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Crystal growth models and Ising models IV. Graphical solutions for correlations

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Abstract. Graphical expansions are used to obtain exact solutions for correlations in symmetric models of crystal growth disorder. These models are equivalent to Ising models with fields and competing multi-spin interactions constrained so as to give an effective reduction in dimensionality. The graphical solutions illustrate the importance of symmetry in these models and indicate the way in which an effective reduction in dimensionality occurs.

It is shown that there are particular temperatures at which all correlations in a first-and-second-neighbour square lattice Ising model and certain correlations in an anisotropic FCC model can be obtained explicitly.

1. Introduction

In the earlier papers in this series (Enting 1977a, b, 1978a, to be referred to as I, II and III) the author has investigated connections between Ising models in statistical mechanics and a class of stochastic lattice models which have been used to model the growth of disordered mixed crystals. In the studies of these models of crystal growth Welberry and co-workers (Welberry and Galbraith 1973, 1975, Welberry 1977a, b, Galbraith and Walley 1976, Welberry and Miller 1977, 1978) used extensive simulations but were also able to obtain a number of exact solutions for various correlations. This was somewhat surprising since the crystal growth models are equivalent to quite complicated Ising models (see I).

An explanation of why these special Ising models turn out to be soluble lies in the observation that the crystal growth models correspond to Ising models with competing interactions and that many of the models correspond to Ising models at the disorder points. Disorder points (Stephenson 1970a) are points at which the competition between interactions leads to a change in the behaviour of the correlations and actually at the disorder point the correlations have a particularly simple structure. Gibberd (1969) was able to obtain graphical techniques for deriving expressions for the correlation functions at the disorder point; these solutions exploited the special simplifications occurring, unlike the general technique used by Stephenson. The present paper extends Gibberd's technique to a wider class of crystal growth models.

There are a number of reasons why correlation solutions in these models are of interest:

(i) In disordered crystals it is the correlations which can be measured experimentally by diffraction techniques.

(ii) Welberry (1977a) has conjectured (on the basis of numerical calculation of short-range correlations) that growth models with rectangular symmetry have exponentially decaying correlations. For the zero-field case this has been confirmed by the exact solution for correlations along the axes (see I) and, for general models with rectangular symmetry, by Pickard (1977). The solutions below confirm Welberry's conjecture.

(iii) It was pointed out in II that the exact solutions of crystal growth models gave constraints for Ising model series expansions. (Such constraints might be used to help derive further series, see Sykes *et al* (1975).)

(iv) The solutions obtained below indicate the type of cancellation obtained and show how crystal growth models have a reduction in the effective dimensionality. Previously this effect has been noted by Stephenson (1970a), Welberry and Miller (1978) and implicitly by Verhagen (1976)

(v) The solutions also illustrate some of the connections between the growth model formulated as a Markov process and the Markov random field characterisation of Ising models. This connection has been discussed by Enting and Welberry (1978). The Markov random field characterisation of Ising models has been exploited by Enting (1977c) in the derivation of triplet order parameters on triangular and honeycomb Ising models.

The layout of the remainder of the paper is as follows. Section 2 describes the crystal growth models and the various possible parametrisations. The exact solutions which have been obtained are reviewed. In §3 the one-dimensional Ising model is described in terms of statistical mechanics, as a Markov random field and as a growth model (or Markov chain). This shows some of the relations between the various characterisations and provides a basis for interpreting results obtained in two-dimensional models. Section 4 generalises the graphical expansion technique used by Gibberd (1969) and applies to systems with particular symmetries. In §5 the method is used to exhibit the special structure of the models considered by Verhagen (1976) and by Welberry and Miller (1977).

This latter model is of considerable interest because it corresponds to an anisotropic FCC model with only two-site interactions (albeit competing interactions).

2. Crystal growth models

The models used by Welberry and co-workers in the study of the growth of mixed disordered crystals had earlier been investigated by a number of statisticians (see for example Whittle 1954, Bartlett 1967, Besag 1974).

In the general form one has a lattice on which a partial ordering or precedence relation is defined on the sites. The basic assumption is that the probabilities for the state of any site depend only on the states of sites preceding it. Although Enting (1978b) has described one application to a system with three-state variables, the present discussion will follow the bulk of previous work in confining itself to binary variables where the variable at site $\boldsymbol{r}$ is denoted by $\sigma_{\boldsymbol{r}} = \pm 1$. We shall use the symbol $\sigma_{\boldsymbol{r}}$ to denote both the random variable $\sigma_{\boldsymbol{r}}$ and its possible values $s_{\boldsymbol{r}}$ so that we write probabilities as $P(\sigma_{\boldsymbol{r}})$ rather than $P(\sigma_{\boldsymbol{r}} = s_{\boldsymbol{r}})$. The whole set of $\sigma_{\boldsymbol{r}}$ is denoted by the vector $\boldsymbol{\sigma}$ of $\sigma_{\boldsymbol{r}}$ values. The probability of a particular set of values $\boldsymbol{\sigma}$ is given by

$$P(\boldsymbol{\sigma}) = \prod_{\boldsymbol{r}} P(\sigma_{\boldsymbol{r}} | \text{predecessors of } \boldsymbol{r}) \tag{2.1}$$

and

$$P(\sigma_r|\text{predecessors}) = \tfrac{1}{2}(1 + \sigma_r \cdot f(\text{predecessors})). \tag{2.2}$$

In practice we shall be interested only in cases where the probability depends only on a small number of neighbouring predecessor sites. In particular we shall consider a square lattice with sites indexed by pairs of integers (i, j) such that (i', j') is a predecessor of (i, j) if $i' \leq i$ and $j' \leq j$ but $(i', j) \neq (i, j)$.

We assume that the probability of σ_{ij} depends only on $\sigma_{i,j-1}$, $\sigma_{i-1,j}$ and $\sigma_{i-1,j-1}$. There are thus 16 conditional probabilities associated with the 16 possible configurations on the set of four sites. Only eight of these are independent. It was shown in I that the probability distribution $P(\boldsymbol{\sigma})$ is (ignoring boundary effects) equivalent to the distribution obtained from an Ising model with multi-site interactions. The interactions were a field, a nearest-neighbour interaction along each axis, a second-neighbour interaction on each diagonal, four three-site interactions and a four-site interaction. Expressions were given for the ten interaction strengths in terms of the conditional probabilities (equation $(7a)$–$(7f)$ of I). Since there are only eight independent probabilities we have two implicit constraints on the interaction strengths. The equations given in I parametrise the Ising interactions J_i in terms of $\exp(-J_i/kT)$. For many purposes it is convenient to use the variables $\tanh(J_i/kT)$ so that we can work with expressions which are linear in the σ_{ij} variables. Without going into details of the parametrisation it is still possible to review the results which have been obtained for correlations.

Pickard (1977) has shown that of the square lattice growth models described above, the models with rectangular symmetry (i.e. mirror lines parallel to both axes) have two-site correlations which decay exponentially. This behaviour had been conjectured by Welberry (1977a) and a graphical derivation of the results is given below. Pickard's solution is based on a comparison of alternative characterisations of the process. An algebraic derivation of the zero-field correlations for rectangular symmetry is given in III.

For the anisotropic triangular lattice at its disorder point (characterised by $\tanh(\beta J_1)\tanh(\beta J_2) = -\tanh(\beta J_3)$) Gibberd (1969) obtained a graphical solution for some of the two-site correlations. This graphical approach is generalised in the following sections.

It should be noted that Welberry and Galbraith (1973) were able to evaluate *all* correlations in the triangular model at its disorder point, by using algebraic techniques. The present paper concentrates on graphical solutions because these techniques exhibit the general properties of the solution which are often more informative than the solutions themselves.

3. The one-dimensional Ising model

The one-dimensional Ising model has its energy given by

$$E = \sum_{n=1}^{N} (-J\sigma_n\sigma_{n+1} - H\sigma_n) \tag{3.1}$$

and from the basic formalism of statistical mechanics the probability of any spin configuration $\boldsymbol{\sigma}$ is given by

$$P(\boldsymbol{\sigma}) = Z^{-1}\exp(-E(\boldsymbol{\sigma})/kT) \tag{3.2}$$

where Z, the partition function, acts as a normalising factor. Using a linearisation technique due to van der Waerden (1941) we can write (3.2) as

$$P(\boldsymbol{\sigma}) = C \prod_{n=1}^{N} (1 + v\sigma_n\sigma_{n+1})(1 + h\sigma_n) \tag{3.3}$$

where $v = \tanh(J/kT)$ and $h = \tanh(H/kT)$ and C is another normalising factor. To convert this expression into a growth model expression we split the field into two contributions so that apart from boundary corrections,

$$\begin{aligned} P(\boldsymbol{\sigma}) &= D \prod_{n=1}^{N} (1 + h_1\sigma_n)(1 + v\sigma_n\sigma_{n+1})(1 + h_2\sigma_{n+1}) \\ &= D \prod_{n=1}^{N} [(1 + h_1 v h_2) + \sigma_n(h_1 + vh_2) + \sigma_{n+1}(h_2 + vh_1) + \sigma_n\sigma_{n+1}(v + h_1h_2)] \end{aligned} \tag{3.4}$$

where

$$(h_1 + h_2)/(1 + h_1h_2) = h \tag{3.5}$$

and D is yet another irrelevant normalising factor.

If we choose h_1 such that

$$h_1 + vh_2 = 0 \tag{3.6}$$

i.e.

$$h_2 = [(v-1) - \sqrt{(v-1)^2 + 4h^2v}]/2hv \tag{3.7}$$

then we can interpret each factor in (3.4) as a growth model conditional probability and we have

$$P(\sigma_{n+1}|\sigma_n) = \tfrac{1}{2}\{1 + \sigma_{n+1}[(h_2 + vh_1) + \sigma_n(v + h_1h_2)]/(1 + vh_1h_2)\} \tag{3.8}$$

and

$$P(\boldsymbol{\sigma}) = \prod_n P(\sigma_{n+1}|\sigma_n). \tag{3.9}$$

Assuming a sufficiently large system so that we have translational invariance we can write

$$M = \langle\sigma_{n+1}\rangle = [(h_2 + vh_1) + \langle\sigma_n\rangle(v + h_1h_2)]/(1 + vh_1h_2)$$

whence

$$M = \frac{h_2 + vh_1}{1 + h_1h_2v - v - h_1h_2} = \frac{h_2 - h_1}{1 - h_1 - h_2} \tag{3.10}$$

using the techniques described by Welberry and Galbraith (1973, 1975) (see also I and III).

An alternative factorisation which can be used to obtain $\langle\sigma_j\rangle$ is to write

$$\begin{aligned} P(\boldsymbol{\sigma}) &\propto \prod_{m\geqslant j} (1 + h_1\sigma_m)(1 + h_2\sigma_{m+1})(1 + v\sigma_m\sigma_{m+1}) \\ &\quad\times \prod_{m<j} [(1 + h_1\sigma_{m+1})(1 + h_2\sigma_m)(1 + v\sigma_m\sigma_{m+1})](1 + h_2\sigma_j)(1 - h_1\sigma_j) \\ &\propto \prod_{m\geqslant j} [1 + \sigma_{m+1}(A + B\sigma_m)] \prod_{m<j} [1 + \sigma_m(A + B\sigma_{m+1})] \\ &\quad\times [1 + \sigma_j(h_2 - h_1)/(1 - h_1h_2)] \end{aligned} \tag{3.11}$$

To evaluate

$$\langle\sigma_j\rangle=\sum_{\{\boldsymbol{\sigma}\}}\sigma_j P(\boldsymbol{\sigma})$$

we have to sum over all terms in the product in which all the σ_i variables appear an even number of times. In fact the only such factor is $\sigma_j\times 1\times 1\ldots\times 1\times 1\ldots\sigma_j(h_2-h_1)/(1-h_1h_2)$. Any attempt to include other factors generates a product which closes (if at all) only at the boundaries. Any contribution other than 1 from the $m=j$ factor brings in σ_{j+1} with an odd power. If this is cancelled by a contribution from the $m=j+1$ factor we bring in σ_{j+2} with power one and so on. For $v<1$ and sufficiently small h such contributions will not be significant if j is sufficiently far from the boundaries. Thus

$$\langle\sigma_j\rangle=(h_2-h_1)/(1-h_1h_2) \tag{3.12}$$

where we have used $\langle 1\rangle=1$ to determine the normalising factor in (3.11).

What we have used is the property that the growth model conditional probabilities are linear in one of the σ_i variables. If one has a symmetry in the model one can factor $P(\boldsymbol{\sigma})$ into expressions corresponding to all growth outward from some central region of interest so that none of the growth model probabilities contribute to expectations in the region. The only factors which do contribute are the corrections. The product of growth probabilities in (3.11) includes $(1+h_1\sigma_j)$ twice and omits $(1+h_2\sigma_j)$ and so we have the final factor as a correction.

Gibberd's graphical analysis is just a two-dimensional analogue of this trick. In this case the overlap or correction region is a line rather than a single point and so correlations correspond to a one-dimensional Ising model in a field.

Using the characterisation (3.8) we have

$$P(\sigma_{n+1}|\sigma_n)=\tfrac{1}{2}[1+\sigma_{n+1}(A+B\sigma_n)] \tag{3.13}$$

whence

$$\langle\sigma_{n+1}\sigma_k\rangle=AM+B\langle\sigma_n\sigma_k\rangle \qquad k\leqslant n$$

or

$$\langle\sigma_{n+1}\sigma_k\rangle-M^2=B(\langle\sigma_n\sigma_k\rangle-M^2) \tag{3.14}$$

so that correlations decay exponentially. This is to be expected since (3.13) simply describes a Markov chain.

This parametrisation of the one-dimensional Ising model is also useful for demonstrating the decimation renormalisation group transformation (see Nelson and Fisher 1975). We wish to demonstrate that if one selects as a new set of sites, every second site from a one-dimensional Ising model, the probability distribution on this new set is simply that of a one-dimensional Ising model.

One puts

$$P(\sigma_{n+1}|\sigma_{n-1})=\sum_{\sigma_n}P(\sigma_{n+1}|\sigma_n)P(\sigma_n|\sigma_{n-1})=\tfrac{1}{2}[1+\sigma_{n+1}(A+AB+B^2\sigma_{n-1})]. \tag{3.15}$$

The parameters of the growth model characterisation transform as $A\to A+AB$; $B\to B^2$. This transformation leaves $M=A/(1-B)$ invariant as it must since the spin distributions on the new lattice are equivalent to those on the original lattice.

The final characterisation of the one-dimensional Ising model is the Markov random field characterisation. If we write the dependence of σ_i on all other sites as

$$P(\sigma_i|\boldsymbol{\sigma}/\sigma_i)=\frac{P(\boldsymbol{\sigma})}{P(\boldsymbol{\sigma}/\sigma_i)}=\frac{P(\boldsymbol{\sigma})}{\sum_{\sigma_i} P(\boldsymbol{\sigma})}$$

$$=\frac{(1+v\sigma_i\sigma_{i-1})(1+v\sigma_i\sigma_{i+1})(1+h\sigma_i)}{1+v^2\sigma_{i-1}\sigma_{i+1}+vh(\sigma_{i+1}+\sigma_{i-1})} \tag{3.16}$$

since all terms not containing σ_i cancel between the numerator and denominator. The Markov random field criterion is that

$$P(\sigma_i|\boldsymbol{\sigma}/\sigma_i)=P(\sigma_i|\sigma_{i-1},\sigma_{i+1}) \tag{3.17}$$

$$=\frac{P(\sigma_i\sigma_{i-1}\sigma_{i+1})}{P(\sigma_{i-1}\sigma_{i+1})} \tag{3.18}$$

Evaluating (3.18) verifies that (3.16) is a Markov random field characterisation of the one-dimensional Ising model.

4. Models with special symmetry

The most common form of graphical expansion for Ising models in the high-temperature regime starts from the van der Waerden linearisation shown in equation (3.3) and represents each term in the expanded product by a graph.

In general if

$$E=-\sum_R K_R\sigma_R \tag{4.1}$$

$$\exp(-E/kT)=\prod_R [\cosh K/kT(1+\sigma_R v_R)] \tag{4.2}$$

where $v_R=\tanh(K_R/kT)$, R denotes arbitrary subsets of sites and σ_R is the product $\Pi_{i\in R}\sigma_i$.

Each term in the expanded product is mapped onto a graph (or hypergraph if any of the sets R contain more than two sites), so that for example factors $v\sigma_i\sigma_j$ are represented by a line from i to j. The only graphs which contribute to the sum over all σ states of $\exp(-\beta E)$ are those with an even number of spin variables associated with each site.

For growth models we use a graphical expansion based on combining the product (4.2) into the form (2.2). If one has a lattice symmetry then one can choose the growth direction implied by (2.2) in several ways. The graphical representation of the terms $\sigma_i f$ (neighbours) for any basic cell of the lattice will be an arrow indicating which is the distinguished site i for that cell.

The next stage in the development is to choose different directions for different regions of the lattice and to obtain correction terms for the boundary between the regions. Figure 1(a) shows how the orientations would be chosen for the factorisation (3.11) used for the one-dimensional Ising model. Figure 1(b) shows such a choice for a lattice with rectangular symmetry. For a growth model with σ_{ij} depending on $\sigma_{i-1,j}$, $\sigma_{i,j-1}$, $\sigma_{i-1,j-1}$ this choice implies:

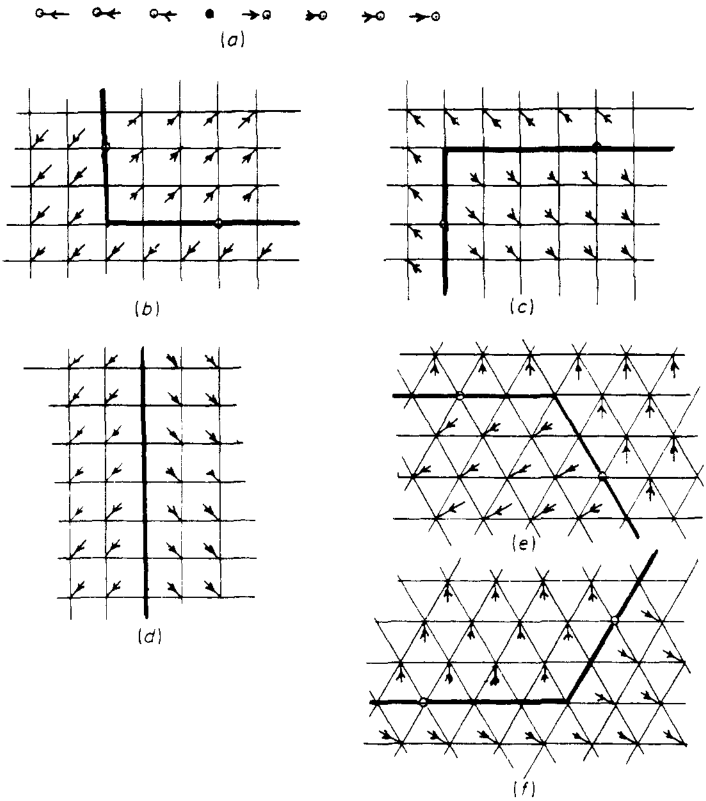

Figure 1. The orientation of cells used in obtaining special growth model solutions. In each cell the arrow points to the spin singled out by the growth model characterisation. Heavy shading shows the boundary region. (*a*) The one-dimensional Ising model; (*b*), (*c*) square lattice models with correlations in two different quadrants; (*d*) linear correlations in a model with reflection symmetry; (*e*), (*f*) triangular lattice models with correlations in two different sectors.

(*a*) The equivalent Ising model interactions which combine to give expressions of the form (2.2) are those within the four-site cells (see I).

(*b*) The only interactions which are overcounted or undercounted by this procedure are those common to two cells on opposite sides of the boundary, i.e. single-site interactions on boundary sites and pairwise interactions along the boundary line.

(*c*) The correction terms in (*b*) are the only factors which contribute either to the partition function or to two-site correlations for sites in the boundary line. Any other contribution, from the cells (represented by a cell with an arrow) will imply an odd spin σ_i at the end of the arrow. If this spin is not to contribute 0 it must be cancelled by one of the spins of a neighbouring cell further from the boundary and this implies another 'odd' spin which must in turn be cancelled by more distant spins. Again this process terminates, if at all, only at the boundary of the whole system. If all the factors involved are of magnitude less than one (and this will be the case if (2.2) is to represent probabilities) then the contributions from the growth model cells becomes negligible as the system becomes arbitrarily large.

If the system had full square lattice symmetry then all sites along the boundary would be equivalent and the 'correction' interactions would be those of the one-dimensional Ising model. (The only site for which this is not obvious and has to be checked by explicitly writing down the interactions is the boundary corner). As shown in the previous section this implies that correlations decay exponentially with distance along the boundary line.

For systems with rectangular symmetry we have different interactions along the two line segments and the correction field at the corner is different from that at other sites. We treat this system as a Markov process using a decomposition of the type (3.8) in each segment. If the boundary sites are indexed $-N$ to N with 0 as the corner site we have

$$P(\boldsymbol{\sigma}_{\text{boundary}}) = \prod_{n<0} \tfrac{1}{2}[1+\sigma_{n+1}(a+b\sigma_n)] \prod_{n>0} (1+\sigma_n(\alpha+\beta\sigma_{n-1}))(1+h\sigma_0) \tag{4.13}$$

where the contribution h is obtained from combining the corner correction described above with a correction arising from having two different Markov parametrisations meeting at the corner. Translational invariance gives

$$\langle\sigma_{-1}\rangle = a + b\langle\sigma_{-2}\rangle = a/(1-b) = \langle\sigma_0\rangle = a + b\langle\sigma_{-1}\rangle + h$$

whence $h=0$. Using the results of equation (3.4) we have

$$\langle\sigma_n\sigma_m\rangle - M^2 = \begin{cases} b(\langle\sigma_n\sigma_{m-1}\rangle - M^2) & n<m\leqslant 0 \\ \beta(\langle\sigma_n\sigma_{m-1} - M^2\rangle) & n\leqslant 0,\ m>0 \\ (1-M^2)b^{|n|}\beta^{|m|} & n\leqslant 0,\ m\geqslant 0. \end{cases} \tag{4.4}$$

Figure 1(b) has only used the symmetry of invariance under reversals of the growth direction but, as shown in figure 1(c), if one requires correlations in the quadrants which contain the growth direction one must have invariance under all rotations of the growth direction. If we have full rectangular symmetry all correlations decay as given by (4.4) while if we have only symmetry under reversal of the growth direction (4.4) applies only in certain sectors. (As found by Gibberd (1969) for the anisotropic triangular Ising model.) If we have invariance under reflection about one of the axes then the construction in figure 1(d) shows that we can expect exponential decays for correlations between pairs of sites lying in the mirror line.

Figures 1(e, f) show how the same techniques can be applied to the fully symmetric triangular growth model studied in II. In this case the only correction interactions are single-site interactions as the cells have no shared edges so that

$$\langle\sigma_{\mathbf{0}}\sigma_{\boldsymbol{r}}\rangle = M^2 \qquad \boldsymbol{r}\neq\mathbf{0}. \tag{4.5}$$

We conclude this section by re-deriving the susceptibility of a second-neighbour Ising growth model. This model was considered in III but the parametrisation given here is more suitable for comparison with series expansions.

The two Ising model interactions are denoted J_1, J_2 and we use the conventional expansion variables

$$v = \tanh(J_1/kT) \tag{4.7a}$$

$$w = \tanh(J_2/kT). \tag{4.7b}$$

So that we can associate a definite energy function to each square cell we divide the interaction J_1 into two contributions K and L:

$$J_1 = K + L \tag{4.8a}$$

$$x = \tanh(K/kT) \tag{4.8b}$$

$$y = \tanh(L/kT) \tag{4.8c}$$

$$v = (x+y)/(1+xy). \tag{4.8d}$$

If we denote the four spins around the square by $a, b, c, d = \pm 1$ then we assume L acts between a and b and between a and c while K acts between c and d and b and d.

The contribution of the cell to $\exp(-\beta E)$ is

$$C(1+yab)(1+yac)(1+xcd)(1+xbd)(1+wad)(1+wbc). \tag{4.9}$$

The construction used in figure 1(b) can be used if expression (4.9) can be written so that all non-constant terms are linear in spin d, i.e. if (4.9) can be written in the form (2.2). We want the coefficient of ab (which is equal to the coefficient of ac) and the coefficient of bc, to vanish, i.e.

$$w = -(x^2+y^2+2xyw+x^2w+y^2w^2+x^2y^2w) \tag{4.10a}$$

$$y = -(xw+yw+yx^2+xw^2+x^2yw+xwy^2+y^2w^2x) \tag{4.10b}$$

and from (4.8d) we have

$$x = v(1+xy)-y. \tag{4.10c}$$

In terms of figure 1(b) the boundary line has been given a contribution L from cells on both sides of the line but has no contribution K and so the 'correction' interaction is $K-L$. The nearest-neighbour interaction for spins on the boundary line is

$$t = \tanh[(K-L)/kT] = (x-y)/(1-xy). \tag{4.11}$$

Since the correlations satisfy (4.4) (with $M=0$) we can sum over all correlations to find

$$\chi = \left(\frac{1+t}{1-t}\right)^2. \tag{4.12}$$

The equations (4.10a)–(4.10c) can be used in the order a, b, c to obtain a series expansion for x, y, w in powers of v. The initial approximation for the iteration is $x = v$, $y = w = 0$. The results are:

$$w = -v^2+2v^4-9v^6+48v^8-289v^{10}+1870v^{12}-12709v^{14}+\dots \tag{4.13}$$

representing the constraint which makes the second-neighbour Ising model a growth model;

$$t = v-2v^3+10v^5-56v^7+350v^9-2326v^{11}+1613v^{13}-\dots \tag{4.14}$$

for the nearest-neighbour correlation;

$$\chi = 1+4v+8v^2+4v^3-16v^4-12v^5+88v^6+108v^7-448v^8-708v^9+2664v^{10} \\ +4908v^{11}-16848v^{12}-34604v^{13}+112376v^{14}+\dots \tag{4.15}$$

for the susceptibility.

In view of the connections between growth models and disorder points (see I and III) it might have been expected that the disorder point of a Union Jack lattice (Stephenson 1970*b*) would involve a simple cancellation of interactions, similar to that described above. This however is not the case since disorder point correlations in the Union Jack model do not have a simple exponential decay.

5. Two special models

Two systems which illustrate applications of the various characterisations described above are those analysed by Verhagen (1976) and Welberry and Miller (1978). In each case the important symmetry is that of invariance under reversal of the growth direction. The earlier discussions have concentrated on the cases which also have the maximum symmetry within the layers orthogonal to the growth direction but this restriction is for reasons of convenience and most of the results described below carry through to less symmetric systems.

Verhagen (1976) considered a 'triangular' type model, i.e. one in which σ_{ij} depended only on $\sigma_{i-1,j}$ and $\sigma_{i,j-1}$. He constructed his probabilities so that the sequence could also be characterised by a Markov chain from σ_{ij} to $\sigma_{i,j-1}$ to $\sigma_{i+1,j-1}$ to $\sigma_{i+1,j-2}$ to $\sigma_{i+2,j-2}$ etc as shown in figure 2(*a*). Once the Markov chain characterisation is obtained the solutions for single-site expectations and correlations within the chain can be found as in §3.

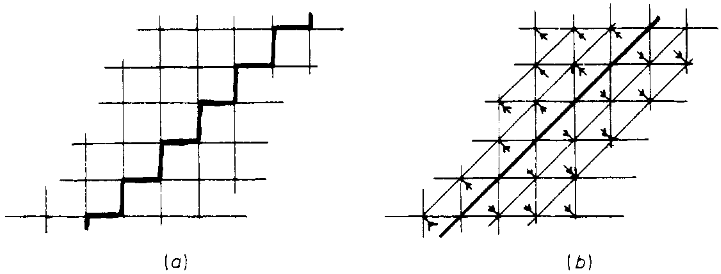

Figure 2. Characterisation of Verhagen's models. (*a*) the line along which Verhagen constructed a Markov chain; (*b*) the cell orientation for the graphical solution. Unlike the system shown in figures 1(*e*, *f*), the absence of three-site interactions enables us to equate triangles of opposite parities.

As pointed out by Enting and Welberry (1978) there are other ways of looking at this model. One can start with the general triangular lattice growth model and require that it be invariant under reversal of the growth direction. In terms of the Ising model parametrisation given in I this is a requirement that there be no three-site interaction between $\sigma_{ij}, \sigma_{i,j-1}$ and $\sigma_{i-1,j}$. From this starting point there are two different ways of solving the model:

(i) The construction in figure 2(*b*) shows how the 'correction' interactions must be those of a one-dimensional Ising model and so one has an Ising model distribution on $\{\sigma_{ij} : i+j=n\}$.

(ii) Because of the reversibility the layer with $i+j=n$ depends on the layer $i+j=n+1$ in the same way as n depends on layer $n+1$ and for an individual spin all this dependence is through its neighbours. This means that layer n and layer $n+1$ together form a Markov random field or equivalently a one-dimensional Ising model.

The results of these two approaches are equivalent to those by Verhagen since, as we have seen in § 3, an Ising model on the set of sites shown in figure 2(a) will give a distribution equivalent to a Markov chain on those sites and the distribution on the set of alternate sites will also be that of a one-dimensional Ising model (see equation (3.15) or Nelson and Fisher 1975).

When we consider three-dimensional models the Markov chain characterisation cannot be used but the other two methods described above can be used virtually unchanged. Welberry and Miller (1977) described a simple cubic lattice with a growth direction along the body diagonal of the cubes so that site i, j, k depended on sites $i-1, j, k, i, j-1, k$ and $i, j, k-1$. They restricted their consideration to zero field so that reversibility of the growth direction implied that the only interactions occurring in a three-dimensional Ising model characterisation were two-site interactions along the cubic axes and two-site interactions within layers orthogonal to the growth direction. As above one can either take the reciprocal dependence of adjacent layers to say that pairs of layers form a Markov random field or equivalently a honeycomb lattice Ising model or one can perform a construction analogous to figure 2(b) and show that the correction interactions are pair interactions in the (111) planes and so the spin distribution on each layer is that of the triangular lattice Ising model. The equivalence of the spin distribution of the alternate sites of a honeycomb Ising model to the distribution for a triangular Ising model is given by the well known star–triangle transformation (see for example Syozi 1972).

Instead of using the (111) planes to divide the space into two regions with opposite growth directions we can also use the {110} or {100} planes. In the former case the correction interactions are those of a rectangular lattice Ising model while in the latter case they are those of an (anisotropic) triangular Ising model. In other words we have a three-dimensional Ising model with only pairwise interactions, but the correlations in a number of planes are those of two-dimensional Ising models. (If we regard the lattice as FCC rather than SC then we have a model with only nearest-neighbour interactions.)

The interactions in the models are most easily described in terms of variables $K_i = J_i/kT$. If one had three variables K_1, K_2, K_3 and regarded them as interactions on a honeycomb lattice then one could use the star–triangle transformation (Syozi 1972) to construct three new variables $K'_1(K_1, K_2, K_3)$, $K'_2(K_1, K_2, K_3)$, $K'_3(K_1, K_2, K_3)$ which are interactions for an 'equivalent' triangular lattice model. We construct a three-dimensional growth model on a simple cubic lattice by using the interactions

K_1 : [100] direction

K_2 : [010] direction

K_3 : [001] direction

$-K'_1$: [011] direction

$-K'_2$: [101] direction

$-K'_3$: [110] direction

Given this prescription we have:

(i) Correlations in a (111) plane are those of triangular Ising model with interactions (K'_1, K'_2, K'_3).

(ii) Correlations in a (100) plane are those of a triangular Ising model with interactions $(K_2, K_3, -K'_1)$. Permuting indices 1, 2, 3 gives the corresponding results for (010) and (001) planes.

(iii) Correlations in a (110) plane are those of a rectangular Ising model with interactions (K_3, K'_3).

(iv) A lattice consisting of a pair of adjacent (111) planes will have the correlations of a honeycomb Ising model with interactions (K_1, K_2, K_3).

Since these various subsystems interset we have a number of equivalences between correlations on different Ising models. The connection between (i), (ii) and (iv) was exploited by Baxter and Enting (1978) in their algebraic solution of the Ising model energy. These connections (in a more general form) have previously been obtained by Baxter (1978).

Going back to the case $K_1 = K_2 = K_3 = K$, $K'_1 = K'_2 = K'_3 = K'$ the growth model constraint is

$$w^2 = (v + v^2)/(1 + v^3) \tag{5.1}$$

$$w = \tanh K \tag{5.2a}$$

$$v = \tanh K'. \tag{5.2b}$$

Working in terms of the energy parameters $J = kTK$ for the $\langle 100 \rangle$ directions and $-J' = -kTK'$ for interactions in the (111) planes, we can fix J, J' and regard the growth constraint (5.1) as giving a temperature at which the correlations are given by two-dimensional solutions. A solution will exist if

$$0 < J'/|J| = R \leq R_{\max} \approx 0{\cdot}655. \tag{5.3}$$

For values of R in the range 0·5 to $R_{\max}$ there will in fact be two solutions for the temperature.

6. Conclusions

The results presented in the preceding sections have shown how, in symmetric crystal growth models, a regrouping of conventional high-temperature expansions for Ising models leads directly to a number of special properties of correlations. The graphical solutions have exhibited the exponential decay found by Pickard (1977) and conjectured by Welberry (1977a), and have also shown how the Markov chain behaviour described by Pickard arises with the formalism of the Gibbs probability distribution. One special case obtained is the confirmation that all two-site correlations vanish in a growth model with full triangular symmetry. The introduction of 'correction' interactions associated with the graphical expansions show how an effective reduction of dimensionality arises in these models. The three-dimensional model described by Welberry and Miller is particularly interesting because the individual layers have the distribution of a two-dimensional Ising model. In other words the time evolution of the growth model corresponds to a Monte Carlo simulation of a two-dimensional Ising model. On the other hand using the methods of I the space–time characterisation of the growth model is equivalent to a conventional Ising model in statistical mechanics and so the normal techniques of equilibrium statistical mechanics can be used to explore the spatial–temporal properties of a simulation procedure. Furthermore, the three-dimensional characterisation is particularly simple involving only two-site interactions. Investigations of this system are currently progressing.

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