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## High-field expansions for multi-state lattice models

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**Abstract.** High-field expansions are obtained for general three-state models on the face-centred cubic lattice. It is then shown that the method of partial generating functions can be extended to give series expansions for general multi-state models, such as the Potts models and the general spin Ising models.

### 1. Introduction

In this paper we discuss methods of deriving high-field (low-temperature) expansions for general multi-state lattice models. The models we consider can be described in the following way.

- (i) At each site there is a variable that can be in any one of a finite number of states.
- (ii) The total energy of any configuration depends on the total number of sites in each state and the total number of nearest-neighbour pairs in each of the possible combinations of states.

Three-state models of this type have been applied to a variety of physical systems such as  $^3\text{He}$ - $^4\text{He}$  and dilute magnets (references to this are given in § 2). Higher-state systems include the general spin Ising model and the various Potts models (Potts 1952). In § 5 we consider the two-layer lattice of Ising spin  $\frac{1}{2}$  as a single-layer four-state system. This enables us to obtain expansions for two-layer systems from existing combinatorial data on two-dimensional systems and, by relaxing conditions (ii) above slightly, to apply the method of partial generating functions to a system with four-spin interactions.

The basic technique for obtaining high-field expansions directly has been described by Domb (1960). The expansion is a perturbation expansion about a fully aligned state and one considers increasing numbers of perturbed sites. Domb provides graphs and lattice constants which enable one to obtain the contributions for up to five perturbed sites. These combinatorial data can be used in multi-state systems such as the Potts model (Enting 1974a) and the general three-state model discussed in § 3, but it is necessary to know the adjacency matrices of the graphs used. For loose-packed lattices § 4 shows how we can extend the method of partial generating functions (Sykes *et al* 1965) and, once we have identified a shadow lattice, we can obtain series expansions for any model of the type described above for up to five perturbed sites by means of algebraic manipulation without detailed lattice combinatorial information. Higher-order perturbation terms do need information on the combinatorial properties of the lattice, but what we present in this work is a way of expressing the combinatorial information so that series expansions for any multi-state model can be obtained by algebraic manipulation.

The layout of the paper is as follows. Section 2 describes the three-state model and various applications that have been made. It illustrates some of the general properties of such multi-state models and the various relations between different models. Section 3 describes direct expansions for these models. The most important point is that since all the states are essentially equivalent, in that any labelling of the states is arbitrary, we can make use of this equivalence to reduce the number of series terms that need be given. This procedure of giving a small number of terms from which all others can be derived by symmetry enables us to extend the method of partial generating functions to arbitrary numbers of states in § 4. Section 5 describes a number of particular multi-state models to which these methods apply. In the appendix we give high-field polynomials for the general three-state model on the fcc lattice. For most other lattices we can use the method of partial generating functions for which general 'codes' are given in § 4 and the appendix. (The triangular lattice is excluded. It can be treated by a decomposition into three sublattices; this will be considered elsewhere.)

## 2. Three-state systems

There have been a number of models considered in which a lattice has sites which may be in any one of three states. The most obvious example is the spin 1 Ising model in which the states are the three possible  $S^z$  components of a spin of magnitude one. With a suitable choice of interaction any three-state model may be expressed as a spin 1 Ising system as shown below. Some of the systems which can be represented by three-state models are quenched dilute spin  $\frac{1}{2}$  magnets (Katsura and Tsujiyama 1966) and  $^3\text{He}$ - $^4\text{He}$  mixtures (Blume *et al* 1971).

Following the basic assumption given in the introduction that the energy depends only upon the number of sites in each state and the number of different types of pairs, we put

$$E = \bar{h}_1 N_a + \bar{h}_2 N_b + \bar{h}_3 N_c + \bar{c}_1 N_{aa} + \bar{c}_2 N_{bb} + \bar{c}_3 N_{ab} + \bar{c}_4 N_{ac} + \bar{c}_5 N_{bc} + \bar{c}_6 N_{cc} \quad (1)$$

where we have denoted the three different states  $a, b, c$ . For comparison with the spin 1 representations given below we represent the interactions in terms of a matrix  $A_{ij}$  so that

$$E = \sum_{(i,j)} N_{ij} A_{ij} \quad (2)$$

where the sum is over the six pairs  $(a, a), (b, b), (c, c), (a, b), (a, c), (b, c)$ .

The existence of the matrix  $A_{ij}$  depends upon the ability to relate  $N_a, N_b$  to the numbers of bonds by

$$zN_a = 2N_{aa} + N_{ab} + N_{ac} \quad (3a)$$

$$zN_b = 2N_{bb} + N_{ab} + N_{bc} \quad (3b)$$

where  $z$  is the lattice coordination number. While we use the relations (3a), (3b) to show that  $A_{ij}$  exists, the more important use is to eliminate  $N_{ac}, N_{bc}$  from (1). We also put

$$\bar{h}_3 = \bar{c}_6 = 0 \quad (4)$$

which corresponds to choosing a fully aligned  $c$  state as having the zero of energy.

We can then write  $E$  in the form

$$E = h_1 N_a + h_2 N_b + c_1 N_{aa} + c_2 N_{bb} + c_3 N_{ab}. \tag{5}$$

This is the form of the linkage rule used by Sykes and Gaunt (1973) and corresponds to an  $A_{ij}$  matrix

$$A_{ij} = \begin{matrix} & \begin{matrix} c & a & b \end{matrix} \\ \begin{matrix} c \\ a \\ b \end{matrix} & \begin{bmatrix} 0 & z^{-1}h_1 & z^{-1}h_2 \\ z^{-1}h_1 & 2z^{-1}h_1 + c_1 & z^{-1}(h_1 + h_2) + c_3 \\ z^{-1}h_2 & z^{-1}(h_1 + h_2) + c_3 & 2z^{-1}h_2 + c_2 \end{bmatrix} \end{matrix}. \tag{6}$$

We now interpret the  $c, a, b$  as the  $1, 0, -1$   $S^z$  values of a spin 1 Ising system and give a list of the  $A_{ij}$  matrices for various interactions:

$$S_i + S_j = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & -2 \end{bmatrix}$$

$$S_i S_j = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$$

$$S_i^2 + S_j^2 = \begin{bmatrix} 2 & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 1 & 2 \end{bmatrix}$$

$$S_i^2 S_j^2 = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix}$$

$$S_i S_j (S_i + S_j) = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

and a 'constant' matrix with all elements equal.

Since the six independent components of each of these matrices correspond to six linearly independent six-dimensional vectors, any symmetric  $3 \times 3$  matrix can be expressed as a sum of these interactions. (It is also possible to consider  $A_{ij}$  that are not symmetric, but this implies an interaction that depends on the direction of the bond. Additional linearly independent matrices correspond to  $S_i - S_j, S_i^2 - S_j^2, S_i S_j (S_i - S_j)$ . A model in which this asymmetry occurs has been considered by Bell and Lavis (1970) and will be investigated elsewhere.)

In terms of the 'linkage rules' the interactions become:

$$S_i \rightarrow -N_a - 2N_b \tag{7a}$$

$$S_i^2 \rightarrow -N_a \tag{7b}$$

$$S_i S_j \rightarrow -zN_a + N_{aa} - 2zN_b + 4N_{bb} + 2N_{ab} \quad (7c)$$

$$S_i^2 S_j^2 \rightarrow -zN_a + N_{aa} \quad (7d)$$

$$S_i S_j (S_i + S_j) \rightarrow 2N_{aa} + 2N_{ab} - 2zN_a - 2zN_b. \quad (7e)$$

These linkage rules correspond to summing  $S_i$ ,  $S_i^2$  interactions over all sites while the other interactions are summed over all bonds. In contrast the use of matrix  $A_{ij}$  includes the  $S_i$ ,  $S_i^2$  terms in the sum over all bonds and so the contributions must be divided by  $z$  as in equation (6).

The linkage rules (7a-e) are based on the correspondence  $(c, a, b) \rightarrow (1, 0, -1)$ . If the ground state has  $S^z = 0$  then the mapping  $(c, a, b) \rightarrow (0, 1, -1)$  gives the linkage rules

$$S_i S_j \rightarrow N_{aa} - N_{ab} + N_{bb} \quad (8a)$$

$$S_i^2 S_j^2 \rightarrow N_{aa} + N_{ab} + N_{bb} \quad (8b)$$

$$S_i S_j (S_i + S_j) \rightarrow 2N_{aa} - 2N_{bb} \quad (8c)$$

$$S_i \rightarrow N_a - N_b \quad (8d)$$

$$S_i^2 \rightarrow N_a + N_b. \quad (8e)$$

The following models are particular systems for which these linkage rules can be used.

### 2.1. Spin 1 Ising model

The linkage rule has been given by Sykes and Gaunt (1973). The interaction  $-JS_i S_j$  gives

$$E = J(zN_a + 2zN_b - N_{aa} - 2N_{ab} - 4N_{bb}). \quad (9)$$

The field term  $-HS_i$  gives

$$E_H = H(N_a + 2N_b) \quad (10)$$

so that in the notation of (5):

$$h_1 = H + Jz, \quad h_2 = 2H + 2Jz, \quad c_1 = -J, \quad c_2 = -2J.$$

### 2.2. ${}^3\text{He}$ - ${}^4\text{He}$ model (Blume-Capel model)

Blume *et al* (1971) added a  $\Delta S_i^2$  term to the spin 1 Ising model to represent a chemical potential  $\Delta$  in the  ${}^3\text{He}$ - ${}^4\text{He}$  model. The energy change is

$$E_\Delta = -\Delta N_a \quad (11)$$

so that  $h_2, c_1, c_2, c_3$  are unchanged but

$$h_1 = H + Jz - \Delta. \quad (12)$$

For  $\Delta > zJ$  the  $S^z = \pm 1$  states are no longer the ground states in zero field and it is appropriate to expand about  $S^z = 0$ .

Using (8a-e) the linkage rule gives

$$E = \Delta(N_a + N_b) - J(N_{aa} - N_{ab} + N_{bb})$$

or

$$h_1 = \Delta, \quad h_2 = \Delta, \quad c_1 = -J, \quad c_2 = -J, \quad c_3 = J.$$

This can be used to interpret the series in the appendix, interpreted by means of (16), (17a–e) to obtain large- $\Delta$  expansions. High-temperature expansions for this model have been obtained by Oitmaa (1971, 1972) and by Saul *et al* (1974), who also obtained high-field (large  $H$ ) expansions. They were able to undertake an extensive analysis of the tricritical region. Their polynomials can be obtained from those in the appendix by making the transformation  $v \rightarrow u^{-1}$ ,  $w \rightarrow u^{-2}$ ,  $u \rightarrow u^{-4}$ . To obtain the full set given by Saul *et al* it is necessary to use relations (19) and (20) so that their  $L_{nm}$  polynomials correspond to the spin  $\frac{1}{2}$  Ising polynomials given by Sykes *et al* (1965). The index system used by the former corresponds to  $(2N_a + N_b, N_b)$  rather than  $(N_a, N_b)$ .

A generalization of the Blume–Capel model has been given by Ditzian (1974) who included a term  $S_j^2 S_j^2$ . She used the same index system as Saul *et al*. Her series can be obtained from those in the appendix by making the transformation

$$v \rightarrow u^{-1}v^{-1}, \quad w \rightarrow u^{-2}, \quad u \rightarrow u^{-4}.$$

This model includes the three-state Potts model as a special case (see equation (15)), but comparison of her series with those of Enting (1974a) shows that it is more efficient to consider the Potts model directly. The series grouping used by Ditzian suppresses some of the information that is potentially available.

### 2.3. Three-state Potts model

The symmetric form of the linkage rule for the three-state Potts model (Potts 1952) has the form

$$E = J(N_{ab} + N_{ac} + N_{bc}) \tag{13}$$

which becomes

$$E = J(zN_a + zN_b - 2N_{aa} - 2N_{bb} - N_{ab}); \tag{14}$$

this corresponds to

$$-\frac{1}{2}JS_i S_j - JS_i^2 S_j^2 + JzS_i^2, \tag{15}$$

the form used by Ditzian and Oitmaa (1974).

For the Potts model the ordering fields used by Enting (1974a) were

$$\begin{aligned} -\bar{h}_1 S_i^2 &\rightarrow \bar{h}_1 N_a, \\ \frac{1}{2}h_2(S_i - S_i^2) &\rightarrow \bar{h}_2 N_b \end{aligned}$$

and the combination

$$-\frac{1}{2}\bar{h}(S_i + S_i^2) \rightarrow \bar{h}(N_a + N_b).$$

Ditzian and Oitmaa used  $-HS_i$ .

A check on the expansions is obtained by interpreting the series in the appendix by

$$h_1 = \bar{h}_1 + zJ, \quad h_2 = \bar{h}_2 + zJ, \quad c_1 = -2J, \quad c_2 = -2J, \quad c_3 = -J$$

and comparing the series to that given by Enting (1974a).

### 3. Series expansion for the three-state model

The series expansions that we consider will be perturbation expansions about a fully aligned  $c$  state and are obtained by considering successively larger numbers of perturbed sites. For each perturbation we add to the configurational partition function  $\Lambda$  a Boltzmann factor  $\exp(-\beta E')$ .

Using

$$E' = h_1 N_a + h_2 N_b + c_1 N_{aa} + c_2 N_{bb} + c_3 N_{ab}$$

we expand as

$$\ln \Lambda = \sum l_{mnpqr} \mu_1^m \mu_2^n u^p v^q w^r \tag{16}$$

with

$$\mu_1 = \exp(-\beta h_1) \tag{17a}$$

$$\mu_2 = \exp(-\beta h_2) \tag{17b}$$

$$u = \exp(-\beta c_1) \tag{17c}$$

$$v = \exp(-\beta c_2) \tag{17d}$$

$$w = \exp(-\beta c_3). \tag{17e}$$

Putting

$$L_{mn}(u, v, w) = \sum_{pqr} l_{mnpqr} u^p v^q w^r \tag{18}$$

we find that

$$L_{mn}(u, v, w) = L_{nm}(v, u, w) \tag{19}$$

and

$$L_{m0}(u, v, w) = u^{mz/2} L_m(u^{-1}) \tag{20}$$

where the  $L_m$  are the high-field polynomials for the spin  $\frac{1}{2}$  Ising model and are given by Sykes *et al* (1965). Other  $L_{mn}$  are given in the appendix for the face-centred cubic lattice. Loose-packed lattices can be treated by the methods of the following section and the triangular lattice will be treated elsewhere.

When using the graphs tabulated by Domb (1960) we have to perform a decoration of the graphs. To show this we represent the perturbation expansion by a hierarchy of summations:

$$\begin{aligned} & \sum_{\text{all perturbations}} \exp(-\beta E) \\ &= \sum_n \left\{ \sum_{\substack{\text{all topologically} \\ \text{distinct arrangements} \\ \text{of } n \text{ sites}}} \left[ \sum_{\substack{\text{all embeddings of} \\ \text{this topology}}} \left( \sum_{\substack{\text{the } 2^n \text{ arrange-} \\ \text{ments of } a, b \text{ spins} \\ \text{on these sites}}} \exp(-\beta E) \right) \right] \right\}. \end{aligned}$$

In this context 'topologically distinct' means having distinct sets of  $E$  from the  $2^n$  arrangements. The contributions from  $h_1, h_2$  depend only upon the numbers  $N_a, N_b$  but the  $c_1, c_2, c_3$  factors depend upon the adjacency matrix  $V_{ij}$  for the graph representing the perturbed sites, since

$$E = \sum_{\{(i,j):V_{ij} \neq 0\}} A_{ij}.$$

Since this summation must include all bonds between all pairs of perturbed sites the required graphs are section graphs or strong embeddings.  $E$  does not depend on how the graph is embedded, so instead of summing over all embeddings we multiply by the lattice constant :

$$\sum_{\text{all perturbations}} = \sum_{\text{strong graphs}} (\text{lattice constant}) \sum_{\substack{2^n \text{ arrangements} \\ \text{of } a, b \text{ sites}}}$$

The series expansion is thus obtained by decorating the vertices of the graphs tabulated by Domb (1960). If we want  $\ln \Lambda$  we replace the lattice constant by the term in the lattice constant that is linear in the number of sites.

The fact that these multi-state models lead to graph decoration problems enables us to generalize the method of partial generating functions. The structure of the partial generating functions has mapped a lattice combinatorial problem on to an algebraic combinatorial problem. The general multi-state models require the same lattice constants as the spin  $\frac{1}{2}$  Ising model, so the generalization of the spin  $\frac{1}{2}$  Ising model becomes in principle a matter of algebraic transformation rather than being an essentially new combinatorial problem. In the following sections we present partial generating function expressions valid for arbitrary multi-state systems.

#### 4. The method of partial generating functions

In § 3 we used the symmetry property (19) to reduce the number of series coefficients that need be given. In this section the symmetry of the system under permutations of the arbitrary labels assigned to the perturbed states enables us to give expressions that can be applied to general multi-state models.

The model is as described in the introduction but we only consider lattices that can be decomposed into two sublattices, A and B, so that any nearest-neighbour bond has one end on each sublattice.

We consider a system of  $n + 1$  states labelled 0 to  $n$ . The interaction energy between states of types  $i$  and  $j$  is denoted by  $J_{ij}$  and the field coupling to state  $i$  by  $h_i$  with

$$\mu_i = \exp(-\beta h_i). \tag{21}$$

The expansions take the form

$$\ln \Lambda = \sum_{\{\mathbf{m}\}} L_{\mathbf{m}}(\{J_{ij}\}) \prod_{i=1}^n \mu_i^{m_i} \tag{22}$$

$$\mathbf{m} = \langle m_1, m_2 \dots m_n \rangle. \tag{23}$$

The  $L_{\mathbf{m}}$  are polynomials in  $\{\exp(-\beta J_{ij})\}$  and  $m_i$  is the number of sites in state  $i$  in the perturbations that contribute to  $L_{\mathbf{m}}$ .

We now consider distinguishing between perturbations on each sublattice and put

$$L_{\mathbf{m}} = \frac{1}{2} \sum_{\mathbf{m}'} \bar{L}_{\mathbf{m}-\mathbf{m}',\mathbf{m}'} \tag{24}$$

where  $\bar{L}_{\mathbf{m},\mathbf{m}'}$  is the sum of perturbations with  $m_i$  of type  $i$  on the A sublattice and  $m'_i$  of type  $i$  on the B sublattice.



We construct the partial generating functions

$$F_m = \sum_{\{m'\}} \bar{L}_{m,m'} \prod_i (\mu_i^{m_i}) \prod_i [\exp(znJ_{i0})]^{m_i} \tag{25}$$

where  $z$  is the coordination number of the (original) lattice. Defining the order of a vector  $m$  as  $\sum m_i$ , a knowledge of all  $F_m$  up to order  $K$  in  $m$  will give all  $L_m$  up to order  $2K + 1$  because of the symmetry property

$$\bar{L}_{m,m'} = \bar{L}_{m',m}. \tag{26}$$

Following the usual procedure in this method we express the partial generating functions as codes. The present notation is

$$k(\lambda/a/b/c \dots) = k(\lambda/a_1, a_2, \dots, a_n/b_{11}, b_{21}, b_{22}, b_{31}, \dots, b_{nn}/c_{111}, \dots) \\ = kf_0^{-\lambda} \prod_i f_i^{a_i} \prod_{(i,j)} f_{ij}^{b_{ij}} \dots \tag{27}$$

The slashes are included since the vectors  $a, b, c$  will be of length  $n, \frac{1}{2}n(n + 1)$  etc which will be undetermined in the general form and truncated after all nonzero coefficients have been given. There are two important properties that enable us to quote codes applicable to general  $n$  and general  $J_{ij}$ .

(i) If  $m$  is of the form  $\langle m_1, \dots, m_i, 0, 0, \dots, 0 \rangle$  then  $F_m$  for the  $(n + 1)$ -state model has the same code expansion as  $F_{m'}$  for the  $(i + 1)$ -state model with  $m' = \langle m_1, m_2, \dots, m_i \rangle$ . This is obvious when it is realized that  $a_i$  is the number of A sites which are neighbours to only one B site of type  $i$  and  $b_{ij}$  is the number of A sites between two B sites of types  $i$  and  $j$ . These definitions make no reference to  $n$ , the number of possible perturbed states.

(ii) An expansion

$$F_m = \sum_{\text{codes}} K(\lambda/a/b/c \dots)$$

is invariant under any permutation of the labels 1 to  $n$ . This means applying the same permutation to the labels of  $m, a, b, c, f_i$  etc and merely reflects the arbitrary nature of the labelling.

The effect of these symmetry properties is that it is sufficient to consider only  $m$  vectors of the forms:

$\langle 1 \rangle$	for 1st order
$\langle 2 \rangle, \langle 1, 1 \rangle$	for 2nd order
$\langle 3 \rangle, \langle 2, 1 \rangle, \langle 1, 1, 1 \rangle$	for 3rd order
$\langle 4 \rangle, \langle 3, 1 \rangle, \langle 2, 1, 1 \rangle, \langle 1, 1, 1, 1 \rangle$	for 4th order.

ie no  $m$  with zero components needs to be considered. Also for vectors  $\langle K \rangle, F_{\langle K \rangle}$  is obtained from  $F_K$  for the spin  $\frac{1}{2}$  Ising model using the mapping of the codes:

$$(\lambda, \alpha, \beta, \gamma, \dots) \rightarrow (\lambda/\alpha, 0 \dots / \beta, 0 \dots / \gamma \dots /).$$

These codes are obtained by considering graphs on what is called a shadow lattice. This has the sites of the B sublattice but its bonds connect any two B sites that have a common A neighbour on the original lattice. For any pair of B sites we define  $w$  as the number of A sites neighbouring both B sites. The different possible  $w_i$  values divide the shadow lattice bonds into equivalence classes denoted by type  $i$ . For any site we denote the number of type  $i$  bonds to the site by  $z_i$ . Presented in table 1 is a list of lattices,

**Table 1.** Loose-packed lattices, their shadow lattices with bonds coordination numbers  $z_i$ , and the number of common neighbours on the original lattice,  $w_i$ .

Lattice	$z$	Shadow lattice	Neighbours	$z_i$	$w_i$
hc	3	tri	1st	6	1
sq	4	sq	1st	4	2
			2nd	4	1
sc	6	fcc	1st	12	2
			2nd	6	1
bcc	8	sc	1st	6	4
			2nd	12	2
			3rd	8	1
diam	4	fcc	1st	12	1
hsc	8	hfcc	1st	24	2
			2nd	8	1
hbcc	16	hsc	1st	8	8
			2nd	24	4
			3rd	32	2
			4th	16	1

their shadows and the various  $w_i, z_i$  with the shadow lattice bonds described as 1st, 2nd, etc neighbours on the shadow lattice.

The notation for four-dimensional lattices follows that of Moore (1970) where, describing lattices in terms of typical nearest neighbours to the origin, we have

$$\text{hsc } (1, 0, 0, 0), \quad \text{hfcc } (1, 1, 0, 0), \quad \text{hbcc } (1, 1, 1, 1).$$

We have not given any detailed proof of the form of the codes but the remarks at the end of the previous section indicate the line of argument. The connected graphs correspond to finite sums which are evaluated explicitly. Disconnected A sites are independent, so we can generalize the  $\mu^z \mu$  in the spin  $\frac{1}{2}$  Ising model to  $\sum_i \mu_i \exp(-\beta J_{0i} z)$ . The structure of the generating functions expressed in terms of codes, especially the form of the contributions from disconnected A sites, gives lattice combinatorial factors in terms of algebraic combinatorial factors. This approach has been discussed by Enting (1974b).

We can write

$$f_0 = 1 + \sum_i \mu_i \exp(-\beta J_{0i} z) \tag{28}$$

$$F_0 = \ln f_0 \tag{29}$$

$$F_{\langle 1 \rangle} = (z; z) \tag{30}$$

$$F_{\langle 2 \rangle} = \left( -\frac{1}{2} + \sum_i z_i/2 \right) (2z/2z) + \sum_i z_i/2 (2z - 2w_i/2z - 2w_i/w_i). \tag{31}$$

$$F_{\langle 1,1 \rangle} = \left( -\frac{1}{2} + \sum_i z_i/2 \right) (2z/2z) + \sum_i z_i/2 (2z - w_i/2z - 2w_i/0, w_i). \tag{32}$$

In the appendix we also give  $F_{21}, F_{111}$  for square, honeycomb, sc and diamond lattices.

The general forms for the  $f$  functions are

$$f_i = 1 + \sum_k \mu_k \exp\{-\beta [J_{k0}(z-1) - J_{i0} + J_{ik}]\} \tag{33}$$

$$f_{ij} = 1 + \sum_k \mu_k \exp\{-\beta[J_{k0}(z-2) - J_{i0} - J_{j0} + J_{ik} + J_{jk}]\} \quad (34)$$

$$f_{ijl} = 1 + \sum_k \mu_k \exp\{-\beta[J_{k0}(z-3) - J_{i0} - J_{j0} - J_{l0} + J_{ik} + J_{jk} + J_{lk}]\}. \quad (35)$$

## 5. Specific models

### 5.1. Standard $q$ -state Potts model

While the possibility of having arbitrary fields (eg  $h_1, h_2$  as described at the end of § 2) would lead to complicated expressions, if we put  $h_i = h, i = 1 \dots n, n = q-1$ , then with  $J_{ij} = J(1 - \delta_{ij})$  (28) becomes

$$f_0 = 1 + (q-1)\mu u^z \quad (\text{denoted } f_1 \text{ by Enting 1974a, b);} \quad (36)$$

(23) becomes

$$f_i = 1 + \mu u^{z-2} + (q-2)\mu u^{z-1} \quad (\text{denoted } f_2); \quad (37)$$

(34) becomes

$$f_{ii} = 1 + \mu u^{z-4} + (q-2)\mu u^{z-2} \quad (\text{denoted } f_3) \quad (38)$$

or

$$f_{ij} = 1 + 2\mu u^{z-3} + (q-3)\mu u^{z-2} \quad (\text{denoted } f_4); \quad (39)$$

(35) becomes

$$f_{iii} = 1 + \mu u^{z-6} + (q-2)\mu u^{z-3} \quad (\text{denoted } f_5) \quad (40)$$

$$f_{iij} = 1 + \mu u^{z-5} + \mu u^{z-4} + (q-3)\mu u^{z-3} \quad (\text{denoted } f_6) \quad (41)$$

$$f_{ijk} = 1 + 3\mu u^{z-4} + (q-4)\mu u^{z-3} \quad (\text{denoted } f_7). \quad (42)$$

( $f_1$  to  $f_7$  are for comparison with the notation of Enting (1974a, b) which will not be used in the following work. Enting (1974b) gives  $f_6$  incorrectly.)

It is possible to combine the expressions to obtain the  $F_n$  given by Enting (1974a, b). The procedure indicates how code expansions can be used for more general models.

$$(a) \quad F_0 = \ln f_0$$

$$(b) \quad F_1 = F_{\langle 1,0,\dots,0 \rangle} + F_{\langle 0,1,0,\dots,0 \rangle} + \dots + F_{\langle 0,\dots,1 \rangle} = (q-1)F_{\langle 1 \rangle}$$

since by (37) all the  $f_i$  are equal.

$$(c) \quad F_2 = F_{\langle 2,0,0,\dots \rangle} + F_{\langle 0,2,\dots,0 \rangle} + F_{\langle 0,\dots,2 \rangle} + F_{\langle 1,1,0,\dots \rangle} + F_{\langle 1,0,1,\dots \rangle} + F_{\langle 0,0,\dots,1,1 \rangle} \\ = (q-1)F_{\langle 2 \rangle} + \frac{1}{2}(q-1)(q-2)F_{\langle 1,1 \rangle}.$$

Similarly

$$(d) \quad F_3 = (q-1)F_{\langle 3 \rangle} + \frac{1}{2}(q-1)(q-2)(q-3)F_{\langle 2,1 \rangle} + \frac{1}{6}(q-1)(q-2)(q-3)F_{\langle 1,1,1 \rangle}.$$

Another simplification that arises in this model is for  $F_{\langle 1,1,\dots,1 \rangle}$ . The only  $f_{ij}, f_{ijk}, f_{ijkl}$  that occur are for  $i, j, k, l$  all different, so the code expansions for  $F_{\langle 1,1,\dots \rangle}$  are the spin  $\frac{1}{2}$  Ising model codes interpreted by

$$(\lambda, \alpha, \beta, \gamma \dots) = f_0^{-\lambda} (1 + \mu u^{z-2} + (q-2)\mu u^{z-1})^\alpha (1 + 2\mu u^{z-3} \\ + (q-3)\mu u^{z-2})^\beta (1 + 3\mu u^{z-4} + (q-4)\mu u^{z-3})^\gamma \dots$$

5.2. Spin  $s$  Ising model

$$n = 2s$$

$$J_{ij} = -J(i - s/2)(j - s/2) + Js^2/4$$

$$\mu_j = \mu^j.$$

This last property shows that after expanding the partial generating functions we need to group somewhat differently from the manner implied by equation (24). The appropriate combined generating functions are

$$F_1 = F_{\langle 1 \rangle}$$

$$F_2 = F_{\langle 2,0 \rangle} + F_{\langle 0,1 \rangle}$$

$$F_3 = F_{\langle 3 \rangle} + F_{\langle 1,1 \rangle} + F_{\langle 0,0,1 \rangle}$$

$$F_4 = F_{\langle 4 \rangle} + F_{\langle 2,1 \rangle} + F_{\langle 0,2 \rangle} + F_{\langle 1,0,1 \rangle} + F_{\langle 0,0,0,1 \rangle}$$

$$F_5 = F_{\langle 5 \rangle} + F_{\langle 1,2 \rangle} + F_{\langle 3,1 \rangle} + F_{\langle 2,0,1 \rangle} + F_{\langle 0,1,1 \rangle} + F_{\langle 1,0,0,1 \rangle} + F_{\langle 0,0,0,0,1 \rangle}.$$

In terms of the order of polynomials that are yielded by a given order of generating function this procedure is a slight improvement on that described by Sykes and Gaunt (1973). Fox and Gaunt (1972) treated the diamond and honeycomb lattices by using the data given by Sykes *et al* (1965) for up to five perturbed sites on the shadow lattice. These gave 11 high-field polynomials as expected from considering up to five perturbed shadow lattice sites, but Fox and Gaunt added the 12th polynomial by noting that the only contributions at order 12 that correspond to 12 perturbed sites will be those with all sites in state 1. The graphs are thus the same as for the spin  $\frac{1}{2}$  Ising model from which series the additional terms may be obtained.

In the present formalism we note that the only contribution to  $F_6$  that involves six perturbed shadow sites is  $F_{\langle 6 \rangle}$ , which is the spin  $\frac{1}{2}$  Ising model code. This will enable 13 high-field polynomials to be obtained from explicit considerations of five perturbed shadow sites. The present method gives the additional polynomial because the information from the spin  $\frac{1}{2}$  Ising model is introduced at the level of the partial generating functions rather than at the level of the final  $L_n$  polynomials.

5.3. A two-layer spin  $\frac{1}{2}$  Ising model

The system considered is a spin  $\frac{1}{2}$  Ising model on two coupled square lattices (ie two planes of a simple cubic lattice). The interactions are  $J_1$  in the upper plane,  $J_2$  in the lower plane. The  $J_1 = J_2 = J_{12}$  case was investigated by Ballentine (1964) using high-temperature expansions. Investigations by Oitmaa and Enting (1975) indicate that the general case has a very complicated behaviour.

We represent this as a four-state model on a square lattice in order to take advantage of the available combinatorial information for this lattice.

We denote the states and their fields as follows.

$$0 \rightarrow (+, +)$$

$$1 \rightarrow (+, -) \quad h_1 = H_2 + 2J_{12}$$

$$2 \rightarrow (-, +) \quad h_2 = H_1 + 2J_{12}$$

$$3 \rightarrow (-, -) \quad h_3 = H_1 + H_2.$$

The energies are

$$J_{10} = 2J_2, \quad J_{20} = 2J_1, \quad J_{30} = 2J_1 + 2J_2, \quad J_{12} = 2J_1 + 2J_2, \\ J_{13} = 2J_1, \quad J_{23} = 2J_2, \quad J_{ii} = 0.$$

Also any of the expansions will be invariant under the transformation state 1  $\rightarrow$  state 2, state 2  $\rightarrow$  state 1,  $J_1 \rightarrow J_2$ ,  $J_2 \rightarrow J_1$ ,  $H_1 \rightarrow H_2$ ,  $H_2 \rightarrow H_1$ .

#### 5.4. Generalized Ashkin–Teller model

This is again a two-layer model, but the two layers have equal interactions and are coupled by a four-spin interaction. The work of Ditzian (1972) indicates that the exponents may be the same as for the eight-vertex model. Since this model can be defined with two fields,  $H$  and  $E$ , as can the eight-vertex model (Barber and Baxter 1973), it may be possible to test the conjectures concerning the exponent  $\beta_e$  that were made by Enting and Gaunt (1974). Again, mapping the two-layer system on to a four-state system (which was the original form given by Ashkin and Teller 1943), we have:

$$\begin{aligned} h_1 &= H + 2E \\ h_2 &= H + 2E \\ h_3 &= 2H \\ J_{10} &= J_{20} = J_{13} = J_{23} = 2J \\ J_{12} &= J_{30} = 4J \\ J_{ii} &= 0. \end{aligned}$$

#### 5.5. A special case

We mention briefly a special class of systems, those in which the lowest energy perturbations can be into either of two equivalent states. Important examples are the planar Potts models (Potts 1952) in which a two-dimensional vector can take up one of  $q$  symmetric directions. The interaction is proportional to the scalar product of pairs of neighbour vectors. If the ordering field is in one of the allowed directions then this defines the lowest energy state (denoted 0). The smallest perturbations which give the lowest order  $L_m$  will be into the two equivalent states denoted by 1 and  $q-1$ . The possible perturbations into these sites give contributions to  $\ln Z$  equivalent to those of the three-state Potts model. When using partial generating functions a major contribution comes from terms in which all perturbed sites on one sublattice are in states 1 and  $q-1$ . Summing over all perturbations on the other sublattice means that we can obtain most of the low-order series terms by reinterpreting the three-state Potts model generating functions given by Enting (1974a). Polynomials  $L_1$  to  $L_9$  have been obtained for the six-state planar Potts model. After using the three-state codes only seven additional terms in the generating function need be calculated separately. The details of these calculations will be given elsewhere.

## 6. Conclusions

The formalism presented in § 4 shows how the method of partial generating functions can be extended to a far more general class of lattice models than has hitherto been

considered. Sykes and Gaunt (1973) gave the basic principles but we feel that the important result is that it is possible to express the combinatorial data in a form that is common to all models. Previous work on the spin 1 Ising model (Fox and Gaunt 1972) and on the Potts model (Enting 1974a) has expressed the code expansions in a form that is applicable only to the model considered, in spite of the fact that these two problems require essentially the same combinatorial information.

In spite of the potential complication of the general form, when particular cases are considered as in § 5, any inherent symmetry can be used at a very early stage to simplify the problem. It is to be hoped that with the calculation of additional code expansions for  $F_m$ , the methods given here will prove useful in the derivation of series expansions.

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### Appendix

#### *A.1. High-field polynomials for three-state model with general linkage rule*

$$L_{11} = 12w - 13$$

$$L_{12} = 24vw^2 + 84vw - 120v + 42w^2 - 240w + 211$$

$$L_{13} = 8v^3w^3 + 48v^3w^2 + 120v^3w - 200v^3 + 48v^2w^3 + 252v^2w^2 + 696v^2w - 1122v^2 \\ + 120vw^3 - 36vw^2 - 4368vw + 4644v + 44w^3 - 1122w^2 + 4644w - 3777$$

$$L_{22} = 12uvw^4 + 96uvw^3 + 252uvw^2 + 564uvw - 1062uv + (u+v)(24w^4 + 240w^3 - 186w^2 \\ - 2244w + 2322) + 6w^4 + 564w^3 - 4368w^2 + 9288w - 5665\frac{1}{2}$$

$$L_{14} = 24v^6w^2 + 24v^6w - 56v^6 + 72v^5w^3 + 144v^5w^2 + 408v^5w - 720v^5 + 54v^4w^4 + 216v^4w^3 \\ + 936v^4w^2 + 2184v^4w - 3882v^4 + 96v^3w^4 + 712v^3w^3 + 1848v^3w^2 - 924v^3w \\ - 2236v^3 + 240v^2w^4 + 552v^2w^3 - 6594v^2w^2 - 62160v^2w + 74574v^2 + 96vw^4 \\ - 2964vw^3 - 15636vw^2 + 146592vw - 137376v + 9w^4 - 1448w^3 + 25284w^2 \\ - 91584w + 71516$$

$$L_{23} = 96uv^3w^4 + 168uv^3w^3 + 408uv^3w^2 + 792uv^3w - 1728uv^3 + 120uv^2w^5 + 288uv^2w^4 \\ + 1080uv^2w^3 + 2184uv^2w^2 + 4632uv^2w - 9732uv^2 + 24uvw^6 + 216uvw^5 \\ + 1032uvw^4 + 936uvw^3 - 7668uvw^2 - 38352uvw + 48012uv + 168uw^5 \\ + 48uw^4 - 6720uw^3 - 804uw^2 + 50568uw - 45792u + 48v^3w^5 + 144v^3w^4 \\ + 352v^3w^3 - 768v^3w^2 - 3792v^3w + 4328v^3 + 12v^2w^6 + 144v^2w^5 + 1152v^2w^4 \\ + 1824v^2w^3 - 3504v^2w^2 - 23232v^2w + 25284v^2 + 288vw^5 + 2856vw^4 \\ - 12480vw^3 - 55368vw^2 + 197160vw - 137376v + 48w^5 + 2550w^4 \\ - 39800w^3 + 171876w^2 - 274752w + 143032.$$

A.2. Expansions for  $F_m$  of third order*Honeycomb*

$$F_{\langle 2,1 \rangle} = 3(7/4, 2/0/0, 1) + 3(6/2, 1/1, 2) + 18(7/3, 2/1, 1) + 9(7/4, 1/0, 2) - 30(8/4, 3/1) \\ - 60(8/5, 2/0, 1) + 58(9/6, 3)$$

$$F_{\langle 1,1,1 \rangle} = 6(7/2, 2, 2/0/0, 0, 0, 0, 1) + (6/1, 1, 1/0, 1, 0, 1, 1) + 18(7/1, 2, 2/0, 1, 0, 1) \\ + 18(7/2, 1, 2/0, 1, 0, 0, 1) + 18(7/2, 2, 1/0, 0, 0, 1, 1) - 60(8/2, 2, 3/0, 1) \\ - 60(8/2, 3, 2/0, 0, 0, 1) - 60(8/3, 2, 2/0, 0, 0, 0, 1) + 116(9/3, 3, 3)$$

*Square*

$$F_{\langle 2,1 \rangle} = 2(8/4, 0/0, 4) + 4(8/2, 2/2, 2) + 4(8/4, 1/0, 2/0, 1) + 8(8/3, 2/1, 1/0, 1) + 8(9/3, 3/2, 1) \\ + 8(9/5, 1/0, 3) + 8(9/4, 2/1, 2) + 6(10/6, 2/0, 2) + 12(10/5, 3/1, 1) \\ - 24(10/4, 4/2) - 48(10/6, 2/0, 2) - 28(11/6, 4/1) - 56(11/7, 3/0, 1) \\ + 97(12/4, 4, 4)$$

$$F_{\langle 1,1,1 \rangle} = 4(8/0, 2, 2/0, 2, 0, 2) + 4(8/2, 0, 2/0, 2, 0, 0, 2) + 4(8/2, 2/0, 0, 0, 2, 2) \\ + 8(8/1, 2, 2/0, 1, 0, 1/0, 0, 0, 0, 1) + 8(8/2, 1, 2/0, 1, 0, 0, 1/0, 0, 0, 0, 1) \\ + 8(8/2, 2, 1/0, 0, 0, 1, 1/0, 0, 0, 0, 0, 1) + 8(9/3, 2, 1/0, 0, 0, 1, 2) \\ + 8(9/3, 1, 2/0, 1, 0, 0, 2) + 8(9/1, 3, 2/0, 1, 0, 2) + 8(9/1, 2, 3/0, 2, 0, 1) \\ + 8(9/2, 3, 1/0, 0, 0, 2, 1) + 8(9/2, 1, 3/0, 2, 0, 0, 1) + 12(10/2, 3, 3/0, 1, 0, 1) \\ + 12(10/3, 2, 3/0, 1, 0, 0, 1) + 12(10/3, 3, 2/0, 0, 0, 1, 1) - 48(10/2, 2, 4/0, 2) \\ - 48(10/2, 4, 2/0, 0, 0, 2) - 48(10/4, 2, 2/0, 0, 0, 0, 2) - 56(11/3, 3, 4/0, 1) \\ - 56(11/3, 4, 3/0, 0, 0, 1) - 56(11/4, 3, 3/0, 0, 0, 0, 1) + 194(12/4, 4, 4).$$

*Diamond*

$$F_{\langle 2,1 \rangle} = 12(10/6, 3/0/0, 1) + 12(9/4, 2/1, 2) + 84(10/5, 3/1, 1) + 42(10/6, 2/0, 2) \\ - 120(11/6, 4/1) - 240(11/7, 3/0, 1) + 211(12/8, 4)$$

$$F_{\langle 1,1,1 \rangle} = 24(10/3, 3, 3/0/0, 0, 0, 0, 0, 1) + 24(9/2, 2, 2/0, 1, 0, 1, 1) + 84(10/2, 3, 3/0, 1, 0, 1) \\ + 84(10/3, 2, 3/0, 1, 0, 0, 1) + 84(10/3, 3, 2/0, 0, 0, 1, 1) - 240(11/3, 3, 4/0, 1) \\ - 240(11/3, 4, 3/0, 0, 0, 1) - 240(11/4, 3, 3/0, 0, 0, 0, 1) + 422(12/4, 4, 4).$$

*Simple cubic*

$$F_{\langle 2,1 \rangle} = 24(13/6, 3/1, 2/0, 1) + 48(15/7, 5/2, 1) + 48(15/8, 4/1, 2) + 48(15/9, 3/0, 3) \\ + 12(14/8, 3/0, 2/0, 1) + 24(14/7, 4/1, 1/0, 1) + 15(16/10, 4/0, 2) \\ + 30(16/9, 5/1, 1) - 168(16/8, 6/2) - 336(16/10, 4/0, 2) - 96(17/10, 6/1) \\ - 192(17/11, 5/0, 1) + 454(18/12, 6) + 30(14/8, 2/0, 4) + 60(14/6, 4/2, 2)$$

$$\begin{aligned}
F_{\langle 1,1,1 \rangle} = & 48(13/3, 3, 3/0, 1, 0, 1, 1/0, 0, 0, 0, 0, 1) + 48(15/5, 4, 3/0, 0, 0, 1, 2) \\
& + 48(15/5, 3, 4/0, 1, 0, 0, 2) + 48(15/4, 5, 3/0, 0, 0, 0, 1) \\
& + 48(15/4, 3, 5/0, 2, 0, 0, 1) + 48(15/3, 4, 5/0, 2, 0, 1) + 48(15/3, 5, 4/0, 1, 0, 2) \\
& + 24(14/3, 5, 5/0, 1, 0, 1/0, 0, 0, 0, 0, 1) \\
& + 24(14/5, 3, 5/0, 1, 0, 0, 1/0, 0, 0, 0, 0, 1) \\
& + 24(14/5, 5, 3/0, 0, 0, 1, 1/0, 0, 0, 0, 0, 1) + 30(16/5, 4, 5/0, 1, 0, 0, 1) \\
& + 30(16/5, 5, 4/0, 0, 0, 1, 1) + 30(16/4, 5, 5/0, 1, 0, 1) \\
& - 336(16/6, 4, 4/0, 0, 0, 0, 2) - 336(16/4, 6, 4/0, 0, 0, 2) - 336(16/4, 4, 6/0, 2) \\
& - 192(17/5, 5, 6/0, 1) - 192(17/5, 6, 5/0, 0, 0, 1) - 192(17/6, 5, 5/0, 0, 0, 0, 1) \\
& + 908(18/6, 6, 6) + 60(14/4, 4, 2/0, 0, 0, 2, 2) + 60(14/4, 2, 4/0, 2, 0, 0, 2) \\
& + 60(14/2, 4, 4/0, 2, 0, 2).
\end{aligned}$$

## References

- Ashkin J and Teller E 1943 *Phys. Rev.* **64** 159  
Ballentine L E 1964 *Physica* **30** 1231  
Barber M N and Baxter R J 1973 *J. Phys. C: Solid St. Phys.* **6** 2913  
Bell G M and Lavis D A 1970 *J. Phys. A: Gen. Phys.* **3** 427  
Blume M, Emery V J and Griffiths R B 1971 *Phys. Rev. A* **4** 1071  
Ditzian R V 1972 *J. Phys. C: Solid St. Phys.* **5** L250  
— 1974 *J. Phys. A: Math., Nucl. Gen.* **7** L152  
Ditzian R V and Oitmaa J 1974 *J. Phys. A: Math., Nucl. Gen.* **7** L61  
Domb C 1960 *Adv. Phys.* **9** 149  
Enting I G 1974a *J. Phys. A: Math., Nucl. Gen.* **7** 1617  
— 1974b *J. Phys. A: Math., Nucl. Gen.* **7** 2181  
Enting I G and Gaunt D S 1974 *J. Phys. A: Math., Nucl. Gen.* **7** L70  
Fox P F and Gaunt D S 1972 *J. Phys. C: Solid St. Phys.* **5** 3085  
Katsura S and Tsujiyama B 1966 *Critical Phenomena* eds M S Green and J V Sengers, Misc., Publ. No. 273  
(Washington: National Bureau of Standards) p 219  
Moore M A 1970 *Phys. Rev. B* **1** 2238  
Oitmaa J 1971 *J. Phys. C: Solid St. Phys.* **4** 2466  
— 1973 *J. Phys. C: Solid St. Phys.* **5** 435  
Oitmaa J and Enting I G 1975 *J. Phys. A: Math., Nucl. Gen.* **8** in the press  
Potts R B 1952 *Proc. Camb. Phil. Soc.* **48** 106  
Saul D M, Wortis M and Stauffer D 1974 *Phys. Rev. B* **9** 4964  
Sykes M F, Essam J W and Gaunt D S 1965 *J. Math. Phys.* **6** 283  
Sykes M F and Gaunt D S 1973 *J. Phys. A: Math., Nucl. Gen.* **6** 643