# Multiple phase coexistence and the scaling transformation



1983 J. Phys. A: Math. Gen. 16 1019

(http://iopscience.iop.org/0305-4470/16/5/020)

J. Phys. A: Math. Gen. 16 (1983) 1019–1033. Printed in Great Britain

# Multiple phase coexistence and the scaling transformation

D W Wood and A H Osbaldestin

Mathematics Department, University of Nottingham, Nottingham, NG7 2RD, UK

Received 23 September 1982

**Abstract.** It is shown that a simple extension of the finite size scaling method in the theory of critical phenomena can yield a sequence of approximants to any point subset of the interaction parameter space where multiple phase coexistence is possible. The method is illustrated by an application to the three-, four- and five-state Potts models, and even in its lowest order of approximation is able to distinguish the difference in the zero-field critical behaviour between the five-state and the three- and four-state models.

## 1. Introduction

The present authors (Wood and Osbaldestin 1982) have shown how the scaling transformation of Kadanoff (Kadanoff *et al* 1967), when adapted for use on semi-infinite lattice model systems (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, Goldfinch and Wood 1982, Blöte and Nightingale 1982), naturally yields a sequence of approximants to the entire phase equilibrium surface of the model in the space of its interaction parameters. The calculations of Wood and Osbaldestin on the two-dimensional Ising and Potts models show that even in the lowest order the approximants yield a coexistence surface $\Sigma$ close to the exact limiting surface. The method has also been demonstrated in a subsequent calculation by Osbaldestin and Wood (1982), who have obtained the form of the phase equilibrium surface of the three-state antiferromagnetic Potts model in the presence of its ordering fields

Once the outline form of $\Sigma$ has been fully obtained in such calculations, one can of course identify subsets of points of $\Sigma$ where various forms of multiple phase coexistence are possible. In constructing phase equilibrium surfaces from calculations of this type where there may be several interaction parameters, it would clearly be very helpful to be able to project independently out of $\Sigma$ the various point subsets on which multiple phase coexistence is possible. Such a technique would also be of interest in its own right. The purpose of the present paper is to show that the scaling transformation and the general technique of the method can be simply extended to provide approximants for each point subset of $\Sigma$ where a given order of multiple coexistence is possible.

The theoretical background to this extension of the finite size scaling calculations is given in § 2, and is then illustrated in § 3 with specific calculations on the three-, four- and five-state ferromagnetic Potts models in their ordering fields (for a review of the Potts model see Wu (1982)). Previous studies of Potts models using finite lattice calculations have been made by Hamer and Barber (1981), Roomany and Wyld

(1980), Hamer (1981) and Herrman (1981). These calculations have been performed in the lowest order of approximation which the technique will allow, and in every case the appropriate point subsets of $\Sigma$ where multiple coexistence is possible are clearly indicated. Some of the boundary points of these subsets are known exactly, and even the lowest approximants seem to yield very good approximations to these points. The results for the five-state Potts model show how powerful the technique is. For the ferromagnetic Potts models all the phase transitions in zero field are first order for $q>4$ (Baxter 1973), and thus along the zero-field line in the five-state model we expect to see just one point where the disordered phase can coexist with the five varieties of ordered phase; this is a point of sixfold phase coexistence. The technique described here faithfully represents this phenomenon, and is thus able to identify the difference in critical behaviour between the $q<5$ and the $q\geqslant 5$ Potts models.

## 2. Coexistence and degeneracy

A general mathematical mechanism to describe a phase transition originally advanced by Kac (1968) is the construction of a linear operator from the Hamiltonian, the largest eigenvalue of which yields the thermodynamic free energy density. Kac argues that the degeneracy of this eigenvalue can be quite generally associated with a phase transition, and marks the appearance of two stable macroscopic states. Kac's illustrations of this view were on long-range force models, where specific types of pair potentials on lattice models naturally produced the above operator as the kernel of a Hilbert–Schmidt integral equation (for a review see Hemmer and Lebowitz (1976)). For latttice model Hamiltonians with short-range forces this operator is the transfer matrix (for reviews of these methods see Lieb and Wu (1972), Thompson (1972) and Wood (1975); for an account of asymptotic degeneracy see Domb (1960)).

Consider an $N$-site lattice model subdivided into a one-dimensional sequence of subsystems of $n$ sites; for example, the successive columns of a square net lattice form such a sequence. If we denote and index the spin configurations of two neighbouring subsystems by $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$ then the transfer matrix elements are given by

$$T_{\sigma,\sigma'}=\exp\{-\beta[U(\boldsymbol{\sigma})/2+U(\boldsymbol{\sigma}')/2+W(\boldsymbol{\sigma},\boldsymbol{\sigma}')]\} \qquad (\beta=1/kT) \quad (1)$$

where $W(\boldsymbol{\sigma},\boldsymbol{\sigma}')$ is the interaction energy between neighbouring subsystems in configurations $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$ and $U(\boldsymbol{\sigma})$ and $U(\boldsymbol{\sigma}')$ are the self-energies of each subsystem. The partition function $Z_N$ and the free energy $F_N$ are given by

$$-\beta F_N(\boldsymbol{K})=\ln Z_N(\boldsymbol{K})=\ln[\lambda_1^{N/n}(\boldsymbol{K})+\lambda_2^{N/n}(\boldsymbol{K})+\ldots+\lambda_\Omega^{N/n}\boldsymbol{K})] \quad (2)$$

where $\Omega$ is the number of configurations possible in a subsystem, and $\boldsymbol{K}$ is the set of reduced interaction parameters of the model. In regions of $\boldsymbol{K}$ space where the largest eigenvalue of $T$ is asymptotically non-degenerate in the thermodynamic limit $(N,n)\to\infty$, the free energy density $f(\boldsymbol{K})$ is given by

$$\beta f(\boldsymbol{K})=\lim_{N\to\infty}\frac{1}{N}\ln Z_N(\boldsymbol{K})=\lim_{n\to\infty}\frac{1}{n}\ln\lambda_1(\boldsymbol{K}) \quad (3)$$

where $\lambda_1$ is the largest eigenvalue of $T$. The probability $P_n(\boldsymbol{\sigma})$ that the $n$ sites of a given subsystem will be in a specific spin configuration $\boldsymbol{\sigma}$ is given by

$$P_n(\boldsymbol{\sigma}) = \sum_j^{\Omega} \lambda_j^{N/n} \varphi_j(\boldsymbol{\sigma})^2 / Z_N \qquad (\lambda_1 > \lambda_2 \geqslant \lambda_3 \geqslant \ldots), \tag{4}$$

where $\varphi_j(\boldsymbol{\sigma})$ are the elements of the eigenvector $\varphi_j$ corresponding to the eigenvalue $\lambda_j$. In the above non-degenerate subspace of $\boldsymbol{K}$

$$\lim_{N\to\infty} P_n(\boldsymbol{\sigma}) = \varphi_1(\boldsymbol{\sigma})^2. \tag{5}$$

Suppose we take a point in $\boldsymbol{K}$ space where the largest eigenvalue of $T$ is asymptotically twofold degenerate, which now has the two corresponding eigenvectors $\varphi_1$ and $\varphi_2$. From (4), on the assumption that

$$Z_N \sim 2\lambda_1^{N/n} \qquad (N/n \text{ large}), \tag{6a}$$

we obtain

$$\lim_{n\to\infty} P_n(\boldsymbol{\sigma}) = \tfrac{1}{2}\varphi_1(\boldsymbol{\sigma})^2 + \tfrac{1}{2}\varphi_2(\boldsymbol{\sigma})^2 = P_\infty(\boldsymbol{\sigma}) \tag{6b}$$

and adopting Kac's viewpoint it seems natural to associate the eigenvectors $\varphi_1$ and $\varphi_2$ with the two possible stable phases (phases **1** and **2** say) which the system can adopt. Thus if we use $P(a)$ and $P(a|b)$ to denote the probability of event $a$, and the conditional probability of event $a$ given $b$ respectively, then our physical interpretation of (6) takes the form

$$P_\infty(\boldsymbol{\sigma}) = P(\mathbf{1})P_\infty(\boldsymbol{\sigma}|\mathbf{1}) + P(2)P_\infty(\boldsymbol{\sigma}|\mathbf{2}) \tag{7}$$

where $P(\mathbf{1}) = P(\mathbf{2}) = \frac{1}{2}$. In the case of regions of $\boldsymbol{K}$ space where the largest eigenvalue of $T$ is asymptotically $l$-fold degenerate, equations (6), (7) and their interpretation generalise to the form

$$P_\infty(\boldsymbol{\sigma}) = 1/l \sum_{i=1}^{l} \varphi_i(\boldsymbol{\sigma})^2 \tag{8}$$

and

$$P_\infty(\boldsymbol{\sigma}) = \sum_{i=1}^{l} P(\boldsymbol{i})P_\infty(\boldsymbol{\sigma}|\boldsymbol{i}) \tag{9}$$

where $\varphi_1, \varphi_2, \ldots, \varphi_l$ are the eigenvectors of the maximum eigenvalue. In terms of our interpretation (6), if $g(\sigma)$ represents some function of a single spin, then the ensemble expectation value of $g$ takes the form

$$\langle g \rangle = \tfrac{1}{2}(\varphi_1, g(\sigma)\varphi_1) + \tfrac{1}{2}(\varphi_2, g(\sigma)\varphi_2) \tag{10}$$

where $\sigma$ is a specific spin in $\boldsymbol{\sigma}$, and again it seems natural to interpret $(\varphi_i, g\varphi_i)$ as the mean value of $g$ in phase $\boldsymbol{i}$.

We will now assume that our lattice models are defined in terms of site variables $\sigma_i$ $(i = 1, 2, \ldots, N)$ which can adopt a finite number of specific values, say $\alpha_1, \alpha_2, \ldots, \alpha_q$. It is convenient to think in terms of the population densities $\langle \delta_{\sigma,\alpha_i} \rangle$; regions where the spin states $\sigma = \alpha_i$ are favoured can be thought of as $i$-rich regions. Here we are interested in the expectation $\langle \delta_{\sigma(0),\alpha_i} \delta_{\sigma(r),\alpha_i} \rangle$ where $\sigma(0)$ and $\sigma(r)$ refer to two corresponding spins in the $n$-site subsystems a distance $r$ apart, thus

$$\langle \delta_{\sigma(0),\alpha_i} \delta_{\sigma(r),\alpha_i} \rangle = P_n(\sigma(r) = \alpha_i \cap \sigma(0) = \alpha_i) \tag{11}$$

and is a measure of the probability that $\sigma(r)$ is in a state $\alpha_i$, and that the corresponding spin at the origin is in a state $\alpha_i$. In the absence of a long-range correlation between the spin states we expect that

$$\lim_{r\to\infty} \langle \delta_{\sigma(0),\alpha_i}\delta_{\sigma(r),\alpha_i}\rangle = \langle \delta_{\sigma(0),\alpha_i}\rangle\langle \delta_{\sigma(r),\alpha_i}\rangle = \langle \delta_{\sigma,\alpha_i}\rangle^2 \tag{12}$$

for translationally symmetric systems. Thus on a lattice of $N$ sites we define the correlation between spins at $\mathbf{0}$ and $\boldsymbol{r}$ by the correlation

$$C_n(r) = \langle \delta_{\sigma(0),\alpha_1}\delta_{\sigma(r),\alpha i}\rangle - \langle \delta_{\sigma,\alpha_i}\rangle^2 \tag{13}$$

which in the case of a system in one homogeneous phase is the same as the so-called correlation of fluctuations

$$C_n(r) = \langle (\delta_{\sigma(0),\alpha_i} - \langle \delta_{\sigma,\alpha_i}\rangle)(\delta_{\sigma(r),\alpha_i} - \langle \delta_{\sigma,\alpha_i}\rangle)\rangle \tag{14}$$

(Kadanoff *et al* 1967). An evaluation of (11) can readily be developed in terms of the transfer matrix and the result is

$$\langle \delta_{\sigma(0),\alpha_i}\delta_{\sigma(r),\alpha_i}\rangle = Z_N^{-1} \sum_{i,j}^{\Omega} \lambda_i^{N/n-r} \lambda_j^r (\varphi_1, \delta_{\sigma,\alpha_i}\varphi_j)^2 \tag{15}$$

where $\delta_{\sigma,\alpha_i}\varphi(\boldsymbol{\sigma})$ is the element $\boldsymbol{\sigma}$ of $\varphi_j$ multiplied by $\delta_{\sigma,\alpha_i}$ for a specific spin in $\boldsymbol{\sigma}$, and $r$ is usually the number of lattice spacings between the corresponding spins $\sigma(0)$ and $\sigma(r)$ in two subsystems. Thus in the subspace of $\boldsymbol{K}$ in which $\lambda_1$ is asymptotically non-degenerate

$$P_\infty(\sigma(r) = \alpha_i \cap \sigma(0) = \alpha_i) = (\varphi_1, \delta_{\sigma,\alpha_i}\varphi_1)^2 + \sum_{j=2}^{\infty} (\lambda_j/\lambda_1)^r (\varphi_1, \delta_{\sigma,\alpha_i}\varphi_j)^2 \tag{16}$$

and hence the limit

$$\lim_{n\to\infty} C_n(r) = \sum_{j=2}^{\infty} (\lambda_j/\lambda_1)^r (\varphi_1, \delta_{\sigma,\alpha_i}\varphi_j)^2 = C_\infty(r) \tag{17}$$

showing that a finite correlation over an infinite range is possible only in regions of $\boldsymbol{K}$ space where $\lambda_1$ is asymptotically degenerate.

Consider now the subspace of $\boldsymbol{K}$ where $\lambda_1$ is asymptotically degenerate. We would like an interpretation of (11) and (12) corresponding to the interpretation of $P_n(\boldsymbol{\sigma})$ in (6*b*); however, the uncorrelated terms corresponding to the limit $r\to\infty$ take on a more complicated structure with respect to the macroscopic phases when these are represented by $\varphi_1$ and $\varphi_2$. In this subspace (15) yields

$$\begin{aligned} P_\infty(\sigma(r) = \alpha_i \cap \sigma(0) = \alpha_i) &= \tfrac{1}{2}(\varphi_1, \delta_{\sigma,\alpha_i}\varphi_1)^2 + \tfrac{1}{2}(\varphi_2, \delta_{\sigma,\alpha_i}\varphi_2)^2 + (\varphi_1, \delta_{\sigma,\alpha_i}\varphi_2)^2 \\ &\quad + \frac{1}{2}\sum_{j=3}^{\infty} \left(\frac{\lambda_j}{\lambda_1}\right)^r [(\varphi_1, \delta_{\sigma,\alpha_i}\varphi_j)^2 + (\varphi_2, \delta_{\sigma,\alpha_i}\varphi_j)^2] \end{aligned} \tag{18}$$

where the correlation between spins $\sigma(0)$ and $\sigma(r)$ is represented by the correlation function

$$C_\infty(r) = P_\infty(\sigma(r) = \alpha_i \cap \sigma(0) = \alpha_i) - \tfrac{1}{2}(\varphi_1, \delta_{\sigma,\alpha_i}\varphi_1)^2 - \tfrac{1}{2}(\varphi_2, \delta_{\sigma,\alpha_i}\varphi_2)^2 - (\varphi_1, \delta_{\sigma,\alpha_i}\varphi_2)^2. \tag{19}$$

In (19) the first two terms clearly represent the expectation that a site is in state $\alpha_i$ in phases **1** and **2** respectively. The mixed term, however, is not an expectation of this type, but could be thought of as a transition probability that a given site remains in state $\alpha_i$ in a transition from one phase to the other. Thus our interpretation of (18) would be

$$\begin{aligned} P_\infty(\sigma(r)=\alpha_i \cap \sigma(0)=\alpha_i) \\ &= P(\mathbf{1})P_\infty(\sigma=\alpha_i|\mathbf{1})^2 + P(\mathbf{2})P_\infty(\sigma=\alpha_i|\mathbf{2})^2 \\ &\quad + P_\infty(\sigma=\alpha_i|\text{a transition } \mathbf{1}\rightleftharpoons\mathbf{2}) + C_\infty(r) \end{aligned} \tag{20}$$

and the measure of the correlation is

$$C_\infty(r) = \frac{1}{2}\sum_{j=3}^{\infty} (\lambda_j/\lambda_1)^r[(\varphi_1, \delta_{\sigma,\alpha_i}\varphi_j)^2 + (\varphi_2, \delta_{\sigma,\alpha_i}\varphi_j)^2]. \tag{21}$$

Suppose that the two stable phases in (20) are $\alpha_1$ and $\alpha_2$ rich phases; then (21) shows that a finite long-range correlation between sites $\sigma(0)$ and $\sigma(r)$ being in a third state $\alpha_k$ is only possible when $\lambda_1$ is asymptotically threefold degenerate. This long-range correlation is precisely how we would describe the emergence of a third coexisting phase. Thus we can take asymptotic threefold degeneracy in $\lambda_1$ to mark out the subspace $\boldsymbol{K}$ where triple points are possible. We can also define the characteristic range of correlation for a third species within the domain of two coexisting phases in the usual way by

$$\xi(\boldsymbol{K}) = -1/\ln(\lambda_3/\lambda_1). \tag{22}$$

The arguments leading to (21) and (22) can obviously be extended to represent $p$ coexisting phases. In a subspace of $\boldsymbol{K}$ where $\lambda_1$ is asymptotically $(p-1)$-fold degenerate, the measure of correlation corresponding to (21), denoted by $C_{p,\infty}(r)$, is

$$C_{p,\infty}(r) = \frac{1}{p-1}\sum_{j=p}^{\infty} (\lambda_j/\lambda_1)^r\left(\sum_{i=1}^{i=p-1} (\varphi_i, \delta_{\sigma,\alpha_i}\varphi_j)^2\right). \tag{23}$$

Thus if $\alpha_1, \ldots, \alpha_{p-1}$ rich phases are the coexisting phases, the emergence of an additional stable phase is possible only if $T$ becomes asymptotically $p$-fold degenerate. We can define the characteristic correlation length associated with the growth of this new phase by $\xi_p$ where

$$\xi_p = -1/\ln(\lambda_p/\lambda_1). \tag{24}$$

Thus $\xi_2$ is the usual coherence length† associated with the correlation of fluctuations in (14).

The application of the above to finite size scaling calculations now follows from (24) and Wood and Osbaldestin (1982). If the system is held at a point in $\boldsymbol{K}$ space where $p$-fold coexistence is possible, then $T$ is asymptotically $(N, n \to \infty)$ $p$-fold degenerate and $\xi_p$ diverges everywhere in $\boldsymbol{K}$ space where such coexistence is possible, and is therefore absolutely invariant to any spacial rescaling of the assembly. In terms of the scaling relation

$$\xi_p(\boldsymbol{K}') = (1/L)\,\xi_p(\boldsymbol{K}) \tag{25}$$

when applied to the various types of coexistence, we can readily use the finite size scaling method to construct a sequence of approximants to point subsets of $\boldsymbol{K}$ space where $p$-fold coexistence is possible.

† Fisher (1969) has given an identification of $\xi_2$ at points on the coexistence sheet in terms of the interfacial surface tension.

## 3. Multiple phase coexistence in the Potts models

To illustrate the above theoretical discussion we have performed finite size scaling calculations based upon (25) for the two-dimensional ferromagnetic Potts model on a square net lattice for the cases $q=3, 4$ and 5. As in previous calculations (Wood and Osbaldestin 1982), the $q^m \times q^m$ transfer matrix is defined by (1) with $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}'$ being neighbouring columns of $m$ sites on an $m\times\infty$ lattice. We denote the correlation length (24) for such a system by $\xi_p(m)$ which is the characteristic length on an $m\times\infty$ lattice. Thus, taking $\xi_p^{(m)}$ and $\xi_p^{(m+1)}$ as $\xi_p(\boldsymbol{K}')$ and $\xi_p(\boldsymbol{K})$ respectively in (25) with $L=1+1/m$, the functions

$$\varphi_{m,p}(\boldsymbol{K}) = m[\xi_p^{(m)}(\boldsymbol{K})]^{-1} - (m+1)[\xi_p^{(m+1)}(\boldsymbol{K})]^{-1} \tag{26}$$

define a sequence on $m$ where the zero contour $\varphi_{m,p}=0$ is an $m$th-order approximant to the point subsets of $\boldsymbol{K}$ space where $p$-fold phase coexistence can occur.

The Hamiltonian of the $q$-state Potts model in the presence of its ordering fields is given by

$$\mathscr{H}_N = -J\sum_{nn}\delta_{\sigma_i,\sigma_j} - \sum_{i=1}^{N}\sum_{j=1}^{q} h_j\delta_{\sigma_i,j} \qquad (J>0) \tag{27}$$

where $\sigma_i$ $(i=1,2,\ldots,N)$ can take the values $1,2,\ldots,q$, $h_j$ is the ordering field of species $j$, and where in addition we impose the condition

$$\sum_{j=1}^{q} h_j = 0. \tag{28}$$

The first summation in (27) is over all nearest-neighbour pairs of sites. To simplify the discussion of phase coexistence we set $h_1=h$ and consider the fields $h_2, h_3, \ldots, h_q$ to be equal; thus

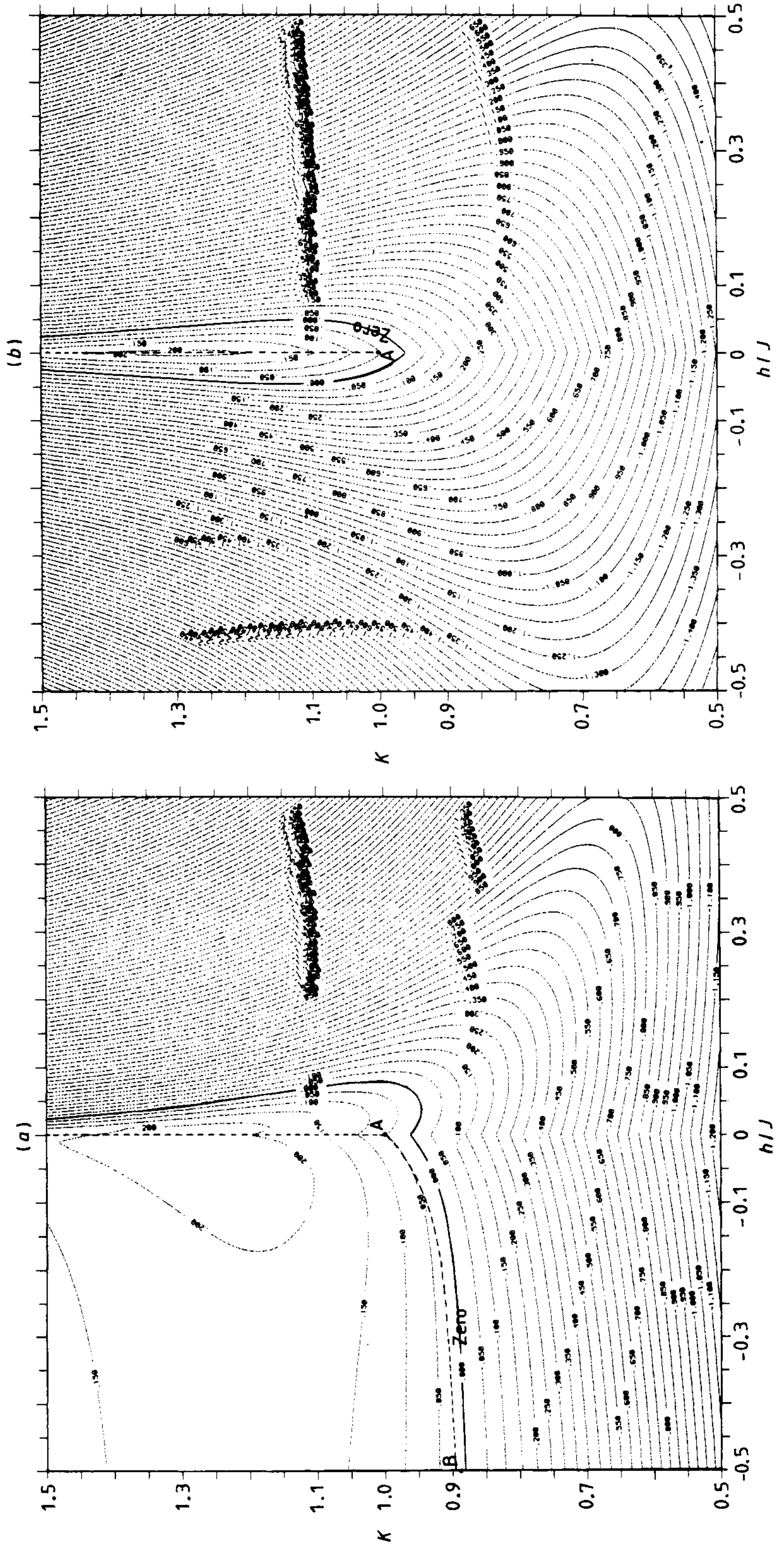
$$\mathscr{H}_N = -J\sum_{nn}\delta_{\sigma_i,\sigma_j} - h\sum_i[\delta_{\sigma_i,1} - (\delta_{\sigma_i,2}+\delta_{\sigma_i,3}+\ldots+\delta_{\sigma_i,q})/(q-1)]. \tag{29}$$

For regions of $(T,h)$ space where $h_1$ is large and negative and where $h_2=h_3=\cdots=h_q$, we expect the thermodynamic behaviour to be close to that of the $(q-1)$-state Potts model in zero field since species 1 is suppressed and the ordering fields of the other species are all equal. In such a region of $(T,h)$ space (at low enough temperatures) we expect to see $(q-1)$-fold phase coexistence, and in the limit $h\to-\infty$ we expect the temperature range over which $(q-1)$ phase coexistence can occur to be that of the $(q-1)$-state Potts model in the zero field (this is the range $0<T<T_c=J\ln[1+(q-1)^{1/2}]/k$). Thus for the model of (29), $h<0$, approximants $\varphi_{m,2}, \varphi_{m,3}, \ldots, \varphi_{m,q-1}$ of (26) should all converge to the same region of $(T,h)$ space. Clearly $q$-fold phase coexistence for the model (27) is only possible for $h=0$, and thus we expect to see the zero contour of the approximant $\varphi_{m,q}$ approximate the line segment $\infty>K>K_c=\ln(1+\surd q)$, $(K=\beta J)$. If the endpoint of this line segment $K_c$ is a first-order transition point, which for $q>4$ it is (in two dimensions, Baxter (1973)), then at this point $(q+1)$-fold phase coexistence is possible, where the additional phase is the high-temperature disordered phase. Attempts to project out all of these point subsets of $(T,h)$ space can be made by using (26) with $p=2,3,\ldots,q+1$. The calculations reported here have been completed for the cases $m=2$ and $q=3$, 4 and 5.

The results for the three-state Potts model are shown in figures 1($a$), ($b$) and ($c$). The contours of figure 1($a$) are those discussed previously (Wood and Osbaldestin 1982). The region of two-phase coexistence, which is the coexistence surface $\Sigma$, is a sheet of points inside $h<0$ bounded by a line of critical points; this is represented by $\varphi_{2,2}$ as the large and almost flat-topped hill enclosed by the zero contour. The broken line is a schematic representation of the exact limiting form of $\Sigma$. We expect the small thumb-like loop inside $h>0$ to converge to the zero-field critical point at A, which is at $K_c = 1{\cdot}0050\dots$ The first example of the claims in § 2 is provided by figure 1($b$) showing the contours of $\varphi_{2,3}(K, h)$ where the zero contour represents an approximation to the line of triple points on $h=0$ given by $K_c<K<\infty$. The approximation even at this low order emerges as a narrow hairpin-like enclosure of the exact line segment. The loop intersects the $h=0$ line in an approximation to $K_c$, and the contour map here is very similar to that obtained for the simple Ising model (Wood and Osbaldestin 1982). We know that $K_c$ is a second-order critical point (Baxter 1973), thus the point $(K_c, 0)$ is not a quadruple point where the disordered phase coexists with the three ordered phases. This 'negative' result is reflected in the contours of $\varphi_{2,4}$ shown in figure 1($c$) where the zero contour does not exist.

The corresponding sequence of results for the four-state Potts model is shown in figures 2($a$), ($b$), ($c$) and ($d$). Again the whole coexistence surface is approximated by $\varphi_{2,2}$ and again is a continuous plateau-like region bounded by the zero contour inside $h<0$. For the four-state Potts model we expect to see three-phase coexistence on $\Sigma$ inside $h<0$: $\varphi_{2,3}$ for this model shown in figure 2($b$) depicts the same plateau-like region as in figure 2($a$) which is a sheet of triple points. Inside $h<0$ the contours of 2($a$) and 2($b$) are identical. Four-phase coexistence is only possible on the zero-field line, and the line segment $K_c<K<\infty$ is again approximated by a hairpin-like enclosure of this segment by the zero contour of $\varphi_{2,4}$, which now shows a marked asymmetry about $h=0$. Again no evidence of five-phase coexistence is obtained, and the contours of $\varphi_{2,5}$ contain no zero contour; these are shown in figure 2($d$). If we accept the interpretation of § 2, then the absence of zero contours in both figures 1($c$) and 2($d$) is of course a statement that the thumb-like extensions of the zero contours in figures 1($a$) and 2($a$) will converge to the single point $K_c$, and that coexistence with the disordered phase is not possible for the three- and four-state Potts models.

The corresponding results for the five-state Potts model are shown in the sequence of figures 3($a$), ($b$), ($c$) and ($d$). The whole $\Sigma$ surface indicated by figure 3($a$) appears to be qualitatively the same as that found for the three- and four-state Potts models, the only slight difference being that the thumb-like extension of the zero contour inside $h>0$ is here slightly larger. Here we would expect that the plateau enclosed by the zero contour is a sheet of quadruple points inside $h<0$. The contours of $\varphi_{2,3}$ and $\varphi_{2,4}$ are indentical for the five-state Potts model and are shown in figure 3($b$), and clearly mark out $\Sigma$ as being a sheet of fourfold coexistence inside $h<0$. Again the contours of figure 3($a$) and 3($b$) inside $h<0$ are identical. Figures 1($a$), 2($a$) and 3($a$) all show the zero contour to be approximating the zero-field critical point of the corresponding $(q-1)$-state Potts model in the limit $h\to-\infty$; these points are marked B on the figures. The same hairpin-like enclosure of the zero-field segment $K_c<K<\infty$ appears in the zero contour of $\varphi_{2,5}$ marking out fivefold phase coexistence. However, when we look for sixfold coexistence in the contours of $\varphi_{2,6}$ we find that this time the technique has detected this as a phenomenon characteristic of this model. Here the


(a)
(b)
K
h/J
Zero
A
B
1.5
1.3
1.1
1.0
0.9
0.7
0.5
-0.5
-0.3
-0.1
0
0.1
0.3
0.5

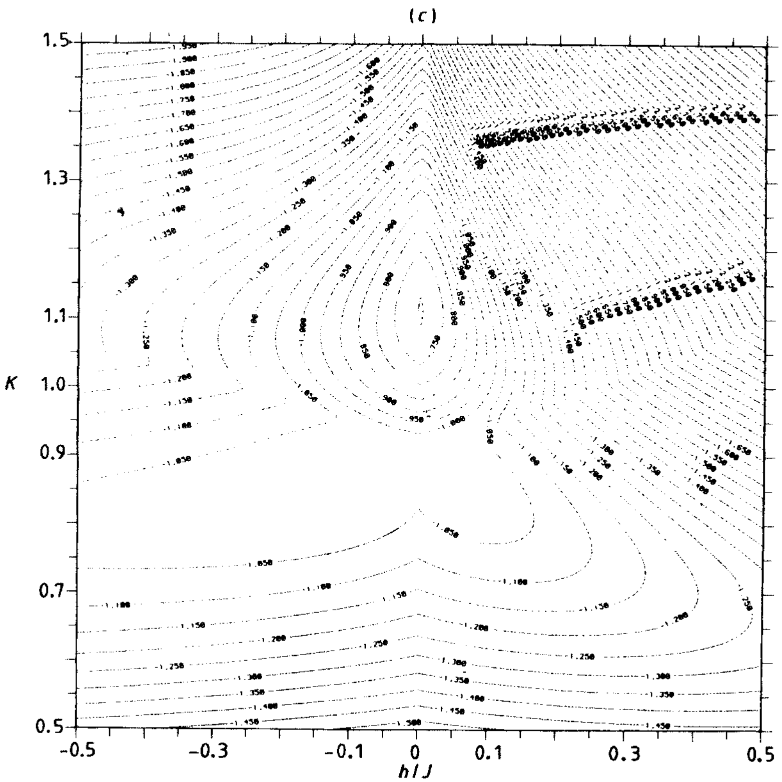
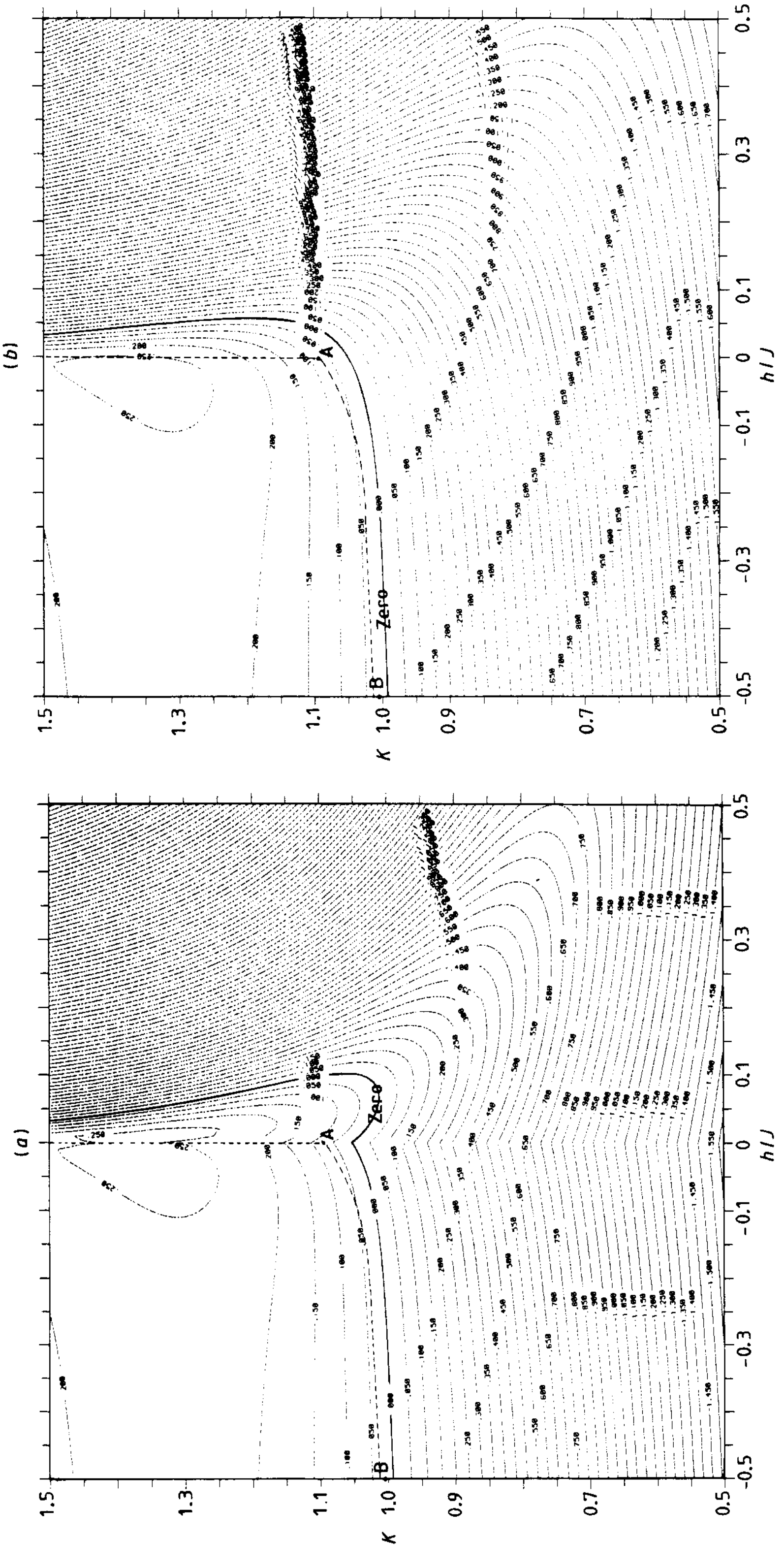



**Figure 1.** This sequence of figures shows the results obtained for the three-state Potts model. In each figure the points marked A and B are the exact zero-field critical points $K_c$ for the three- and two-state Potts models respectively, and the broken lines are schematic representations of the exact point subsets of $(K, h)$ space where coexistence is possible. (*a*) The zero contour of $\varphi_{2,2}(K, h)$ is the approximation to $\Sigma$, and marks off a plateau inside $h<0$. (*b*) The contours of $\varphi_{2,3}(K, h)$; three-phase coexistence on the zero-field line segment $1.0050\ldots<K<\infty$ is approximated by the hairpin-like enclosure of the zero contour of $\varphi_{2,3}(K, h)$. (*c*) The contours of $\varphi_{2,4}(K, h)$; the absence of a zero contour shows that there is no point in $(K, h)$ space where four-phase coexistence is possible, and thus that the thumb-like extensions of the zero contour of (*a*) inside $h>0$ will converge to the point A.


(b)
(a)
K
h/J
Zero
A
B

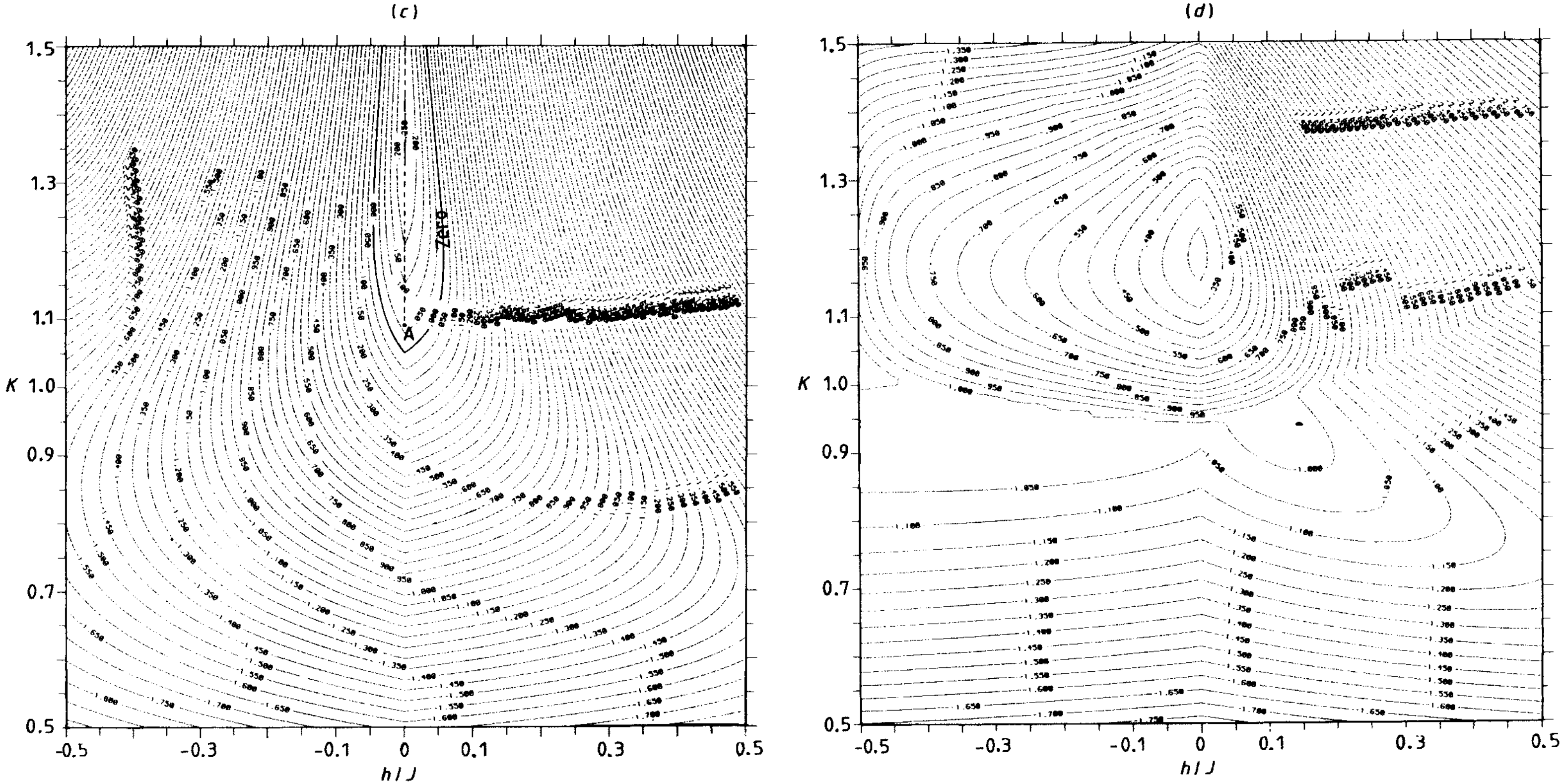
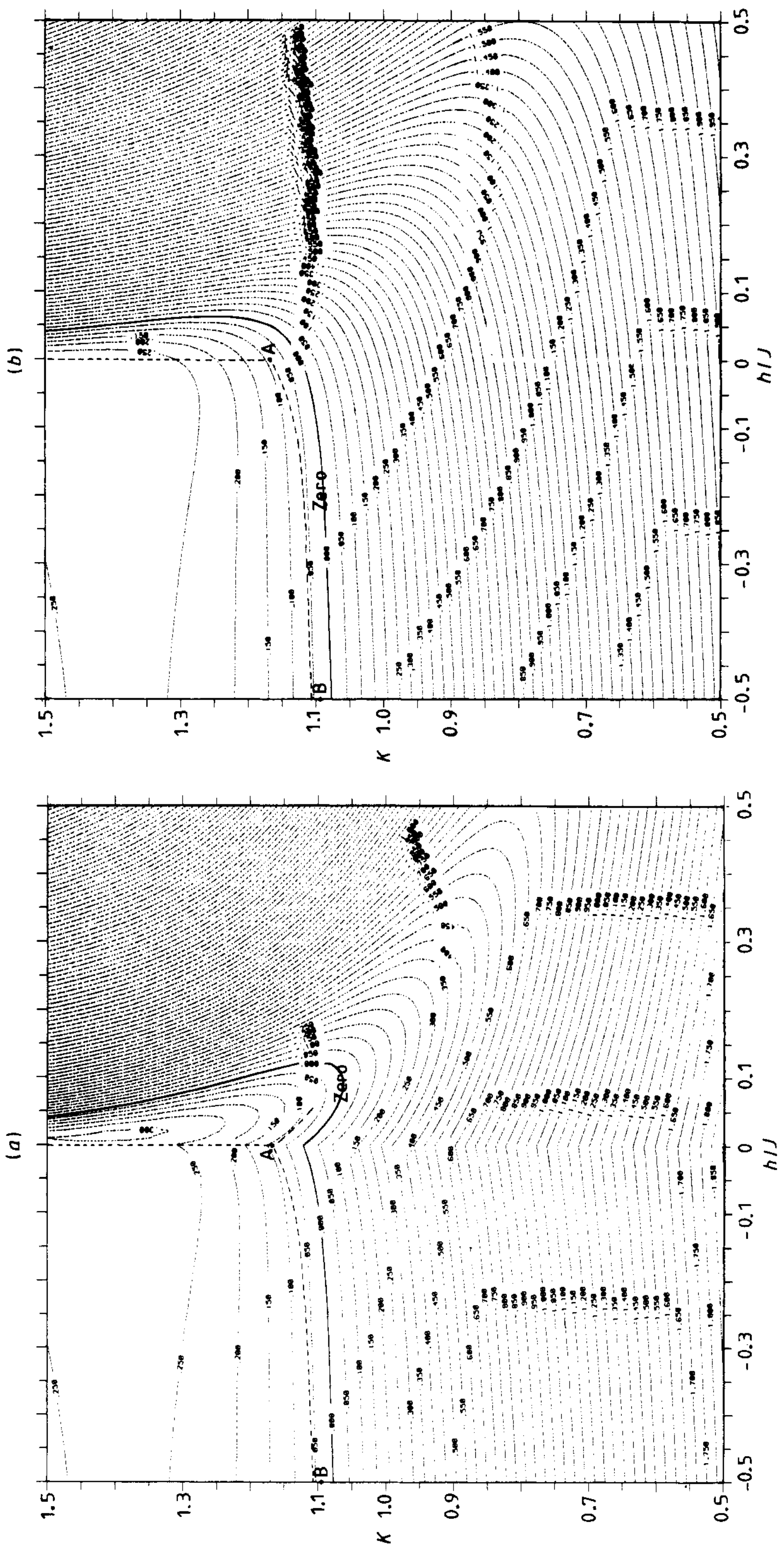



**Figure 2.** This figure sequence shows the results obtained for the four-state Potts model. Points A and B are the exact zero-field critical points for the four- and three-state models respectively. The broken lines are schematic representations of the point subsets of $(K, h)$ space where coexistence is possible. (*a*) The zero contour of $\varphi_{2,2}(K, h)$ is the approximation to $\Sigma$ and marks off a plateau inside $h<0$. (*b*) The contours of $\varphi_{2,3}(K, h)$. Inside $h<0$ these contours are identical to those of $\varphi_{2,2}$, showing that this region of $\Sigma$ is a sheet of triple points. In the limit $h \to \infty$ the model is equivalent to a three-state Potts model in zero field (point B), hence the boundary line of three-phase phase coexistence represented by the zero contour is probably a line of anomalous tricritical points. (*c*) The contours of $\varphi_{2,4}(K, h)$. The hairpin-like zero contour is the approximation to the line segment on the zero-field line $1.0986\ldots<K<\infty$ where fourfold phase coexistence is possible. (*d*) The contours of $\varphi_{2,5}(K, h)$. The absence of a zero contour shows that the zero-field point $K_c = 1.0986\ldots$ is not a first-order transition point, and that the thumb-like extension of the zero contour of $\varphi_{2,2}$ inside $h>0$ will converge to the one point at $K_c$.


(a)
(b)
K
h/J
Zero
A
B
1.5
1.3
1.1
1.0
0.9
0.7
0.5
-0.5
-0.3
-0.1
0
0.1
0.3
0.5

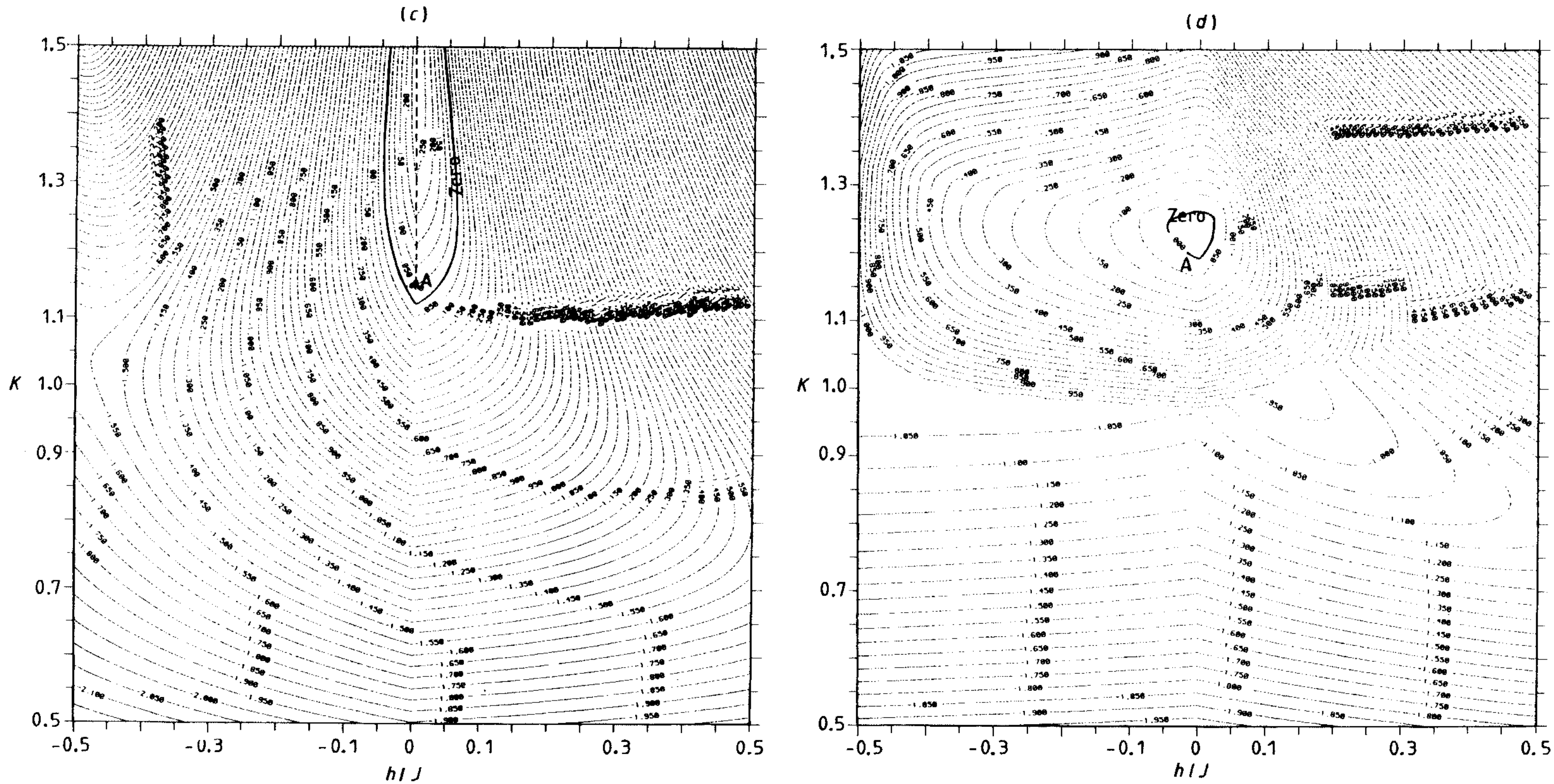



**Figure 3.** This figure sequence shows the results obtained for the five-state Potts model. Points A and B are the transition points for the five- and four-state models respectively, and the broken lines are schematic representations of the point subsets of $(K, h)$ space where coexistence is possible. ($a$) The zero contour of $\varphi_{2,2}(K, h)$ is similar to the previous cases and $\Sigma$ is a sheet of points approximated by the enclosure of the zero contour. There is no indication at this stage that the thumb-like extension inside $h>0$ is any different from those obtained for three- and four-state Potts models. ($b$) The contours of $\varphi_{2,3}(K, h)$ and $\varphi_{2,4}(K, h)$ are identical, and also identical to those of $\varphi_{2,2}$ inside $h<0$. The coexistence sheet of $\Sigma$ inside $h<0$ is clearly seen to be a sheet of quadruple points. ($d$) The contours of $\varphi_{2,5}(K, h)$. As in the previous cases the hairpin-like zero contour is the approximation to the line segment on the $h=0$ line, $1.1743\ldots<K<\infty$, where fivefold coexistence is possible. ($d$) The contours of $\varphi_{2,6}(K, h)$. This time the approximant detects the presence of a zero contour. It appears as a small ring about a zero-field transition point, which we interpret as an approximation to a point on the zero-field line. Thus the technique has detected the phenomena of sixfold phase coexistence occuring in this model, where the high-temperature disordered phase can coexist with the five ordered phases. We expect that the small ring given by $\varphi_{2,6}=0$ will rapidly converge to the point $K_c=\ln(1+\sqrt{5})=1.1743\ldots$ in the higher-order approximants. Figures. 1($c$), 2($d$) and 3($d$) show that the method has represented the essential differences in the zero-field critical behaviour the five-state Potts model and the three- and four-state models.

zero contour of $\varphi_{2,6}$ exists and appears as a small ring centred on the zero-field point $K_c$, and thus faithfully records the model to have only first-order transitions in zero field. We expect the sequence of zero contours of $\varphi_{m,6}$ to converge rapidly onto the point $K_c = \ln(1+\sqrt{5})$.

## 4. Summary

The authors have shown that the finite size scaling method, apart from being a method which naturally yields a sequence of approximants to the whole phase coexistence surface $\Sigma$, can be simply extended into a technique giving a parallel sequence of approximants for any point subset of $\Sigma$ where multiple phase coexistence is possible. The scheme has been illustrated by applications to the three-, four- and five-state Potts models on the two-dimensional quadratic lattice. Even in the lowest order of approximation, the scheme gives overall results which are clearly very close to the exact results, and also yields a faithful representation of the important qualitative differences between the five-state and three- and four-state Potts models.

We have now shown that the method of finite size scaling analysis based upon Kadanoff's simple scaling relation (25), as originally implemented by Nightingale (1976), does not select in its solutions simply the critical points of the phase diagram. These solutions are really approximations to points on the boundary of the whole coexistence surface. Our appraisal of the finite size scaling technique with regard to the present application and its extension to obtaining very accurate exponents (Blöte and Nightingale 1982, Wood and Goldfinch 1980) is that it is potentially the most powerful computational method in the theory of phase transitions.

## Acknowledgments

One of us (AHO) would like to thank the SERC for the award of a maintenance grant.

## References

Baxter R J 1973 *J. Phys. C: Solid State Phys.* **6** L445–8
Blöte H W J, Nightingale M P 1982 *Physica* **112A** 405–65
Blöte H W J, Nightingale M P and Derrida B 1981 *J. Phys. A: Math. Gen.* **14** L45–9
Domb C 1960 *Phil. Mag. Adv. Phys.* **9** 149, 175
Fisher M E 1969 *J. Phys. Soc. Japan Suppl.* **26** 87–93
Goldfinch M C and Wood D W 1982 *J. Phys. A : Math. Gen.* **15** 1327–38
Hamer C J 1981 *J. Phys. A: Math Gen.* **14** 2982–3003
Hamer C J and Barber M N 1980 *J. Phys. A: Math. Gen.* **13** L169–74
——1981 *J. Phys. A: Math. Gen.* **14** 2009–25
Hemmer P C and Lebowitz J L 1976 *Phase transitions and critical phenomena* vol 5b eds C Domb and M S Green (New York: Academic)
Herrman H J 1981 *Z. Phys.* B **43** 55–60
Kac M 1968 *Mathematical Mechanisms of Phase Transitions, Brandeis Lectures* 1966 (New York: Gordon and Breach)
Kadanoff L P, Gotze W, Hamblen D, Hecht R, Lewis E A S, Palciauskas V V, Rayl M, Swift J, Aspnes D and Kane J 1967 *Rev. Mod. Phys.* **39** 359–431
Lieb E H and Wu F Y 1972 *Phase transitions and critical phenomena* vol 2 eds C Domb and M S Green (New York: Academic)

Nightingale M P 1976 *Physica* **83A** 561–72
——1977 *Phys. Lett.* **59A** 486–8
Nightingale M P and Blöte H W J 1980 *Physica* **104A** 352–7
Osbaldestin A H and Wood D W 1982 *J. Phys. A: Math. Gen.* **15** 3593–8
Roomany H H and Wyld H W 1980 *Phys. Rev.* B **23** 1357–61
Roomany H H, Wyld H W and Holloway L E 1980 *Phys. Rev.* D **21** 1557–63
Sneddon L 1978 *J. Phys. C : Solid State Phys.* **11** 2823–8
Sneddon L and Stinchcombe R B 1979 *J. Phys. C: Solid State Phys.* **12** 3761–70
Thompson C J 1972 *Mathematical Statistical Mechanics* (New York: Macmillan)
Wood D W 1975 *Statistical Mechanics* vol 2 (London: Chem. Soc)
Wood D W and Goldfinch M C 1980 *J. Phys. A: Math Gen.* **13** 2781–94
Wood D W and Osbaldestin A H 1982 *J. Phys. A: Math. Gen.* **15** 3579–91
Wu F Y 1982 *Rev. Mod. Phys.* **54** 235–68