

# Critical behaviour of a two-dimensional bonded lattice model

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**Abstract.** The Bell–Lavis model of a two-dimensional bonded lattice fluid is investigated by real space renormalisation group methods. All the fixed points in a restricted parameter subspace are obtained, but their stability is analysed in the full parameter space of the system. Within the subspace melting is predicted to occur via a second-order transition in the same universality class as the 3-state ferromagnetic Potts model. This contrasts with the predictions of mean-field theory. There is however a weakly relevant eigenvalue whose corresponding eigenvector is in a direction out of the subspace, so the fixed point may not be a critical point for the full model. A second result of interest is that the fixed point, found by Schick and Griffiths for the 3-state antiferromagnetic Potts model on a triangular lattice, also describes the transition in the more general case of an antiferromagnetic spin-one Ising model (the Blume–Emery–Griffiths model) on the same lattice. Some interesting symmetry properties of the subspace are also discussed.

## 1. Introduction

Bell and Lavis (1970) (hereafter referred to as BL) introduced a triangular lattice model for the fluid phases of the water system, in which hydrogen bonding was represented by attributing to each molecule preferential bonding directions. Using a closed-form approximation they were able to reproduce a first-order phase transition with the characteristic density maximum along isobars in the liquid phase. Using the same approximation method Lavis (1973) extended the model to include a long-range ordered ice-like phase. This phase was attained via a first-order transition in which the solid phase was less dense than the liquid phase. The properties of the thermodynamic response functions along the liquid–vapour transition curve were investigated by Lavis (1975). These exhibited water-like properties.

In the present paper we begin a study of this model by real space renormalisation group (RSRG) methods (for a review see Niemeijer and van Leeuwen 1976). One motivation for attempting this problem with renormalisation group (RG) methods is the recent realisation that various types of sublattice ordering in Ising models can involve transitions which are in different universality classes from the ferromagnetic transition (Alexander 1975, Domany *et al* 1977, Krinsky and Mukamel 1977). As we shall show in § 3, long-range order in the BL model, which corresponds to the ice phase, also involves a type of sublattice ordering in the Ising representation of the model. The question arises, then, as to whether the fluid–solid transition in the BL model (which as

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we shall see is possibly of second order) falls into one of the already established universality classes or is in a new class. An interesting feature of the model is that it does not have the usual inversion symmetry when the signs of all the spins are changed. This again raises the possibility of new universality classes.

The BL model has a rich and complicated phase diagram and reduces to several other interesting models in limiting cases. For example, for certain values of the parameters, the BL model reduces to the 3-state Potts model (Potts 1952) which is rather similar to the spin-one Ising model except that all three possible spin states are equivalent. The ferromagnetic transition in this model is predicted by Landau theory to be first order, whereas it is known exactly (Baxter 1973) to be continuous. The 3-state Potts model with sublattice ordering on a triangular lattice has already been studied by Schick and Griffiths (1977) (hereafter referred to as SG). Another special case of the BL model is a modified 3-state Potts model which includes the term in the spin Hamiltonian which breaks the inversion ( $S \leftrightarrow -S$ ) symmetry. Since this term is the main new feature of the model and because the full model is very complicated we restrict our attention here to this special subspace.

The antiferromagnetic groundstate of this subspace is the same as the ordered ground state (solid phase) of the BL model so we expect our results to be of some relevance to the full model. In the restricted parameter space the full fixed point structure is determined and thus in this subspace the phase diagram can be constructed. The stability of these fixed points is analysed, leading to predictions for the critical exponents. This we are able to do in the *full* parameter space of the BL model. Consequently we are able to estimate whether the fixed points which we find really correspond to critical points of the BL model.

Within our 3-parameter subspace the fixed point which describes the antiferromagnetic transition lies in an invariant plane of the transformation, where the symmetry is *again* that of the 3-state Potts model. As a result the antiferromagnetic transition, which corresponds to the melting transition in this subspace of the BL model, is second order, in contrast to mean-field theory (Lavis 1973) which predicts a first-order change, and is in the same universality class as the *ferromagnetic* transition in the 3-state Potts model (see SG). However we find a weakly relevant eigenvalue which takes one out of the subspace so this fixed point may not correspond to an ordinary critical point of the full BL model. The order of a transition may depend on spatial dimensionality and we suspect that second-order melting found in this study is a consequence of the low dimensionality of the BL model. In three dimensions, for example, the 3-state Potts model probably has a *first-order* transition (Aharony *et al* 1977, Mukamel *et al* 1976) in agreement with mean-field theory but in contrast to Baxter's exact prediction for the same model in two dimensions.

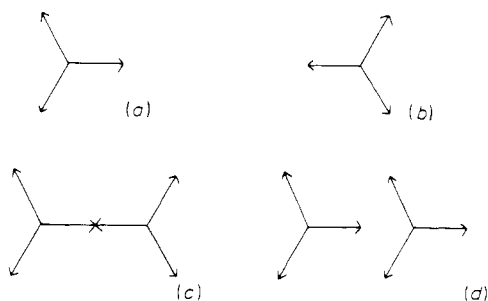
We introduce the model and discuss the restricted (extended Potts) subspace in § 2. In § 3 Landau theory and the symmetry properties are considered and the RG transformation is constructed in § 4, where results for fixed points and exponents are also given. Our conclusions are summarised in § 5.

## 2. The model

### 2.1. General form

The BL model is an extension of the simpler lattice fluid models to the case where the molecules have some 'structure'. A triangular lattice is assumed and a molecule is

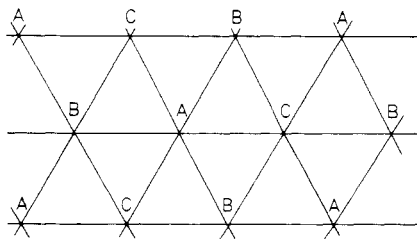
represented by three arrows (bonding arms) radiating from a point, the angles between the arrows being  $120^\circ$  (see figure 1(a)). Each lattice site is either vacant or has a molecule, centred at the site, with the arrows directed towards three of the six nearest-neighbour sites. There are therefore two possible orientations for a molecule which are shown in figures 1(a) and (b).



**Figure 1.** (a) and (b) denote the two possible orientations of the molecule on a triangular lattice in the BL model. They will be designated as states  $S = 1$  and  $S = -1$ , respectively, of a spin-one Ising model. The state  $S = 0$  corresponds to there being no molecule on the site. (c) represents a configuration of two neighbouring molecules which form a bond while (d) shows one of the non-bonding arrangements. Configurations (c) and (d) have energies  $-(\epsilon + w)$  and  $-\epsilon$  respectively.

Molecules on adjacent sites can either form a bond, if they have arrows which meet as in figure 1(c), or not, as in figure 1(d). These two configurations have energies  $-(\epsilon + w)$  and  $-\epsilon$  respectively. The mean density of molecules is fixed most conveniently for the present calculation by using the grand canonical distribution with chemical potential as an independent variable.

For RSRG calculations it is useful to rewrite the Hamiltonian in spin language. Each site can be in one of three possible states: no molecule, a molecule with the orientation of figure 1(a) or a molecule with the orientation of figure 1(b). With these we associated the spin states  $S = 0$ ,  $S = 1$  and  $S = -1$  respectively of a spin-one Ising model. We also need to define three sublattices A, B and C, on the triangular lattice, whose locations are indicated in figure 2. Bonding between adjacent sites on A and B sublattices can occur only if  $S_A = -1$  and  $S_B = 1$ . For bonding between B and C sublattices we need  $S_B = -1$  and  $S_C = 1$  and for bonding between C and A sublattices we need  $S_C = -1$  and  $S_A = 1$ . Noting that the projection operators which pick out the states  $S = \pm 1$  are  $\frac{1}{2}(S^2 \pm S)$ , the



**Figure 2.** The convention adopted for labelling the three sublattices A, B and C.

Hamiltonian  $\mathcal{H}$  may be written in the form

$$\mathcal{H} = -\frac{1}{2}\epsilon \sum_i (S_{iA}^2 S_{iB}^2 + S_{iB}^2 S_{iC}^2 + S_{iC}^2 S_{iA}^2) - \frac{1}{8}w \sum_i [(S_{iA}^2 - S_{iA})(S_{iB}^2 + S_{iB}) + (S_{iB}^2 - S_{iB})(S_{iC}^2 + S_{iC}) + (S_{iC}^2 - S_{iC})(S_{iA}^2 + S_{iA})] \quad (1)$$

where  $i$  denotes a particular triangle and  $S_{i\alpha}$  ( $\alpha = A, B$  or  $C$ ) denotes the spin of the site on sublattice  $\alpha$  in triangle  $i$ . The mean density of molecules is  $\langle S^2 \rangle$  so a chemical potential term  $-\mu S^2$  is added for each site giving in all an additional term

$$\mathcal{H}_\mu = -\frac{1}{6}\mu \sum_i (S_{iA}^2 + S_{iB}^2 + S_{iC}^2), \quad (2)$$

the factor of  $\frac{1}{6}$  arising because each site is shared between six triangles. We define  $H = -\beta\mathcal{H}$  where  $\beta = 1/k_B T$  and rearranging the terms in equation (1) we have  $H = H_1 + H_2$ , where

$$H_1 = \frac{1}{2}\bar{J} \sum_i (S_{iA}S_{iB} + S_{iB}S_{iC} + S_{iC}S_{iA}) - \frac{1}{6}\bar{\Delta} \sum_i (S_{iA}^2 + S_{iB}^2 + S_{iC}^2) + \frac{1}{2}\bar{K} \sum_i (S_{iA}^2 S_{iB}^2 + S_{iB}^2 S_{iC}^2 + S_{iC}^2 S_{iA}^2) \quad (3)$$

and

$$H_2 = -\frac{1}{4}P \sum_i (S_{iA} - S_{iB})(S_{iB} - S_{iC})(S_{iC} - S_{iA}). \quad (4)$$

The interactions  $\bar{J}$ ,  $\bar{K}$ ,  $\bar{\Delta}$  and  $P$  are related to the original parameters by

$$\begin{aligned} \bar{J} &= -\frac{1}{4}\beta w \\ \bar{K} &= \beta(\epsilon + \frac{1}{4}w) \\ \bar{\Delta} &= -\beta\mu \\ P &= \frac{1}{2}\beta w. \end{aligned} \quad (5)$$

Although  $P = -2\bar{J}$  for the BL model, this relationship no longer holds after a RG transformation so we need to make use of different symbols for these two quantities.  $H_1$  corresponds to the Blume–Emery–Griffiths (1971) model which has been studied by mean field (Blume *et al* 1971, Lajzerowicz and Sivardière 1975) and RSRG methods (Berker and Wortis 1976). A new feature of the present model is that the spin-spin coupling  $\bar{J}$  is antiferromagnetic, since bonding occurs only if the molecules have different orientations, which is important for the triangular lattice discussed here. The crucial role of the sign of the interaction for the triangular lattice can be gauged from the fact that a spin  $-\frac{1}{2}$  Ising antiferromagnet has no transition on a triangular lattice (Wannier 1950). In fact the BL model is isomorphic to the spin  $-\frac{1}{2}$  Ising antiferromagnet in the high-density limit ( $\bar{\Delta} \rightarrow -\infty$ ) (see Bell and Lavis 1970, appendix) since the  $S = 0$  states are suppressed,  $H_2$  is zero and the  $\bar{K}$  and  $\bar{\Delta}$  terms in  $H_1$  are constants.

The most interesting feature of the model is, however, the appearance of  $H_2$ , which does not have the usual inversion ( $S \leftrightarrow -S$ ) symmetry. It is clear why the model in its original form does not have this symmetry since changing the orientations of each member of a pair of bonded molecules always breaks the bond.  $H_2$  is non-vanishing only when the spins around the triangle are in different states. The energy is  $\frac{1}{2}P$  if the A,

B and C spins are in states +, 0 and - respectively, or any even permutation of this and it is  $-\frac{1}{2}P$  for an odd permutation.

In the RSRG calculation which follows it will be necessary to include all interactions compatible with the symmetry of the model which can be fitted into an elementary triangle. We therefore add to the Hamiltonian a term  $H_3$  given by

$$H_3 = \bar{L} \sum_i S_{iA}^2 S_{iB}^2 S_{iC}^2 + \bar{M} \sum (S_{iA}^2 S_{iB} S_{iC} + S_{iB}^2 S_{iC} S_{iA} + S_{iC}^2 S_{iA} S_{iB}). \quad (6)$$

We will generalise the term 'Blume-Emery-Griffiths model' to include systems with Hamiltonian  $H_1 + H_3$ , since  $H_3$  is generated from  $H_1$  by RG transformations (whereas  $H_2$  is not).

### 2.2. The Potts and extended Potts subspaces

The full Hamiltonian  $H_1 + H_2 + H_3$  has an extremely complex phase diagram so we shall consider, in this paper, a restricted subspace involving only three instead of six parameters. The stability of the fixed points will, however, be analysed in the full space of six parameters.

Suppose initially we set  $P = 0$  and assume the following relationships between the remaining five parameters:

$$\begin{aligned} \bar{J} &= \frac{1}{2}K \\ \bar{K} &= -\frac{3}{2}K + M \\ \bar{\Delta} &= 3(M - K) \\ \bar{M} &= \frac{1}{8}(M - 3K) \\ \bar{L} &= -\frac{3}{8}(M - 3K). \end{aligned} \quad (7)$$

It is now straightforward to show that the three states +, 0 and -, which henceforth will be denoted by a, b and c respectively, are completely equivalent. The Hamiltonian can be expressed in the form

$$H_1 = \frac{1}{2}K \sum_i \sum_l (p_{iA}^l p_{iB}^l + p_{iB}^l p_{iC}^l + p_{iC}^l p_{iA}^l - 3p_{iA}^l p_{iB}^l p_{iC}^l) + \frac{1}{2}M \sum_i p_{iA}^l p_{iB}^l p_{iC}^l, \quad (8)$$

where  $p_{iA}^l$  ( $l = a, b$  and  $c$ ) is a projection variable which takes the value one if the spin  $iA$  is in state  $l$  and zero otherwise. The Hamiltonian described by equation (8) is a straightforward generalisation of the usual 3-state Potts model and a RG treatment of it has been given by SG. The range of parameters which satisfies equations (7), together with the condition  $P = 0$ , will therefore be called the *Potts subspace*.

$H_2$ , written in spin notation in equation (4), can be re-expressed in terms of the Potts variables as

$$H_2 = \frac{1}{2}P \sum_i \sum_{l_1, l_2, l_3} \epsilon_{l_1 l_2 l_3} p_{iA}^{l_1} p_{iB}^{l_2} p_{iC}^{l_3}, \quad (9)$$

where  $\epsilon_{lmn}$  is the Levi-Civita tensor which has the value one if  $l, m$  and  $n$  are a, b and c or an even permutation of this, the value minus one for an odd permutation and the value zero otherwise. The range of parameters which satisfy equation (7), but with  $P \neq 0$ , will be called the *extended Potts subspace*. The corresponding Hamiltonian  $H_{EP}$  is given by

$$H_{EP} = H_P + H_2, \quad (10)$$

with  $H_P$  and  $H_2$  given by equations (8) and (9) respectively. The rest of this paper is devoted to a discussion of  $H_{EP}$ .

### 3. Symmetry properties and Landau theory

One of the most important criteria for choosing a RG transformation is that it preserves, as far as possible, the symmetries of the Hamiltonian. SG have discussed the symmetry properties of  $H_P$  and our treatment of the more general case  $P \neq 0$  follows largely their approach.

First of all we observe that if we replace  $P$  by  $-P$  and invert the spins on all the lattice sites the Hamiltonian is invariant. The phase diagram must therefore be symmetric about the plane  $P = 0$ . Our transformation will satisfy this condition so  $P = 0$  will be an invariant plane.

In the plane  $P = 0$  the Hamiltonian is invariant under relabelling of the states a, b, c simultaneously on all lattice sites. (Notice that the configurations in figures 3(c) and 3(d) have the same energy for  $P = 0$ .) The corresponding group is the permutation group of three objects,  $S_3$ , which is isomorphic to the point group  $C_{3v}$ . In the plane  $P = 0$  the Hamiltonian is also invariant under any permutation of the sublattice labels, which also corresponds to the group  $S_3$ . The full symmetry group, which we denote by  $G_0$ , is therefore the direct product  $S_3(\text{states}) \otimes S_3(\text{sublattices})$ . We have summarised the relevant symmetry information in table 1.

The line  $M = 0$  is a special line in the plane  $P = 0$  because the configurations shown in figure 3(a) have the same energy as those shown in figures 3(c) and 3(d). There is, therefore, a new symmetry element  $\tau$  (SG) where  $\tau$  involves making the replacement  $a \rightarrow b \rightarrow c \rightarrow a$  on sublattice B,  $a \rightarrow c \rightarrow b \rightarrow a$  on sublattice C and leaving the spins on sublattice A unchanged. The enlarged symmetry group is called  $G_1$  (see table 1).

The transformation of SG ensures that  $P = 0, M = 0$  is an invariant line and, since our transformation reduces to theirs for  $P = 0$ , ours will also have this property. It will be seen below that this line will correspond to the intersection of *three* invariant planes in the extended Potts space with  $P \neq 0$ .

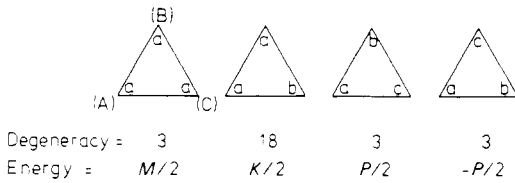
If  $P \neq 0$  an odd permutation of the states changes the sign of  $H_2$  as does also an odd permutation of sublattice labels. On the other hand a combination of these operations leaves  $H_2$  and hence  $H_{EP}$  unchanged. The symmetry operations are therefore combinations of an even permutation of states together with an even permutation of

**Table 1.** Symmetry properties of subspace ( $K, M, P$ )

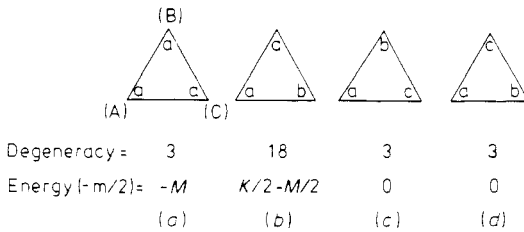
| Region of parameter subspace   | Symmetry   |
|--------------------------------|--|
| $P \neq \pm M, P \neq 0$       | $H_0$ : Elements are combinations of an even permutation of states together with an even permutation of sublattice labels plus combinations of an odd permutation of states together with an odd permutation of sublattice labels. |
| Planes $P = 0$ and $P = \pm M$ | $G_0$ : Symmetry of Potts model $G_0 = S_3(\text{states}) \otimes S_3(\text{sublattices})$ .   |
| Line $P = M = 0$               | $G_1$ : Elements are those of $G_0$ together with $\tau$ (see text) and $\tau^2$ plus all products of $\tau$ and $\tau^2$ with elements of $G_0$ .   |

sublattice labels plus combinations of an odd permutation of states together with an odd permutation of sublattice labels. The corresponding group is denoted by  $H_0$  (table 1).

The plane  $M = P$  is special because in this plane the configurations of figure 3(a) and 3(c) have the same energy. If we now redefine the states according to the SG symmetry element  $\tau$  (i.e.  $a \rightarrow b \rightarrow c \rightarrow a$  on sublattice B,  $a \rightarrow c \rightarrow b \rightarrow a$  on sublattice C, the states on sublattice A remaining unchanged) the possible configurations and their energies are shown in figure 4 (for  $M = P$ ). Denoting by a prime the values of the parameters in the plane  $M = P$ , we see that if  $K' = K - \frac{1}{2}M$  and  $M' = P' = -\frac{1}{2}M$  the states in figure 4 are in



**Figure 3.** Possible states of a single triangle and their energies in the extended Potts subspace. The sublattices are labelled in (a). The degeneracies refer to the number of distinct arrangements which for (a) have all states the same, for (b) have two states the same and one different, for (c) have the states on sublattices A, B, C an even permutation of a, b, c and for (d) an odd permutation of a, b, c.



**Figure 4.** As figure 3 except that now  $P = M$  and we have performed the relabelling  $a \rightarrow b \rightarrow c \rightarrow a$  on sublattice B,  $a \rightarrow c \rightarrow b \rightarrow a$  on sublattice C while leaving unchanged the states on sublattice A. We have also subtracted  $\frac{1}{2}M$  from the energy of each configuration. The states are now in one-to-one correspondence with those of figure 3 with  $P = 0$ .

one-to-one correspondence with the states in the Potts subspace (figure 3 with  $P = 0$ ) apart from an overall shift in energy. It follows that the plane  $M = P$  also has the Potts symmetry and for every point  $(K, M, 0)$  in the plane  $P = 0$  there is a point  $(K', M', P')$ , given by

$$K' = K - \frac{1}{2}M \tag{11a}$$

$$M' = -\frac{1}{2}M \tag{11b}$$

$$P' = -\frac{1}{2}M \tag{11c}$$

in the plane  $P' = M'$  which has the same free energy apart from an additive constant.

Similarly, for  $M = -P$ , configurations given by figures 3(a) and 3(d) have the same energy, so we conclude that there is Potts symmetry in this plane also and we have a mapping which is the same as that given by equations (11) except that now equation (11(c)) becomes  $P' = \frac{1}{2}M$ .

Since the planes  $M = \pm P$  have a Potts symmetry, which is higher than the symmetry of an arbitrary point in the parameter space, it is desirable that the transformation

leaves these planes invariant and preserves the mapping of equations (11). The transformation described in § 4 has this property.

SG have discussed the order parameters for the case  $P = 0$  and have shown that, for the ferromagnetic phase, the order parameter is two-dimensional with components

$$\psi_1 = 3^{-1/2}(\psi_{1A} + \psi_{1B} + \psi_{1C}), \quad \psi_2 = 3^{-1/2}(\psi_{2A} + \psi_{2B} + \psi_{2C}), \quad (12)$$

where

$$\psi_{1\alpha} = \frac{3}{2}n_\alpha^a - \frac{1}{2}, \quad \psi_{2\alpha} = \frac{1}{2}3^{1/2}(n_\alpha^b - n_\alpha^c) \quad (13a)$$

and

$$n_\alpha^l = \langle p_\alpha^l \rangle \quad (13b)$$

for  $l = a, b, c$  and  $\alpha = A, B, C$ . They have also shown that the antiferromagnetic order parameter is four-dimensional with components

$$\begin{aligned} \phi_1 &= (2/3)^{1/2}(\psi_{1A} - \frac{1}{2}\psi_{1B} - \frac{1}{2}\psi_{1C}) & \phi_2 &= (2/3)^{1/2}(\psi_{2A} - \frac{1}{2}\psi_{2B} - \frac{1}{2}\psi_{2C}) \\ \phi_3 &= 2^{-1/2}(\psi_{1B} - \psi_{1C}) & \phi_4 &= 2^{-1/2}(\psi_{2B} - \psi_{2C}). \end{aligned} \quad (14)$$

The symmetry group for  $P = 0$  is, as noted above,  $S_3(\text{states}) \otimes S_3(\text{sublattices})$  and  $(\psi_1, \psi_2)$  transforms according to the representation  $E(\text{states}) \otimes A_1(\text{sublattices})$ , whereas  $(\phi_1, \phi_2, \phi_3, \phi_4)$  transforms according to the representation  $E(\text{states}) \otimes E(\text{sublattices})$ , where  $A_1$  and  $E$  are respectively the identity and doubly-degenerate representations of  $S_3 (C_{3v})$ .

When  $P \neq 0$  the symmetry is lowered from  $G_0$  to  $H_0$  (table 1). The ferromagnetic order parameter remains unchanged and the antiferromagnetic order parameter given by equations (14) splits into two doublets  $E^+ = (\theta_1^+, \theta_2^+)$  and  $E^- = (\theta_1^-, \theta_2^-)$  which are order parameters for the paramagnetic-antiferromagnetic transitions when  $P > 0$  and  $P < 0$  respectively. We find that

$$\theta_1^+ = 2^{-1/2}(\phi_1 + \phi_4) = \frac{1}{2}(n_A^a + n_B^b + n_C^c - 1) \quad (15a)$$

$$\theta_2^+ = 2^{-1/2}(\phi_2 + \phi_3) = 12^{-1/2}(n_A^b + n_B^c + n_C^a - n_A^c - n_B^a - n_C^b) \quad (15b)$$

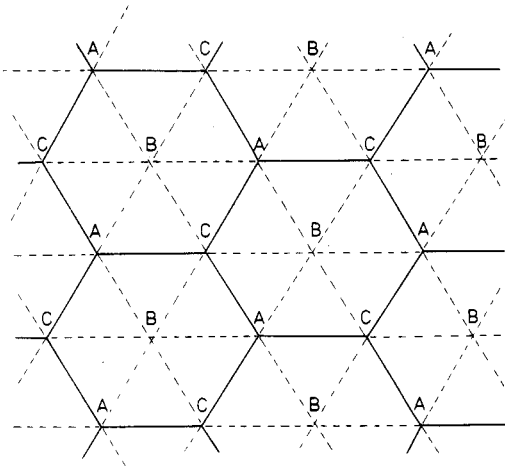
$$\theta_1^- = 2^{-1/2}(\phi_1 - \phi_4) = \frac{1}{2}(n_A^a + n_B^c + n_C^b - 1) \quad (15c)$$

$$\theta_2^- = 2^{-1/2}(\phi_2 - \phi_3) = 12^{-1/2}(n_A^c + n_B^b + n_C^a - n_A^b - n_B^a - n_C^c) \quad (15d)$$

The molecule arrangement which corresponds to ordering of  $\theta_1^+$  is shown in figure 5. It is just the low-density solid phase of the BL model. Although we have made a number of simplifications of the original model by working in a three-parameter subspace we see nevertheless that the ordered antiferromagnetic phase with  $P > 0$  is a phase of the actual model.

In the planes  $M = \pm P$  the symmetry is that of the Potts model. We find that for  $M = P$  the four order parameters  $\psi_1, \psi_2, \theta_1^-, \theta_2^-$  transform like a four dimensional representation analogous to  $(\phi_1, \phi_2, \phi_3, \phi_4)$ . For  $M = -P$  it is the set of parameters  $\psi_1, \psi_2, \theta_1^+, \theta_2^+$  which form the four dimensional representation. In a similar way we see for  $M = P$  that  $(\theta_1^+, \theta_2^+)$  transforms like the ferromagnetic order parameter  $(\psi_1, \psi_2)$ . We shall show in § 4 that the fixed points which govern the paramagnetic-antiferromagnetic transition with  $P \neq 0$  lie in the symmetry planes  $M = \pm P$ . It follows that this transition lies in the same universality class as ferromagnetic ordering in the 3-state Potts model. For this transition Landau theory predicts a first-order transition (see SG) in contradiction to Baxter's (1973) exact result that the transition is continuous.

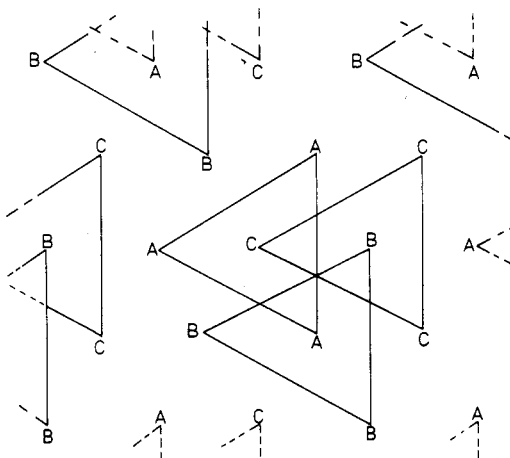




**Figure 5.** The low-density ice phase of the BL model. This corresponds to sublattices A, B and C being in states  $(a, b, c)$  (i.e.  $S = (1, 0, -1)$ ) or any even permutation of this.

**4. The RG transformation and results.**

Since the restricted subspace in which we are working is just a slight extension of the Potts model investigated by SG it is natural to use the same transformation scheme as they do. In order to preserve the sublattice structure three cells are used and the block spin for a given sublattice is related to the single spins on that sublattice only. The structure of the three interpenetrating three-spin cells is shown in figure 6. Periodic boundary conditions are applied so that the ratio of the number of nearest-neighbour pairs to the number of sites is correct both for the original spins and for the block spins. This ensures that the ground state is correctly predicted. If at least two of the spins in a cell are in the same state then the block spin is assigned that state. For configurations with the spins all in different states the block spin is assigned to each of the three states with weight one third.



**Figure 6.** The assignment of spins to cells.

The recursion relations have been evaluated analytically and in terms of the variables  $x = \exp(K/2)$ ,  $y = \exp(M/2)$  and  $q = \exp(P/2)$  they are

$$x' = [(Z^{aab})^2 / (Z^{abc} Z^{acb})]^{1/12} \quad (16a)$$

$$y' = [(Z^{aaa})^2 / (Z^{abc} Z^{acb})]^{1/12} \quad (16b)$$

$$q' = [Z^{acb} / Z^{abc}]^{1/12} \quad (16c)$$

where

$$\begin{aligned} Z^{aaa} = & \frac{2}{3}x^{18} + 12x^{15}y + 18x^{14}y^2(q^2 + q^{-2}) + 72x^{13}y^3 + 60x^{12}y^6 + 36x^{12}y^4(q^2 + q^{-2}) \\ & + 66x^{12}y^2 + 108x^{11}y^5 + 36x^{11}y^3(q^2 + q^{-2}) + 54x^{10}y^8 \\ & + 36x^{10}y^4 + \frac{40}{3}x^9y^3 + 27x^8y^8(q^2 + q^{-2}) + 54x^8y^6 + 18x^6y^{12} + y^{18} \end{aligned} \quad (17a)$$

$$\begin{aligned} Z^{aab} = & \frac{32}{3}x^{18} + 9x^{16}y^2 + 9x^{16}(q^2 + q^{-2}) + 30x^{15}y + 45x^{14}y^4 + 21x^{14}y^2(q^2 + q^{-2}) \\ & + 3x^{14}[7 + 15(q^4 + q^{-4})] + 24x^{13}y^3 + 24x^{13}y(q^2 + q^{-2}) + 5x^{12}y^6 \\ & + 12x^{12}y^4(q^2 + q^{-2}) + 12x^{12}y^2(7 + q^4 + q^{-4}) + x^{12}[12(q^2 + q^{-2}) \\ & + 5(q^6 + q^{-6})] + 42x^{11}y^3(q^2 + q^{-2}) + 42x^{11}y + 3x^{10}y^4[4 + 3(q^4 + q^{-4})] \\ & + 12x^{10}y^2(q^2 + q^{-2}) + 9x^{10} + \frac{94}{3}x^9y^3 \end{aligned} \quad (17b)$$

$$\begin{aligned} Z^{acb} = & \frac{2}{3}x^{18} + 12x^{15}y + 18q^2x^{14}y^2 + 18x^{14} + 72q^2x^{13}y + 6x^{12}y^2(6q^4 + 11) \\ & + 12x^{12}(3q^2 + 5q^6) + 36q^2x^{11}y^3 + 36x^{11}y(3q^4 + 1) + 36q^2x^{10}y^2 \\ & + 54q^8x^{10} + \frac{40}{3}x^9y^3 + 27q^4x^8y^2(q^4 + 2) + 27q^6x^8 + 18q^{12}x^6 + q^{18} \end{aligned} \quad (17c)$$

and

$$Z^{abc}(x, y, q) = Z^{acb}(x, y, q^{-1}). \quad (17d)$$

Equations (17a-d) have the following easily established symmetry properties:

$$Z^{aaa}(x, 1, 1) = Z^{abc}(x, 1, 1) \quad (18a)$$

$$Z^{aaa}(x, y, q) = Z^{aaa}(x, y, q^{-1}) \quad (18b)$$

$$Z^{aab}(x, y, q) = Z^{aab}(x, y, q^{-1}) \quad (18c)$$

$$Z^{aaa}(x, y, y) = Z^{acb}(x, y, y) \quad (18d)$$

$$Z^{aaa}(x, y, 1) = y^9 Z^{abc}(x/y^{1/2}, 1/y^{1/2}, 1/y^{1/2}) \quad (18e)$$

$$Z^{aab}(x, y, 1) = y^9 Z^{aab}(x/y^{1/2}, 1/y^{1/2}, 1/y^{1/2}) \quad (18f)$$

$$Z^{abc}(x, y, 1) = y^9 Z^{acb}(x/y^{1/2}, 1/y^{1/2}, 1/y^{1/2}). \quad (18g)$$

Equations (18b,c) and (17d) imply that the  $(K, M, P)$  phase diagram is symmetric about  $P = 0$ , so  $P = 0$  is an invariant plane. This together with equation (18a) shows that  $M = P = 0$  is an invariant line. It follows from equation (18d) that  $M = P$  is an invariant plane, while equations (18e-g) indicate that the mapping defined by equations (11) is preserved by the transformation.

The recursion relations have *fifteen* fixed points, all of which lie in the three invariant planes  $P = 0, \pm M$ . Of these *four* are sinks for the four possible phases, paramagnetic (p), ferromagnetic (f) and antiferromagnetic with  $P > 0$  and  $P < 0$  ( $af^+$  and  $af^-$ ), *three* are discontinuity fixed points (Nienhuis and Nauenberg, 1975) at zero temperature which

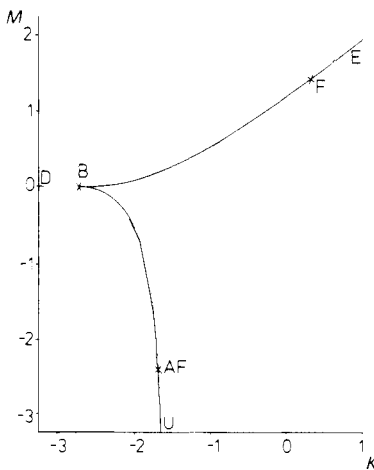
control the first-order phase transitions between the three ordered phases and *one* is a higher order discontinuity fixed point at zero temperature, where all three ordered phases meet. This latter is at  $M = P = 0, K \rightarrow -\infty$  and is the discontinuity fixed point referred to by SG. The locations of the remaining *seven* fixed points are given in table 2.  $AF^+(AF^-)$  is the fixed point for the p-af<sup>+</sup> (p-af<sup>-</sup>) transition and controls behaviour on the critical surface between these two phases. F describes the p-f transition both for  $P = 0$  and  $P \neq 0$  and is discussed in SG. The p-f critical surface intersects the p-af<sup>+</sup> (p-af<sup>-</sup>) critical surface along a bicritical line whose critical behaviour is controlled by the fixed point  $B^+$  ( $B^-$ ). The p-af<sup>+</sup> and p-af<sup>-</sup> critical surfaces intersect along a bicritical line controlled by AF, which in the  $P = 0$  plane is the antiferromagnetic fixed point studied by SG (where appropriate we use their notation for fixed points). In the enlarged space, with  $P \neq 0$ , AF now appears however as a bicritical point. Finally all three ordered phases and the paramagnetic phase come together at B, which in SG was a bicritical point. Now it is a higher order multicritical point which alternatively can be considered as the intersection of the three bicritical lines.

The phase boundaries in the planes  $P = 0$  and  $M = P$  are shown respectively in figures 7 and 8. The ferromagnetic phase is bounded by the line  $P = M = 0$ , the planes  $P = \pm M$  (for  $M > 0$ ) and a surface spanned between the line  $BB^+S$  (figure 8) and the corresponding line on the plane  $M = -P$ . The critical surface separating the paramagnetic phase from the various ordered phases is shown, projected on to a plane perpendicular to the  $K$  axis, in figure 9. For given  $P$  and  $M$  the paramagnetic phase occurs for  $K$  larger than the critical value  $K_c(P, M)$ .

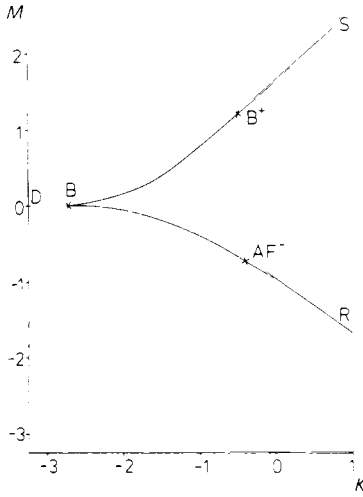
Once the fixed points have been located the recursion relations can be linearised about the fixed points and the stability matrix ( $R_{\omega\gamma}$ ), defined by

$$\delta Q'_\omega = \sum_\gamma R_{\omega\gamma} \delta Q_\gamma \tag{19}$$

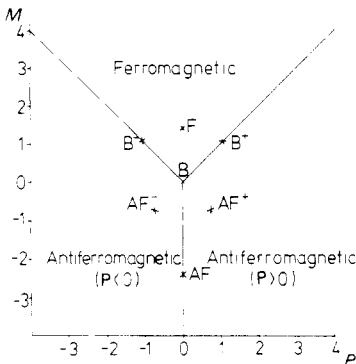
obtained. Here  $Q_\omega = K, M$  or  $P$  and  $\delta Q_\omega = Q_\omega - Q_\omega^*$ , where  $Q_\omega^*$  is the value at the fixed point. The eigenvalues  $\lambda_i$  are written  $b^{y_i}$ , where  $b$  is the scale change,  $3^{1/2}$  in the present example, and the  $y_i$  for various fixed points are listed in table 2. A critical fixed point



**Figure 7.** Phase diagram in the plane  $P = 0$ . The region to the right of the line EBU is paramagnetic, above EBD is ferromagnetic and below DBU is the surface of coexistence of the antiferromagnetic phases with  $P > 0$  and  $P < 0$ .



**Figure 8.** Phase diagram in the plane  $P = M$ . The region to the right of the line  $SBR$  is paramagnetic, below  $DBR$  is antiferromagnetic with  $P < 0$  and above  $DBS$  is the surface of coexistence of the ferromagnetic phase and the antiferromagnetic phase with  $P > 0$ . The phase diagrams of figures 7 and 8 are related by the mapping given by equations (11).



**Figure 9.** A projection of the surface separating the paramagnetic phase from the various ordered phases on to the  $M$ - $P$  plane.

should have just one relevant (i.e. positive) exponent,  $y_1$  say. The coefficient of the corresponding eigenvector is then proportional to  $T - T_c$  and  $y_1$  is the inverse of the correlation length exponent  $\nu$ , (see e.g. Ma, 1976 p 143).

For F, B and AF we denote by a superscript ' $P$ ' in table 2 the exponent  $y_P$  corresponding to the eigenvector in the direction of the  $P$  axis. We see that the  $P$  direction is irrelevant for F (i.e.  $y_P < 0$ ) so the SG fixed point describes the ferromagnetic ordering even for  $P \neq 0$ . On the other hand the  $P$  direction is strongly relevant for AF and as a result the antiferromagnetic transitions with  $P > 0$  ( $< 0$ ) are described by different fixed points  $AF^+$  ( $AF^-$ ).

Because of the exact mapping, given by equations (11), the fixed points F,  $AF^+$  and  $AF^-$  have the same exponents, which are those of the 3-state Potts model. Similarly  $B^+$ ,  $B^-$  and AF have the same exponents. However the exponents for F and AF are

**Table 2.** Properties of non-trivial fixed points in subspace  $(K, M, P)$

| Region of parameter space | Designation                        | Location $(K^*, M^*, P^*)$                           | Exponents within subspace        | Exponents outside subspace |
|---------------------------|------------------------------------|--|----------------------------------|----------------------------|
| Line $M = P = 0$          | B<br>(higher-order multi-critical) | $(-2.72, 0, 0)$                                      | $(1.99, 0.87, 1.99^P)^\dagger$   | $(1.99, -0.64, -1.38)$     |
|                           | F (critical)                       | $(0.32, 1.44, 0)$                                    | $(1.04, -1.79, -1.58^P)^\dagger$ | $(1.61, 0.29, -1.16)$      |
| Plane $P = 0$             | AF (bicritical)                    | $(-1.68, -2.39, 0)$                                  | $(1.11, -1.90, 1.87^P)^\dagger$  | $(-0.17, -0.58, -2.10)$    |
|                           | AF <sup>-</sup> (critical)         | $(-0.40, -0.72, -0.72)$                              | $(1.04, -1.79, -1.58)$           | $(0.33, -0.99, -2.14)$     |
| Plane $P = M$             | B <sup>+</sup> (bicritical)        | $(-0.48, 1.19, 1.19)$                                | $(1.11, -1.90, 1.87)$            | $(1.90, 0.28, -0.87)$      |
|                           | AF <sup>+</sup> (critical)         |  |                                  |                            |
| Plane $P = -M$            | B <sup>-</sup> (bicritical)        | As for plane $P = M$ but with sign of $P^*$ changed. |                                  |                            |

<sup>†</sup> The superscript  $P$  denotes the eigenvalues whose eigenvector is in the  $P$  direction.

different (although numerically the difference is rather small) as is to be expected from the symmetry arguments of SG and § 3.

Finally we have derived the recursion relations in the six-dimensional parameter space of the full BL model. The formulae are too complicated to be given here so we quote, in the last column of table 2, simply the exponents, at the fixed points of the subspace, corresponding to eigenvectors in directions out of the subspace. We observe that with  $P = 0$ , AF has only one relevant eigenvalue in the full space. It therefore represents a critical point describing antiferromagnetic ordering in the  $S = 1$  Ising model (Blume–Emery–Griffiths model) on a triangular lattice. This fixed point, first found by SG, is therefore applicable to a wider range of problems than the one which they considered. Fixed points AF<sup>+</sup> and AF<sup>-</sup> have a second weakly relevant eigenvalue which takes one out of the subspace. If this result is correct it implies that AF<sup>+</sup> and AF<sup>-</sup> do not describe critical points in the full parameter space and melting in the BL model is described by another fixed point. It should be pointed out, however, that RSRG methods seem relatively unreliable for subleading exponents, particularly with rather loosely connected clusters such as we have here. In fact a closely analogous treatment of the spin  $\frac{1}{2}$  Ising antiferromagnet on a triangular lattice by Schick, Walker and Wortis (1977) leads to predictions of the number of relevant exponents at the so-called Baxter–Wu fixed point which disagree with the virtually exact results of Barber (1976). Consequently it is possible that the second relevant exponent at AF<sup>+</sup> and AF<sup>-</sup> is an artefact of the approximation, in which case melting in the BL model would be *second*-order and described by the 3-state ferromagnetic Potts model. This discussion also puts into question, however, the above conclusions regarding the stability of the fixed point AF in the full  $S = 1$  Blume–Emery–Griffiths parameter space.

### 5. Conclusions

We have discussed the BL model using RSRG methods within a subspace of three parameters  $(K, M, P)$ . Within this subspace there are three planes which have Potts symmetry and all the fixed points lie on these planes. There is a simple mapping (equations (11)) between a point on one plane and a corresponding point on another

plane which has the same free energy. If the second relevant exponent at fixed points  $AF^+$  and  $AF^-$ , which leads out of the subspace, is an artefact of the approximation, melting in the BL model is second-order and corresponds to the paramagnetic-ferromagnetic transition on the 3-state Potts model. The antiferromagnetic fixed point AF found by SG actually applies to a wider class of models than they discuss. The nature of the phase transitions in the BL model should be more fully understood when the fixed points and their exponents have been determined in the full parameter space. This is a problem which we intend to pursue.

### Addendum

After this paper was submitted for publication we became aware of related work by Adler, Aharony and Oitmaa (1978) and Mahan and Girvin (1978). Adler *et al* investigated the BEG model on the triangular lattice using a RSRG method similar to that of Niemeijer and van Leeuwen (1976) but did not consider antiferromagnetic ordering which is the main subject of the present study. Mahan and Girvin do consider the possibility of antiferromagnetic order on the triangular lattice and use a RSRG scheme similar to the one discussed here. Unfortunately they do not give their results for the fixed point describing the second-order antiferromagnetic transition in the BEG model, which we have argued should correspond to the fixed point AF.

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