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A renormalisation group investigation of the Ashkin–Teller–Potts model

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Abstract. The Ashkin–Teller–Potts model is examined using two renormalisation group methods: (*a*) the cluster expansion; and (*b*) the lower bound variational method. The critical surface is found to be in agreement with that conjectured by Wu and Lin. We find a very strong indication of a line of fixed points along which we obtain a continuous variation of the specific heat exponent with the four-spin coupling. A comparison is made with the eight-vertex model.

1. Introduction

The Ashkin–Teller model of statistical mechanics was introduced (Ashkin and Teller 1943) as a generalisation of the Ising model to the case where each lattice site may be occupied by one of four different types of atom: A, B, C, D. The interaction energies between neighbouring pairs of atoms are given by:

types of interaction	energy
A–A, B–B, C–C, D–D	ϵ_0
A–B, C–D	ϵ_1
A–C, B–D	ϵ_2
A–D, B–C	ϵ_3

(1.1)

and the Boltzmann weights by

$$\omega_i = \exp(-\epsilon_i/kT) \qquad i = 0, 1, 2, 3. \tag{1.2}$$

The model definition does not make any distinction between the atoms and therefore all four types are treated on equal footing. The special case in which $\epsilon_1 = \epsilon_2 = \epsilon_3$ was also considered by Potts (1952) and the general model is often known as the Ashkin–Teller–Potts (ATP) model. This particular Potts model satisfies a duality relation (Ashkin and Teller 1943, Potts 1952) enabling the critical temperature of the model—assuming there to be one transition only—to be located at

$$\omega_0/\omega = 3 \tag{1.3}$$

where $\omega = \omega_1 = \omega_2 = \omega_3$.

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Fan (1972a) showed that the ATP model could also be considered in terms of Ising spins on two superimposed lattices. Thus, at each point of the lattice we have two spins (σ, s) (figure 1), and the four atoms may be represented as

$$A \equiv (+,+) \qquad B \equiv (+,-) \qquad C \equiv (-,+) \qquad D \equiv (-,-). \tag{1.4}$$

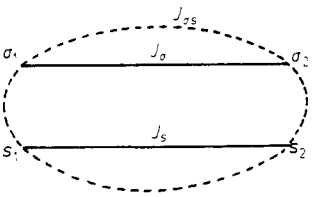

Figure 1. The interactions between a nearest-neighbour pair of sites on the ATP lattice.

The energy of interaction is then given in terms of coupling constants

$$\begin{aligned}
\epsilon_0 &= J_0 + J_\sigma + J_s + J_{\sigma s} \\
\epsilon_1 &= J_0 + J_\sigma - J_s - J_{\sigma s} \\
\epsilon_2 &= J_0 - J_\sigma + J_s - J_{\sigma s} \\
\epsilon_3 &= J_0 - J_\sigma - J_s + J_{\sigma s}
\end{aligned} \tag{1.5}$$

where J_0 is a constant. The equivalence of atoms A, B, C, D then implies the equivalence of $\epsilon_1, \epsilon_2, \epsilon_3$ and also of $J_\sigma, J_s, J_{\sigma s}$.

In a similar manner we may also represent the eight-vertex model (see, e.g., Lieb and Wu 1972) in terms of interactions J^+, J^- and J between Ising spins on a square lattice (figure 2). The Boltzmann constants, a, b, c, d corresponding to the possible vertex types, are then given by (Kadanoff and Wegner 1971):

$$\begin{aligned}
a &= A \exp(K^+ + K^- + \lambda) \\
b &= A \exp[-(K^+ + K^-) + \lambda] \\
c &= A \exp(K^+ - K^- - \lambda) \\
d &= A \exp[-(K^+ - K^-) - \lambda]
\end{aligned} \tag{1.6}$$

where A is a constant and $K^\pm = J^\pm / kT$, $\lambda = JkT$.

When the ATP and the eight-vertex models are both written in their Ising representations it may be seen that they have similar symmetry properties (Fan

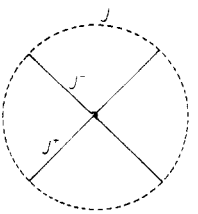

Figure 2. The interaction constants of the Ising representation of the eight-vertex model: J^+ between next-nearest neighbours on the positive diagonal; J^- between next-nearest neighbours on the negative diagonal; J coupling the four spins around a unit square.

1972b). Due to this similarity Fan suggested that the two models might be related in some manner. Wegner (1972) showed that, in fact, the relationship was between the ATP model and the staggered eight-vertex model (having weights a, b, c_+, d_+ and a, b, c_-, d_- on the two sublattices) with $c_+ = d_-$, $c_- = d_+$. He proved this by applying a duality transformation to the spins of one layer (the s layer) of the ATP lattice, thereby obtaining the equivalence of the following expressions:

$$J_{\sigma s} = J_s \qquad b = 0 \tag{1.7}$$

$$J_\sigma = J_s \qquad a = b + c_+ + d_+ \tag{1.8}$$

$$\omega_0 = \omega_1 + \omega_2 + \omega_3 \qquad c_+ = c_- = d_+ = d_-. \tag{1.9}$$

The transformation does not, however, enable us to determine any of the exponents from a knowledge of the equivalent eight-vertex ones.

Using the known exact information about the Ising (Onsager 1944) and the eight-vertex (Baxter 1972) models, Wu and Lin (1974) conjectured that the ATP model should, in general, have two phase transitions—the exception to this being the cases $J_i = J_j > J_k$. Then under the assumption (without loss of generality)

$$\omega_0 = 1 \qquad 0 \leqslant \omega_1, \omega_2, \omega_3 \leqslant 1 \tag{1.10}$$

they proposed a form for the critical surface of the model (see figure 3) consisting of three symmetrically placed cups meeting each other along lines for which two of the

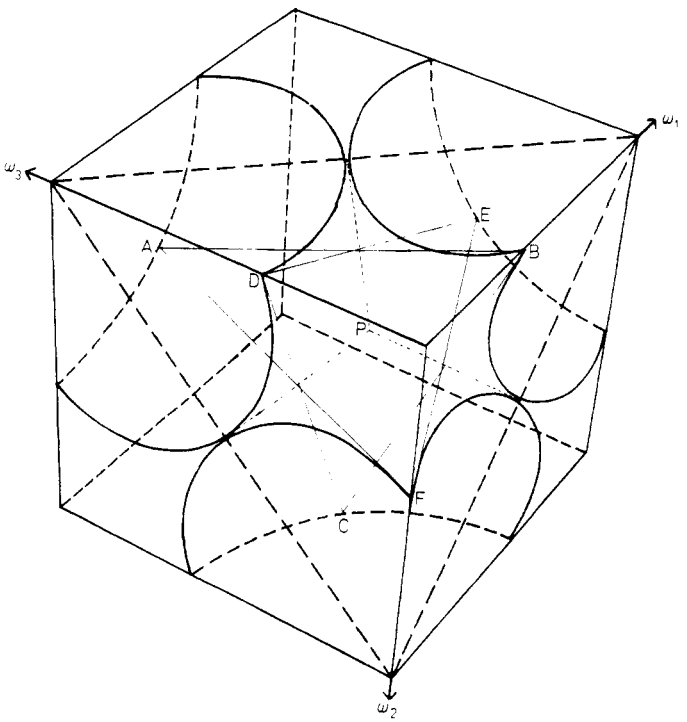

Figure 3. The critical surface of the ATP model, as conjectured by Wu and Lin. The lines joining ABCDEF are the lines of criticality of the Ising model, and the point P is the critical point of the four-state Potts model.

interactions $J_\sigma, J_s, J_{\sigma s}$ become equal. (These are the three lines meeting at P in figure 3.)

Baxter's solution of the eight-vertex model showed that the critical exponents varied continuously as a function of the four-spin coupling, λ, thereby contradicting the universality hypothesis. Kadanoff and Wegner (1971) showed that this variation could, in fact, be accounted for within scaling arguments which are the basis of universality. Due to the similarity of the two models, and in particular to the fact that both models contain a four-spin coupling, it seems possible that the ATP model could be a second candidate for continuously varying exponents. For this reason much attention has been centred on the ATP model.

Recently many statistical mechanical problems have been studied using the renormalisation group introduced by Wilson (1971) as a transformation in momentum space, and later extended to real space by several authors (Niemeyer and Van Leeuwen 1974, Kadanoff and Houghton 1975.) These transformations have given a relatively simple and accurate method of studying the critical properties of various models. In this paper we report the results of renormalisation group (RNG) studies of the ATP model. In § 2 we use symmetry arguments to consider the expected form of the critical surface and in § 3 we describe the results obtained for this surface using the cluster expansion of Niemeyer and Van Leeuwen. In § 4 we have used the lower bound RNG transformation of Kadanoff and Houghton (1975) (which proved to be remarkably accurate for the simple Ising model) to study the possibility of varying exponents for the ATP model and also to obtain numerical estimates for these exponents. Some of these results have previously been reported (Ashley and Green 1976).

2. The expected form of the critical surface

From a study of the known exact results on the Ising and eight-vertex models and their relationship with the ATP system, Wu and Lin (1974) were able to propose a form for the critical surface of the Ashkin–Teller model. This surface is shown in figure 3, and shows clearly the expectation of two phase transitions except in the cases

$$\omega_i = \omega_j \geqslant \omega_k.$$

The existence of these two phase transitions was also noted by Wegner (1972) who reasoned that, because the symmetry group of the system has three non-trivial subgroups, the model should undergo first a partial, and then a complete disordering.

We consider the two-layered Ising lattice representation of the model in which there are two spins (σ, s) at each lattice site. We distinguish between three (not independent) layers: the σ and s layers consisting of the lattices of σ and s spins respectively, and the σs layer whose spins are the product of the σ and s spins at each site. Assuming that there are no external fields, the model may be described in terms of three nearest-neighbour couplings J_σ, J_s and $J_{\sigma s}$. The ATP symmetry then implies that the model is unchanged under any permutation of $(J_\sigma, J_s, J_{\sigma s})$. Under the assumption (1.10) we may write the Boltzmann factors as

$$\begin{aligned} \omega_\sigma &= \exp[-2(K_s + K_{\sigma s})] \\ \omega_s &= \exp[-2(K_\sigma + K_{\sigma s})] \\ \omega_{\sigma s} &= \exp[-2(K_\sigma + K_s)] \end{aligned} \tag{2.1}$$

and the coupling constants

$$K_\sigma = \ln(\omega_\sigma/\omega_s\omega_{\sigma s})/4$$
$$K_s = \ln(\omega_s/\omega_\sigma\omega_{\sigma s})/4 \tag{2.2}$$
$$K_{\sigma s} = \ln(\omega_{\sigma s}/\omega_\sigma\omega_s)/4$$

where $K_i = J_i/kT$. Over the whole of the region $0 < \omega_i \leqslant 1$ this correspondence is one-to-one, but this is no longer true if any of the ω_i are equal to zero. (We assume this to be physical.) For example if $\omega_\sigma = \omega_s = 0$, $\omega_{\sigma s} \neq 0$ then all the $\boldsymbol{K}$ points subject to the restrictions

$$K_{\sigma s}\text{`} = \text{'}\infty \qquad K_\sigma + K_s = -\tfrac{1}{2}\ln\omega_{\sigma s} \tag{2.3}$$

correspond to the single $\boldsymbol{\omega}$ point $(0, 0, \omega_{\sigma s})$. This one-to-many correspondence is important since we will find points of the critical surface on the ω axes.

We start by considering the critical behaviour of the model having K_σ, K_s, $K_{\sigma s}$ all different. We take

$$|K_\sigma| > |K_s| > |K_{\sigma s}|$$

and note that other equivalent parts of the critical surface may be described by taking a permutation on $(\sigma, s, \sigma s)$. As always, at high temperatures, the spins are randomly aligned. As the temperature is lowered, K_σ, being the largest of the three couplings, forces the σ layer to order first at a temperature T_{1c}. At this point the s and σs layers have no overall order. On lowering the temperature still further the effect of K_s will be enough to force layer s to order at a temperature T_{2c}. Since, at this point, the σs layer is the product of two ordered layers it will also be ordered and there can be no further transition. This analysis is true even if $|K_\sigma| > |K_s| = |K_{\sigma s}|$. However, if $|K_\sigma| = |K_s| \geqslant |K_{\sigma s}|$ then layers σ and s will order first and together. Thus, with the first two layers ordering together we go straight from the high to the low temperature phase and there is only one transition.

We now consider the case in which one of the interaction constants, say $K_{\sigma s}$, is negative. The conditions (1.10) imply that at most one of the K_i may be negative and that this one must have a smaller modulus than the others. In this case we have two ferromagnetic interactions competing with a less powerful antiferromagnetic interaction, and since the three layers are not independent it is only possible to achieve a ground state at low temperatures on two of the layers. For given K_σ and K_s and $K_{\sigma s} \leqslant 0$ the model giving the minimum energy ground state has $K_{\sigma s} = 0$, this being the limiting model for which all three layers achieve their respective ground states. The philosophy of the renormalisation group is to do an averaging over the short-range detail of the system at each iteration. Thus, it seems likely that some of the detail to be lost in an approximate scheme would be that concerned with the instability due to one of the layers of a system with a negative coupling constant not being in its ground state at low temperatures. This would imply that a fixed point governing the low temperature behaviour (as well as that governing the high temperature behaviour and any other stable fixed point) of such a system would have a corresponding zero coupling constant, $K_{\sigma s} = 0$. Also, since all stable fixed points have $K_{\sigma s} = 0$ any fixed point corresponding to critical behaviour will have $K_{\sigma s} = 0$. Under this assumption it is impossible to have continuously varying exponents for negative $K_{\sigma s}$, since this would require a line of fixed points having negative $K_{\sigma s}$ values. Finally, since any fixed point

having one of the $K_l = 0$ will be of Ising form, we therefore expect the negative $K_{\sigma s}$ model to having Ising behaviour and exponents.

If, in particular we have $K_\sigma > K_s > 0$, $K_{\sigma s} = -K_s$ then after layer σ has ordered there will be no further transition, since there is no energy advantage in the other layers ordering. So, in this case, there is only one transition and the low temperature state is governed by a fixed point at $K_\sigma \to \infty$, K_s, $K_{\sigma s} = 0$.

The above results are summarised in table 1 which shows the values of the interaction constants K_σ, K_s, $K_{\sigma s}$ at the stable fixed points of all the ATP models.

Table 1. The stable fixed points governing all types of ATP model.

Description of model	High temperature fixed point	Stable fixed point for partial ordering	Low temperature fixed point	Number of transitions
(1) $K_\sigma = K_s = K_{\sigma s} > 0$	$K_l = 0 \quad l = \sigma, s, \sigma s$	——	$K_l \to \infty \quad l = \sigma, s, \sigma s$	1
(2) $K_i = K_j > K_j \geqslant 0$	$K_l = 0 \quad l = \sigma, s, \sigma s$	——	$K_l \to \infty \quad l = \sigma, s, \sigma s$	1
(3) $0 \leqslant K_i \leqslant K_j < K_k$	$K_l = 0 \quad l = \sigma, s, \sigma s$	$K_k \to \infty \quad K_i, K_j = 0$	$K_l \to \infty \quad l = \sigma, s, \sigma s$	2
(4) $K_i < 0 \quad K_j, K_k > 0$ $\lvert K_i \rvert < K_j < K_k$	$K_l = 0 \quad l = \sigma, s, \sigma s$	$K_k \to \infty \quad K_i, K_j = 0$	$K_k, K_j \to \infty \quad K_i = 0$	2
(5) $K_i = K_j > \lvert K_k \rvert$ $K_k < 0$	$K_l = 0 \quad l = \sigma, s, \sigma s$	——	$K_i, K_j \to \infty \quad K_k = 0$	1
(6) $K_i > K_j = -K_k$	$K_l = 0 \quad l = \sigma, s, \sigma s$	——	$K_i \to \infty \quad K_i, K_k = 0$	1

3. The critical surface found by cluster expansion calculations

After Wilson's development of the momentum-space RNG, Niemeyer and Van Leeuwen (NVL) introduced a real-space RNG which has proved to be particularly convenient for the study of many statistical mechanical problems. In their paper NVL developed two methods— the cumulant and the cluster expansions. In this report we consider only the cluster expansion.

In this theory the lattice is blocked into cells such that each spin is in exactly one cell and the cell pattern has the same symmetry as the original lattice. A new spin, μ, is then placed within each cell and the renormalised coupling constants calculated by a partial trace method.

NVL, working with the Ising model on the plane triangular lattice, found that the most suitable definition for the cell spin was given by the sign rule

$$\mu_i = \mathrm{sgn}(\sigma_{i_1} + \sigma_{i_2} + \sigma_{i_3}).$$

In applying the transformation to the square lattice Nauenberg and Nienhuis (1974) used a similar definition for the cell spin by allocating three of the configurations for which $\Sigma\sigma_i = 0$ to positve cell spin and the other three, obtained by reversal of all spins, to negative cell spin.

In this section we extend the cluster expansion to the ATP model using the two-layered Ising representation. We follow Nauenberg and Nienhuis in choosing cells of four sites each (see figure 4). Since we have two layers of Ising spins we must define two new spins per cell—μ in the σ layer and t in the s layer. From the symmetry of the ATP model these two spins are equivalent and also equivalent to a new interlayer spin μt, in the σs layer. The fact that the new spins μ, t and μt are not independent imposes restrictions on the cell spin definition. It is not possible, for

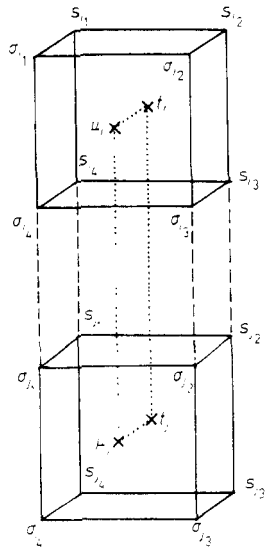

Figure 4. A cluster of two four-site cells on the square ATP lattice.

instance, to use the definition of Nauenberg and Nienhuis within the σ and s layers separately, since this leads to a contradiction in the definition of the interlayer spin, μt. For consistency and in order to retain the ATP model symmetry, we find that the only possible cell spin definitions are:

(*a*) $\mu_i = \pm\sigma_{i_j}$ $\quad t_i = \pm s_{i_j}$ $\quad (\mu t)_i = \pm(\sigma s)_{i_j}$ $\quad j = 1, 2, 3, 4$

(*b*) $\mu_i = \pm\sigma_{i_j}\sigma_{i_k}$ $\quad t_i = \pm s_{i_j}s_{i_k}$ $\quad (\mu t)_i = \pm(\sigma s)_{i_j}(\sigma s)_{i_k}$ $\quad j$ and k distinct

(*c*) $\mu_i = \pm\sigma_{i_1}\sigma_{i_2}\sigma_{i_3}\sigma_{i_4}/\sigma_{i_j}$ $\quad t_i = \pm s_{i_1}s_{i_2}s_{i_3}s_{i_4}/s_{i_j}$

(*d*) $\mu_i = \pm\sigma_{i_1}\sigma_{i_2}\sigma_{i_3}\sigma_{i_4}$ $\quad t_i = s_{i_1}s_{i_2}s_{i_3}s_{i_4}$ $\quad (\mu t)_i = (\sigma s)_{i_1}(\sigma s)_{i_2}(\sigma s)_{i_3}(\sigma s)_{i_4}$.

In choosing a suitable definition, we impose the restriction that under the transformation

$$\sigma_i \to -\sigma_i \qquad s_i \to -s_i \qquad \text{for all } i$$

we have

$$\mu_i \to -\mu_i \qquad t_i \to -t_i.$$

We are thus left only with types (*a*) and (*c*). Symmetry arguments show that each definition within a given type gives the same results. The effects of the definitions of types (*a*) and (*c*) on the Ising and Potts model fixed points were investigated (using a two-cell cluster). The results are shown in table 2 and although it can be seen that the results do depend on the definition used, there does not appear to be any criterion for the choice. In this work we have defined the cell spins by

$$\mu_i = \sigma_{i_1} \qquad t_i = s_{i_1}.$$

With this form of the cluster expansion we cannot get good quantitative results due to the size of the cluster used and to the difficulty in defining a suitable cell spin. The cluster expansion does, however, seem to give good qualitative results and we expect this to be carried over into our adaptation of the transformation to the ATP model.

Table 2. The fixed points of the Ising and Potts models for the two possible definitions of cell spin.

Model	Definition of cell spin μ	$K_\sigma^* = K_s^*$		$K_{\sigma s}^*$		Specific heat exponent	
		cluster expansion	exact	cluster expansion	exact	cluster expansion	exact/ series
Ising	$\mu = \pm\sigma_i$ $i = 1, 2, 3, 4$	0·69711	0·44064	0·0	0·0	0·00440	0·0
	$\mu = \pm\sigma_1\sigma_2\sigma_3\sigma_4/\sigma_i$ $i = 1, 2, 3, 4$	0·88366	0·44064	0·0	0·0	0·0928	0·0
Potts	$\mu = \pm\sigma_i$ $i = 1, 2, 3, 4$	0·41088	0·27465	0·41088	0·27465	0·34147	0·64 ± 0·05[a]
	$\mu = \pm\sigma_1\sigma_2\sigma_3\sigma_4/\sigma_i$ $i = 1, 2, 3, 4$	0·49290	0·27465	0·49290	0·27465	0·38967	0·64 ± 0·05

[a] From Enting (1975).

The renormalisation group transformation, R, transforms one set of coupling constants, $\{K\}$, to a new set $\{K'\}$

$$R(\{K\}) = \{K'\}$$

and a fixed point is given by

$$R(\{K^*\}) = \{K^*\}.$$

The transformation is linearised about the fixed point

$$\{K'\} = R(\{K\}) = R(\{K^*\} + \epsilon\{K\}) = \{K^*\} + \epsilon R^{\mathrm{L}}(\{K\}) + \mathrm{O}(\epsilon^2)$$

and the eigenvalues, λ_i, and eigenfunctions, $u_i(\{K\})$, of R^{L} are calculated:

$$R^{\mathrm{L}} u_i(\{K\}) = \lambda_i u_i(\{K\}).$$

By applying the transformation R to the function $\{K^*\} + u_i(\{K\})$ it is seen that an eigenvalue λ_i greater than one corresponds to an instability in the fixed point, the direction of which is given by the eigenfunction, u_i. We expect the fixed points corresponding to high and low temperature behaviour, to be stable with respect to a small change in the temperature, and we therefore refer to these as the stable fixed points. The fixed point corresponding to critical behaviour, will, however, be unstable to a small temperature change, and will be denoted an unstable, or critical fixed point.

Application of the transformation leads to unstable fixed points of only two types—the Potts model fixed point and fixed points of Ising type. Results for these are shown in Table 2.

By iterating the transformation from a given starting Hamiltonian, $H(K_\sigma, K_s, K_{\sigma s})$, we move along flow lines of the transformation to a stable fixed point describing the state of ordering of the initial Hamiltonian. By taking a series of starting Hamiltonians with a given ratio $R \equiv K_\sigma : K_s : K_{\sigma s}$ and finding their flow lines we, in effect, study the behaviour of the model as the temperature is varied. Thus if one starting Hamiltonian $H_1(R; T_1)$ flows to the high temperature fixed point (all $K_i \to 0$) we conclude that H_1 represents a system in a disordered state at temperature T_1. By varying T from 0 to ∞ (or equivalently by varying K_σ from ∞ to 0) we find the temperatures which give an ordered, a partially ordered and a disordered state, and

therefore by finding the boundary values T_c of T for these regions, we find the temperature at which phase transitions take place. A graph of the flow lines (K_s against $K_{\sigma s}$) for the ratio

$$R \equiv K_\sigma : K_s : K_{\sigma s} = 1 : 1{\cdot}3 : 1{\cdot}6$$

is given in figure 5. (A similar graph is obtained for K_σ against $K_{\sigma s}$). The broken lines in this graph are the lines between two regions and thus form a part of the critical surface. The end points of these critical lines are unstable fixed points which govern the critical behaviour of the particular ATP model under consideration. From figure 5 we see that the model, having ratio R, undergoes two phase transitions as expected.

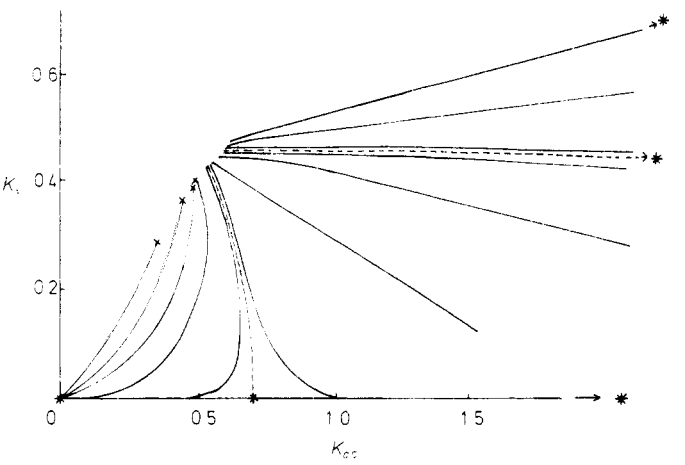

Figure 5. The flow lines for the cluster expansion for the ratio $R \equiv K_\sigma : K_s : K_{\sigma s} = 1 : 1{\cdot}3 : 1{\cdot}6$.

The above procedure was carried out for a set of values of R. The critical lines found by this method gave a critical surface consisting of three equivalent cups touching each other along lines for which $K_i = K_j \geq K_k$, in qualitative agreement with that found by Wu and Lin (figure 3). We should not be surprised at this agreement since the shape of the critical surface was arrived at by symmetry arguments and we know that the RNG is defined so that all lattice symmetries are maintained.

The critical surface for $K_\sigma = K_s$ is shown in figure 6, confirming that for $K_{\sigma s} > K_\sigma = K_s$ we do find two transitions, but only one for the case $K_\sigma = K_s \geq K_{\sigma s}$ as expected.

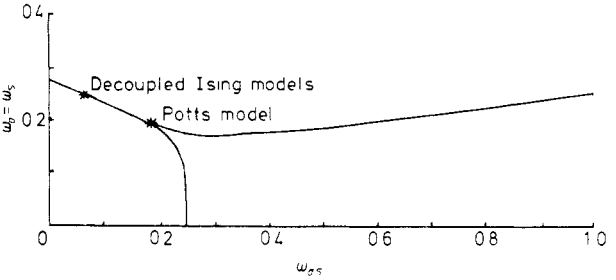

Figure 6. The cross section of the critical surface of the ATP model for which $K_\sigma = K_s$.

Under iteration all Hamiltonians, with the single exception of the Potts model Hamiltonian, were governed by Ising-like fixed points. Thus, this method of analysis gives no indication of a line of fixed points and therefore no continuously varying exponents. However, the simpler we make an approximation, the less likely it is to find a given fixed point and so we should not be surprised that our crude approximation found only the fixed points of special symmetry.

As expected the model with three different interactions gave two transitions. The transition away from the high temperature phase was governed, in all cases, by Ising model fixed points—$K_i = S$, $K_j = K_k = 0$, where S is the critical temperature of the Ising model The second transition was governed by fixed points at $\omega_i = r = e^{-2S}$, $\omega_j = \omega_k = 0$, which as noted before is a one-to-many correspondence of the ω–K transformation. In terms of the coupling constants different models are governed by different fixed points. However, since these fixed points are approached along lines of constant K_j and K_k it can easily be shown that, at least within the RNG of nearest neighbour couplings only, all these fixed points give Ising exponents. Therefore the cluster expansion leads us to expect Ising exponents for all ATP models except the single case of the Potts model.

4. Analysis of the ATP model using the lower bound renormalisation transformation

In 1975 Kadanoff first introduced a real-space RNG using a variational approximation. The basic philosophy being that a set of transformations could be defined, using a number of free parameters, to give either an upper or a lower bound to the free energy. The best transformation was then defined to be that for which the choice of free parameters gave an optimal bound on the free energy. In practice there is no guarantee that these optimal transformations need either give a value of the free energy close to its true value or that the exponent values—found from the derivatives of the free energy—need be close to their values. However, when Kadanoff and co-workers applied the transformation to the square Ising model they obtained remarkably accurate results. In view of the accuracy of these results we thought it worthwhile to apply this transformation to the ATP model.

A full description of the lower bound transformation is given in Kadanoff *et al* (1976), but for completeness we give a brief description of the main points of the transformation as extended to the ATP system.

We consider a system of $2N$ Ising spins, two, (σ, s), being placed at each vertex of a two-layered lattice. The system is then described by a Hamiltonian H, which is a function of some set of coupling constants $\{K\}$, including, in particular, the nearest-neighbour couplings K_σ, K_s, $K_{\sigma s}$. The RNG transformation, R, will then take us to a new set of spins $\{\mu, t\}$ described by a Hamiltonian, H', and coupled by a set of coupling constants $\{K'\}$. The condition on the exact transformation is that the free energy is unchanged in the transformation. In practice, however, we are unable to find such an exact transformation and we must resort to some approximation. Kadanoff *et al* did this by forming lower bounds on the free energy:

$$F_{N'}(R^1(H_K)) \leqslant F_{N'}(R(H_K)) = F_N(H_K) \tag{4.1}$$

where R^1 represents the approximate RNG transformation. In defining this lower bound transformation we introduce a set of variational parameters $\boldsymbol{p}$. Then the exact

transformation is given by

$$H'(\mu, t) = -\ln \sum_{\{\sigma, s\}} \exp(-H(\sigma, s) + T(\mu, t, \sigma, s, \boldsymbol{p})) \tag{4.2}$$

where, in order that the free energy is unchanged, we must have

$$\sum_{\{\mu, t\}} \exp(T(\mu, t, \sigma, s, \boldsymbol{p})) = 1 \tag{4.3}$$

and the lower bound transformation is

$$H^{\mathrm{l}}(\sigma, t) = -\ln \sum_{\{\sigma, s\}} \exp(-H(\sigma, s) + T(\mu, t, \sigma, s, \boldsymbol{p}) + V(\sigma, s)) \tag{4.4}$$

where, by choosing V to be a sum of terms, each odd under some lattice symmetry, we have ensured that the free energy is, in fact, a lower bound on the exact free energy.

Now define

$$H(\sigma, s) = -\sum_{\text{squares}} \sum_{i} K_i S_i(\sigma, s) \tag{4.5}$$

where the S_i are a complete set of spin functions $\{S\}$ obeying all the lattice symmetries. We find that there are 55 of these spin functions. However, in applying the transformation, we follow Kadanoff in performing an initial decimation thus obtaining a permutation symmetry between the sites of a square. In this way we restrict the spin functions to a set of 35, thus making the problem more manageable. The symmetry of the transformation will imply that $H'(\mu, t)$ may be written in a similar form to $H(\sigma, s)$.

We now consider the lattice to be coloured as shown in figure 7. The new set of spins, $\{\mu, t\}$ are placed within the red squares. Choose

$$T(\mu, t, \sigma, s, \boldsymbol{p}) = \sum_{\substack{\text{red} \\ \text{squares}}} (\mu p_\sigma S_{\sigma_1} + t p_s S_{s_1} + \mu t p_{\sigma s_1} S_{\sigma s_1} - U) \tag{4.6}$$

where

$$S_{\sigma_1} = \sigma_1 + \sigma_2 + \sigma_3 + \sigma_4$$

$$S_{s_1} = s_1 + s_2 + s_3 + s_4$$

$$S_{\sigma s_1} = \sigma_1 s_1 + \sigma_2 s_2 + \sigma_3 s_3 + \sigma_4 s_4$$

σ_i, s_i, $i = 1, \ldots, 4$, are the spins around a red square and U is such that (4.3) is satisfied, i.e.

$$U = \ln(\mathrm{e}^{a+b+c} + \mathrm{e}^{a-b-c} + \mathrm{e}^{-a+b-c} + \mathrm{e}^{-a-b+c}) \tag{4.7}$$

where $a = p_\sigma S_{\sigma_1}$, $b = p_s S_{s_1}$, $c = p_{\sigma s} S_{\sigma s_1}$ p_σ, p_s, $p_{\sigma s}$ are our variational parameters.

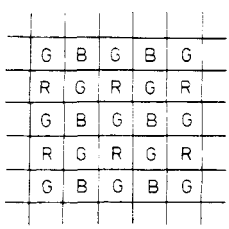

Figure 7. The division of the square lattice into red, blue and green squares. Renormalised spins are placed in the red squares.

Finally V is chosen so that all the interactions within the red and green squares are moved to the blue squares. This enables the sum in (4.4) over all squares of the lattice to be separated into a product of sums over the spins around the blue squares. Each sum is now only over 256 terms and the transformation is manageable. The transformation may be written

$$H'(\mu, t) = -\sum_i K_i' S_i(\mu, t)$$

$$= -\ln \sum_{\{\sigma,s\}} \exp\Big(p_\sigma \sum_{i=1}^{4} \mu_i\sigma_i + p_s \sum_{i=1}^{4} t_i s_i + p_{\sigma s} \sum_{i=1}^{4} \mu_i t_i \sigma_i s_i + 4 \sum_i K_i S_i(\sigma, s) \Big)$$

$$\times (e^{a+b+c} + e^{a-b-c} + e^{-a+b-c} + e^{-a-b+c})^{-1}$$

where the first sum within the large parentheses is over all cell spins surrounding the blue cell and the last is over all the coupling constants K_i.

As usual the critical properties of the system are determined by the eigenvalues, λ_i, of the derivative matrix

$$T_{ij} = \partial K_i / \partial K_j.$$

From the eigenvalues we calculate a further set of quantities a_i:

$$a_i = \frac{\ln \lambda_i}{d \ln l}$$

where d is the dimension of the system and l is a new lattice spacing in terms of the old. Thus in our case $a_i = \ln \lambda_i / \ln 4$. We assume, along scaling argument lines, that the free energy F, is a homogeneous function of the reduced temperature t, the magnetic field h, and any other property x, showing singular behaviour:

$$\lambda F(t, h, x) = F(\lambda^a t, \lambda^b h, \lambda^c x)$$

where a, b and c may be identified with the a_i defined above. Scaling now allows us to write the exponents α and δ as $\alpha = 2 - (1/a)$, $\delta = b/(1-b)$ and also to express the critical exponents corresponding to the singularity in the property x, in terms of a, b, c.

Due to the two-layered nature of the system, the ATP model has two order parameters:

magnetisation	$M = \langle \sigma_i \rangle = \langle s_i \rangle$
polarisation	$P = \langle \sigma_i s_i \rangle$.

Thus in addition to the normal magnetisation exponents δ_m and β_m corresponding to the singular behaviour of the spin function S_{σ_1} (or S_{s_1}) $= \Sigma\sigma_i$ as $H \to 0 (t = 0)$ and $t \to 0 (H = 0)$ respectively, we expect to find critical exponents δ_e and β_e corresponding to the critical behaviour of the spin function $S_{\sigma_1 s_1} = \Sigma_{\sigma_i s_i}$.

Although our definition of the RNG transformation allows us to include external fields, we have, for simplicity, only studied the ATP model in the absence of any such fields. In effect this reduces the dimension of the space in which we are searching for fixed points to an eleven-dimensional space of coupling constants. The coupling constants, together with the corresponding spin functions are given in table 3.

As in the case of the cluster expansion, successive applications of the transformation lead us along flow lines to a stable fixed point. By obtaining these flow lines for a given p_σ, p_s and $p_{\sigma s}$ the approximate position of a line of critical surface was

Table 3. The coupling constants and corresponding spin functions.

Coupling constant	Corresponding spin function
K_σ	$S_{\sigma 2} = \sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1 + \sigma_1\sigma_2 + \sigma_2\sigma_4$
K_s	$S_{s2} = s_1s_2 + s_2s_3 + s_3s_4 + s_4s_1 + s_1s_3 + s_2s_4$
$K_{\sigma s}$	$S_{(\sigma s)2} = \sigma_1s_1\sigma_2s_2 + \sigma_2s_2\sigma_3s_3 + \sigma_3s_3\sigma_4s_4 + \sigma_4s_4\sigma_1s_1 + \sigma_1s_1\sigma_3s_3 + \sigma_2s_2\sigma_4s_4$
$K_{\sigma 4}$	$S_{\sigma 4} = \sigma_1\sigma_2\sigma_3\sigma_4$
K_{s4}	$S_{s4} = s_1s_2s_3s_4$
$K_{(\sigma s)4}$	$S_{(\sigma s)4} = \sigma_1s_1\sigma_2s_2\sigma_3s_3\sigma_4s_4$
$K_{\sigma 2s2}$	$S_{\sigma 2s2} = \sigma_1\sigma_2s_3s_4 + \sigma_2\sigma_3s_4s_1 + \sigma_3\sigma_4s_1s_2 + \sigma_4\sigma_1s_2s_3 + \sigma_1\sigma_3s_2s_4 + \sigma_2\sigma_4s_1s_3$
$K_{s2(\sigma s)2}$	$S_{s2(\sigma s)2} = s_1s_2s_3s_4(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1 + \sigma_1\sigma_3 + \sigma_2\sigma_4)$
$K_{\sigma 1s1(\sigma s)1}$	$S_{\sigma 1s1(\sigma s)1} = \sigma_1s_2\sigma_3s_3 + \sigma_1s_2\sigma_4s_4 + \sigma_1s_3\sigma_2s_2 + \sigma_1s_3\sigma_4s_4 + \sigma_1s_4\sigma_2s_2$ $+ \sigma_1s_4\sigma_3s_3 + \sigma_2s_1\sigma_3s_3 + \sigma_2s_1\sigma_4s_4 + \sigma_2s_3\sigma_1s_1 + \sigma_2s_3\sigma_4s_4$ $+ \sigma_2s_4\sigma_1s_1 + \sigma_2s_4\sigma_3s_3 + \sigma_3s_1\sigma_2s_2 + \sigma_3s_1\sigma_4s_4 + \sigma_3s_2\sigma_1s_1$ $+ \sigma_3s_2\sigma_4s_4 + \sigma_3s_4\sigma_1s_1 + \sigma_3s_4\sigma_2s_2 + \sigma_4s_1\sigma_2s_2 + \sigma_4s_1\sigma_3s_3$ $+ \sigma_4s_2\sigma_1s_1 + \sigma_4s_2\sigma_3s_3 + \sigma_4s_3\sigma_1s_1 + \sigma_4s_3\sigma_2s_2$
K_0	$S_0 = 1$

found. It was then possible, by taking as our starting point a Hamiltonian on the approximate critical line and using numerical convergence techniques, to find a fixed point Hamiltonian

$$H(\boldsymbol{K}, p_\sigma, p_s, p_{\sigma s}) = H^*(\boldsymbol{K}^*, p_\sigma, p_s, p_{\sigma s}) \tag{4.9}$$

having instabilities in certain directions. The best fixed point was then found by optimising over the free parameters according to the prescription given by Kadanoff *et al* (1976), so that

$$H^*(\boldsymbol{K}^*, p_\sigma, p_s, p_{\sigma s}) = H^*(\boldsymbol{K}^*, p_\sigma^*, p_s^*, p_{\sigma s}^*). \tag{4.10}$$

We first describe the results obtained for the particular case $K_{\sigma s} = 0$, of the ATP model which decouples into two simple Ising models. Although this case is rather trivial we use it as an illustration of the accuracy of the method. For $K_\sigma \neq K_s$ we find two transitions at temperatures T_{1c} and T_{2c}. We take $T_{1c} > T_{2c}$. As the temperature is varied we find several regimes:

(*a*) $T > T_{1c}$. The model is completely disordered and there are no relevant eigenvalues at the fixed point (corresponding to the fixed point being stable in all directions).

(*b*) $T_1 = T_{1c} > T_{2c}$. This is controlled by a fixed point having relevant temperature and magnetic eigenvalues $\lambda_{T\sigma}$ and $\lambda_{H\sigma}$ corresponding to instabilities in the fixed point in these directions in the σ lattice.

(*c*) $T_{2c} < T < T_{1c}$. We find a magnetic eigenvalue due to the σ lattice being in an ordered state.

(*d*) $T = T_{2c}$. In this case the fixed point has temperature and magnetic eigenvalues for the s lattice.

(*e*) $T < T_{2c}$. This is governed by the low temperature fixed point and we have magnetic eigenvalues for both lattices. If, in particular we have $K = K_s$ then the types (*b*), (*c*), (*d*) are replaced by a single type:

(*f*) $T = T_{1c} = T_{2c}$. The model has one transition only and its critical properties are governed by a fixed point with two equal magnetic eigenvalues. In this case we

find a marginal eigenvalue, $\lambda = 1$, corresponding to a neutral stability in the $K_{\sigma s}$ direction.

In addition to the above mentioned eigenvalues we find crossover exponents ϕ_1, ϕ_2, ϕ_3 corresponding to the critical behaviour of the spin functions

$$S_1 = \sum_{i,j} \sigma_i \sigma_j \qquad S_2 = \sum_{k \neq i,j} \sigma_i \sigma_j s_k \qquad S_3 = \sum_{k \neq i,j} \sigma_k s_i s_j \tag{4.11}$$

for various values of the ratio T_{1c}/T_{2c}. Since, in this case, the two lattices are decoupled we may express these functions as a product of the functions on the two lattices separately. Thus

$$S_1 = S_{\sigma_1} S_{s_1} \qquad S_2 = S_{\sigma_2} S_{s_1} \qquad S_3 = S_{\sigma_1} S_{s_2}. \tag{4.12}$$

From the Ising model results we will then know the exact values of ϕ_1, ϕ_2 and ϕ_3.

Table 4 gives the values of the fixed point couplings and free parameters, and table 5 the a_i values corresponding to the magnetic and temperature eigenvalues together with the exact results for comparison. Table 6 shows the crossover exponents for the two cases: (i) $T_{1c} > T_{2c}$; (ii) $T_{1c} = T_{2c}$.

The method of finding the flow lines of various starting Hamiltonians with a given ratio $R \equiv K_\sigma : K_s : K_{\sigma s}$ and fixed p_σ, p_s, $p_{\sigma s}$ was used to confirm that we do indeed find

Table 4. The coupling constant and variational parameter values at the fixed points of the decoupled ATP model ($K_{\sigma s} = 0$).

Fixed point	K_σ^*	K_s^*	p_σ^*	p_s^*	$p_{\sigma s}^*$
a	0	0	0	0	0
b	0·1397	0	0·766	0	0
c	∞	0	∞	0	0
d	∞	0·1397	∞	0·766	0
e	∞	∞	∞	∞	0
f	0·1397	0·1397	0·766	0·766	0

Table 5. The a_i corresponding to magnetic and temperature eigenvalues for all fixed points of the decoupled ATP model ($K_{\sigma s} = 0$).

Fixed point	$a_{H\sigma}$ calculated/ exact	a_{Hs} calculated/ exact	$a_{T\sigma}$ calculated/ exact	a_{Ts} calculated/ exact
a	——	——	——	——
b	0·9377	——	0·5005	——
	0·9375		0·5	
c	1·00	——	——	——
	1·00			
d	1·00	0·9377	——	0·5005
	1·00	0·9375		0·5
e	1·00	1·00	——	——
	1·00	1·00		
f	0·9377	0·9377	0·5005	0·5005
	0·9375	0·9375	0·5	0·5

Table 6. The crossover exponents at temperature T_{1c} for two decoupled Ising systems having transition temperatures T_{1c} and T_{2c}. ϕ_{ic}, $i = 1, 2, 3$ represent the exponents calculated by the LBRNGT and ϕ_{iE} the corresponding exact values.

	ϕ_{1c}	ϕ_{1E}	ϕ_{2c}	ϕ_{2E}	ϕ_{3c}	ϕ_{3E}
$T_{1c} > T_{2c}$	0·1247	0·125	0·9991	1·0	0·1247	0·125
$T_{1c} = T_{2c}$	0·2494	0·25	1·124	1·125	1·124	1·125

two phase transitions for the general case of the ATP model. In order to obtain any numerical results by this method, however, would entail the variation of the p_i to their optimum values at each iteration of the transformation. Due to the extremely time consuming nature of this process, this was not done.

For the particular case $K_\sigma = K_s \geqslant K_{\sigma s}$ in which the ATP model undergoes one transition only, we do find an indication of a line of fixed points when $K_{\sigma s} \geqslant 0$. As expected we find no fixed points having one of the nearest-neighbour couplings negative. Strictly speaking, for a best transformation and therefore a fixed point, we should require that the transformation be optimal with respect to p_σ, p_s and $p_{\sigma s}$ simultaneously. In practice, we find that this is only true exactly in the cases of special symmetry, e.g. the Potts model in which all three parameters are constrained to be equal, and the decoupled Ising lattices model in which $p_{\sigma s}$ is constrained to be zero. However, it was found possible to obtain a line of fixed points for $0 \leqslant K_{\sigma s} \leqslant K_\sigma = K_s$ in the two cases: (1) for optimal $p_1 = p_2$; (2) for optimal p_3.

We find that for $K_{\sigma s}/K_\sigma$ small and also for $K_{\sigma s}/K_\sigma$ close to 1 the fixed points are sufficiently close to being optimal for all three parameters simultaneously that in these regions we may infer a line of fixed points within the eleven-dimensional space of coupling constants. A graph of $K_{\sigma s}$ against K_σ for the two cases described above is shown in figure 8. From this we may see that while the p_σ–p_s curve is smooth and well behaved, there appears to be a singularity in the $p_{\sigma s}$ curve. At each of the fixed points,

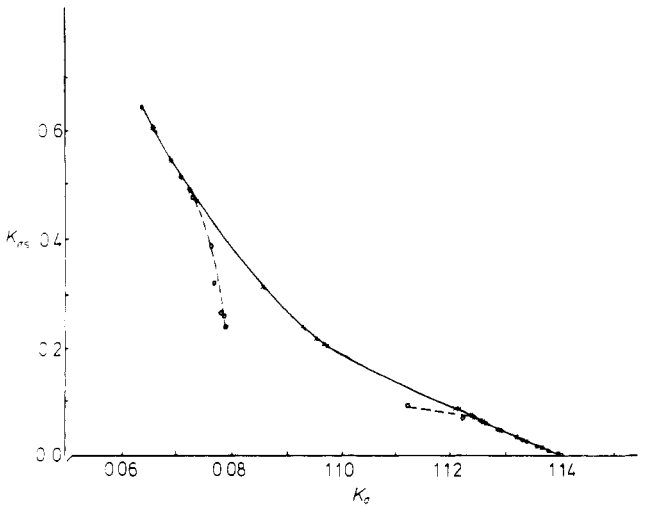

Figure 8. A graph of $K_{\sigma s}$ against K_σ for the region $0 \leqslant K_{\sigma s} \leqslant K_\sigma (= K_s)$ in the two cases: (i) optimal p_1 and p_2 (ii) optimal p_3 (broken curve with open circles). Fixed points which may be considered to be optimal for all three parameters are denoted by asterisks.

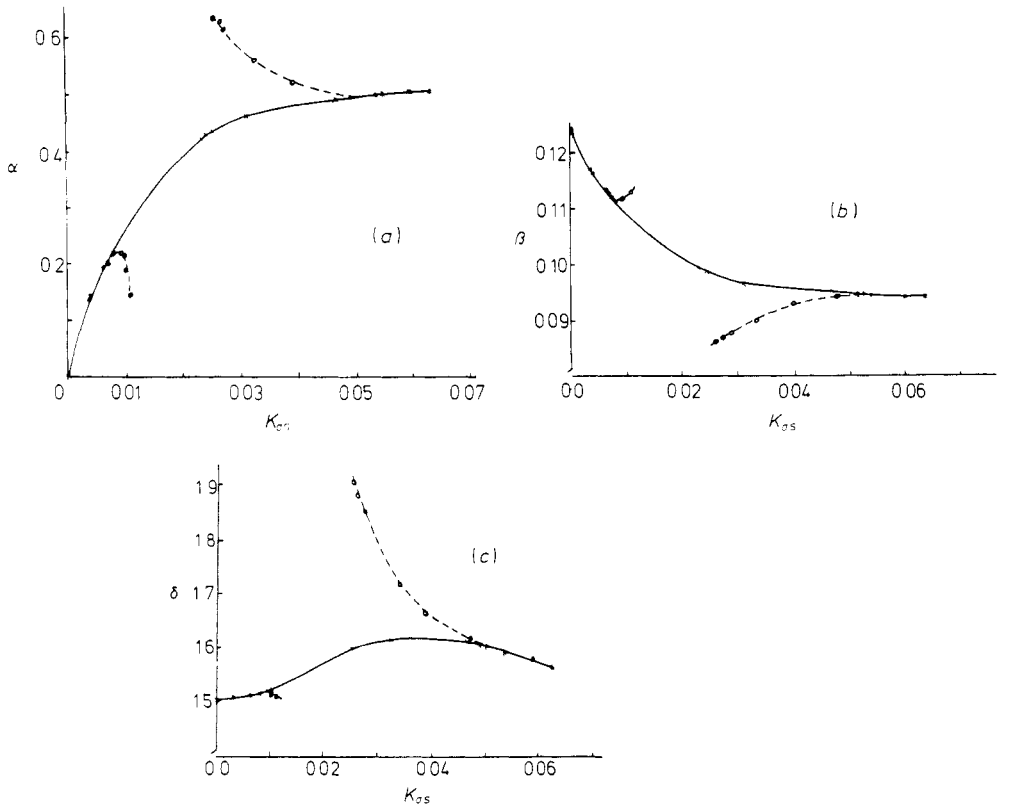

Figure 9. Graphs against $K_{\sigma s}$ of: (a) the specific heat exponent, α; and the magnetic exponents (b) β and (c) δ; for the region $0 \leq K_{\sigma s} \leq K_{\sigma}(=K_s)$ in the two cases: (i) optimal p_1 and p_2 (full curve with crosses); (ii) optimal p_3 (broken curve with open circles).

values of the critical exponents were calculated and graphs of α, β and δ against $K_{\sigma s}$—the four-spin coupling—in the same two cases as above are shown in figures 9(a), (b), (c). Again the singularity in the $P_{\sigma s}$ curve shows up clearly while the p_{σ}–p_s curve is well behaved. It is worth noting here, that although the δ curve does appear to vary considerably, this exponent is extremely sensitive to the exact position of the fixed point and thus our results need not contradict the hypothesis that $\delta = 15$ for all values of $K_{\sigma s}$.

The reason for the singularity in the $p_{\sigma s}$ curve is not clear, but due to the smoothness of the p_{σ}–p_s curve it is tempting to treat this set of fixed points as a true line of fixed points and compare our results with those of the eight-vertex model. We note that the values of the specific heat component α, are the same for the two models in the two cases:

(i) the symmetric case $K_{\sigma} = K_s = K_{\sigma s}$ and $\lambda = K^+ = K^-$, $\alpha = \frac{1}{2}$;

(ii) the decoupled case $K_{\sigma s} = 0$ and $\lambda = 0$, $\alpha = 0$.

It therefore seems possible that α takes the same values in the two models for the same ratio of the four-spin coupling to the two-spin couplings.

In order to make a direct comparison though, it would be necessary to find the critical temperatures (i.e. $K_{\sigma sc}$) corresponding to all the fixed points. However, as previously mentioned, the procedure necessary to find the critical temperature

involves optimisation over $p_\sigma, p_s, p_{\sigma s}$ at each iteration and is therefore not feasible. Thus it is only possible for us to make the comparison using the fixed point values of the couplings, K_σ^* and K_s^*. This comparison is shown in figure 10 from which it may be seen that the conjecture of equivalent α values for the two models is unlikely to be true. It would, however, be interesting to see how much difference a true comparison using the ATP critical temperatures would make.

Finally it seems worthwhile to compare our results for the decoupled model with exact results, and the Potts model results with series expansion results. This comparison is given in table 7.

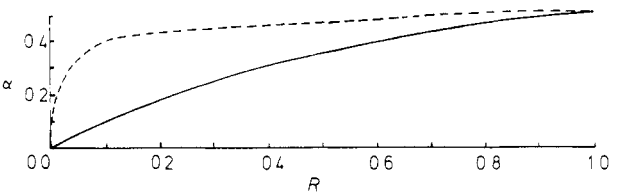

Figure 10. A comparison of the variation of α with the ratio R = four-spin coupling/two-spin couplings for the eight-vertex model (full curve) and for the ATP model (broken curve). For the ATP model the values of the couplings are the fixed point values.

Table 7. Comparison of the Ising model and Potts model exponents with exact or series results.

	Ising model		Potts model	
Critical exponent	renormalisation group	exact results	renormalisation group	series expansion
α	0·0017	0·0	0·5009	$0{\cdot}64 \pm 0{\cdot}05$[a]
δ_m	15·040	15·0	15·65	$15{\cdot}8 \pm 0{\cdot}8$[b]
δ_e	7·021	7·0	15·65	$15{\cdot}8 \pm 0{\cdot}8$[b]
β_m	0·1246	0·125	0·09005	$0{\cdot}089 \pm 0{\cdot}003$[a]
β_e	0·2494	0·25	0·09005	$0{\cdot}089 \pm 0{\cdot}003$[a]

[a] Enting (1975).
[b] Enting (1976).

5. Summary

We have examined the ATP model, in the absence of any external fields, using two distinct RNG transformations. The cluster expansion, used to give easily obtainable and good qualitative results, gave a description of the critical surface in accordance with that conjectured by Wu and Lin (1974). Our adaptation of the cluster expansion to the ATP model was however, a very simple one and the two-cell cluster used was not large enough to give good numerical results.

The Kadanoff LBRNGT was not suitable for a study of the whole of the critical surface due to the enormity of the calculations required for this, but it was used to give numerical results for the critical exponents. We found a very strong indication of a

line of fixed points giving varying exponents for the cases $K_i = K_j \geq K_k \geq 0$ and a comparison of these results was made with the exact eight-vertex model results.

Away from the lines of fixed points our study leads us to believe that the ATP model has Ising behaviour and therefore Ising exponents.

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