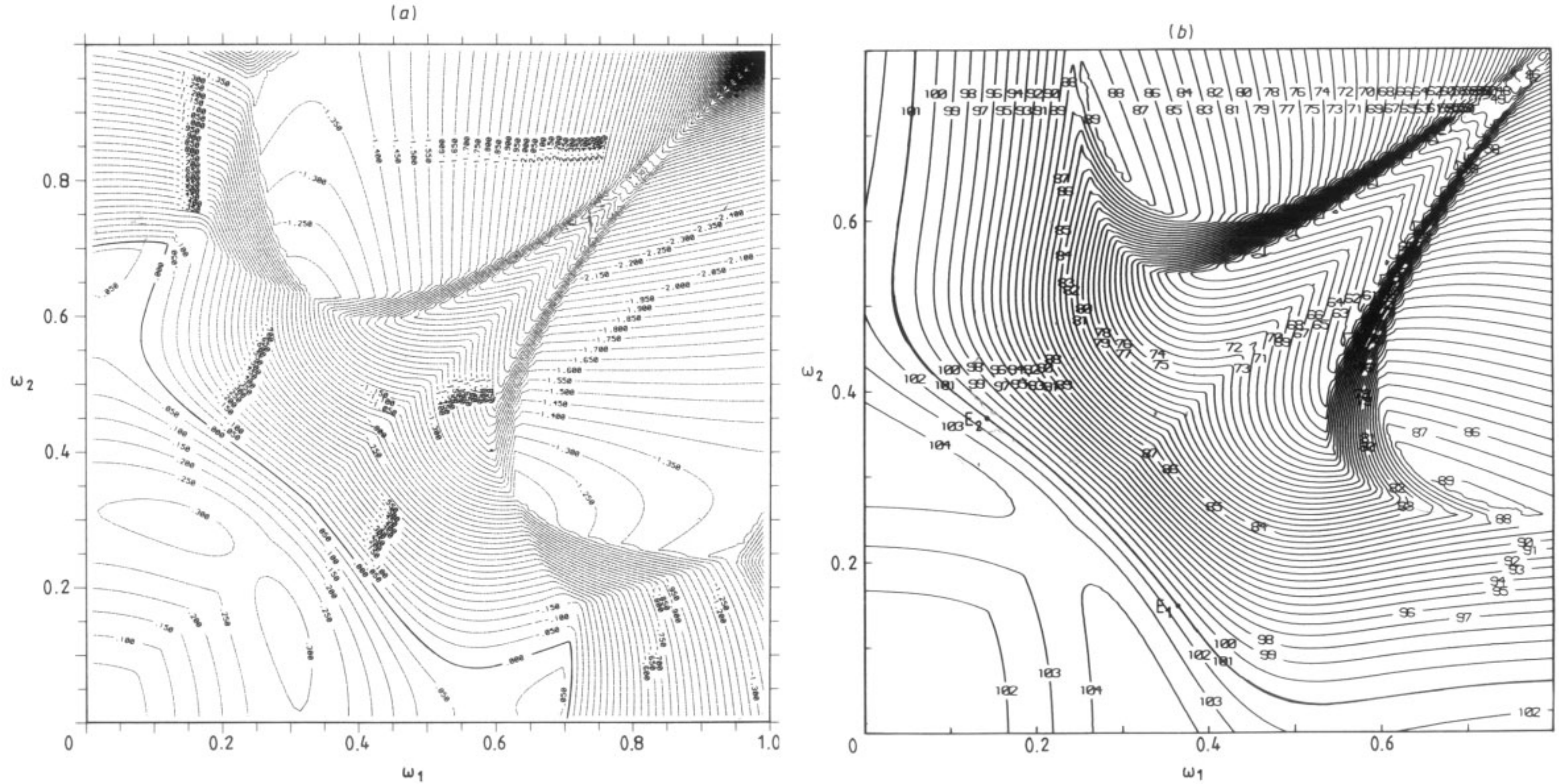


Figure 7. The contours of $\phi_{2,4}$ and $\phi_{3,4}$ for the Z_5 model. The zero contours approximate the low-temperature phase boundary and a possible coexistence with the disordered phase (corresponding to the section E_1E_2 in figure 5) respectively, the zero contour of $\phi_{3,4}$ is labelled 101, and the contour continues smoothly to intersect the edge at $\omega_1 = 1$.

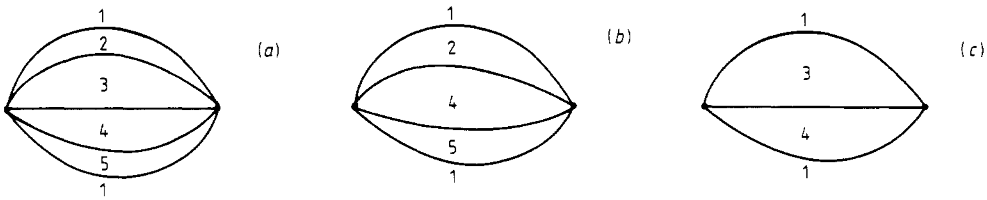


Figure 8. The three types of vortex–antivortex pairs which can be formed in the Z_5 model.

Our intepretation of these contours is that the LT phase boundary will ultimately intersect the axes ω_1, and ω_2 and that in view of the above the LT and HT phases will meet at the end of the dual line; thus our view of the phase diagram is represented by the bulb shaped region shown in figure 5; we think it particularly significant that no transition of any type is detected on the lines $\omega_1 = 1$, and $\omega_2 = 0$ (see also Ruján *et al* 1981).

An alternative view of the KT phase giving some evidence of its existence can be obtained by giving a specific Z_5 model some form of single site ordering field. We have taken the special case of the vector Potts model in a field h with a Hamiltonian

$$= -J\sum_{ij}\cos(\theta_i - \theta_j) - h\sum_i \cos\theta_i \qquad J > 0. \tag{7}$$

In zero field the model lies along the thermodynamic trajectory $\omega_1 = \omega_2^{(3-\sqrt{5})/2}$ and is shown in figure 5. In the limit $h \to -\infty$ the model reduces to a simple zero field Ising model in which two coexisting phases are phases of preferred alignment along $\theta_i = 4\pi/5$ and $6\pi/5$ with a critical point at $2K_c$ (Ising)/$[1-\cos(2\pi/5)] = 1.275\ldots$. The contours of $\phi_{2,2}(K, h)$ are shown in figure 9, and as expected the zero contour marks off a region of two phase coexistence inside $h < 0$, in which the two phases are perturbed versions of the phases at $h = -\infty$ whose exact critical point is marked at A. Here again the location of the contours inside ± 0.05 are quite sensitive to the values of the approximant, however an entirely new feature is the very pronounced lobe-like extension centred on the zero field axis (compare the corresponding scalar Potts models, Wood and Osbaldestin (1983)). A schematic interpretation of the exact phase boundary which the zero contour represents is drawn on figure 9 (broken curve), where the section BC is the KT phase.

4. Three-body interactions on the triangular lattice

Here we consider a generalisation of the Ising model which incorporates three spin terms into the Hamiltonian in the form

$$= -J_2\sum_{ij}\sigma_i\sigma_j - J_3\sum_{ijk}\sigma_i\sigma_j\sigma_k - H\sum_i \sigma_i \qquad J_{2,3} > 0 \tag{8}$$

where the variables σ_i are Ising-like with values ± 1, and the interactions J_2 and J_3 are on nearest-neighbour pairs and nearest-neighbour triangles respectively. The pure triplet model ($J_2 = 0$) in zero field has been solved exactly by Baxter and Wu (1973, 1974), other studies of mixed interactions have used series expansions and real space renormalisation techniques (Wood and Griffiths 1974, Griffiths and Wood 1973, Barber 1976, Imbro and Hemmer 1976). Baxter and Enting (1976) showed that the pure triplet

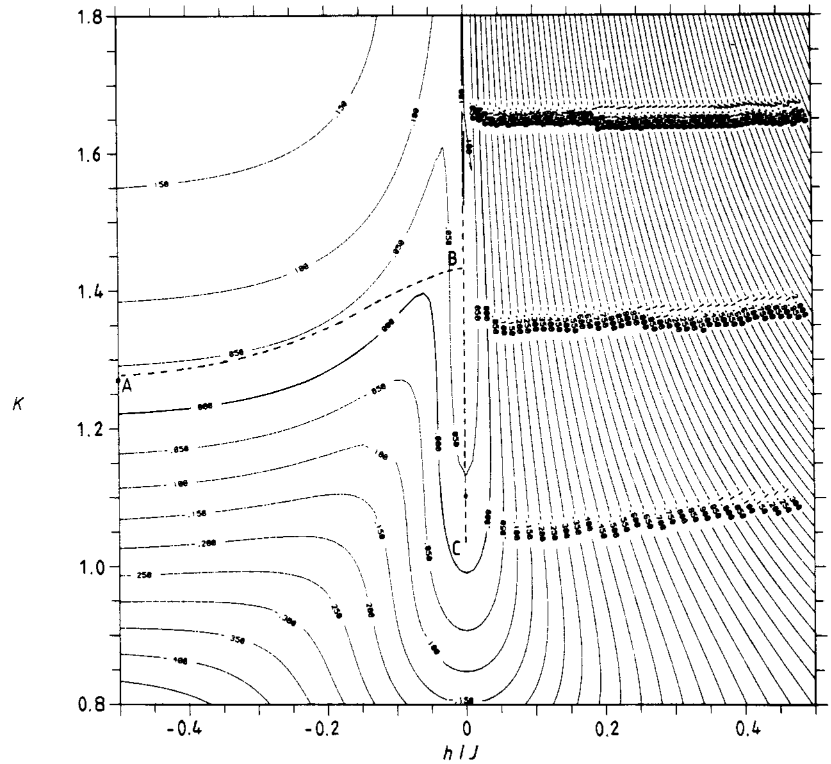


Figure 9. The contours of the vector Potts model in a field h. The large lobe-like extension near to the zero field axis denotes the effect of the KT phase. A is the exact critical point at $h = -\infty$ and the broken curve is a schematic representation of the exact phase diagram.

model is a special case of the symmetric eight-vertex model, and vertex model representations and duality properties of triplet models have been discussed by Wood and Pegg (1977). No exact information of the phase equilibrium of the triplet model in relation to its ordering field H or the pair field J_2 is known.

The exact solution of the pure triplet model in zero field reveals a single critical point at the self dual point $K_{3,c}(=\beta J_3) = 0.440\,68\ldots$ where $\langle\sigma_i\rangle = 0$, $K_3 \leq K_{3,c}$. The model does *not* have inversion symmetry, the zero field low-temperature ground state is fourfold degenerate; the four ground state configurations are shown in figure 10, these characterise the four coexisting phases below the critical point. In a small negative field these states split, the three phases characterised by spin reversals on two of the three equivalent sublattices (figures 10(b), (c), and (d)) remain degenerate and characterise a region of three phase coexistence which opens up in the negative field region. At zero temperature there is a critical field at $H = -6J_3$ beyond which the ground state has all spins reversed ($\sigma_i = -1$), hence we expect $h = -6J_3$ to be the end point of a line of critical points inside the negative field region bordering a sheet of three phase coexistence.

All of these features are beautifully revealed in the scaling contours shown in figure 11. The approximants in this case must be constructed using $3n \times \infty$ strips, this preserves the ground state symmetries on finite systems. The approximants $\phi_{3,k}(K_2, K_3, H)$ have been formed using the transfer matrices of $6 \times \infty$ and $3 \times \infty$ strips. The contours of

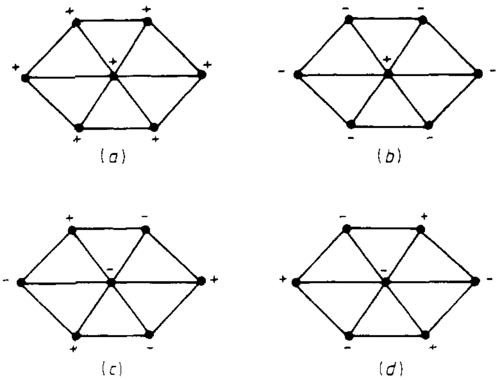


Figure 10. The four zero temperature ground state configurations of the pure triplet model on a triangular lattice.

$\phi_{3,2}$ and $\phi_{3,3}$ are practically indistinguishable, and give an amazingly clear resolution (in intervals of 0.5) of the region of three phase coexistence (figure 11(*a*)). The zero field edge of this region terminates almost exactly at the correct critical point. The contours of $\phi_{3,4}$ in figure 11(*b*) represent the fourfold phase coexistence along $H = 0$ by a thin hairline loop almost exactly equal to the coexistence line. In figure 11(*b*) the scale has been enlarged to show the loop. This has cut off the appearance of a rogue zero contour inside the three phase region (such contours are also seen in figure 4). It differs from the contours which have so far represented boundaries of phase coexistence in that it lies on the 'hillside' and does not form an edge to a plateau or broad summit. However we have no rationale for labelling this contour or those in figure 4 as spurious.

The contours in figure 11 for the case of a mixed Hamiltonian at the ratio $\gamma = J_2/J_3 = \frac{1}{3}$ are shown in figure 12. The Hamiltonian (6) retains the fourfold degenerate ground state shown in figure 10 at a value of the field given by $H = -J_3$; for $H > -J_3$ figure 10(*a*) is the ground state. In general if $\gamma > 0$ it is simple to show that for $\gamma < \frac{2}{3}$ the ground state is fourfold degenerate at $H = -3\gamma J_3$, and that in the region $-6J_3(1-\gamma) < H < -3\gamma J_3$ the ground state is threefold degenerate through the states in figure 10(*b*), (*c*), and (*d*). The phase structure revealed in the case $\gamma = \frac{1}{3}$ shows a copy of the pure triplet case but of reduced size. The remarkable feature is the preservation of a fourfold phase coexistence *line* at the constant field value $H = -3J_2$. It would certainly appear that at this value of γ the model is equivalent to the pure triplet model but in a critical field $H = -3J_2$ and with a reduced critical temperature. The observation here rather suggests that the critical behaviour of the mixed Hamiltonian is likely to remain that of the pure triplet model with an effective translational shift to small negative fields, which seems to conflict with conclusions reached in renormalisation group studies.

We have performed numerous calculations in which the nearest-neighbour coupling J_2 is antiferromagnetic, some of these are shown in figure 13 where the contours obtained from $\phi_{3,2}$ and $\phi_{3,3}$ are identical, hence in every case the large plateau humps represent regions of three phase coexistence. It is well known that the simple antiferromagnetic Ising model on a triangular lattice has no critical or phase coexistence at $H = 0$ (Domb 1974) and that the ground state is infinitely degenerate. For $H \neq 0$ the ground states are the three configurations in figures 10(*b*), (*c*) and (*d*) when $H < 0$, and their spin inversions when $H > 0$. The critical fields for zero temperature transitions

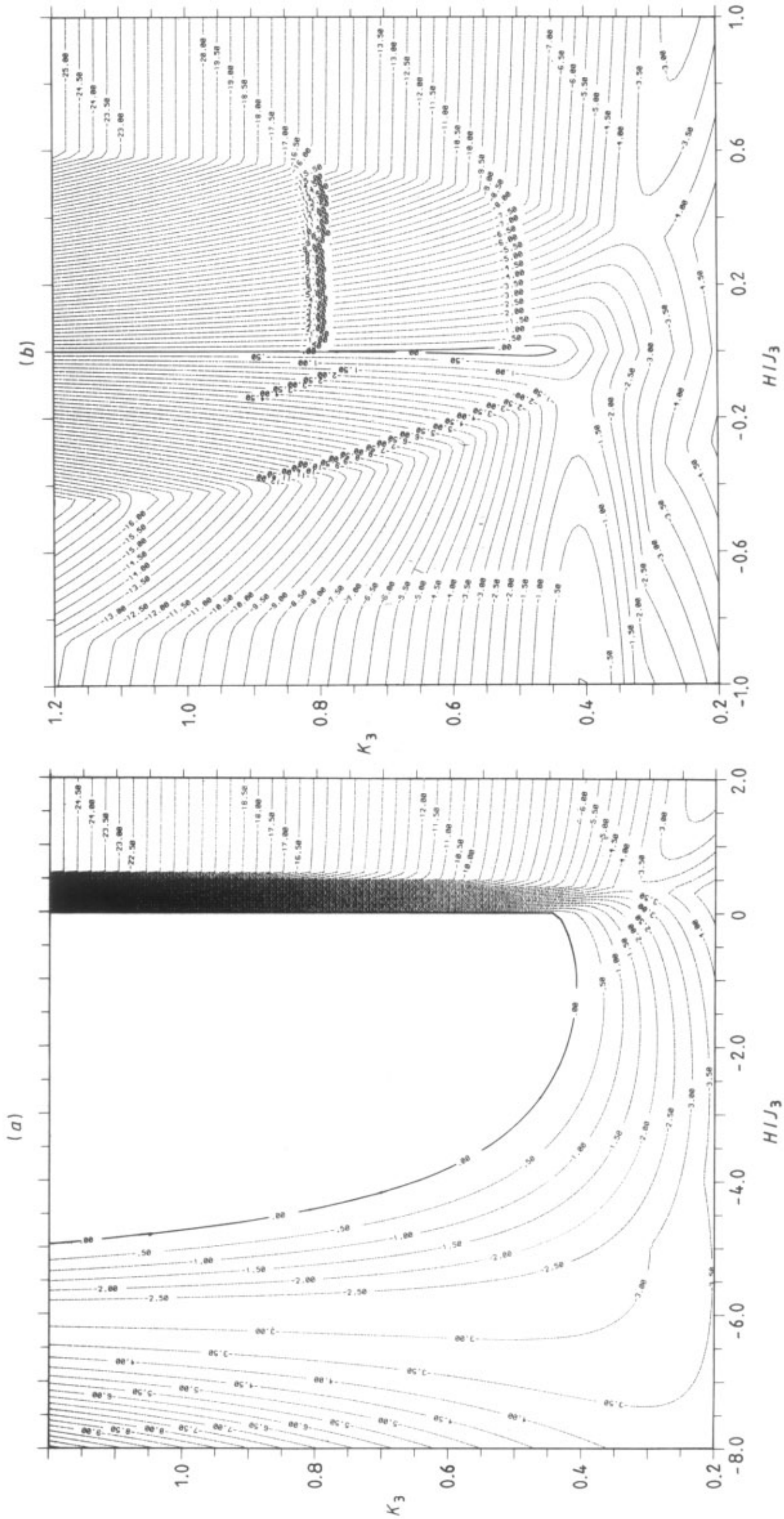


Figure 11. (a) The contours of $\phi_{3,2}$ for the pure triplet model in a field, obtained from $6\times\infty$ and $3\times\infty$ strips. The zero contour encloses a region of three phase coexistence. (b) The contours of $\phi_{3,4}$ for the pure triplet model, the fourfold phase coexistence in zero field is almost exactly represented by the hairpin loop enclosing a section of the zero field axis.

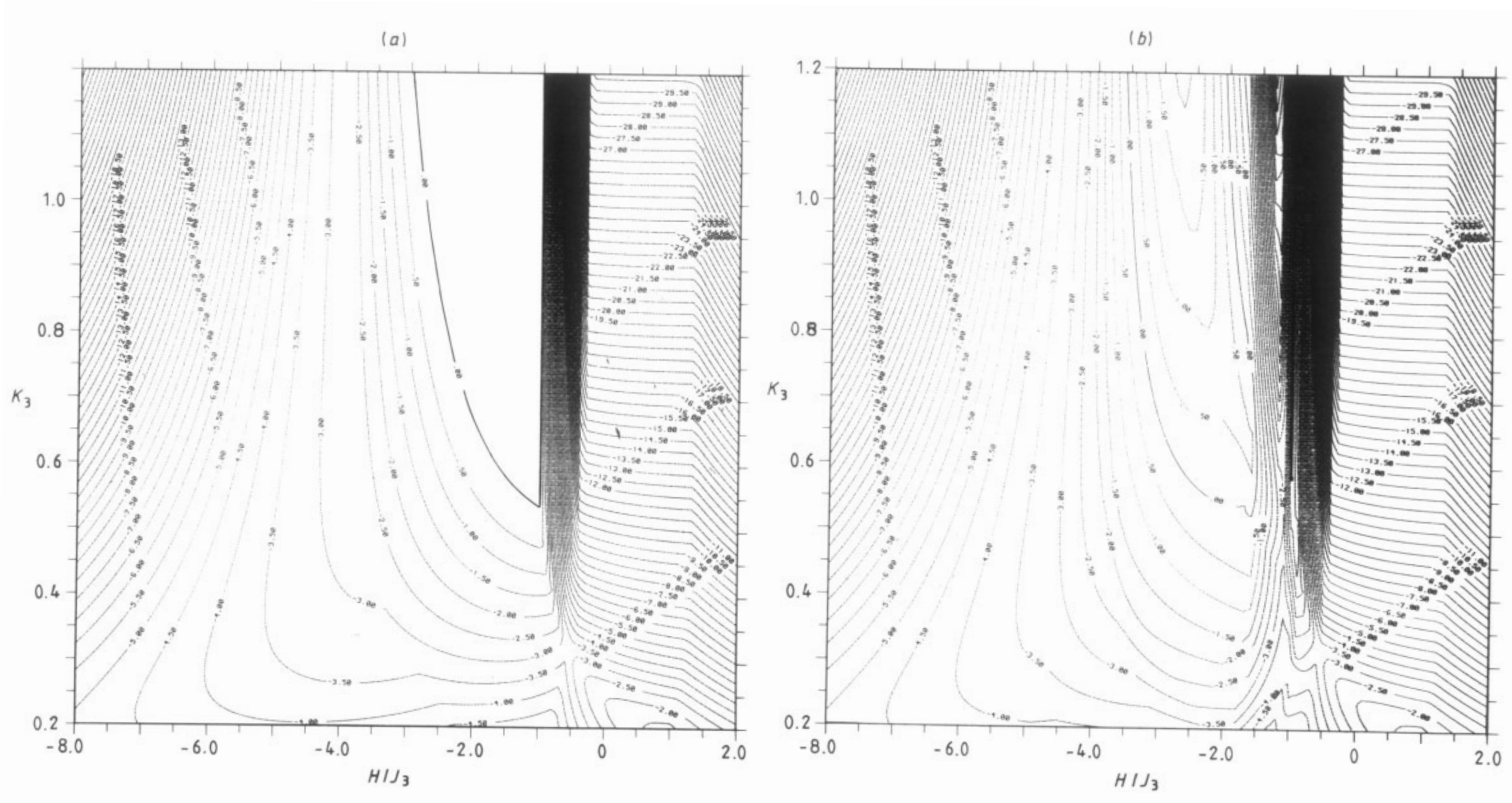
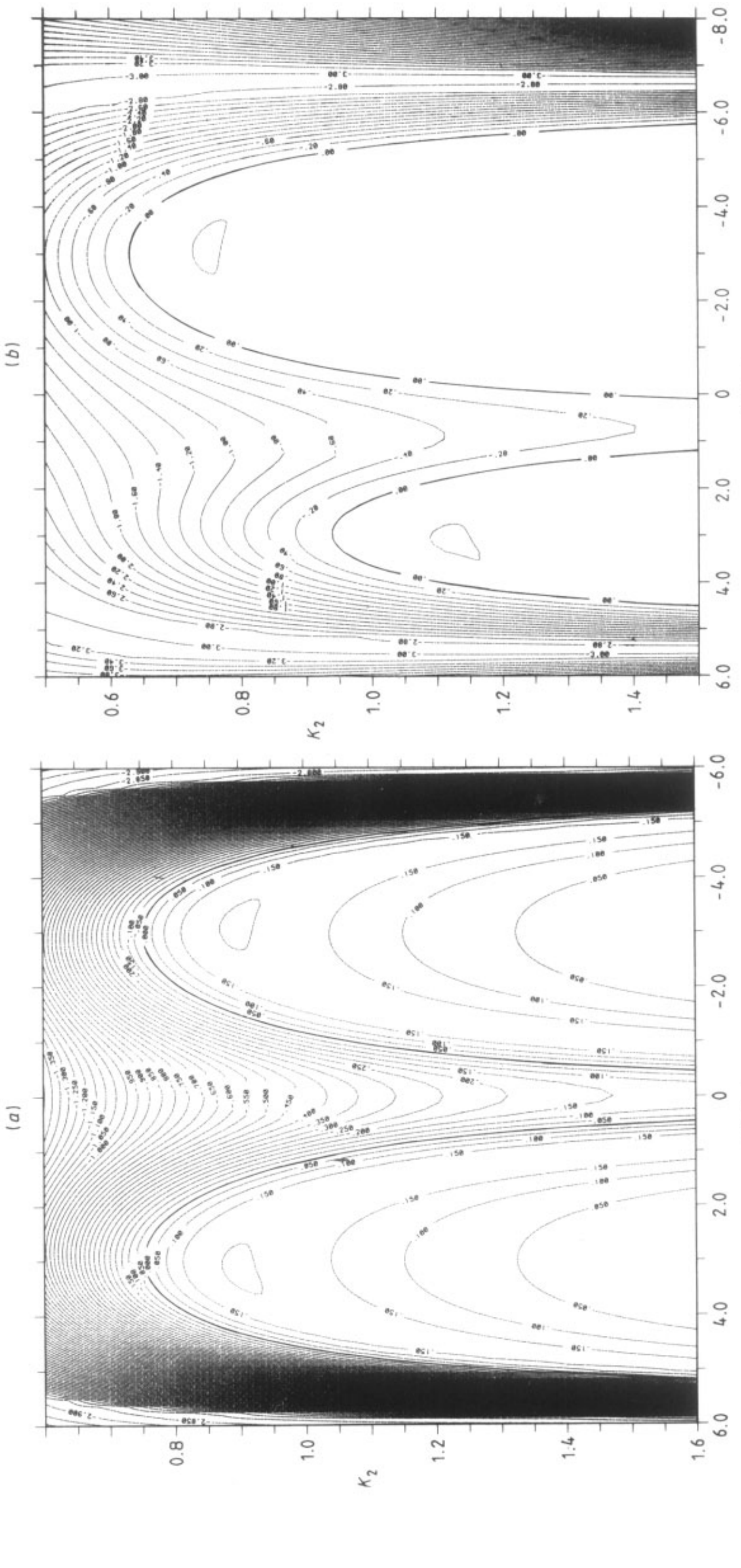


Figure 12. The contours corresponding to those f the pure triplet model in **figure** 11 for the case f a mi ed interaction at $J_2/J_3=\frac{1}{3}$


(a)
(b)
K2
H/|J2|

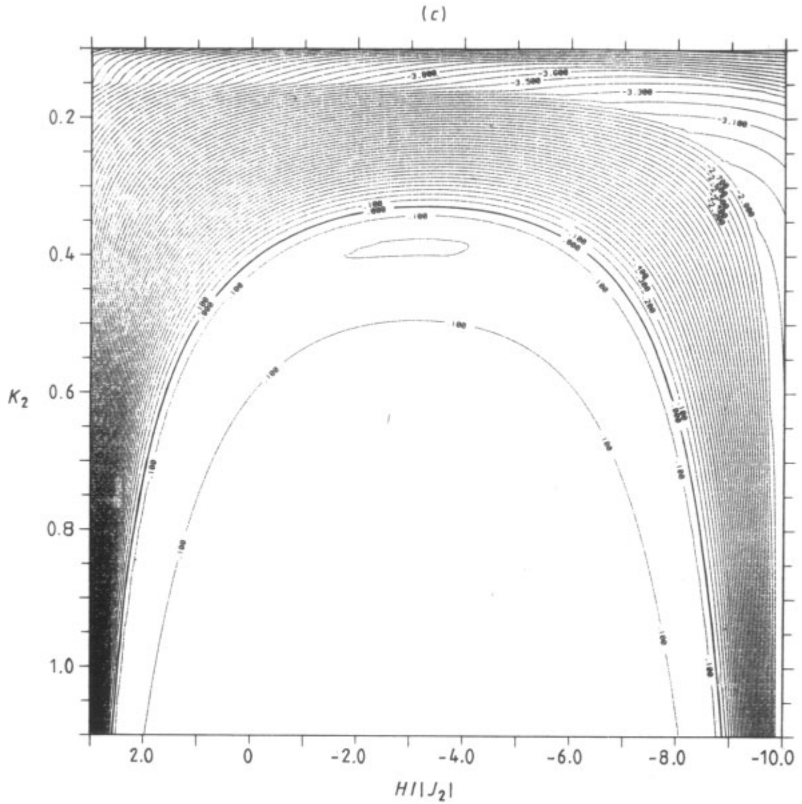


Figure 13. (*a*) The contours of $\phi_{3,2}$ and $\phi_{3,3}$ for the simple antiferromagnetic Ising model on a triangular lattice. The two humps in non-zero field mark off regions of three phase coexistence. (*b*) The contours of $\phi_{3,2}$ and $\phi_{3,3}$ for the mixed antiferromagnetic model with $J_3/|J_2| = 1/10$. The hump lying inside the positive field moves further into the positive field region, and diminishes in size. (*c*) The contours of $\phi_{3,2}$ and $\phi_{3,3}$ for the mixed antiferromagnetic model with $J_3/|J_2| = \frac{2}{3}$. The spin inversion transition between the two regions of three phase coexistence has vanished, a single three phase region remains characterised by the configurations corresponding to the region inside the negative field in (*a*).

into states of all spins positive or negative are at $H = \pm 6J_2$. Figure 13(*a*) reveals all of these features very clearly. The critical line of order-disorder transitions has been studied by Kinzel and Schick (1981). A triplet spin field removes the multiple degeneracy of the ground state in zero field which is now threefold degenerate. The two humps of figure 13(*a*) remain in the phase diagram when $J_3/|J_2| < \frac{1}{2}$ and $J_3 > 0$; the area of coexistence lying within a positive field shrinks with increasing J_3 and vanishes altogether at $J_3/|J_2| = \frac{1}{2}$. These features are illustrated by the contours in figure 13(*b*) at $J_3/|J_2| = 1/10$; at $T = 0$ the critical fields are given by $H/|J_2| = -6(1 - J_3/|J_2|)$, and $6(1 + J_3/|J_2|)$, and the spin inversion transition between the two areas of three phase coexistence occurs at $H = 6J_3$ ($J_3/|J_2| < \frac{1}{2}$). The phase diagram for $J_3/|J_2| = \frac{2}{3}$ is shown in the contours of figure 13(*c*), the spin inversion transition has now vanished, phase coexistence originally inside the negative field hump has taken over the whole phase equilibrium surface.

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