Crystal growth models and Ising models. II. Constraints on high-field expansions

1977 J. Phys. A: Math. Gen. 10 1023

(http://iopscience.iop.org/0305-4470/10/6/021)

J. Phys. A: Math. Gen., Vol. 10, No. 6, 1977. Printed in Great Britain. © 1977

Crystal growth models and Ising models II. Constraints on high-field expansions

I G Enting

Department of Theoretical Physics, Research School of Physical Sciences, The Australian National University, Canberra, ACT, 2600, Australia

Received 18 November 1976

Abstract. High-field expansions for the Ising model on a honeycomb lattice have been given in terms of mixed one-spin/two-spin/three-spin Ising models on the triangular lattice. It is pointed out that a two-parameter subset of these mixed models has been solved and that the series expansions are thus subject to a large number of constraints.

1. Introduction

High-field expansions for Ising models have been very important in the study of critical phenomena. One of the reasons for this is that these series are appropriate for studying the approach to the critical point along the zero-field line from low temperatures and also along the critical isotherm. They can also be transformed to give high-temperature expansions.

One of the most significant advances in techniques of deriving such series expansions was the method of partial generating functions (Sykes *et al* 1965, to be referred to as I). One of the simplest applications of this method is the honeycomb lattice Ising model which can be transformed by a star-triangle transformation into a triangular lattice Ising model with a field, H, a nearest-neighbour interaction, J, and a three-spin interaction, J_3, on half the triangles. These techniques have been developed in a series of papers (Sykes *et al* 1973a, b, c, 1975a, b, c, to be referred to as II, III, IV, VII, VIII and IX) and extensive tables of series coefficients for this mixed model have been given (I, III, IX). The most recent refinement of these techniques used a number of consistency requirements on the series as constraints to reduce the amount of combinatorial information needed.

Some months after the publication of IX a solution for the magnetization and nearest-neighbour correlation of a subset of the one-spin/two-spin/three-spin triangular model was given by Welberry and Galbraith (1975). The solutions applied to the surface in H–J–J_3 space sketched in figure 1. (Actually Welberry and Galbraith solved a model with an additional free parameter corresponding to a lattice anisotropy—we shall consider only the isotropic case). The solutions of these crystal growth models resulted from work by statisticians and theoretical chemists (Bartlett 1967, 1968, Welberry and Galbraith 1973). The work is not expressed in Ising model terminology and in fact makes no mention of the Ising model. The independent development of these growth model solutions simultaneously with extensive series work on the corresponding Ising models is a remarkable coincidence.

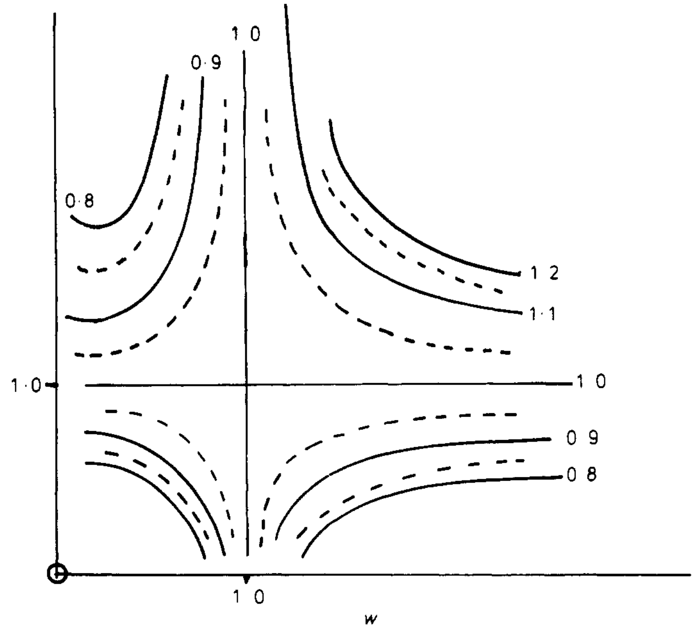

Figure 1. The surface in the space of $\mu = \exp(-2H/kT)$, $u = \exp(-2J/kT)$, $w = \exp(-2J_3/kT)$ on which the mixed triangular lattice model corresponds to a crystal growth model and can be solved. Contours of fixed u are shown at intervals $\Delta u = 0{\cdot}1$ with auxiliary contours sketched at $\Delta u = 0{\cdot}05$. As viewed from the direction of the u axis the surface shows a saddle at $(\mu, u, w) = (1, 1, 1)$.

The correspondence between crystal growth models and Ising models has been described by Enting (1977). Enting considered an eight-parameter subset of a class of ten-parameter square lattice Ising models, including the mixed triangular lattice model as a special case. The derivation for the special case is given in § 2 with a slight change of emphasis from the original derivation and a considerable simplification in the detailed mathematics. Section 3 gives an alternative derivation of the exact solutions and expresses these in Ising model terms. Section 4 shows how these solutions can be compared with the published Ising model series data. Section 5 concludes the paper with a discussion of the problems involved in using these constraints in the derivation of series expansions.

2. Crystal growth models and Ising models

This section repeats the discussion given by Enting (1977) and gives detailed transformations for the triangular lattice one-spin/two-spin/three-spin model. The original paper of Enting gives a more general transformation, discusses boundary conditions and investigates other special cases with particular emphasis on disorder-point phenomena.

Both the crystal growth models and the Ising models can be regarded as models of random systems with spatial interactions. Since each model was introduced in connection with problems in solids, the spatial framework used is generally a regular crystal lattice. In each model the variation has been simplified so that each site $\boldsymbol{r}$ of the lattice has a two-state variable $\sigma_r = \pm 1$. The states represent occupation by one of the two types of molecule when modelling the growth of disordered mixed crystals or of one of two types of atom in the Ising model description of binary alloys. Other interpretations of the Ising model variables are as presence or absence of a gas molecule (lattice gas) or as the value of the z component of a spin $\frac{1}{2}$ (magnetic models).

To make the connection between crystal growth models and Ising models we consider the overall configuration represented by $\boldsymbol{\sigma}$, a vector of σ_r variables. This has a probability which is denoted $P(\boldsymbol{\sigma})$. In the statistical mechanics of the Ising model one has

$$P(\boldsymbol{\sigma}) = \exp(-E(\boldsymbol{\sigma})/kT)/Q. \tag{1}$$

We consider the energy defined on a square lattice of sites (i, j) by

$$E(\boldsymbol{\sigma}) = -\sum_{(i,j)} (H\sigma_{ij} + J\sigma_{ij}\sigma_{i-1,j} + J\sigma_{ij}\sigma_{i,j-1} + J'\sigma_{i-1,j}\sigma_{i,j-1} + J_3\sigma_{ij}\sigma_{i,j-1}\sigma_{i-1,j}). \tag{2}$$

The J and J' interactions define a triangular lattice with three-spin interactions J_3 on all triangles of one parity. The crystal growth model is defined by

$$P(\boldsymbol{\sigma}) = \prod_{(i,j)} P_{ij} \tag{3}$$

$$P_{ij} = \tfrac{1}{2} + \sigma_{ij}[\alpha - \tfrac{1}{2} + \beta(x_{i-1,j} + x_{i,j-1}) + \delta x_{i,j-1}x_{i-1,j}]. \tag{4}$$

Equation (4) corresponds to equation (1) of Welberry and Galbraith (1975) with $\beta = \gamma$. The occupation variables are

$$x_{ij} = \tfrac{1}{2}(\sigma_{ij} + 1) = 0 \qquad \text{or} \qquad 1. \tag{5}$$

The α, β, δ parameters are transformed to variables X, Y, Z as indicated in table 1. In crystal growth models the factors P_{ij} are interpreted as conditional probabilities of a site (i, j) having state σ_{ij} given the state of neighbours $(i-1, j)$ and $(i, j-1)$.

Table 1. The conditional probabilities P_{ij} for various spin configurations, expressed in two different parametrizations before the imposition of constraints (8a), (8b).

Spin configuration			Probability $P(\sigma_{ij}\|\sigma_{i-1,j}\sigma_{i,j-1}) = P_{ij}$	
(i, j)	$(i-1, j)$	$(i, j-1)$	Welberry and Galbraith	Present paper
1	1	1	$\alpha+2\beta+\delta$	X
−1	1	1	$1-\alpha-2\beta-\delta$	$1-X$
−1	−1	−1	$1-\alpha$	Z
1	−1	−1	α	$1-Z$
−1	1	−1	$1-\alpha-\beta$	Y
−1	−1	1	$1-\alpha-\beta$	Y
1	1	−1	$\alpha+\beta$	$1-Y$
1	−1	1	$\alpha+\beta$	$1-Y$

Enting has shown that (3), (4) is equivalent to (1), (2). Given the existence of an equivalence the transformation can be defined in terms of

$$\mu = \exp(-2H/kT) \tag{6a}$$

$$u = \exp(-2J/kT) \tag{6b}$$

$$v = \exp(-2J'/kT) \tag{6c}$$

$$w = \exp(-2J_3/kT) \tag{6d}$$

by evaluating $P(\boldsymbol{\sigma})$ for simple configurations of $-$ sites surrounded by a sea of $+$ sites. Dividing each expression by the probability of all sites being $+$ removes the need to evaluate Q in (1).

For one $-$ site:

$$\mu u^4 v^2 w^3 = (1-X)(1-Y)^2/X^3. \tag{7a}$$

For (i, j), $(i-1, j)-$:

$$\mu^2 u^6 v^4 w^4 = (1-X)Y(1-Y)^3/X^5. \tag{7b}$$

For $(i-1, j)$ and $(i, j-1)-$:

$$\mu^2 u^8 v^2 w^4 = (1-X)^2(1-Y)^2(1-Z)/X^5. \tag{7c}$$

For $(i-1, j)$, $(i, j-1)$ and $(i, j)-$:

$$\mu^3 u^8 v^4 w^7 = (1-X)^2(1-Y)^4 Z/X^7. \tag{7d}$$

To impose triangular lattice symmetry we require $J = J'$, i.e. $u = v$, or from (7*b*), (7*c*)

$$(1-X)(1-Z) = Y(1-Y) \tag{8a}$$

or in terms of the Welberry and Galbraith variables

$$-\alpha\delta = \beta - \beta^2. \tag{8b}$$

Equation (8*b*) is equivalent to the $\beta = \gamma$ case of equation (6) of Welberry and Galbraith (1975) defining their special case 1 (SC1). Thus for $\beta = \gamma$ imposing the SC1 constraint is equivalent to imposing triangular lattice symmetry on the corresponding triangular lattice Ising model. Equations (7*a*), (7*b*), (7*d*), (8*a*) define a surface in μ–u–w space, on which the multispin Ising model (2) is equivalent to a crystal growth model. This surface is sketched in figure 1.

3. Solutions for crystal growth models

The derivation of solutions starts from equation (4):

$$P_{ij} = \tfrac{1}{2} + (2x_{ij} - 1)[\alpha - \tfrac{1}{2} + \beta(x_{i-1,j} + x_{i,j-1}) + \delta x_{i-1,j}x_{i,j-1}]. \tag{4}$$

Now

$$\langle x_{ij}\rangle = \sum_{\text{configurations}} x_{ij} \prod_{(m,n)} P_{mn} \tag{9a}$$

$$= \sum\nolimits^{(1)} x_{ij} \prod\nolimits^{(1)} P_{mn} \tag{9b}$$

$$= \sum\nolimits^{(1)} x_{ij}P_{ij} \prod\nolimits^{(2)} P_{mn} \tag{9c}$$

$$= \sum\nolimits^{(2)} [\alpha + \beta(x_{i-1,j} + x_{i,j-1}) + \delta x_{i,j-1}x_{i-1,j}] \prod\nolimits^{(2)} P_{mn} \tag{9d}$$

$$= \alpha + \beta\langle x_{i-1,j}\rangle + \beta\langle x_{i,j-1}\rangle + \delta\langle x_{i,j-1}x_{i-1,j}\rangle. \tag{9e}$$

The product $\Pi_{(m,n)}$ is over all sites in the system; the sum $\Sigma^{(1)}$ and the product $\Pi^{(1)}$ include all sites (m, n) such that $m \leq i$; $n \leq j$, the sum being over all configurations of x_{mn} on these sites. The sum $\Sigma^{(2)}$ and product $\Pi^{(2)}$ exclude (i, j). Equation $(9b)$ follows from $(9a)$ because the terms removed are factors which are sums of probabilities, i.e. 1. Equation $(9d)$ follows from $(9c)$ since the case $x_{ij} = 0$ contributes zero to $\Sigma^{(1)}$. Equation $(9d)$ is a sum of terms having the same structure as equation $(9b)$ (with a shift of origin and inclusion of some additional P_{nm} that give factors of 1) and so $(9d)$ is itself a sum of expectations as indicated in $(9e)$.

Similarly, using $x_{mn}^2 = x_{mn}$,

$$\langle x_{i-1,j}x_{ij}\rangle = \alpha\langle x_{i-1,j}\rangle + \beta\langle x_{i-1,j}\rangle + \beta\langle x_{i-1,j}x_{i,j-1}\rangle + \delta\langle x_{i-1,j}x_{i,j-1}\rangle. \tag{10}$$

We now wish to compare stationary solutions of triangular symmetry for growth models and the multispin Ising model of equation (2). This comparison can be made in a naive manner without considering what type of limiting process is actually needed to achieve a stationary distribution. For a stationary distribution

$$\langle x_{ij}\rangle = \langle x_{i-1,j}\rangle = \langle x_{i,j-1}\rangle = \theta. \tag{11}$$

For triangular lattice symmetry we require

$$-\alpha\delta = \beta - \beta^2 \tag{8b}$$

so that

$$\langle x_{ij}x_{i-1,j}\rangle = \langle x_{ij}x_{i,j-1}\rangle = \langle x_{i-1,j}x_{i,j-1}\rangle = \phi. \tag{12}$$

Thus

$$\alpha = \theta(1-2\beta) - \phi\delta \tag{13a}$$

$$0 = \theta(\alpha+\beta) + \phi(\beta+\delta-1). \tag{13b}$$

Eliminating ϕ, δ from $(8b)$, $(13a)$, $(13b)$ gives

$$\theta = \alpha/(1-\beta) \tag{14a}$$

$$\phi = \theta^2 \tag{14b}$$

as found by Welberry and Galbraith (1975).

It should be noted that equations $(9e)$ and (10) can only be solved in this manner if we impose triangular lattice symmetric by use of constraint $(8b)$. The technique used by Welberry and Galbraith (1975) also required the use of constraint $(8b)$ for reasons that appear to be connected with the property $\phi = \theta^2$ leading to distributions on one diagonal being characterized only by θ, rather than using any symmetry.

Simulations performed by Welberry and Galbraith indicate that all two-site correlations 'decouple' to be equal to θ^2. This conjecture is confirmed by the series expressions for susceptibility considered in the following section which indicate

$$\chi = 4\sum_{\text{sites}} (\langle x_{00}x_{ij}\rangle - \theta^2) = 4(\theta - \theta^2) \tag{15}$$

since the only contribution comes from $(i, j) = (0, 0)$.

4. Constraints on Ising model series

Sykes and co-workers have given coefficients in the series expansions for the isotropic ($J' = J$) case of model (2). The reduced free energy has the form

$$-kT \ln \Lambda_{\mathrm{T}} = -kT \sum_{pqr} a_{pqr} \bar{\mu}^p \bar{\mu}^q \bar{w}^r \tag{16}$$

with

$$\bar{\mu} = \mu u^6 w^3 \tag{17a}$$

$$\bar{u} = u^{-2} w^{-2} \tag{17b}$$

$$\bar{w} = u^{-6} w^{-2}. \tag{17c}$$

The coefficients are actually quoted in the context of the alternative interpretation on the honeycomb lattice:

$$-kT \ln \Lambda_{\mathrm{H}} = -kT \sum_{pqr} a_{pqr} \mu^p (6p - q - 2r, 6p - 2q - 3p, p, q) \tag{18}$$

where the expressions (a, b, c, d) denote coded partial generating functions of the form $f_1^{-a} f_2^b f_3^c f_4^d$. The sum of terms with a common p value is denoted F_p.

The actual coefficients are given in I, III and IX. We have also calculated $a_{13,2,8} = 3$, $a_{13,1,8} = 6$, $a_{14,1,9} = 3$ and $a_{15,0,10} = 1$.

To compare series expansions with the exact solutions we need an appropriate pair of expansion variables x, y. One such pair is defined by

$$x = 1 - X \tag{19a}$$

$$y = Y/x \tag{19b}$$

so that constraint ($8a$) leads to

$$1 - Z = y(1 - xy). \tag{19c}$$

The expansion variables then become

$$\bar{\mu} = x(1 - xy)^2/(1 - x)^3 \tag{20a}$$

$$\bar{u} = y(1 - x)/(1 - xy) \tag{20b}$$

$$\bar{w}\bar{\mu} = (1 - y + xy^2)/(1 - x). \tag{20c}$$

The expressions that can be compared are

$$M = \langle \sigma_{ij} \rangle = 1 - 2 \sum_{pqr} p a_{pqr} \bar{\mu}^p \bar{u}^q \bar{w}^r$$

$$= 2\theta - 1 = (1 - x - xy)/(1 + x - xy) \tag{21}$$

$$\tau = \langle \sigma_{ij} \sigma_{i-1,j} \rangle = 1 - \tfrac{2}{3} \sum_{pqr} (6p - 2q + 6r) a_{pqr} \bar{\mu}^p \bar{u}^q \bar{w}^r = M^2 \tag{22}$$

$$\chi = \sum_{(m,n)} (\langle \sigma_{ij} \sigma_{mn} \rangle - M^2) = 4 \sum_{pqr} p^2 a_{pqr} \bar{\mu}^p \bar{u}^q \bar{w}^r$$

$$= 1 - M^2 \qquad \text{(conjected on the basis of simulation).} \tag{23}$$

The four coefficients given above together with 74 other coefficients from I, III, IX are sufficient to give M, τ, χ correct to order x^5 for all powers of y, when expressions (20a, b, c) are substituted into the series expansions in (21), (22), (23). The agreement gives a consistency check on the derivation of the Ising model coefficients and the growth model solutions. To order x^5 the conjecture that $\chi = 1 - M^2$ is confirmed. It is possible to replace x, y by other variables that lead to alternative groupings of the a_{pqr} coefficients.

When the exact solutions are expanded in powers of x and y, non-zero coefficients occur only when the exponent of y is less than or equal to the power of x so that up to order x^n there are $\frac{1}{2}(n+1)(n+2)$ coefficients that are generally non-zero. In addition to these $\frac{1}{2}(n+1)(n+2)$ constraints arising from each of the three exact solutions, the zero coefficients also represent constraints on the series since individual terms $a_{pqr}\bar{\mu}^p\bar{u}^q\bar{w}^r$ can have non-zero contributions to $x^n y^m$ with $m > n$ (for example $a_{10,0,6}$).

5. Conclusions

In the work of Welberry and Galbraith (1975), the special growth model (SC1) studied above was of comparatively little interest because all the two-site correlations 'decoupled' and so these models could not give any behaviour indicative of ordering in diffraction simulation studies. The SC1 model is however of considerable interest in connection with Ising model series since the constraints demonstrated above suggest several questions.

Firstly, is it possible to use such constraints in conjunction with the techniques of Sykes *et al* VII, VIII, IX? For this to be possible, the growth model constraints must be at least partly independent of the constraints used in IX. This question of independence cannot be easily answered.

Secondly, there is the possibility of these solutions leading to entirely new techniques of series derivation. Generally series expansions represent a perturbation about a special point such as $T = 0$ or $T = \infty$. The ability to calculate correlations means that in principle we can calculate perturbation expansions about all points on the surface shown in figure 1.

The occurrence of constraint (8b) as being necessary for the derivation of solutions by two rather different techniques remains puzzling since in one case the constraint represents a symmetry requirement while in the other case it appears to be the condition for decoupling described by (14b). As discussed by Enting (1977) the use of symmetry properties arises from the Ising model interpretation of the crystal growth models since the growth models themselves are formulated in terms that disguise lattice symmetries. Application of the Ising model viewpoint in the derivation of symmetries has led to solutions for growth models that had not been solved by other methods (T R Welberry, private communication).

References

Bartlett M S 1967 *J. R. Statist. Soc.* A **130** 457–74
—— 1968 *J. R. Statist. Soc.* A **131** 579–80
Enting I G 1977 *J. Phys. C: Solid St. Phys.* **10**
Sykes M F, Essam J W and Gaunt D S 1965 *J. Math. Phys.* **6** 283–98

Sykes M F, Gaunt D S, Essam J W and Hunter D L 1973a *J. Math. Phys.* **14** 1060–5
Sykes M F, Gaunt D S, Mattingly S R, Essam J W and Elliott C J 1973b *J. Math. Phys.* **14** 1066–70
Sykes M F, Gaunt D S, Martin J L, Mattingly S R and Essam J W 1973c *J. Math. Phys.* **14** 1071–4
Sykes M F, Watts M G and Gaunt D S 1975a *J. Phys. A: Math. Gen.* **8** 1441–7
—— 1975b *J. Phys. A: Math. Gen.* **8** 1448–60
Sykes M F, McKenzie S, Watts M G and Gaunt D S 1975c *J. Phys. A: Math. Gen.* **8** 1461–8
Welberry T R and Galbraith R 1973 *J. Appl. Cryst.* **6** 87–96
—— 1975 *J. Appl. Cryst.* **8** 636–44