GENERALISED ISING LATTICES

by

R. G. J. MILLS B.Sc. (Hons.)

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Department of Mathematical Physics,
University of Adelaide,
South Australia.

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CONTENTS.

SUMMARY

A general two dimensional Ising lattice with a periodic lattice cell structure in which there are f spins to each cell is considered. Each cell has 2^f states and an interaction energy between the states of neighbouring cells is defined in terms of the state of each cell. The conditions which the state of a cell must satisfy if the interaction energy is to be due to interactions between pairs of spins places certain restrictions on the state of the cell. It is found that the state of the cells must be invariant under total spin reversal. The interaction energy reduces to an expression which is quadratic in the spin variables and this allows the partition function to be transformed into a combinatorial problem in which there are single bonds between spins. However, due to the generality of the model considered, there are multiple bonds between cells and this feature distinguishes it from those previously solved.

The Pfaffian method of solving the combinatorial problem is valid only when the lattice is planar. This condition reduces the class of lattices which are exactly soluble and it is shown that the widest soluble class of lattices by this method corresponds to a triangulation of the lattice. The case of multiple bonds between cells is not precluded by this condition. The Pfaffian method is extended to solve this class of lattices and a method of expanding the resulting determinant in terms of weight factors associated with the cell is given. For a particular lattice the weight factors are easily calculated and the partition function can be written down immediately in terms

of these weight factors. It is shown how the known results for several lattices can be derived by this method. Then the method is used to illustrate how the weight factors can be found for a complicated cell with single bonds between cells. The partition functions and the critical condition of this lattice for varying bond weights are investigated. Finally a lattice with two spins to a cell and multiple bonds between cells is considered and the partition function is calculated.

In the latter part of the thesis the model proposed is compared to other generalised models. The model is found to include all other exactly soluble lattices with the exception of the lattices which contain arbitary spins considered by Fisher. However, Fisher shows how to transform his lattices into lattices which are contained in the model proposed. The conclusion is that the model proposed generates a new class of exactly soluble Ising lattices.

STATEMENT

This thesis contains no material which has been accepted for the award of any other degree or diploma in any University and to the best of my knowledge and belief, contains no material previously published or written by another person except where reference is made in the text of the thesis.

R. G. J. MILLS.

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CHAPTER 1

INTRODUCTION.

This work deals with a method of finding the partition function and investigating the critical behaviour of generalised Ising lattices. We shall restrict the discussion to two dimensional lattices and exact evaluations of the partition function. The aim is to describe the most general class of lattices which are exactly soluble. To carry out this aim it is necessary to give a more general discussion of the classification of Ising lattices than is customary and in particular to consider the conditions under which such lattices are soluble.

Interest in Ising lattices began in 1925 when Ising[1] formulated a model of a ferromagnet with a spin variable occupying two possible states at each point of the lattice. He found the partition function for the one dimensional case and showed that it did not have a transition point. Peierls[2] showed that the corresponding two dimensional lattice did have a transition point, which was subsequently located by Kramers and Wannier[3]. Onsager[4] evaluated the partition function and formed the critical temperature of the square lattice using an algebraic method. Following Onsager, the triangular and hexagonal[5,6,7], the Kagomé[8,9], the Yamamoto[10], and the Utijama[11] lattices were solved by the algebraic method. Kac and Ward[12] found the partition function for a square lattice by using a combinatorial method and Potts[13] investigated the triangular lattice using this method.

Fisher[14] has shown that a wide class of Ising lattices which are exactly soluble can be derived from the triangular lattice by means of the dual, decorating and star-triangle transformations.

In recent years[15,16] the combinatorial method has been simplified and made rigorous by the use of Pfaffians. Kasteleyn[17,18] has clarified the counting process by showing the relationship between the Ising problem and the Dimer problem. Hurst[19] has shown that the Pfaffian method is applicable to periodic Ising lattices provided they do not contain crossed bonds which is equivalent to the statement that the lattices are planar. Also Hurst[20] has classified plane Ising lattices and described the partition function and critical behaviour of a subclass of plane Ising lattices which includes all the above lattices except those derived by Fisher. In this work we show how the partition function and the critical behaviour of Hurst's full class of plane Ising lattices can be described.

The Ising problem can be formulated in terms of a cell structure. The region considered is divided into congruent cells and these cells are distributed at points whose position vector is

$$j_2\underset{\sim}{a} + j_1\underset{\sim}{b}$$

where j_1, j_2 are integers and $\underset{\sim}{a}$, $\underset{\sim}{b}$ are basis vectors. The cells are numbered from 1 to N = mn such that the cell in the j_1^{th} row and the j_2^{th} column is $(j_1 - 1)n + j_2$. Thus the model considered is an m × n array of N fixed cells which form a two dimensional lattice of N f spins where

f is the number of spins in each cell.

In the usual model[21] there is associated with each cell one spin variable σ_j ($j = 1, 2, \ldots N$) which is a scalar number that has two possible values +1 or -1 depending on whether it is in the +, up state or the -, down state. The 2^N states of the whole system can be specified by the set of N numbers $\{\sigma_j\}$ where $j = 1, 2, \ldots N$. Each spin is postulated to interact with its nearest neighbour spins in such a way that the preferred spin orientation in the ferromagnetic case is the parallel one. Thus the lowest energy state between nearest neighbour spins σ_i and σ_j is that in which they are parallel. The interaction energy between the i^{th} and the j^{th} cell is

$$E_{ij} = - J_{ij} \sigma_i \sigma_j \qquad (1.1)$$

The total energy of the system in the state specified by $\{\sigma_j\}$ is

$$E\{\sigma_j\} = - \Sigma J_{ij} \sigma_i \sigma_j \qquad (1.2)$$

where the sum is taken over all pairs of spins i and j that are nearest neighbours on the lattice. This expression implies that the ground state energy is $- \Sigma |J_{ij}|$ rather than zero. As the cells are all identical the J_{ij} depend on i-j only and if further the lattice is symmetric under inversions then J_{ij} depends on $|i - j|$ rather than i-j so there are $\frac{1}{2}qN$ terms in the sum where q is the number of nearest neighbours. The geometry of the lattice enters the problem through q and J_{ij}. Usually the lattice is periodic with period $q/2$ so there are at most $q/2$ independent J_{ij}. The partition function for the system is

$$Z(T, J_{ij}) = \sum_{\{\sigma_j = \pm 1\}} \exp(-\beta E\{\sigma_j\}) \qquad (1.3)$$

where there are 2^N terms in the summation and where $\beta = \frac{1}{kT}$ with T, the absolute temperature and k, Boltzmann's constant. The thermodynamic functions can be obtained in the usual manner from derivatives of the partition function.

The interaction energy (1.1) can be derived by an alternative method which we shall find useful later when the state of each cell depends on several spins. We denote the interaction energy between the i^{th} cell in the state σ_i and the j^{th} cell in the state σ_j by $E^{\sigma_i\sigma_j}$. The interaction energy between the i^{th} cell and j^{th} cell is postulated to be

$$\begin{aligned} E_{ij} = {} & \tfrac{1}{4} E^{++}(1 + \sigma_i)(1 + \sigma_j) \\ & + \tfrac{1}{4} E^{+-}(1 + \sigma_i)(1 - \sigma_j) \\ & + \tfrac{1}{4} E^{-+}(1 - \sigma_i)(1 + \sigma_j) \\ & + \tfrac{1}{4} E^{--}(1 - \sigma_i)(1 - \sigma_j) \end{aligned} \qquad (1.4)$$

$$\begin{aligned} = {} & \tfrac{1}{4}(E^{++} + E^{+-} + E^{-+} + E^{--}) \\ & + \tfrac{1}{4}(E^{++} + E^{+-} - E^{-+} - E^{--})\,\sigma_i \\ & + \tfrac{1}{4}(E^{++} - E^{+-} + E^{-+} - E^{--})\,\sigma_j \\ & + \tfrac{1}{4}(E^{++} - E^{+-} - E^{-+} + E^{--})\,\sigma_i\sigma_j \end{aligned}$$

If we now assume that the interaction energy is due to interactions between pairs of spins then we require only the quadratic term in (1.4). If the ++ and the -- are the preferred states then the condition

$$E^{++} = E^{--} = -E^{+-} = -E^{-+} = -J_{ij} \qquad (1.5)$$

reduces (1.4) to (1.1). Thus we see that the postulate (1.1) is equivalent to (1.4) plus the requirement that only terms quadratic in the spin variables are retained.

The methods of evaluating the partition function are either algebraic, or combinatorial. Recently Schultz[23] et al have simplified Onsager's algebraic approach by expressing the transfer operator from one row to the next as a product of exponents of quadratic forms in creation and annihilation fermion operators. Using a transformation that diagonalise the transfer operator they obtain Onsager's results. The combinatorial approach was first used by Kac and Ward but today the counting is done by means of Pfaffians. Hurst[22] has compared the two methods and shown that their range of application to exactly soluble lattices is the same. In this work we shall consider only the Pfaffian method.

It is well known[26] that the transformation

$$\exp K_{ij}\,\sigma_i\sigma_j = \cosh K_{ij}(1 + x_{ij}\,\sigma_i\sigma_j) \qquad (1.6)$$

where $x_{ij} = \tanh K_{ij}$ with $K_{ij} = \beta J_{ij}$, reduces the partition function (1.3) to the combinatorial problem

$$Z = (\cosh K_1 \ \ldots \ \cosh K_{q/2})^N \sum_H \ldots \sum_V g(H, D, \ldots, V) x_1^H \ \ldots \ x_{q/2}^V \qquad (1.7)$$

where $g(H, D, \ldots, V)$ is the number of closed polygons which can be drawn on the lattice with H bonds of the type x_1, D bonds of the type x_2, ..., and V bonds of the type $x_{q/2}$.

Hurst and Green[15] were the first to solve this combinatorial

problem by a Pfaffian method. They represent the bonds between cells as the creation of a particle at one cell and its annihilation at the other cell. The generating function for closed polygons on the lattice

$$Z_1 = \sum_H \cdots \sum_V g(H, \ldots, V) x_1^H \cdots x_{q/2}^V \qquad (1.8)$$

is then compared with the expression

$$Z' = (\Omega, \prod_{j=1}^{N} P_j(a)\, \Omega) \qquad (1.9)$$

where $P_j(a)$ is the operator polynomial of the j^{th} cell in the creation and annihilation operators a* and a and Ω is the vacuum state for all operators. They show that Z_1 and Z' are equivalent if the operators are boson operators since onl terms which pair together remain when the expectation value is taken and hence only closed polygons survive. However, for (1.9) to be evaluated as a Pfaffian it is necessary that the operators be fermion operators, and that $P_j(a)$ be factorized into a product of linear fermion operators. They show that, provided the lattice is planar, q terminals can be introduced to each cell and internal operators can be defined such that the Pfaffian correctly counts the closed polygons. If the lattice is non-planar the Pfaffian method breaks down due to negative signs appearing in (1.9).

Kasteleyn[17] has shown that the counting of closed polygons on an Ising lattice is related to the distribution of dimers on an associated dimer lattice. There is a one to one correspondence between the configurations of dimers and the terms of a Pfaffian and all dimers are correctly counted if

the lattice is planar. Although a one to one correspondence does not exist between the closed polygons on an Ising lattice and the configuration of dimers on a dimer lattice, Kastelyn has shown that the elements of the Pfaffian can be assigned to count correctly the closed polygons provided the lattice is planar. The sign of the elements of the Pfaffian are determined once the dimer lattice has been orientated.

The Ising problem has been extended to lattices in which there is more than one spin to each cell. The hexagonal and the Yamamoto lattices are examples in which there are two spins to each cell. Hurst[20] has classified Ising lattices according to the number of spins to each cell and has found the partition function for planar lattices with single bonds between cells. He considers a periodic two dimensional lattice and classifies each spin of the lattice according to the bond connections to the spin. All the spins with the same bond connections form a set $\{P\}$ and due to the periodic nature of the lattice there is a finite number of such sets $\{P_1\}$, $\{P_2\}$, ..., $\{P_f\}$. The spins of the i^{th} set are located at points given by

$$\underset{\sim}{P}_i = j_2\underset{\sim}{a} + j_1\underset{\sim}{b} + \underset{\sim}{c}_i$$

where j_1, j_2 are integers and $\underset{\sim}{a}$, $\underset{\sim}{b}$ are vectors such that $\underset{\sim}{a}$ is the smallest vector with the period of the lattice and $\underset{\sim}{b}$ is the smallest vector non-parallel to $\underset{\sim}{a}$ and $\underset{\sim}{c}_i$ is the vector from the origin to the point of the set $\{P_i\}$ with $j_1 = j_2 = 0$. For particular values of j_1 and j_2 the f spins form a cell of the lattice. Thus the original lattice with interactions between spins which did not all have the same

bond connections has been transformed to a lattice with interactions between cells all of which have the same bond connections. In this work a "generalised lattice" refers to a m × n array of cells each of which contains f spins and all cells have the same bond interactions.

In chapter 2 we consider a model in which there are f spins to each cell. Each cell has 2^f states and we define an interaction energy between the states of neighbouring cells. We investigate the conditions which we must impose on the interaction energy between states for the interaction to give rise to a combinatorial problem which the Pfaffian method of solution can handle. The condition that the interaction energy is quadratic in the spin variables gives rise to a combinatorial problem in which there are only single bonds between spins. A necessary condition for this is that the interaction energy between states is invariant under total spin reversal. Although only single bonds exist between spins it is found that multiple bonds exist between cells and these are the characteristic feature of the generalised lattices. Then we consider the application of the Pfaffian method to the solution of the generalised lattices. Although Kastelyn's method leads more directly to the Pfaffian than the method of Hurst and Green, the latter method is preferred, since the elements of the Pfaffian can be found by a general method. The application of the Pfaffian method requires the lattice to be planar and this condition restricts the class of generalised lattices which are exactly soluble by

the Pfaffian method. We find that a necessary condition that the generalised lattices be planar is that the maximum number of bonds associated with each cell be equal or less than 3f. The soluble lattices with the greatest number of bonds correspond to a triangulation of the lattice. Multiple bonds exist between the cells of the lattice even when the lattice is planar.

In the third chapter we apply the Pfaffian method to the evaluation of the partition function and this gives rise to an anti-hermitian determinant. A general method is given for the expansion of this determinant in terms of certain weight factors which are associated with the cell. In principle the partition function for the generalised lattice can be written down immediately the bond connections to a cell are given and the weight factors calculated.

In chapter 4 we first show how the established results for the Yamamoto hexagonal and triangular lattice can be obtained by our method. Then we investigate the behaviour of a lattice whose cells contain a large number of spins. This is an extension of the lattices with single bonds between cells which have been considered by Hurst.[20] Finally we consider a lattice with multiple bonds between cells.

In the final chapter the relationship between the model proposed in this thesis and other generalised models is considered. Domb[27] has suggested a model with general S having 2S + 1 states to each cell. This model gives rise

to a combinatorial problem in which there are multiple bonds between cells and no exact solution is possible. We find that our model also breaks down when the condition that the interaction energy be due to interactions between pairs of spins is removed since the combinatorial problem then has multiple point interactions. Green[25] has considered a model similar to ours in which there are f spins to each cell but he restricts his lattices to single bonds between cells. We show his lattices to be a subset of our generalised lattices. Potts[28] has derived the critical temperature for a four state model and we show how his result may be obtained by our method. Fisher[14] has derived Ising lattices from known lattices by means of the dual, decorating and star triangle transformations. We show that Fisher's derived lattices can be solved by our method but our most general lattices cannot be derived from known lattices because of the complexity of the bond weights. Also, Fisher solves exactly the partition function for lattices decorated with arbitary spins by transforming the lattice into a simpler lattice. Although the decorated lattice cannot be solved by our method the transformed lattice can.

CHAPTER 2

A MULTIPLE STATE MODEL.

In this chapter we consider a model in which there are f spins to each cell of the lattice. Similar models have been considered indirectly and directly by other authors.[20,25] We have seen in chapter 1 that such a model naturally arises in the classification of periodic two dimensional Ising lattices by Hurst. He solves the hexagonal lattice by considering a cell which contains two spins. Green[25] has also formulated a model in which there are f spins to each cell. His aim in introducing more than one spin variable to represent the configuration of a cell is to consider a wider range of order-disorder phenomena than the theory of magnetism. The spin variables serve only to distinguish the different states of the lattice and need not necessarily represent electronic spin. In a physical situation where the number of states is at all large, more than one spin variable will be needed and for this reason more complicated lattices are of interest. All of these remarks apply equally to the model considered in this chapter. We compare Green's development of the model to our own in chapter 5.

2.1. Interaction energy for 2^f states to each Cell.

Each spin of the system can occupy two states and is represented by a scalar spin variable σ which has values +1 or -1 according to whether it is in the up or the down state respectively. We consider a model in which there are f spins to each cell so there are 2^f states for each

cell. The state of the i^{th} cell is represented by the co-ordinates $\sigma_{i_1}, \sigma_{i_2}, \ldots, \sigma_{i_f}$ or by the projection operators

$$\omega_i^{(k)} = \frac{1}{2^f}(1 \pm \sigma_{i_1})(1 \pm \sigma_{i_2}) \ldots (1 \pm \sigma_{i_f}) \qquad (2.1)$$

where the $\pm$ signs are chosen according to the state k of the cell and $k = 1, 2, \ldots, 2^f$. The energy of interaction between the i^{th} cell and the j^{th} cell is defined to be

$$E_{ij} = \sum_{k=1}^{2^f} \sum_{l=1}^{2^f} \omega_i^{(k)} E^{\sigma_{i_1}\sigma_{i_2} \ldots \sigma_{i_f},\sigma_{j_1}\sigma_{j_2} \ldots \sigma_{j_f}} \omega_j^{(l)} \qquad (2.2)$$

The projection operators ensure that the energy is in the appropriate state. The state of the whole lattice is represented by the co-ordinates σ_{i_r} where $i = 1, 2, \ldots, N$ and $r = 1, 2, \ldots, f$ or by $\omega_i^{(k)}$ where $i = 1, 2, \ldots, N$ and $k = 1, 2, \ldots, 2^f$. We consider interactions only between nearest neighbour cells so that the energy of a particular state of the lattice is

$$E = \sum_i (E_{i\,i+1} + E_{i\,i+n+1} + E_{i\,i+n}) \qquad (2.3)$$

To obtain the partition function we sum over all states of the lattice to obtain

$$Z = \sum_{\omega_1} \ldots \sum_{\omega_N} \exp(-\beta E) \qquad (2.4)$$

where the summations are over the 2^f states of each cell.

The expression (2.2) for the interaction energy between cells is a generalisation of the expression (1.4) to the case of f spins to a cell. If (2.1) is substituted into (2.2) and the expression rearranged in terms of the σ's,

then the interaction energy between cells can be written as

$$E_{ij} = -\sum_{a=0}^{1}\sum_{b=0}^{1}\cdots\sum_{g=0}^{1} J_{ij}^{(ab..c,de..g)}\sigma_{i_1}^{a}\sigma_{i_2}^{b}\cdots\sigma_{i_f}^{c}\sigma_{j_1}^{d}\sigma_{j_2}^{e}\cdots\sigma_{j_f}^{g}$$

where $\sigma^0 = 1$, and

$$J_{ij}^{(ab..c,de..g)} = \frac{1}{4^f}\sum_{k=1}^{2^f}\sum_{l=1}^{2^f}(-1)^P E^{(\sigma_{i_1}\sigma_{i_2}..\sigma_{i_f},\sigma_{j_1}\sigma_{j_2}..\sigma_{j_f})} \tag{2.5}$$

with $P = 1 + \frac{1}{2}a(1 - \sigma_{i_1}) + \frac{1}{2}b(1 - \sigma_{i_2}) + \ldots + \frac{1}{2}g(1 - \sigma_{j_f})$.

In the next section we shall consider the conditions the J_{ij} must satisfy if the partition function is to transform to a combinatorial problem. We note that any restrictions imposed upon J_{ij} will also place restriction on the interaction energies between the states of the cells.

The consistency of the 2^f state model can be demonstrated by showing that the four state model reduces to the two state model if the +- and the -+ states are removed from every cell of the lattice. The partition function (2.4), which is the sum of 2^{fN} terms will not contain contributions from those states if we allow the interaction energy between cells in the unwanted states to become infinite. It is not sufficient to make the interaction energies zero as the states could still exist on the lattice. For f = 2 the partition function is

$$Z = \sum_{\sigma_{i_1}=\pm 1}\cdots\sum_{\sigma_{N_2}=\pm 1}\exp\left\{-\beta\sum_{i=1}^{N}\sum_{j=\begin{cases} i+1 \\ i+n+1 \\ i+n \end{cases}} E_{ij}\right\}$$

where the interaction energy between the i^{th} and j^{th} cell has 16 terms.

$$E_{ij} = \tfrac{1}{4}(1 + \sigma_{i_1})(1 + \sigma_{i_2})E^{++,++}\ \tfrac{1}{4}(1 + \sigma_{j_1})(1 + \sigma_{j_2})$$
$$+ \tfrac{1}{4}(1 + \sigma_{i_1})(1 + \sigma_{i_2})E^{++,+-}\ \tfrac{1}{4}(1 + \sigma_{j_1})(1 - \sigma_{j_2})$$
$$+ \ldots\ldots\ldots\ldots\ldots$$
$$+ \tfrac{1}{4}(1 - \sigma_{i_1})(1 - \sigma_{i_2})\ E^{--,--}\ \tfrac{1}{4}(1 - \sigma_{j_1})(1 - \sigma_{j_2})$$

Allowing $E^{++,+-}$, $E^{++,-+}$, $E^{+-,++}$, $E^{-+,++}$, $E^{--,+-}$, $E^{--,-+}$, $E^{+-,--}$, $E^{-+,--}$ to become infinite after the summation has been taken is the same as limiting the summation to $\sigma_{i_1}\sigma_{i_2} = +1$. In this case

$$Z = \sum_{\sigma_{i_1}\sigma_{i_2} = 1} \exp(-\beta \sum_i \sum_j E_{ij})$$

where

$$E_{ij} = \tfrac{1}{4}(1 + \sigma_{i_1})(1 + \sigma_{i_2})\ E^{++,++}\ \tfrac{1}{4}(1 + \sigma_{j_1})(1 + \sigma_{j_2})$$
$$+ \tfrac{1}{4}(1 + \sigma_{i_1})(1 + \sigma_{i_2})\ E^{++,--}\ \tfrac{1}{4}(1 - \sigma_{j_1})(1 - \sigma_{j_2})$$
$$+ \tfrac{1}{4}(1 - \sigma_{i_1})(1 - \sigma_{i_2})\ E^{--,++}\ \tfrac{1}{4}(1 + \sigma_{j_1})(1 + \sigma_{j_2})$$
$$+ \tfrac{1}{4}(1 - \sigma_{i_1})(1 - \sigma_{i_2})\ E^{--,--}\ \tfrac{1}{4}(1 - \sigma_{j_1})(1 - \sigma_{j_2})$$

If we define

$$\delta_j = \tfrac{1}{4}\{(1 + \sigma_{i_1})(1 + \sigma_{i_2}) - (1 - \sigma_{i_1})(1 - \sigma_{i_2})\}$$
$$= \tfrac{1}{2}(\sigma_{i_1} + \sigma_{i_2})$$

then δ_j has values ± 1 and the interaction energy is

$$E_{ij} = \tfrac{1}{16}(E^{++,++} + E^{++,--} + E^{--,++} + E^{--,--})$$
$$+ \tfrac{1}{16}(E^{++.++} + E^{++,--} - E^{--,++} - E^{--,--})4\ \delta_i$$
$$+ \tfrac{1}{16}(E^{++,++} - E^{++,--} + E^{--,++} - E^{--,--})4\ \delta_j$$
$$+ \tfrac{1}{16}(E^{++,++} - E^{++,--} - E^{--,++} + E^{--,--})4\ \delta_i\delta_j$$

corresponding to (1.4) for the two state model, when we make the transformation

$$E^{\sigma_{i_1}\sigma_{i_2},\sigma_{j_1}\sigma_{j_2}} = E^{\delta_i,\delta_j}$$

2.2 Reduction to a Combinatorial Problem.

We have seen in Chapter 1 that the transformation (1.6) gives rise to single bonds between spins when the exponent is a quadratic expression in the spin variables. If we attempt to generalise this transformation to an arbitrary product of spin variables then using $\sigma_i^2 = 1$ we obtain

$$\exp K \sigma_{i_1}\sigma_{i_2} \cdots \sigma_{j_f} = \cosh K + \sigma_{i_1}\sigma_{i_2} \cdots \sigma_{j_f} \sinh K$$
$$= \cosh K(1 + x\, \sigma_{i_1}\sigma_{i_2} \cdots \sigma_{j_f}) \quad (2.6)$$

where $x = \tanh K$. However, x can no longer be interpreted as a bond representing the interaction between a pair of spins, but rather as a multiple point interaction between all the spins in the product. When the summation over the states of the lattice is performed only the terms in which all the σ's have an even exponent are non-zero. This means that each spin must take part in an even number of multiple point interactions. This combinatorial problem is beyond the scope of present methods and we are restricted to interactions between pairs of spins. We now investigate the conditions which this restriction places on the interaction energies between the states of the i^{th} and j^{th} cell.

The condition that only interactions between pairs of spins are allowed means that (2.5) must be a quadratic function of the spin variables.

$$E_{ij} = -\sum_{k=1}^{f}\sum_{l=1}^{f} J_{ij}^{(kl)}\sigma_{i_k}\sigma_{j_l} - \sum_{k=l} J_{ii}^{(kl)}\sigma_{i_k}\sigma_{i_l} - \sum_{k=l} J_{jj}^{(kl)}\sigma_{j_k}\sigma_{j_l} \tag{2.7}$$

where J_{ij}^{kl} is the energy of interaction between the k spin in the i^{th} and the l^{th} spin in the j^{th} cell, and $J_{ii}^{(kl)}$ is the interaction energy between the k^{th} spin and the l^{th} spin in the i^{th} cell. The set of 4^f equations relating the interaction between spins to the interactions between the states of cell in (2.5) can be solved giving

$$E^{(\sigma_{i_1}\sigma_{i_2}\cdots\sigma_{i_f},\sigma_{j_1}\sigma_{j_2}\cdots\sigma_{j_f})} = \sum_{a=0}\sum_{b=0}\cdots\sum_{g=0}(-)^P J_{ij}^{(ab..c,de..g)} \tag{2.8}$$

where P is again given by (2.5). Since all except the quadratic terms are zero then (2.8) becomes

$$E^{(\sigma_{i_1}\sigma_{i_2}\cdots\sigma_{i_f},\sigma_{j_1}\sigma_{j_2}\cdots\sigma_{j_f})} = \sum_{a+b+..+g=2}(-)^P J_{ij}^{(ab..c,de..g)} \tag{2.9}$$

showing that only $\binom{2^f}{2}$ of the interaction energies between the states of the cells are independent in this case.

If all the spins are reversed then

$$E^{(-\sigma_{i_1} - \sigma_{i_2} \cdots -\sigma_{i_f},-\sigma_{j_1} - \sigma_{j_2} \cdots -\sigma_{j_f})} = \sum_{a+b+\ldots+g=2}(-)^{P'} J^{(ab..c,de..g)}$$

where $P' = 1 + \frac{1}{2}a(1 + \sigma_{i_1}) + \frac{1}{2}b(1 + \sigma_{i_2}) + \ldots + \frac{1}{2}g(1 + \sigma_{j_f})$

Now

$$P - P' = \tfrac{1}{2}a(1 + \sigma_{i_1} - 1 + \sigma_{i_1}) + \ldots + \tfrac{1}{2}g(1 + \sigma_{j_f} - 1 + \sigma_{j_f})$$

$$= a\,\sigma_{i_1} + b\,\sigma_{i_2} + \ldots + g\,\sigma_{j_f}$$

$$= \pm 1 \quad \pm 1$$

$$= 0 \pmod 2$$

since only two of the set a, b, .., g can occur and

$\sigma_i = \pm 1$. Thus $E(-\sigma_{i_1} - \sigma_{i_2} \cdots -\sigma_{j_f}) = E(\sigma_{i_1}\sigma_{i_2} \cdots \sigma_{j_f})$ (2.10)

This means that the interaction energy between the states of the i^{th} and j^{th} cells is invariant under total spin reversal.

The energy of a particular state of the lattice when interactions are allowed only between nearest neighbour cells and when the interaction energy between cells quadratic in the spin variables is found by substituting (2.7) in (2.3) giving

$$E = -\sum_i \Big\{ \sum_k \sum_l J^{(kl)}_{ii+1}\, \sigma_{i_k}\sigma_{(i+1)_l} + \sum_k \sum_l J^{(kl)}_{ii+n+1}\, \sigma_{i_k}\sigma_{(i+n+1)_l} + \sum_k \sum_l J^{(kl)}_{ii+n}\, \sigma_{i_k}\sigma_{(i+n)_l} + 6 \sum_{k\neq l} J^{(kl)}_{ii}\, \sigma_{i_k}\sigma_{i_l} \Big\} \qquad (2.11)$$

where we have put $J^{(kl)}_{ii} = J^{(kl)}_{i+1\, i+1} = J^{(kl)}_{i+n+1\, i+n+1} = J^{(kl)}_{i+n\, i+n}$ since all the cells are congruent. Using the transformation (1.6) we have

$$\exp(-\beta E) = \prod_{i=1}^{N} \Big\{ \Big\{ \prod_{\substack{j = i+1 \\ i+n}}^{i+n+1} \prod_k^f \prod_l^f \cosh K^{(kl)}_{ij} \,(1 + x^{(kl)}_{ij}\sigma_{i_k}\sigma_{j_l}) \Big\} \times \Big\{ \prod_{\substack{k=1 \\ k\neq l}}^{f} \prod_{l=1}^{f} \cosh K^{kl}_{ii}\,(1 + x^{(kl)}_{ii}\,\sigma_{i_k}\sigma_{i_l}) \Big\} \Big\} \qquad (2.12)$$

where $K^{(kl)}_{ij} = \beta\, J^{(kl)}_{ij}$, $x^{(kl)}_{ij} = \tanh K^{(kl)}_{ij}$, and $K^{(kl)}_{ii} = 6\,\beta\, J^{(kl)}_{ii}$. The $x^{(kl)}_{ij}$ represent bonds between the k^{th} spin of the i^{th} cell and the l^{th} spin of the j^{th} cell and will be called external bonds. The $x^{(kl)}_{ii}$ represent the bonds between the k^{th} and l^{th} spins of the i^{th} cell and

will be called internal bonds. If we assume that $J_{ij}^{(kl)}$ depends upon k, l and |i - j| then there are three classes of external bonds given by |i - j| = 1, n + 1, n. These bonds will be called horizontal, diagonal, and vertical and the maximum number of each type will be denoted by h, d, and v respectively. Since no restriction has been placed on the interactions between the spins of neighbouring cells, each spin of a particular cell can interact with every spin of the same cell and the six neighbouring cells. Thus the maximum number of bonds entering and leaving a cell in a given direction is f^2 and the number of internal bonds is $\binom{f}{2}$. Since all the cells are congruent, the bonds entering a cell must be the same type as those leaving the cell. Thus the maximum number of external bonds associated with a cell of f spins is $3f^2$.

When the sum over the states of the cells is taken in (2.12) the only non-vanishing terms are those in which an even number of bonds are connected to each spin of the lattice because $\Sigma\, \sigma_{i_k}^{\text{odd}} = 0$ and $\Sigma\, \sigma_{i_k}^{\text{even}} = 1$. Therefore the partition function is

$$Z = C\, Z_1$$

$$Z_1 = \sum_H \sum_D \sum_V \sum_I y(H, D, V, I) x_{1_1}^{H_1} x_{1_2}^{H_2} \cdots x_{6_{\binom{f}{2}}}^{I_{\binom{f}{2}}} \qquad (2.13)$$

where C is a product of the $\cosh K_{ij}^{(kl)}$. The g(H, D, V, I) is the number of closed polygons which can be drawn on the lattice with H_1 bonds of the type x_1, ..., V_{f^2} bonds of the type x_{f^2}, and $I_{\binom{f}{2}}$ bonds of

the type $x_o{}_{\binom{f}{2}}$. Thus the evaluation of the partition function has become a combinatorial problem.

We now replace each cell of the lattice by a group of 2(h + d + v) terminals labelled according to the following convention.

(1) Terminals labelled from 1 to h, which connect horizontal bonds entering the j^{th} cell from the $j - 1^{th}$ cell.

(2) Terminals labelled from h + 1 to h + d, which connect diagonal bonds entering the j^{th} cell from the $j - n - 1^{th}$ cell.

(3) Terminals labelled from h + d + 1 to h + d + v = g, which connect vertical bonds entering the j^{th} cell from j - n.

(4) Terminals labelled from g + 1 to g + h, which connect horizontal bonds leaving the j^{th} cell for the $j + 1^{th}$ cell.

(5) Terminals labelled from g + h + 1 to g + h + d, which connect diagonal bonds leaving the j^{th} cell for the $j + n + 1^{th}$ cell.

(6) Terminals labelled from g + h + d + 1 to 2g, which connect vertical bonds leaving the j^{th} cell for the $j + n^{th}$ cell.

The ordering of the terminals is as shown in Fig. 2.1 for f = 2.

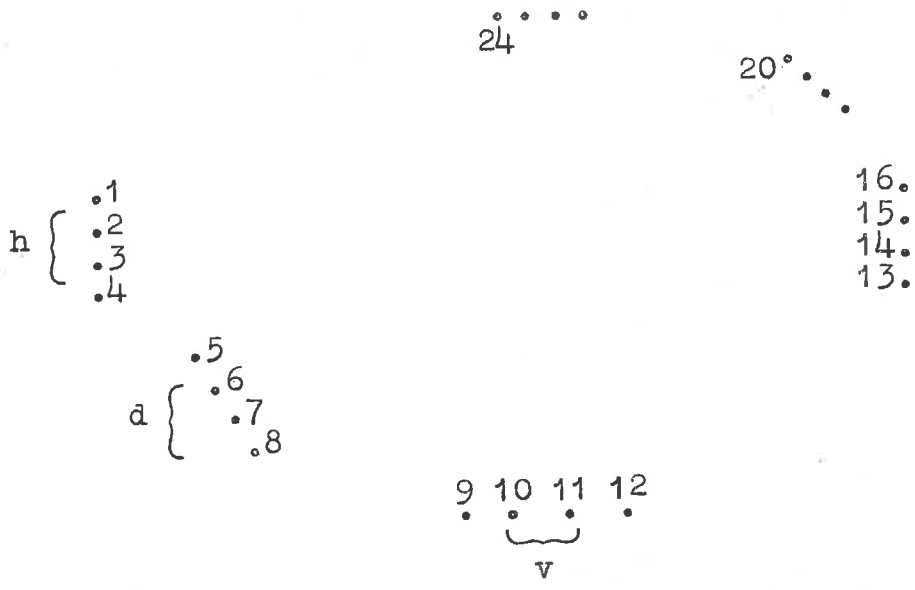


Fig. 2.1

The external bonds can be labelled according to the terminal to which they connect out of the set {1, 2, ..., g}. The assumption that $J_{ij}^{(kl)}$ depends on |i - j| implies that the bond labelled i entering the j^{th} cell from a given direction must also leave the cell in the same direction. We define the terminals from which the i^{th} bond leaves the cell by i' where

$$\begin{aligned} i' &= g + h - i + 1 && \text{if} \quad 1 \leqslant i \leqslant h \\ i' &= g + 2h + d - i + 1 && \text{if } h + 1 \leqslant i \leqslant h + d \\ i' &= g + 2h + 2d + v - i + 1 && \text{if } h + d + 1 \leqslant i \leqslant g \end{aligned} \qquad (2.14)$$

We say that i' is the associated terminal of i.

With the external bonds labelled according to the convention described above the internal bonds can be incorporated in terms of weight factors. We denote by $c_{rst...w}$ the cell weight factor corresponding to the set of diagrams which can be constructed on the cell with the spins connected to the terminals rst...w and among

themselves by internal bonds in such a way that there are an even number of bonds connected to each spin of the cell. The weight factors are functions of the internal bond weights $x_0^{(kl)}$. Because we are concerned only with an even number of bonds connected to each cell then there will always be an even number of terminals rst...w associated with the weight factors. The weight factors have the property that they count the number of paths through the cell consistent with the external bond connections. The usefulness of the weight factor is due to the fact that all the cells are congruent and hence the weight factors are the same for all cells. This means that we need concern ourselves with the external bonds only. Following Hurst and Green[16] we represent the external bonds between cells as the creation of a particle at a terminal of one cell and its annihilation at a terminal of the neighbouring cell. In this way a cell polynomial $P_j(a)$ can be defined which represents all possible bond connections to the cell.

$$P_j(a) = \sum_c \sum c_{rs\ldots w}\, a_r\, a_s \ldots a_w \qquad (2.15)$$

where the first summation is over all even numbers of external bonds connected to the cell and the second summation is over the internal weight factors consistent with the external bond connections. If $r > g$ then a_r is the creation operator a_i^* while if $r < g$ it is an annihilition operator for a_{i-1}, a_{i-n-1}, or a_{i-n}.

Consider the expression

$$Z' = (\Omega, \prod_{i=1}^{N} P_i(a)\ \Omega) \qquad (2.16)$$

where Ω is the vacuum expectation of all operators. When the expectation value is taken the non-zero terms will be those in which all the creation and annihilation operators pair together. From the construction of $P_i(a)$ the non-zero terms will correspond to closed polygons drawn on the lattice. If the operators are boson operators which commute then all the terms in (2.16) will be positive and the polygons will be counted with the correct sign and (2.16) will be the same as (2.13). However, to evaluate (2.16) as a Pfaffian it is necessary that the operators be fermion operators which anti-commute, and hence all the terms of (2.16) may not be positive. It has been shown[16] that all the terms are positive if the lattice is planar. Thus the next condition which we place on the energy is that it gives rise to planar lattices. In the next section we shall consider the limitations which have to be placed on the bonds and hence on the energies if the lattice is to be planar.

2.3 Classification of Planar lattices.

Since the cells of the lattice are congruent, we can classify the lattices according to the bond connections to each cell. We denote the class of lattices such that each cell has f spins, h horizontal bonds, d diagonal bonds, v vertical bonds, and i internal bonds by (f, h, d, v, i).

A planar graph is one in which bonds meet only where spins are located. We have seen that for interactions between nearest neighbour cells the maximum value of h, d and v is f^2 while that of i is $\frac{1}{2}f(f-1)$. Clearly for $f \geq 2$ such a lattice will have bonds crossing at points other than where spins are located and therefore will be non-planar.

We now show that a necessary (but not sufficient) condition for the lattice to be planar is that

$$h + d + v + i \leq 3f. \tag{2.23}$$

For a planar graph[24] we have the Euler formula

$$V + F = E + 2, \text{ and} \tag{2.24}$$

$$3F \leq 2E, \tag{2.25}$$

where F, E, and V are the number of faces edges and vertices respectively. For a generalised lattice with free edge connections in the limit of large N

$$V \to Nf, \text{ and}$$

$$E \to N\,\tfrac{1}{2}(2h + 2d + 2v + 2i)$$

Combining (2.24) and (2.25), F can be eliminated to give

$$E + 6 \leq 3V$$

Thus in the limit of large m and n we have

$$h + d + v + i \leq 3f$$

if the lattice is to be planar. The condition is not sufficient as the lattice (2, 4, 0, 1, 1) of Fig. 2.2 has crossed bonds in the horizontal direction.

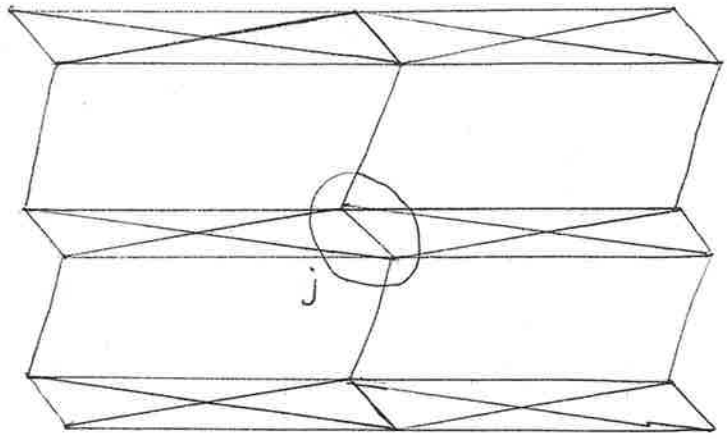
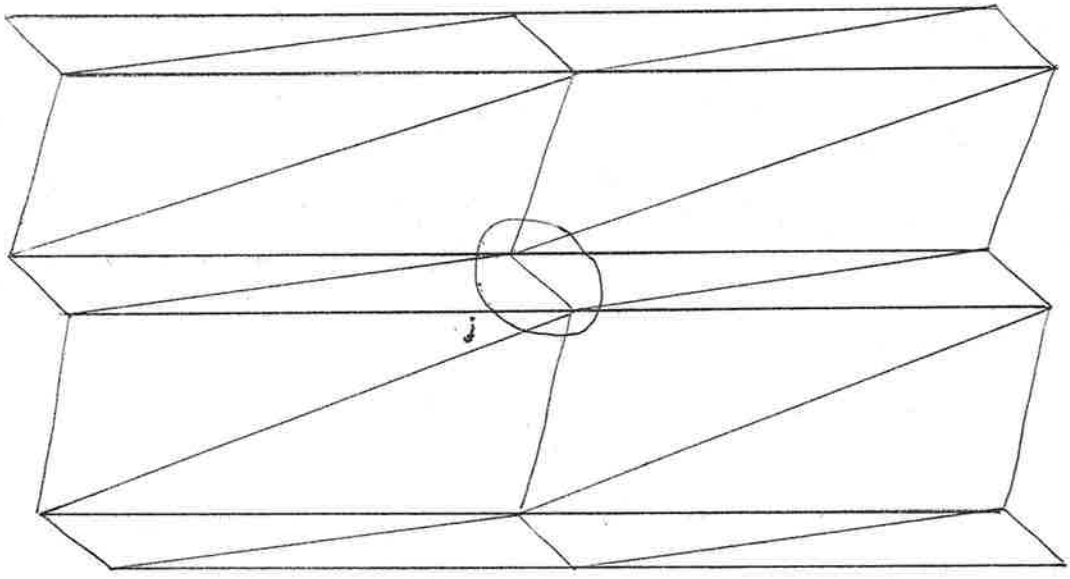


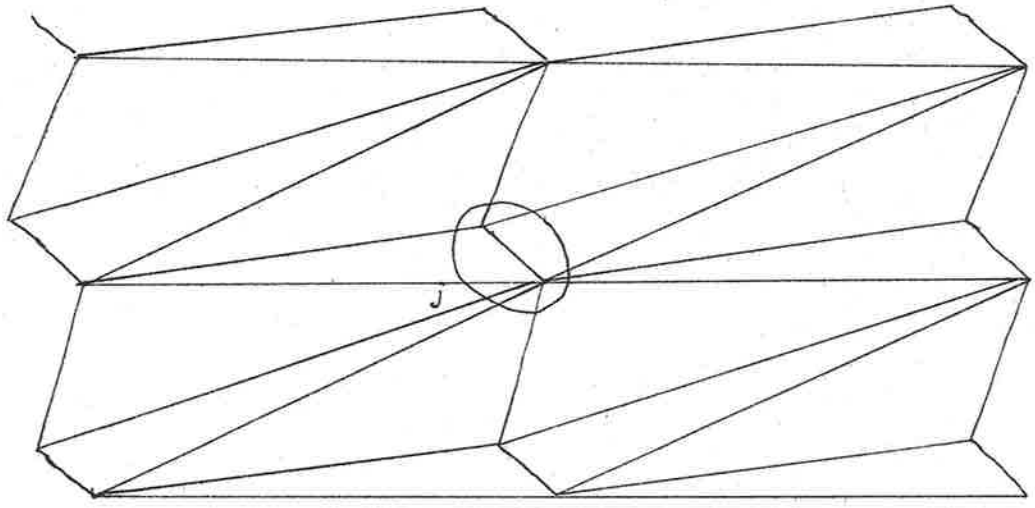
Fig. 2.2 (2, 4, 0, 1, 1)

In Fig. 2.3, some of the planar lattices for f = 2 in which h + d + v + i = 6 are illustrated. It can be seen that these cases correspond to a triangulation of the lattice, since the number of bonds associated with each cell of the lattice is 2h + 2d + 2v + i = 6f - i, and this is the number of bonds when f spins each with 6 nearest neighbours are grouped together. It should, however, be noted that a particular spin may have more than 6 nearest neighbours as shown in (2, 2, 2, 1, 1) for example. Although the lattice (2, 2, 2, 2, 0) appears to have crossed bonds there is no internal bond and it is planar. This lattice is the superposition of two non-interacting triangular lattices.

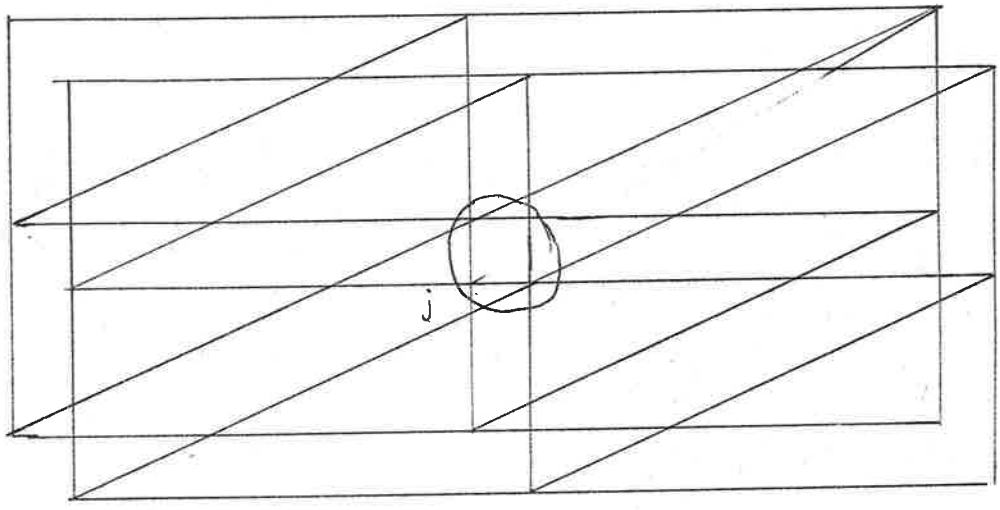
The main characteristic of the multiple state model is that it gives rise to multiple bonds between cells. The number of different bonds which can exist on a planar lattice with f spins to each cell is 3f and the maximum number of bonds in any given direction is 2f - 1. In the next chapter we see how the partition function for such lattices can be evaluated.



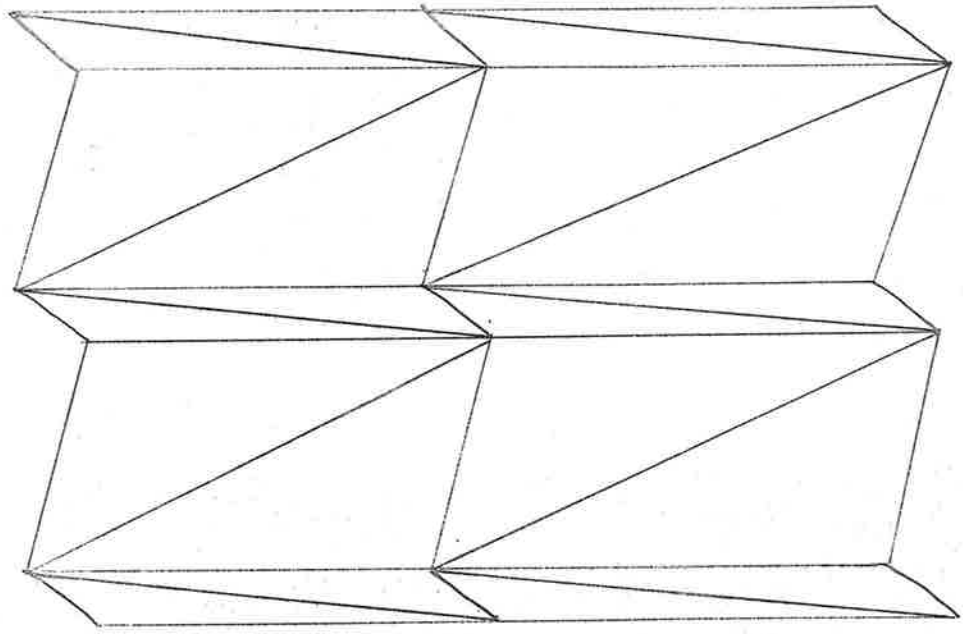
(a) (2, 3, 1, 1, 1)



(b) (2, 2, 2, 1, 1)



(c) (2, 2, 2, 2, 0)



(d) (2, 3, 1, 1, 1)

Fig. 2.3

There is a distinction between the triangular (1, 1, 1, 1, 0) lattice with equal bonds and the (2, 3, 1, 1, 1) lattice shown in Fig. 2.3(a) with all the bonds equal. In appearance they are alike, but the former has 2 states to a cell and single bonds between cells while the latter has 4 states to a cell and multiple bonds between cells. The partition function will be different for each lattice as can be seen by putting all the bonds equal in equation (4.5). The determinant does not reduce to that of a triangular lattice. This distinction is shown in that both Figs. 2.3(a) and (d) are examples of the (2, 3, 1, 1, 1) class of lattices.

CHAPTER 3

SOLUTION OF GENERALISED PLANAR LATTICES BY THE PFAFFIAN METHOD.

3.1 REDUCTION OF THE PARTITION FUNCTION TO A PFAFFIAN.

In this section we shall solve the combinatorial problem of counting closed polygons on the planar lattices of section 2.3 by using the Pfaffian method of Hurst and Green[16]. The essential step needed to evaluate (2.16) as a Pfaffian is the factorization of $P_j(a)$ into a product of linear fermion operators. This is done by introducing internal operators b_{jt} which represent bonds connecting the $2g = 2(h + d + v)$ terminals of the cell. We then write (2.16) as

$$Z' = (\Omega, \prod_{i=1}^{N} \prod_{j=1}^{2g} A_i^{(j)} \Omega)$$

where

$$A_i^{(j)} = \sum_{t=1}^{2g} (b_{jt} + x_j a_j) \qquad (3.1)$$

and Ω is the vacuum state of both the internal and external operators. Hurst[19] has shown that this step is only possible if the weight factors of the cell polynomial (2.15) satisfy the so called consistency conditions. The notation introduced above for the weight factors is most convenient when considering the external bonds to a cell, but for subsequent work it is better to define new coefficients which represent internal connections within a cell. Thus we define

$$C_{ab..h} = C_{rst..w} \qquad (3.2)$$

where a, b, c, .., h is that subset of the 2g terminals which is complementary (in the set theoretical sense) to the subset r, s, t, .., w. In terms of the new coefficients the consistency conditions are

$$(C_{ab..d})^{\nu - \mu - 1} C_{ab..h} = \left| C_{ab..dij} \right| \qquad (3.3)$$

where $C_{ab..h}$ is a coefficient with 2ν indices, $C_{ab..d}$ is a coefficient with 2μ indices which are a subset of the set ab..h, and $C_{ab..dij}$ are coefficients with $2(\mu + 1)$ indices. These indices are restricted by the inequalities $a < b < c < d < i < j < .. < h$, and the Pfaffian on the right hand side of (3.3) is of order $2(\nu - \mu)$. It is formed by taking all pairs of indices i and j which satisfy the above inequalities. The definition and some of the important properties of Pfaffians are given in appendix A.

The expression (3.1) can be written as a Pfaffian by using Wick's theorem, which expresses the product of linear fermion operators as a series of normal products with pairings. The only non-zero terms on taking the expectation value are those with gN pairings and this corresponds to an element of a Pfaffian of order 2gN. Thus

$$Z' = P = \left| P^{(pq)}_{ij} \right|$$

where the non-zero elements of the Pfaffian are

$$\begin{aligned}
P^{(pq)}_{ii} &= \Delta_{pq} = b_{pq} b^{*}_{pq} = (-)^{p+q-1} C_{pq} \\
P^{(pq)}_{ii+1} &= -x^{(p)}_{1} \delta_{qp'} \quad \text{for} \quad 1 \leq p \leq h \\
P^{(pq)}_{ii+n+1} &= -x^{(p)}_{n+1} \delta_{qp'} \quad \text{for} \quad h < p \leq h + d \\
P^{(pq)}_{ii+n} &= -x^{(p)}_{n} \delta_{qp'} \quad \text{for} \quad h + d < p \leq g
\end{aligned} \qquad (3.4)$$

The i, j range from 1 to N with i < j and the p, q range from 1 to 2g with p < q.

The usual method[16] of evaluating the Pfaffian is to write it as the square root of the corresponding antisymmetric determinant and evaluate the determinant as the product of its eigenvalues. One assumes a cyclic boundary condition and the determinant reduces to the product of N determinants of order 2g. Taking the logarithm and replacing the resulting summation by a double integral as m and n are large we have

$$N^{-1} \log Z' = \frac{1}{4\pi^2} \int_0^{2\pi} d\theta \int_0^{2\pi} d\phi \log \Delta(e^{i\theta}, e^{i\phi})$$

where $\Delta = C_o^2 \Delta'$ is a determinant of order 2g with elements

$$\Delta'_{ij} = A_{ij} + \Gamma_{ij}$$

where $A_{ij} = -A_{ji} = (-)^{i+j-1} C'_{ij}$

and $\Gamma_{ij} = -\Gamma^*_{ji}$

$$\begin{aligned} &= -x_i e^{i\theta} \delta_{ji'} && \text{for} \quad 1 \leq i \leq h \\ &= -x_i e^{i(\theta+\phi)} \delta_{ji'} && \text{for} \quad h < i \leq h+d \\ &= -x_i e^{i\phi} \delta_{ji'} && \text{for} \quad h+d < i \leq g \end{aligned} \tag{3.5}$$

for $i < j$, $C'_{ij} = C_{ij}/C_o$

and $\delta_{ji'} \begin{cases} 1 \text{ if } j = i' \\ 0 \text{ otherwise} \end{cases}$ *where i' is the associated label of i*

The bond weights have been redefined such that $x_i = x_1^i$ for for $1 \leq i < h$ and $x_i = x_{n+1}^{(i)}$ for $h < i \leq h+d$ and $x_i = x_n^{(i)}$ for $h+d < i \leq g$.

The determinant can be written so that all the C'_{ij} have

a positive sign factor by using $C_{ij} = -C_{ji}$ for $i > j$ and then multiplying the odd columns and the even rows by -1 giving

$$\Delta = C_0^2 \left| C'_{ij} + (-)^{P'} x_i e^{i\psi} \delta_{ji'} \right|$$

$$\text{where } P' = \begin{cases} i + i' & \text{if } i < j \\ i + i' - 1 & \text{if } i > j \end{cases} \qquad (3.6)$$

and ψ is the appropriate angle given in (3.5).

The consistency of the model on changing from a lattice of the type (f, h, d, v, i) to a lattice of the the type (f, h - 1, d, v, i) by removing one of allowed bond connections will now be demonstrated. For the (2, 3, 1, 1, 1) lattice shown in fig. 3.1 the weight factors can be calculated by connecting an even number of external and internal bonds to the spins. We find

$C_0 = C_{12} = C_{18} = C_{19} = C_{110} = x_0$,

$C_{13} = C_{14} = C_{15} = C_{16} = C_{17} = 1$, etc. and the elements of the determinant are given by $C'_{ij} = C_{ij}/C_0$.

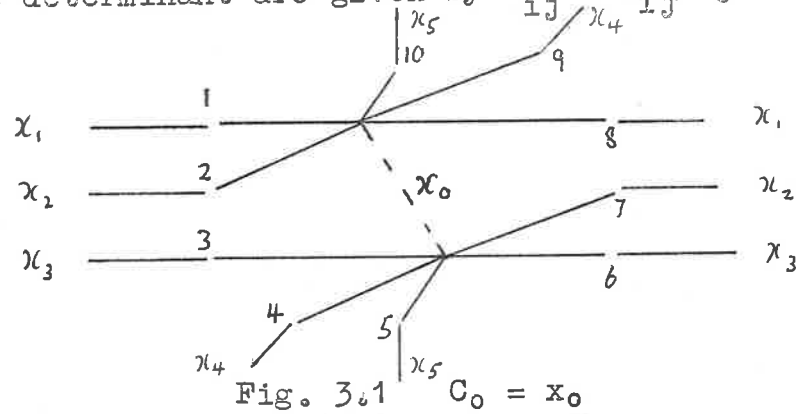


Fig. 3.1 $C_0 = x_0$

For the lattice (2, 2, 1, 1, 1) obtained by putting $x_2 = 0$ we have from Fig. (3.2) that $C_0 = C_{16} = C_{17} = C_{18} = 1$, $C_{12} = C_{13} = C_{14} = C_{15} = x_0$, etc. We wish to show that on removing a bond and reordering the lattice

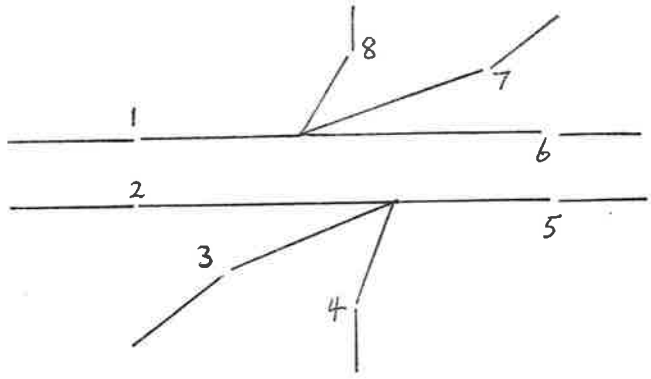


Fig. 3.2 $C_o = 1$

terminals, the determinant Δ is consistent. If we remove an external bond from the lattice by putting $x_a = 0$ then the a, a' rows and columns of determinant are antisymmetric. For definiteness we choose a from the set $\{1, 2, \ldots, h\}$. By using the element $C'_{aa'}$ as a pivot the determinant can be reduced to a determinant of order $2g - 2$ whose elements are Pfaffians of order 4 by the method given in appendix A, equation (A.6). Thus (3.6) becomes

$$\Delta = C_o^2 (C'_{aa'})^{4-2g} \begin{vmatrix} C'_{aa'} & C'_{aj} & C'_{ia} \\ & C'_{a'j} & C'_{ia'} \\ & & C'_{ij} + (-)^{P'} x_i \delta_{ji'} e^{i\psi} \end{vmatrix}$$

where the indices i, j range over 1, 2, ..., 2g excluding a, a'. The Pfaffian elements of the determinant can be expanded and the consistency condition (3.3) then gives

$$\Delta = C_o^2 (C'_{aa'})^{4-2g} \left| C'_{aa'ij} + (-)^{P'} x_i \, C'_{aa'} \, \delta_{ji'} \, e^{i\psi} \right|$$

$$= C_o^2 \, C_o^{2g-4} (C_{aa'})^{4-2g} C_o^{2-2g} \left| C_{aa'ij} + (-)^{P'} x_i C_{aa'} \delta_{ji'} e^{i\psi} \right|$$

$$= (C_{aa'})^2 \left| \frac{C_{aa'ij}}{C_{aa'}} + (-)^{P'} x_i \, \delta_{ji'} \, e^{i\psi} \right|$$

Since $C_{aa'}$ is the weight factor for the set of diagrams, which can be drawn on (f, h, d, v, i) when a, a' are

not connected, this corresponds to C_o for the lattice (f, h - 1, d, v, i). Therefore we define

$$D'_{k\,1} = \frac{D_{kl}}{D_o} = \frac{C_{aa'ij}}{C_{aa'}} \qquad (3.7)$$

and reorder the lattice terminals by changing the complement of {a, a'} to {1, 2, ..., g - 2}. In the new ordering

$$\Delta = D_o^2 \left| D_{kl} + (-)^{P' + Q'} x_k \, \delta_{lk'} \, e^{i\psi} \right|$$

where Q' is the sign change to x_i on reordering. In appendix B we show that $P' + Q' = k + k'$ for $k < l$ and so establish the consistency of the model.

3.2 EXPANSION OF THE DETERMINANT IN TERMS OF THE WEIGHT FACTORS.

In this section we show how the determinant (3.6) can be expanded as a compact expression which is quadratic in the weight factors. From equation (3.5) it can be seen that Δ is the determinant of a matrix which is the sum of a real antisymmetric and an antihermitian matrix. The latter matrix is such that all elements above the main diagonal have row indices which range from 1 to g and column indices which range from g + 1 to 2g. Hence the row and column indices of Γ_{ij} for i < j form disjunct sets. Furthermore because Δ is an even order antihermitian determinant, it is a real number. Hence the phase factors can only contribute to Δ in the form $\cos(p\theta + q\phi)$ where $-(h + d) \leq p \leq (h + d)$ and $-(d + v) \leq q \leq (d + v)$. For the moment we shall put

$(\theta + \phi) = \chi$ and consider the coefficient of

$$\exp i\{(p_1 - q_1)\theta + (p_2 - q_2)\chi + (p_3 - q_3)\phi\}$$

with $0 \leqslant p_1; q_1 \leqslant h$, $0 \leqslant p_2; q_2 \leqslant d$, $0 \leqslant p_3; q_3 \leqslant v$. The integers p_i define the number of phase factors of the various types which come from the portion of Δ above the diagonal whilst the numbers q_i give the number of phase factors which come from below the diagonal.

In order to evaluate the determinant we consider the coefficient of $x_1^{\alpha_1} x_2^{\alpha_1} \ldots x_g^{\alpha_g}$ where $0 \leqslant \alpha_i \leqslant 2$. Let $l_1, l_2, \ldots, l_n$ denote the indices i for which $\alpha_i = 2$; $i_1, i_2, \ldots, i_p$ denote the indices i corresponding to $\alpha_i = 1$ and a positive sign in the phase factor; $j_1, j_1, \ldots, j_q$ denote the indices i corresponding to $\alpha_i = 1$ and a negative sign in the phase factor; and $k_1, \ldots, k_m$ denote the indices i corresponding to $\alpha_i = 0$. All the indices satisfy the inequality $1 \leqslant l, i, j, k \leqslant g$ and associated with the indices are the associated indices l', i', j' and k' which satisfy $g < k', i', j', l' \leqslant 2g$. Let n_i, p_i, q_i and m_i denote the number of bonds selected such that $1 \leqslant n_1, p_1, q_1, m_1 \leqslant h$; $1 \leqslant n_2, p_2, q_2, m_2 \leqslant d$ and $1 \leqslant n_3, p_3, q_3, m_3 \leqslant v$. The required coefficient can be uniquely denoted by

$$D(l;i;j;k) = D(l_1,\ldots,l_n;\ i_1,\ldots,i_p;\ j_1,\ldots,j_q;\ k_1,\ldots,k_m) \tag{3.8}$$

and the determinant can be expanded as

$$\Delta = \sum_{p_i}\sum_{q_i}\sum_{m+n=g-p-q} \exp i\{(p_1 - q_1)\theta + (p_2 - q_2)\chi + (p_3 - q_3)\phi\}$$
$$x_1^{\alpha_1}, \ldots, x_g^{\alpha_g}\, D(l, i, j, k) \tag{3.9}$$

The coefficient (3.8) can be geometrically represented by a cluster of 2g terminals ordered from 1 to 2g as described in section 2.3. The labels denoted by 1 and 1' represent the bonds from one of the cells $j - 1$, $j - m - 1$, $j - m$ to j and from j to one of the cells $j + 1$, $j + m + 1$, $j + m$. The labels denoted by i are for bonds from j to one of $j + 1$, $j + m + 1$, $j + m$ while the labels j represent bonds from $j - m$, $j - m - 1$, $j - 1$ to j. The labels k and k' represent no bond connections to these points.

The first case to consider is the one for which $p_1 = h$, $p_2 = d$, $p_3 = v$ and $q_1 = q_2 = q_3 = 0$. Here $\alpha_1 = \alpha_2 = \ldots = \alpha_g = 1$ and $m = n = 0$ so that the coefficient of $x_1, x_2, \ldots, x_g$ is

$$D(0, 1, 2, \ldots, g; 0; 0)$$

$$= (-)^{S} C_0^2 \begin{vmatrix} C'_{1g+1} & C'_{2g+1} & & C'_{gg+1} \\ C'_{1g+2} & C'_{2g+2} & & C'_{gg+2} \\ & & & \\ C'_{12g} & C'_{22g} & & C'_{g2g} \end{vmatrix}$$

where $S = \frac{1}{2}h(h + 1) + \frac{1}{2}d(d + 1) + \frac{1}{2}v(v + 1)$.

The determinant (3.10) when expanded out gives a set of terms which are a subset of the terms when the Pfaffian of order 2g

$$(-)^{S + g - 1} C_0^2 \begin{vmatrix} C'_{12} & C'_{13} \cdots & C'_{1g+1} \cdots C'_{12g} \\ & & \vdots \quad\quad \vdots \\ & & C'_{gg+1} \cdots C'_{g2g} \\ & & \text{- - - - - - - - - -} \\ & & C'_{2g-1\,2g} \end{vmatrix} \qquad (3.11)$$

is expanded, and the terms containing any of the elements C'_{ab} with a, b both chosen from the set $\{i'\} = \{g + 1, \ldots, 2g\}$ are put equal to zero. The fact that the row and column indices of (3.10) form disjunct sets is essential for this to hold. From the consistency condition (3.3) and the definition of C'_{ij} it can be seen that the Pfaffian (3.11) is just $C_0^{-1}\, C_{12\ldots 2g}$ (apart from the sign factor $(-)^{S + \frac{g}{2}(g-1)}$) and any minor obtained by deleting the rows and columns r, s, t, ..., w is $(-)^P\, C_0^{-1}\, C_{ab\ldots h}$ where P is the parity of the permutation to arrange 1, 2, ..., 2g in the order r, s, t, ..., w, a, b, ..., h. Thus we find

$$D(0;\, 1, 2, \ldots, g;\, 0;\, 0)$$
$$= (-)^{S + \frac{g}{2}(g-1)}\, C_0 C_{12, \ldots, 2g} - \Sigma(-)^P C_{r's'}\, C_{ab, \ldots, h}$$
$$+ \Sigma\Sigma(-)^P C_{r's't'w'}\, C_{cd, \ldots, h} + \ldots\} \quad (3.12)$$

The indices r's't' ... w' are to be chosen from the set $\{i'\}$ and the indices a, b, ..., h are those remaining from the set $\{i, i'\}$ when the former are removed. The structure of (3.12) indicates what is to be expected in the general case.

In the general case the coefficient $D(1;\, i;\, j;\, k)$ is a determinant of order $2g - 2n - p - q = 2m + p + q$, which is obtained from Δ' by striking out the rows and columns containing the factors x_i appearing in the product $x_1^{\alpha_1}, \ldots, x_g^{\alpha_g}$. The striking out of the 2n rows and columns for which $\alpha_i = 2$ eliminates the 1_n, $1'_n$ indices from the determinant. The striking out of the p rows and columns above the diagonal and the q rows and columns below the diagonal for which $\alpha_i = 1$ removes an i, i', j, j'

index from the determinant. All indices occur twice in the original determinant so these indices are still present but only occur once. The rows of the determinant are labelled by j k k' i' and the columns by i k k' j' and from the manner of construction the sets {j, i'} and {i, j'} are disjunct. The rows and columns labelled by k, k' for which $\alpha_i = 0$ form a real anti-symmetric submatrix of D(1; i; j; k) and the determinant can be reduced with respect to these rows and columns by the method shown in appendix A, equation (A.6) and already used in section 3.1. The sign factor arising from these operations is discussed in appendix C. The determinant is first reduced to order 2n + p + q - 2 by selecting the lowest k_1 with $k_1 < k_1'$ such that both $C'_{kk'}$ and $C'_{k'k'}$ are present in the determinant.

$$D = (C_{k_1'k_1'})^{4 - 2m - p - q} C_o^2 \begin{vmatrix} C_{k'k'} & C_{k'j} & C'_{ik_1} \\ & C'_{k'j} & C'_{ik_1'} \\ & & C_{ij} \end{vmatrix} (-)^R \qquad (3.13)$$

$$= (-)^R (C'_{k_1k_1'})^{4 - 2m - p - q} C_o^2 \left| C'_{kk_1'ij} \right|$$

where R is the sign of the determinant on performing the operations described above. The consistency conditions have been used to write the Pfaffian elements in terms of a weight factor. The consistency conditions can be written in terms of the C' by dividing (3.3) through by $C_o^{\nu - \mu}$ giving

$$(C'_{ab,\ldots,d})^{\nu - \mu - 1} C'_{ab,\ldots,h} = \left| C'_{abdij} \right| \qquad (3.3)'$$

This reduction is repeated by selecting the lowest

$k_2 < k_2'$ such that $C'_{k_1 k_1' k_2 k_2'}$ and $C'_{k_1 k_1' k_2' k_2}$ are both present giving a determinant of order $2m + p + q - 4$.

$$D = (-)^R C_o^2 (C'_{k_1 k_1'})^{4 - 2m - p - q} (C_{k_1 k_1' k_2 k_2'})^{6 - 2m - p - q} \times \begin{vmatrix} C'_{k_1 k_1' k_2 k_2'} & C'_{k_1 k_1' k_2 j} & C'_{k_1 k_1' i k_2} \\ & C_{k_1 k_1' k_2' j} & C_{k_1 k_1' i k_2'} \\ & & C_{k_1 k_1' i j} \end{vmatrix}$$

The Pfaffian elements of the determinant can be written as $C'_{k_1 k_1'}\ C_{k_1 k_1' k_2 k_2' i j}$ by using the consistency conditions (3.3)' so that on cancellation of the $C'_{kk'}$ we have,

$$D = (-)^R C_o^2\ (C_{k k_1' k_2 k_2'})^{6 - 2m - p - q} \left| C_{k_1 k_1' k_2 k_2' i j} \right|$$

In like manner this reduction can be continued until all the anti-symmetric part of the determinant has been removed giving a determinant of order $p + q$ with the columns labelled by $\{i, j'\}$ and the rows labelled by $\{j, i'\}$ in numerical order.

$$D = (-)^R\ C_o^2\ (C'_{k_1 k_1' \ldots k_m k_m'})^{4 - 2m - p - q + 2m - 2} \times \left| C'_{k_1 k_1' \ldots k_m k_m' i j} \right|$$

In terms of the original weight factors

$$D = (-)^R\ (C_{k\ k' \ldots k_m k_m'})^{2 - (p + q)} \left| C_{k k' \ldots k_m k_m' i j} \right| \qquad (3.14)$$

From the manner in which the reduction has been performed we know that $k_1 < k_2 < k_3 \ldots < k_m$ and $k_i < k_i'$. We denote the indices $\{k, k'\}$ by $\underline{k}$.

As in the particular case considered above, the terms of the determinant of order $(p + q)$ form a subset of the terms of the Pfaffian of order $2(p + q)$

$$\backslash C_{\underline{k}'rs}|$$

where the indices r, s range over the combined set {i, j, i', j'}. Thus the determinant is equal to the Pfaffian, if the terms in the Pfaffian with both the indices r, s from the set {i, j'} are made zero. Thus

$$\begin{aligned} |C_{\underline{k}ij}| = (-1)^{T+Q}\Big\{ & \underset{2(p+q)}{\backslash C_{\underline{k}rs}|} \\ & - \Sigma \underset{2}{\backslash C_{\underline{k}ab}|} \underset{2(p+q-1)}{\backslash C_{\underline{k}rs}|} \\ & + \Sigma\Sigma \underset{4}{\backslash C_{\underline{k}ab}|} \underset{2(p+q-2)}{\backslash C_{\underline{k}rs}|} \\ & + \ldots\ldots\ldots\Big\} \end{aligned} \qquad (3.15)$$

where Q is parity of the permutation to combine the sets {ji'}{ij'} in numerical order, and where T is the difference in sign between the terms of the determinant and the terms of the Pfaffian $\backslash C_{k_1,\ldots,k'_m\ r\ s}|$. The summations are over the 0, 1, 2, ... pairs of indices a, b which can be selected from the set {i, j'}. By using the consistency conditions (3.3) the Pfaffian can be replaced by weight factors

$$\begin{aligned} \underset{2(p+q)}{\backslash C_{\underline{k}rs}|} &= C_{\underline{k}}^{p+q-1}\, \underset{2(m+p+q)}{C_{\underline{k}\{i,j,i',j'\}}} \\ \underset{2}{\backslash C_{\underline{k}ab}|}\ \underset{2(p+q-1)}{\backslash C_{\underline{k}rs}|} &= (-)^{P} C_{\underline{k}\{ab\}}\, C_{\underline{k}}^{p+q-2}\, \underset{2(m+p+q-1)}{C_{\underline{k}\{ab\}'}} \\ \underset{4}{\backslash C_{\underline{k}ab}|}\ \underset{2(p+q-1)}{\backslash C_{\underline{k}rs}|} &= (-)^{P} C_{\underline{k}}\, \underset{2(m+2)}{C_{\underline{k}\{abcd\}}}\, C_{\underline{k}}^{p+q-3}\, \underset{2(m+p+q-2)}{C_{\underline{k}\{abcd\}'}} \end{aligned} \qquad (3.16)$$

where the subscripts on the left hand side denote the order of the Pfaffian; the subscripts on the right hand side denote the number of indices in the weight factors; P is

the parity of the permutation to rearrange {a, b}, {a, b}' in numerical order; and { }' denotes the complementary set to { }. Finally we combine equations (3.14) and (3.15) and rearrange {$\underline{k}$jii'j'} in numerical order (sign factor Y) giving

$$D = (-)^{R+T+Q+Y}\Big\{C_{\{\underline{k}\}_N} C_{\{\underline{k},i,j,i'j'\}_N} - \Sigma(-)^P C_{\{\underline{k}ab\}_N} C_{\{\underline{k}\{ab\}'\}_N} + \Sigma(-)^P C_{\{\underline{k}abcd\}_N} C_{\{\underline{k}\{abcd\}'\}_N} + \ldots\Big\} \qquad (3.17)$$

where $\{\quad\}_N$ denotes the set to be in numerical order. The sign factors are discussed in appendix C where we show that

$$\begin{aligned} W = R + T + Q + Y = {} & \tfrac{1}{2}(p_1 + q_1)(2h - 2m_1 - p_1 - q_1) \\ & + \tfrac{1}{2}(p_2 + q_2)(2d - 2m_2 - p_2 - q_2) \\ & + \tfrac{1}{2}(p_3 + q_3)(2v - 2m_3 - p_3 - q_3) \\ & + \tfrac{1}{2}(p + q)(g - m - p - q) \end{aligned} \qquad (3.18)$$

when $p + q > 0$; $W = 0$ if $p = q = 0$. We note that the sign factor is symmetric in p_i and q_i as it should be.

If $p_1 = h$, $p_2 = d$, $p_3 = v$, $q_1 = q_2 = q_3 = 0$ then $W = S + \frac{g}{2}(g - 1)$ and (3.17) reduces to (3.12). Thus the coefficients of Δ have been reduced to quadratic expressions in the weight factors.

Equation (3.17) can be rewritten in terms of the original weight factors by using equation (3.2)

$$D = (-)^{W}\Big\{c_{\{l_n i_p j_q l'_n i'_p j'_q\}_N}\, c_{\{l_m l'_n\}_N} - \Sigma(-)^{P} c_{\{l,l'\{a,b\}'\}_N}\, c_{\{ll'ab\}_N} + \Sigma(-)^{P} c_{\{l,l'\{abcd\}'\}_N}\, c_{\{l,l',a,b,c,d\}_N}\Big\} \qquad (3.17)'$$

where

$$W = \tfrac{1}{2}(p_1 + q_1)(2n_1 + p_1 + q_1) + \tfrac{1}{2}(p_2 + q_2)(2n_2 + p_2 + q_2) + \tfrac{1}{2}(p_3 + q_3)(2n_3 + p_3 + q_3) + \tfrac{1}{2}(p + q)(2n + p + q) \qquad (3.18)'$$

The structure of (3.17)' can best be seen by giving a geometric representation. The terms on the right hand side can be represented by two clusters of 2g terminals labelled as in Fig. 2.1. The first term corresponds to all the terminals l_n, i_p, j_q, l'_n, i'_p, j'_q and l_n, l'_n being connected by external bonds in the first and second cluster respectively. The second term corresponds the terminals l, l', {a, b}' and l, l', a, b being connected by external bonds in the first and second cluster respectively. The second term differs from the first in that the terminals a, b are connected by external bonds in the second cluster rather than the first.

As an example we consider the lattice whose cell structure is given in Fig. 3.1. The coefficient of $x_1 x_2^2 x_3^0 x_4 x_5 \cos\{\theta - \chi + \phi\}$ is D(2;1,5;4;3) where $n_1 = 1$, $p_1 = 1$, $p_3 = 1$, $q_2 = 1$, and $m_1 = 1$. From equation (3.18)' the sign factor is

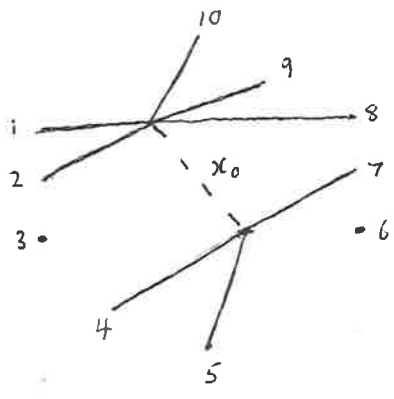
$W = \frac{1}{2}\,1.3 + \frac{1}{2}\,1.1 + \frac{1}{2}\,1.1 + \frac{1}{2}\,3.5$

which is even. Since $1' = 8$, $2' = 7$, $3' = 6$, $4' = 9$, $5' = 10$, equation (3.17)' becomes

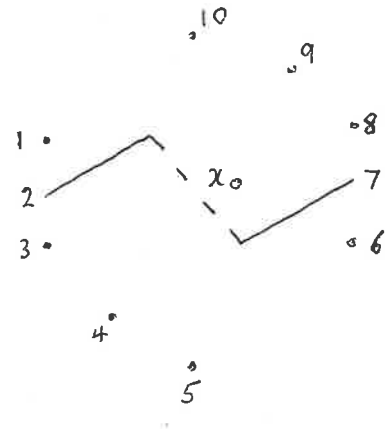
$$D(2;1,5;4;3) = +\left\{c_{124578910}\, c_{27} + c_{2478910}\, c_{1257} + c_{2457810}\, c_{1279} + c_{1247810}\, c_{2579}\right\}$$

where the signs of the second, third and fourth terms are positive because (489,10,15), (458,10,19), and (148,10,59) are odd permutations of (14589,10). The terms in the expansion of D(2;15;4;3) are illustrated in Fig. 3.3. It can be seen that

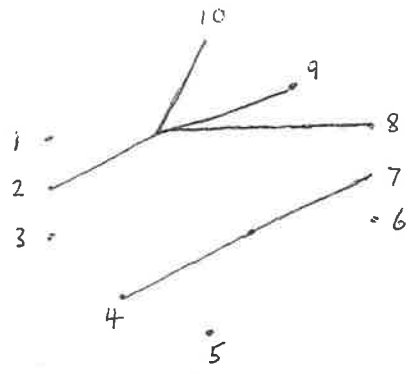
$$D(2;15;4;3) = 2(1 + x_0^2)$$



$c_{124578910} = x_0$

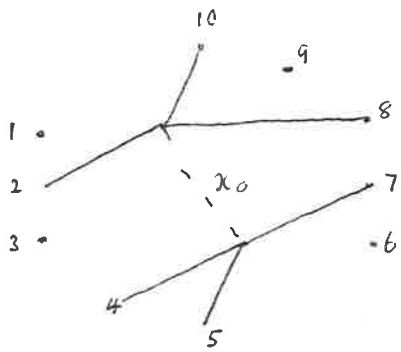


$c_{27} = x_0$

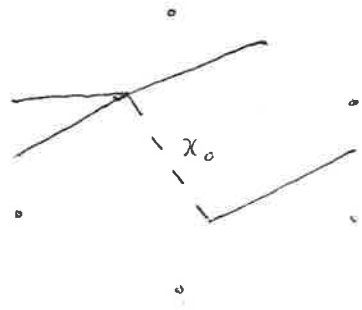


$c_{2478910} = 1$

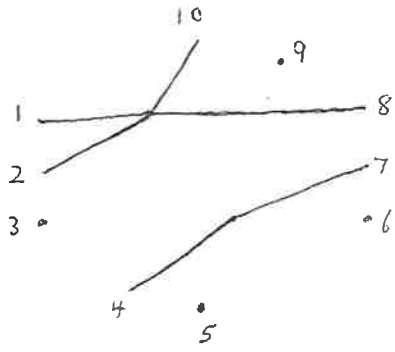
$c_{1257} = 1$



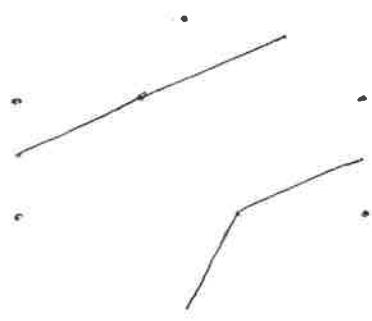
$c_{2457810} = x$



$c_{1279} = x_0$



$c_{1247810} = 1$



$c_{2579} = 1$

Fig. 3.3

The weight factors are found by connecting the external bonds to the spins in such a way that there are an even number of external and internal bonds to each spin. It can be seen that x_2 is always connected in both clusters whereas x_3 is never connected. The result of combining both clusters is a bond weight $x_1 x_2^2 x_4 x_5$.

Summing up we have that the determinant can be expanded as

$$\Delta = \sum_{m+n=g} D(l_n;0;0;k_m) x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_g^{\alpha_g}$$

$$+ \sum_{p\,q} \sum_{m+n=g-p-q} D(l_n;i_p;j_q k_m) x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_g^{\alpha_g}$$

$$\exp i\left\{(p_1 + p_2 - q_1 - q_2)\phi + (p_2 + p_3 - q_2 - q_3)\phi\right\} \qquad (3.19)$$

$$+ 2\sum_{p\,q} \sum_{p\ m+n=g-p-q} D(l_n;i_p;g_q;k_m) x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_g^{\alpha_g}$$

$$\cos\{(p_1 + p_2 - q_1 - q_2)\theta + (p_2 + p_3 - q_2 - q_3)\phi\}$$

where D is given by (3.17)'. The first summation is over the 2^g ways in which the bonds $x_1, \ldots, x_g$ can be separated into two groups $l_1, \ldots, l_n$ with $\alpha_i = 2$ and $k_1, \ldots, k_m$ with $\alpha_i = 0$. In the second summations the p bonds $i_1 \ldots i_p$ can be selected from above the diagonal in $\binom{g}{p}$ ways; the bonds $j_1 \ldots j_p$ can be selected from below the diagonal in $\binom{g-p}{p}$ ways; and the remaining g - 2p bonds can be separated into the $l_1 \ldots l_n$ and $k_1 \ldots k_m$ group in 2^{g-2p} ways. For a given selection $D(l_n;i_p;j_p;k_m)$ there is another selection $D(l_n;j_p;i_p;k_m)$ and these terms combine together to give a cosine term. The third summations is over the $\binom{g}{p}\binom{g-p}{q} 2^{g-p-q}$ ways in which $D(l_n;i_p;j_q;k_m)$ can be selected.

3.3 CRITICAL BEHAVIOUR OF THE MODEL.

The partition function, equation (3.5), is an analytic function of the bond weights and the temperature. For a given lattice the bond weights are fixed but the temperature can vary. The value of the temperature at which the partition function has a singularity is the critical temperature of the lattice. Thus the critical temperature can be found by investigating the position of the singularities of (3.5). Hurst[20] has shown that the integral in (3.5) is singular when the determinant Δ and its derivatives with respect to θ and ϕ vanish.

$$\begin{aligned} \Delta &= 0 \\ d\Delta/d\theta &= 0 \\ d\Delta/d\phi &= 0 \end{aligned} \qquad (3.20)$$

For the model considered by Hurst with only single bonds between cells, the second and third equations gave physical solutions when $\theta, \phi = 0, \pi$. All other solutions to the equations were found to be non-physical. When these values of θ and ϕ were substituted in the first equation, Hurst obtained four equations involving the bond weights and the temperature corresponding to the four different ways a singularity may occur at the end points of the range of integration.

In our model, where there are multiple bonds between cells, we have found, equation (3.19), that Δ is a sum of cosine terms in multiple angles of θ and ϕ, whose coefficients are functions of the bond weights and the temperature. Thus the derivatives of Δ with respect to θ

and ϕ will involve the sum of sine terms in multiple angles of θ and ϕ. Therefore the second and third equations of (3.20) will certainly be satisfied when $\theta, \phi = 0, \pi$. Other solutions to the second and third equations may exist but the fact that they were non-physical in the simpler model considered by Hurst suggests that they will be non-physical in our model also. We will confine our attention to the solution of the first equation of (3.20) for $\theta, \phi = 0, \pi$.

When $\theta = \phi = 0$ are substituted in (3.6) the determinant becomes

$$\Delta = C_0^2 \left| C'_{ij} + (-)^{P'} x_i \, \delta_{ji'} \right| \qquad (3.21)$$

since $e^{i\chi} = e^{-i\chi} = 1$ where $\chi = 0$. Since $P = i + i'$ if $i < j$ and $i + i' + 1$ if $i > j$ the determinant is anti-symmetric and hence it can be written as a Pfaffian.

$$\Delta^{\frac{1}{2}} = C_0 \left| C_{ij} + (-)^{i + i'} x_i \, \delta_{ji'} \right| \qquad (3.22)$$

This Pfaffian can be expanded as a sum of terms $x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_g^{\alpha_g}$ where $\alpha_i = 0, 1$. Let $i_1, \ldots i_{n_1}, i_{n_1 + 1} \ldots i_{n_1 + n_2}, i_{n_1 + n_2 + 1} \ldots i_{n_1 + n_2 + n_3}$ denote the indices for which $\alpha_i = 1$, where n_1 are chosen such that $1 \leqslant i \leqslant h$; n_2 are chosen such that $h < i \leqslant h + d$; n_3 are chosen such that $h + d < i \leqslant g$. Let the coefficient of $x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_g^{\alpha}$ be denoted by $P(i_1 \ldots i_n)$ where $n = n_1 + n_2 + n_3$. Then the required expansion is

$$\Delta^{\frac{1}{2}} = \sum_{\alpha_1 = 0} \ldots \sum_{\alpha_g = 0} P(i_1 \ldots i_2) \, x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_g^{\alpha_g} \qquad (3.23)$$

The coefficient $P(i_1 \ldots i_n)$ is the cofactor of the Pfaffian when the rows and columns containing the indices $i_1 \ldots i_n$ and their associated indices $i' \ldots i'_n$ are removed from the Pfaffian and the bonds weight for which $\alpha_i = 0$ are made zero. The cofactor itself is a Pfaffian of order $2(g - n)$ with elements C'_{ab}, whose rows and columns are labelled by the set of indices $\{i, i'\}'_N$ which is the complement of the set $\{i, i'\}$ in the set $\{1, 2, \ldots, 2g\}$.

$$P(i_1 \ldots i_n) = (-)^Q \, C_o \setminus C'_{ab}|$$

where Q is the sign factor to remove the bonds weights for which $\alpha_i = 1$.

By the consistency conditions (3.3)' the Pfaffian$\setminus C_{ab}|$ can be replaced by

$$(C'_o)^{g-n-1} C'_{\{i,i'\}'} = \left(\frac{C_o}{C_o}\right)^{g-n-1} \frac{C_{\{i,i'\}'_N}}{C_o}$$

From the relation (3.2) we have $C_{\{i,i'\}'_N} = C_{\{i,i'\}_N}$

so that

$$P(i_1 \ldots i_n) = (-)^Q \, C_{\{i,i'\}_N}$$

Thus the first equation of (3.20) for $\theta = \phi = 0$ is

$$\Delta^{\frac{1}{2}} = \sum_{\alpha_i = 0,1} (-)^Q \, C_{\{i,i'\}_N} \, x_1^{\alpha_1} \, x_2^{\alpha_2} \ldots x_g^{\alpha_g} = 0 \qquad (3.24)$$

In appendix D we show that

$$Q = n + n_1 n_2 + n_2 n_3 + n_1 n_3 \qquad (3.25)$$

The form of the determinant for the other values of θ and ϕ can be found from the case $\theta = \phi = 0$ by transformation of the bond weights. From the structure of the determinant in (3.5) we see that the change $\theta = 0$ to $\theta = \pi$ has the effect of changing x_i to $-x_i$ if $1 \leq i \leq h + d$.

Similarly the change $\phi = 0$ to $\phi = \pi$ has the effect of changing x_i to $-x_i$ if $h < i \leqslant g$. The sign transformation of the bond weights to obtain the equations for $\Delta = 0$ from the equation (3.24) is

$$T(x_i) = \begin{cases} -x_i \text{ if } 1 \leqslant i < h + d \text{ for } \theta = \pi, \phi = 0 \\ -x_i \text{ if } h < i \leqslant g \quad \text{for } \theta = 0 \ \phi = \pi \\ -x_i \text{ if } h < i \leqslant h + d \text{ for } \theta = \pi \ \phi = \pi \end{cases} \qquad (3.26)$$

As an example we shall show how this method can be applied to the triangular lattice (1, 1, 1, 1, 0) with one spin to each cell. For $\theta = \phi = 0$ the expression (3.22) is

$$\Delta^{\frac{1}{2}} = C_0 \backslash C'_{12} \quad C'_{13} \quad -C'_{14} - x_1 \quad C'_{15} \quad C'_{16} \;\Big|$$
$$C'_{23} \quad C'_{24} \quad C'_{25} - x_2 \quad C'_{26}$$
$$C'_{34} \quad C'_{35} \quad C'_{36} - x_3$$
$$C'_{45} \quad C'_{46}$$
$$C'_{56}$$

The coefficient of $x_1^0 \ x_2^0 \ x_3^0$ is found by putting $x_1 = x_2 = x_3 = 0$. The sign is positive since $\mathfrak{m} = 0$.

$$\therefore P(0) = C_0 \backslash C'_{12} \ C'_{23} \ C'_{34} \ C'_{45} \ C'_{56} \;\Big|$$

The consistency conditions (3.3)' can be used to reduce this Pfaffian of order C to a weight factor

$$\begin{aligned} P(0) &= C_0 (C'_0)^{3-1} \ C'_{123456} \\ &= C_{123456} \\ &= C_0 \end{aligned}$$

The coefficient of x_1 is obtained by putting $x_2 = x_3 = 0$ and removing the rows and columns containing the indices 1 and 4. A negative sign is produced because $\mathfrak{m} = \mathfrak{m}_1 = 1$.

$$P(1) = C_0(-1)\begin{vmatrix} C'_{23} & C'_{25} & C'_{26} \\ & C'_{35} & C'_{36} \\ & & C'_{56} \end{vmatrix}$$

$$= C_0\,(-1)\,(C'_0)^{2-1}\,C'_{2356}$$

$$= -C_{2356}$$

$$= -c_{14}$$

Again the consistency conditions have been used on the Pfaffian and then the relation (3.2). The coefficients of x_2 and x_3 can be found in like manner. The coefficient of x_1x_2 is found by putting $x_3 = 0$ and removing the rows and columns containing the indices 1245. The sign is negative since $\mathfrak{n} = 2$ and $\mathfrak{n}_1 = \mathfrak{n}_2 = 1$.

i.e. $$P(1,2) = C_0(-1)\begin{vmatrix} C'_{36} \end{vmatrix}$$

$$= -C_{36}$$

$$= -c_{1245}$$

The coefficients of x_1x_3 and x_2x_3 can be found in like manner. Finally the coefficient of $x_1x_2x_3$ removes all the rows and columns from the Pfaffian giving

$$P(1,2,3) = C_0(+1) = C_{123456}$$

The sign is positive since $\mathfrak{n} = 3$, $\mathfrak{n}_1 = \mathfrak{n}_2 = \mathfrak{n}_3 = 1$. Thus the critical equation for the triangular lattice for $\theta = \phi = 0$ is

$$c_0 - x_1c_{14} - x_2c_{25} - x_3c_{36} - x_1x_2c_{1245} - x_1x_3c_{1346} - x_2x_3c_{2356} + x_1x_2x_3c_{123456} = 0.$$

The critical equations corresponding to other values of θ and ϕ can be found by the transformation (3.26). For example the case $\theta = \pi$, $\phi = 0$ can be found by the transformation $x_1 \to -x_1$, $x_2 \to -x_2$ giving

$$c_0 + x_1c_{14} + x_2c_{25} - x_3c_{36} - x_1x_2c_{1245} + x_1x_3c_{1346} + x_2x_3c_{2356} + x_1x_2x_3c_{123456} = 0.$$

CHAPTER 4

SOME EXAMPLES OF GENERALISED LATTICES.

In this chapter we shall show how the partition function and critical equations for the class of lattices described in section 2.3, can be written down by using the results of the previous chapter. The power of the method lies in the fact that the calculations are straight forward although tedious. In general only the method of calculation will be given.

4.1 TWO SPINS TO A CELL.

We consider the lattice from the (2, 3, 1, 1, 1) class of lattices which is shown in Fig. 2.3 (a). This lattice has five external bonds and one internal bond. We replace the cell with two spins by a group of 10 terminals, one for each of the external bonds entering and leaving the cell. These terminals are labelled according to the convention shown in Fig. 2.1. The external bonds are labelled x_1, x_2, x_3, x_4, x_5, according to the terminal which they connect to of the set $\{1, 2, \ldots, 5\}$. The cell for this class of lattices is shown in Fig. 4.1.

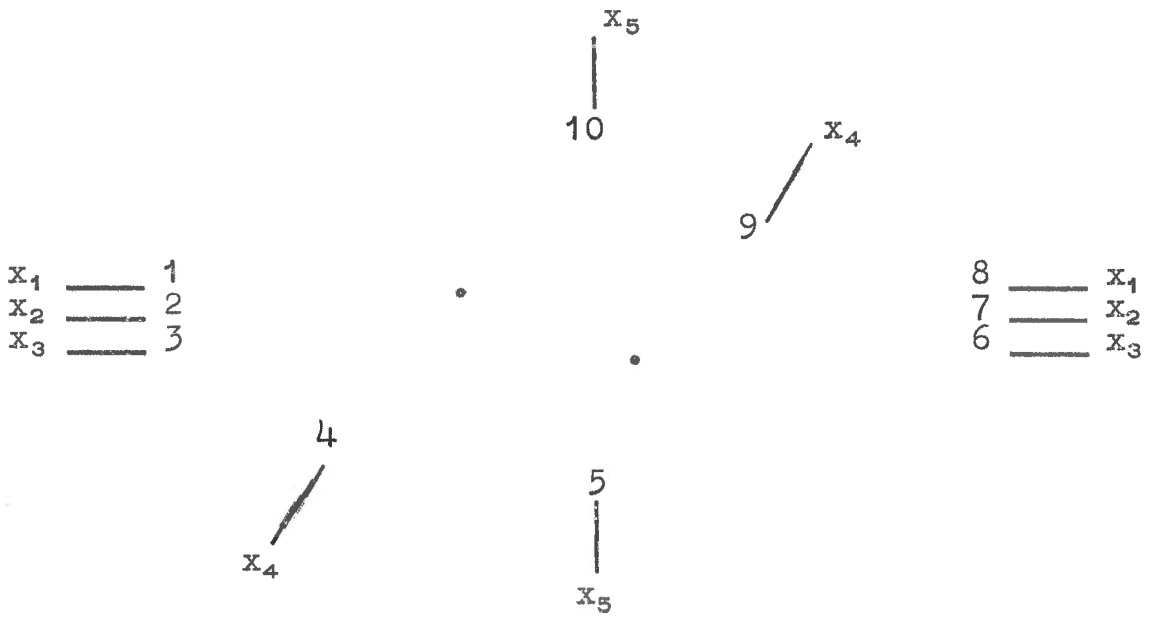
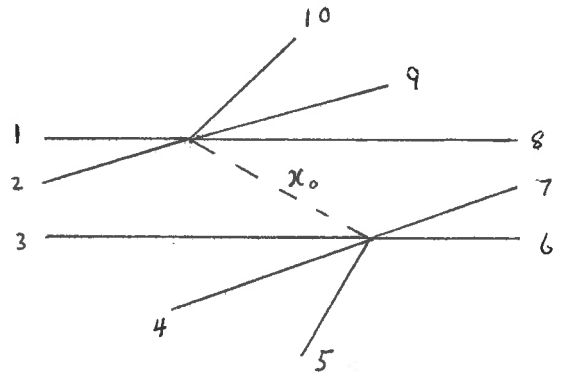


Fig. 4.1

It can be seen that the pairs of terminals (1, 8), (2, 7), (3, 6), (4, 9) and (5, 10) are the associated terminals defined by equation (2.14). The bonds $x_1 x_2 x_3$ represent horizontal bonds between cells x_4 represents a diagonal bond between cells, and x_5 represents a vertical bond between cells.

In order to represent the lattice of Fig. 2.3 (a) we must specify the way in which the external bonds connect to the spins of the cell. There is a weight factor for each way in which the external bonds are connected to the cell. This weight factor describes the ways in which the internal bonds can be arranged so that there is an even number of external and internal bonds to each spin. The way in which the external bonds connect to the spins for the lattice of Fig. 2.3 (a) is shown by the weight factor $c_{12345678910}$ shown in Fig. 4.2.



$C_0 = C_{12345678910} = x_0$

Fig. 4.2

It can be seen that in order to have an even number of bonds to each spin it is necessary for the internal bond to be present.

For this lattice the determinant (3.6) is of order 10 × 10

$\Delta = C_o^2 \times$

$$
\begin{vmatrix}
0 & C'_{12} & C'_{13} & & & & & & & C'_{18}-x_1e^{i\theta} \\
 & 0 & & & & & & & C'_{27}-x_2e^{i\theta} & \\
 & & 0 & & & & & C'_{36}-x_3e^{i\theta} & & \\
 & C'_{ij} & & 0 & & & & & C'_{49}-x_4e^{i(\theta+\phi)} & \\
 & & & & 0 & & & & & C'_{510}-x_5e^{i\phi} \\
 & & C'_{63}+x_3e^{-i\theta} & & & 0 & & & & \\
 & C'_{72}+x_2e^{-i\theta} & & & & & 0 & & C'_{ij} & \\
C'_{81}+x_1e^{-i\theta} & & & & & & & 0 & & \\
 & & C'_{94}+x_4e^{-i(\theta+\phi)} & & & & C'_{ij} & & 0 & \\
 & & & C'_{105}+x_5e^{-i\phi} & & & & & & 0
\end{vmatrix}
\qquad (4.1)
$$

The weight factors $C'_{ij} = C_{ij}/C_0$ can easily be found from Fig. 4.2. We have

$$C'_{ij} = \begin{cases} \frac{1}{x_0} & \text{if } ij \text{ contains an odd number of the set } \{3,4,5,6,7\} \\ 1 & \text{if } ij \text{ contains an even number of the set } \{3,4,5,6,7\} \end{cases} \qquad (4.2)$$

for $i < j$. Thus the determinant to be evaluated is

$$\Delta = x_0^2 \times$$

$$\begin{vmatrix}
0 & 1 & \frac{1}{x_0} & \frac{1}{x_0} & \frac{1}{x_0} & \frac{1}{x_0} & \frac{1}{x_0} & 1-x_1 e^{i\theta} & 1 & 1 \\
-1 & 0 & \frac{1}{x_0} & \frac{1}{x_0} & \frac{1}{x_0} & \frac{1}{x_0} & \frac{1}{x_0}-x_2 e^{i\theta} & 1 & 1 & 1 \\
-\frac{1}{x_0} & -\frac{1}{x_0} & 0 & 1 & 1 & 1-x_3 e^{i\theta} & 1 & \frac{1}{x_0} & \frac{1}{x_0} & \frac{1}{x_0} \\
-\frac{1}{x_0} & -\frac{1}{x_0} & -1 & 0 & 1 & 1 & 1 & \frac{1}{x_0} & \frac{1}{x_0}-x_4 e^{i(\theta+\phi)} & \frac{1}{x_0} \\
-\frac{1}{x_0} & -\frac{1}{x_0} & -1 & -1 & 0 & 1 & 1 & \frac{1}{x_0} & \frac{1}{x_0} & \frac{1}{x_0}-x_5 e^{i\phi} \\
-\frac{1}{x_0} & -\frac{1}{x_0} & -1+x_3 e^{-i\theta} & -1 & -1 & 0 & 1 & \frac{1}{x_0} & \frac{1}{x_0} & \frac{1}{x_0} \\
-\frac{1}{x_0} & -\frac{1}{x_0}+x_2 e^{-i\theta} & -1 & -1 & -1 & -1 & 0 & \frac{1}{x_0} & \frac{1}{x_0} & \frac{1}{x_0} \\
-1+x_1 e^{-i\theta} & -1 & -\frac{1}{x_0} & -\frac{1}{x_0} & -\frac{1}{x_0} & -\frac{1}{x_0} & -\frac{1}{x_0} & 0 & 1 & 1 \\
-1 & -1 & -\frac{1}{x_0} & -\frac{1}{x_0}+x_4 e^{-i(\theta+\phi)} & -\frac{1}{x_0} & -\frac{1}{x_0} & -\frac{1}{x_0} & -1 & 0 & 1 \\
-1 & -1 & -\frac{1}{x_0} & -\frac{1}{x_0}-\frac{1}{x_0}+x_5 e^{-i\phi} & -\frac{1}{x_0} & -\frac{1}{x_0} & -\frac{1}{x_0} & -1 & -1 & 0
\end{vmatrix} \qquad (4.3)$$

A method of expanding this determinant in terms of the bond weights and the weight factors has been described in Chapter 3. We notice that if x_1 and x_2 are selected from above the diagonal and not selected from below the diagonal the 1st and 2nd columns of the determinant remaining, when 1st and 2nd rows and the 7th and 8th columns have been removed, are equal. No matter which further selections are made the 1st and 2nd columns will

remain equal so that D(1;1,2,i;j;k) will be zero for all 1, i, j, k. Similarly we find that

$$D(1;1,2,i;j;k) = D(1;i;1,2,j;k) = 0$$
$$D(1;2,3,i;j;k) = D(1;i;2,3,j;k) = 0$$
$$D(1;3,4,i;j;k) = D(1;i;3,4,j;k) = 0$$
$$D(1;4,5,i;j;k) = D(1;i;4,5,j;k) = 0$$
$$D(1;1,4,i;j;k) = D(1;i;1,4,j;k) = 0$$
$$D(1;5,i;3,j;k) = D(1;3,i;5,j;k) = 0$$
$$D(1;5,i;1,j;k) = D(1;1,i;5,j;k) = 0$$

These relationships reduce the number of terms in (3.19) considerably.

The first summation in (3.19) is over the $2^5 = 32$ terms which arise on selecting the 5 external bonds into two groups $l_1, \ldots, l_n$ and $k_1, \ldots, k_m$. The coefficient of $x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_5^{\alpha_5}$ where $\alpha_i = 0$ or 2 is found from (3.17)' as

$$D(l_n;0;0;k_m) = c^2_{\{l_1,..,l_n,l'_1,..,l'_n\}} \qquad (4.4)$$

From Fig. 4.2 $c^2_{\{l_1,..,l'_n\}}$ is x_0^2 or 1 if $\{l_1,..,l'_n\}$ contains an odd or even number of the elements from the set{3,4,5,6,7} respectively.

The second summation corresponds to selecting p bonds from above the diagonal and the same number q = p of different bonds from below the diagonal. Since there are only 5 bonds altogether, only p = q = 1 and p = q = 2 need be considered for this lattice. Furthermore we have D(1;i;j;k) = D(1;j;i;k) since by (3.17)' the coefficient depends on the set $\{i_1..i_p\ j'_1\ ..j'_q\}$ for a given $l_1..l_n$. Thus the coefficients combine together to give cosine terms.

For selections such that $p_i = q_i$ the angle $\{(p_1 + p_2 - q_1 - q_2)\theta + (p_2 + p_3 - q_2 - q_3)\phi\}$ is zero. The third summation corresponds to selecting p bonds from above the diagonal and $q < p$ different bonds from below the diagonal. For selections such that $p_1 + p_2 = q_1 + q_2$ and $p_2 + p_3 = q_2 + q_3$ the above angle is again zero.

The coefficients D(1;i;j;k) are evaluated by the method illustrated in section 3.2 and after some tedious algebraic manipulations the determinant is found to be

$$
\begin{aligned}
\Delta = {} & \tfrac{1}{2}(1 + x_1^2)(1 + x_3^2)\{(1 + x_0^2)(1 + x_2^2)(1 + x_4^2)(1 + x_5^2) \\
& + (1 - x_0^2)(1 - x_2^2)(1 - x_4^2)(1 - x_5^2)\} \\
& + 4x_0x_2(1 + x_4^2)(1 + x_5^2)\{x_1(1 + x_3^2) + x_3(1 + x_1^2)\} \\
& + 2x_1x_3(1 + x_0^2)(1 + x_2^2)(1 + x_4^2)(1 + x_5^2) \\
& + 4x_4x_5(1 + x_0^2)(1 + x_2^2)\{x_1(1 + x_3^2) + x_3(1 + x_1^2)\} \\
& + 8x_0x_2x_4x_5(1 + x_1^2)(1 + x_3^2) + 32x_0x_1x_2x_3x_4x_5 \\
& - \{x_1(1 + x_3^2) + x_3(1 + x_1^2)\}\{(1 + x_0^2)(1 + x_2^2)(1 - x_4^2)(1 - x_5^2) \\
& + (1 - x_0^2)(1 - x_2^2)(1 + x_4^2)(1 + x_5^2)\} \cos\theta \\
& - 2(1 + x_1^2)(1 + x_3^2)\{x_0x_2(1 - x_4^2)(1 - x_5^2) \\
& + x_4x_5(1 - x_0^2)(1 - x_2^2)\} \cos\theta \\
& - 8x_1x_3\{x_0x_2(1 - x_4^2)(1 - x_5^2) + x_4x_5(1 - x_0^2)(1 - x_2^2)\} \cos\theta \\
& - 2(1 - x_1^2)(1 - x_3^2)\{x_0x_4(1 - x_2^2)(1 - x_5^2) \\
& + x_2x_5(1 - x_0^2)(1 - x_4^2)\} \cos(\theta + \phi) \\
& - 2x_0x_5(1 - x_1^2)(1 - x_2^2)(1 - x_3^2)(1 - x_4^2) \cos\phi \\
& + 2x_1x_3(1 - x_0^2)(1 - x_2^2)(1 - x_4^2)(1 - x_5^2) \cos 2\theta \\
& - 2x_2x_4(1 - x_0^2)(1 - x_1^2)(1 - x_3^2)(1 - x_5^2) \cos(2\theta + \phi)
\end{aligned}
\tag{4.5}
$$

This result can be checked against the known results for the rectangular, triangular hexagonal and Yamamoto lattices. A particular bond x_i of a lattice can be removed by putting $x_i = 0$. A bond can also be made redundant if we coalesce the spins which form the end points of the bonds by putting $x_i = 1$. From Fig. 4.1 we can see that $x_0 = 1$ and $x_2 = x_3 = x_4 = 0$ or $x_0 = 1$ and $x_1 = x_3 = x_4 = 0$ or $x_0 = 1$ and $x_1 = x_2 = x_4 = 0$ or $x_0 = 1$ and $x_2 = x_3 = x_5 = 0$ will produce a rectangular lattice. For the first case the determinant is

$$\Delta = (1 + x_1^2)(1 + x_5^2) - 2x_1(1 - x_5^2)\cos\theta - 2x_5(1 - x_1^2)\cos\phi$$

A triangular lattice may be obtained if we put $x_0 = 1$ and $x_2 = x_3 = 0$ or $x_0 = 1$ and $x_1 = x_3 = 0$ or $x_0 = 1$ and $x_1 = x_2 = 0$. For the first case the determinant is

$$\Delta = (1 + x_1^2)(1 + x_4^2)(1 + x_5^2) - 2x_1(1 - x_4^2)(1 - x_5^2)\cos\theta - 2x_4(1 - x_1^2)(1 - x_5^2)\cos(\theta + \phi) - 2x_5(1 - x_1^2)(1 - x_4^2)\cos\phi + 8x_1x_4x_5.$$

A hexagonal lattice may be obtained by putting $x_1 = x_3 = x_5 = 0$ or $x_1 = x_3 = x_4 = 0$ and the determinant for the latter case is

$$\Delta = 1 + x_0^2x_2^2 + x_0^2x_5^2 + x_2^2x_5^2 - 2x_0x_2(1 - x_5^2)\cos\theta - 2x_0x_5(1 - x_2^2)\cos\phi - 2x_2x_5(1 - x_0^2)\cos(\theta + \phi)$$

The Yamamoto lattice can be obtained by putting $x_1 = x_3 = 0$. Here

$$\Delta = 1 + x_0^2x_2^2 + x_0^2x_4^2 + x_0^2x_5^2 + x_2^2x_4^2 + x_2^2x_5^2 + x_4^2x_5^2$$
$$+ x_0^2x_2^2x_4^2x_5^2 + 8x_0x_2x_4x_5 - 2x_4x_5(1 - x_0^2)(1 - x_2^2)\cos\theta$$
$$- 2x_0x_2(1 - x_4^2)(1 - x_5^2)\cos\theta - 2x_0x_4(1 - x_2^2)(1 - x_5^2)\cos(\theta + \phi)$$
$$- 2x_0x_5(1 - x_2^2)(1 - x_4^2)\cos\phi - 2x_2x_4(1 - x_0^2)(1 - x_5^2)\cos(2\theta + \phi)$$
$$- 2x_2x_5(1 - x_0^2)(1 - x_4^2)\cos(\theta + \phi)$$

All these results agree with those obtained by other authors[2] In the case of the Yamamoto lattice it is necessary to transform the angle $\theta + \phi$ to χ to give the usual result.

The critical equations for this lattice can be found by the method of section 3.3. For a singularity at $\theta = \phi = 0$ the critical equation is given by equation (3.24). For the lattice of Fig. 4.2 this equation is

$$c_0 - c_{18}x_1 - c_{27}x_2 - c_{36}x_3 - c_{49}x_4 - c_{510}x_5 + c_{1278}x_1x_2$$
$$- c_{1368}x_1x_3 - c_{1489}x_1x_4 + c_{15610}x_1x_5 - c_{2367}x_2x_3$$
$$- c_{2479}x_2x_4 - c_{25710}x_2x_5 - c_{3469}x_3x_4 - c_{35810}x_3x_5$$
$$- c_{45910}x_4x_5x - c_{123678}x_1x_2x_3 - c_{124789}x_1x_2x_4$$
$$- c_{1257810}x_1x_2x_5 - c_{134689}x_1x_3x_4 + c_{1356810}x_1x_3x_5$$
$$- c_{1458910}x_1x_4x_5 - c_{234679}x_2x_3x_4 + c_{2356710}x_2x_3x_5$$
$$+ c_{2457910}x_2x_4x_5 - c_{3456910}x_3x_4x_5 - c_{12346789}x_1x_2x_3x_4$$
$$- c_{123567810}x_1x_2x_3x_5 - c_{124578910}x_1x_2x_4x_5 - c_{134568910}x_1x_3x_4x_5$$
$$- c_{2345679910}x_2x_3x_4x_5 + c_{12345678910}x_1x_2x_3x_4x_5 = 0 \qquad (4.6)$$

where the signs of the terms have been found by using equation (3.25). The weight factors are found from Fig. 4.2 to be x_0 if the indices contain an odd number of elements of the set {3, 4, 5, 6, 7} and 1 otherwise. After some algebraic manipulation the critical equation can be written as

$$(1 - x_0x_2)(1 - x_4x_5)(1 - x_1)(1 - x_3)$$
$$- (x_0 + x_2)(x_4 + x_5)(1 + x_1)(1 + x_3) = 0 \qquad (4.7)$$

The other critical equations corresponding to the other values of θ and ϕ at which a singularity may occur can be found by transforming the bond weights according to equation (3.26). One can show that (4.7) gives the correct equation for the rectangular, triangular, hexagonal and Yamamoto lattices by the same method as used in the previous paragraph. For example, if we put $x_1 = x_3 = 0$ we obtain the equation

$$1 + x_0x_2x_4x_5 = x_0x_2 + x_4x_5 + x_0x_4 + x_0x_5 + x_2x_4 + x_2x_5$$

which corresponds to the equation (47a) obtained by Hurst[20] for the Yamamoto lattice.

We note here the distinction between the 2 state and the 4 state model. For $x_0 = 1$ there is no internal bond and the lattice reduces to either the rectangular or the triangular lattice. For $x_0 \neq 1$ the lattice can be reduced to the hexagonal and Yamamoto lattice by appropriate selection of the other bond weights. It is therefore apparent that the latter correspond to multiple state models even though multiple bonds are not present. Our model corresponds to a generalisation of these lattices to the widest class of planar graphs.

4.2 SINGLE BONDS BETWEEN CELLS WITH MANY SPINS.

In this section we consider a lattice in which there are many spins to a cell but only single bonds between cells. This lattice contrasts with the case considered in section 4.1 where we had multiple bonds between cells with only two spins to each cell. In particular we shall consider a lattice where the j^{th} cell has single bond connections to the $j - 1^{th}$, $j - n^{th}$, $j + 1^{th}$, and $j + n^{th}$ cell. Hurst[20] has discussed this case and derived quite general expressions for the partition function and the critical conditions in terms of the weight factors associated with each cell. Here we shall investigate the critical behaviour of more complex cells than those considered by Hurst. The complexity of the cell allows certain of the internal bonds to be while anti-ferromagnetic which others are ferromagnetic. For the lattice investigated it is shown that only one critical temperature exists for each choice of interaction energies.

We consider a lattice which has nine spins to each cell as shown in Fig. 4.3. The cell has two types of external bonds x and y. The internal bonds and the terminals associated with each cell are shown in Fig. 4.4.

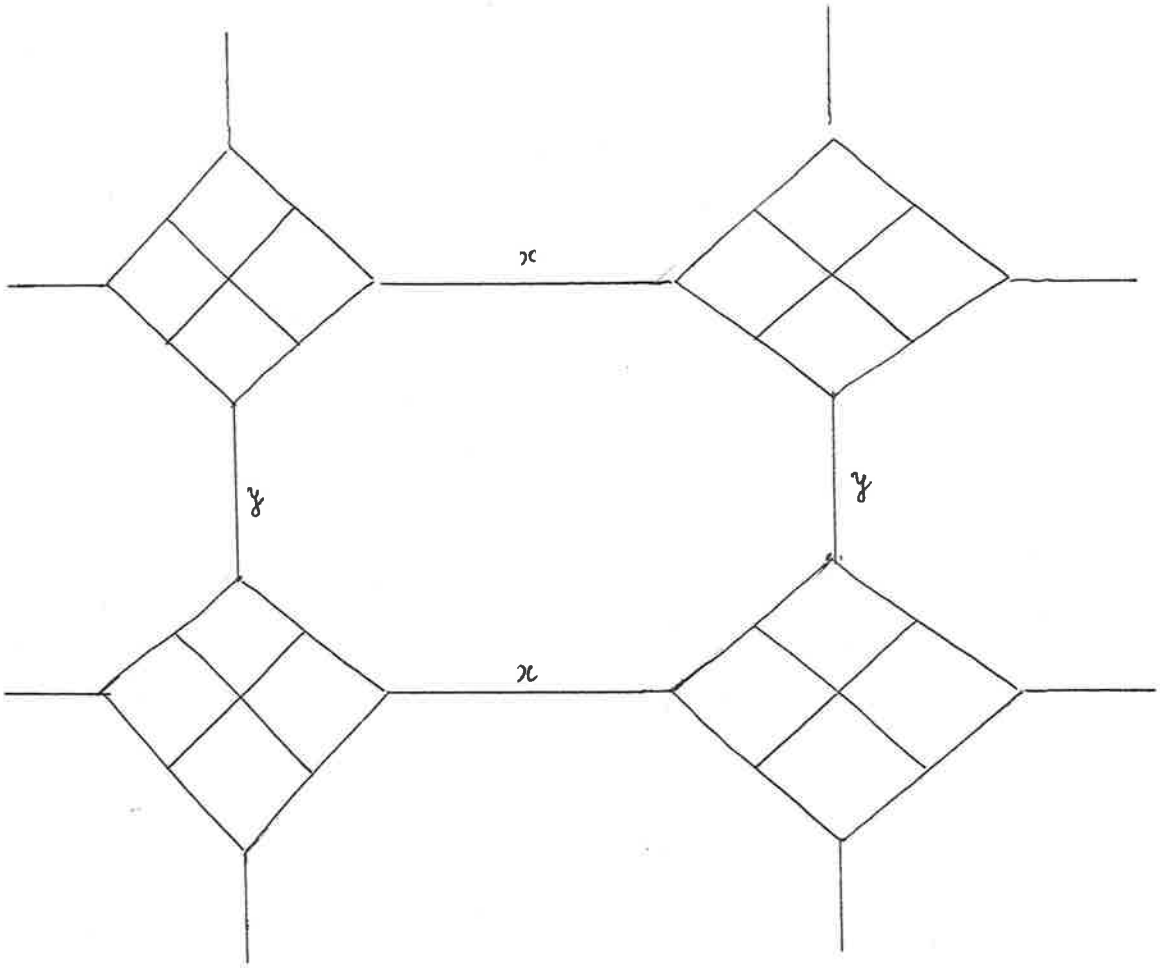


Fig. 4.3

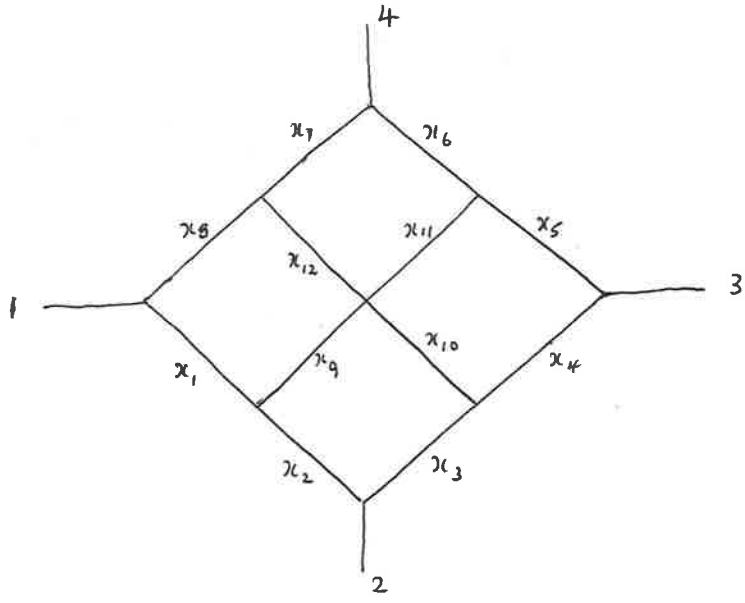


Fig. 4.4

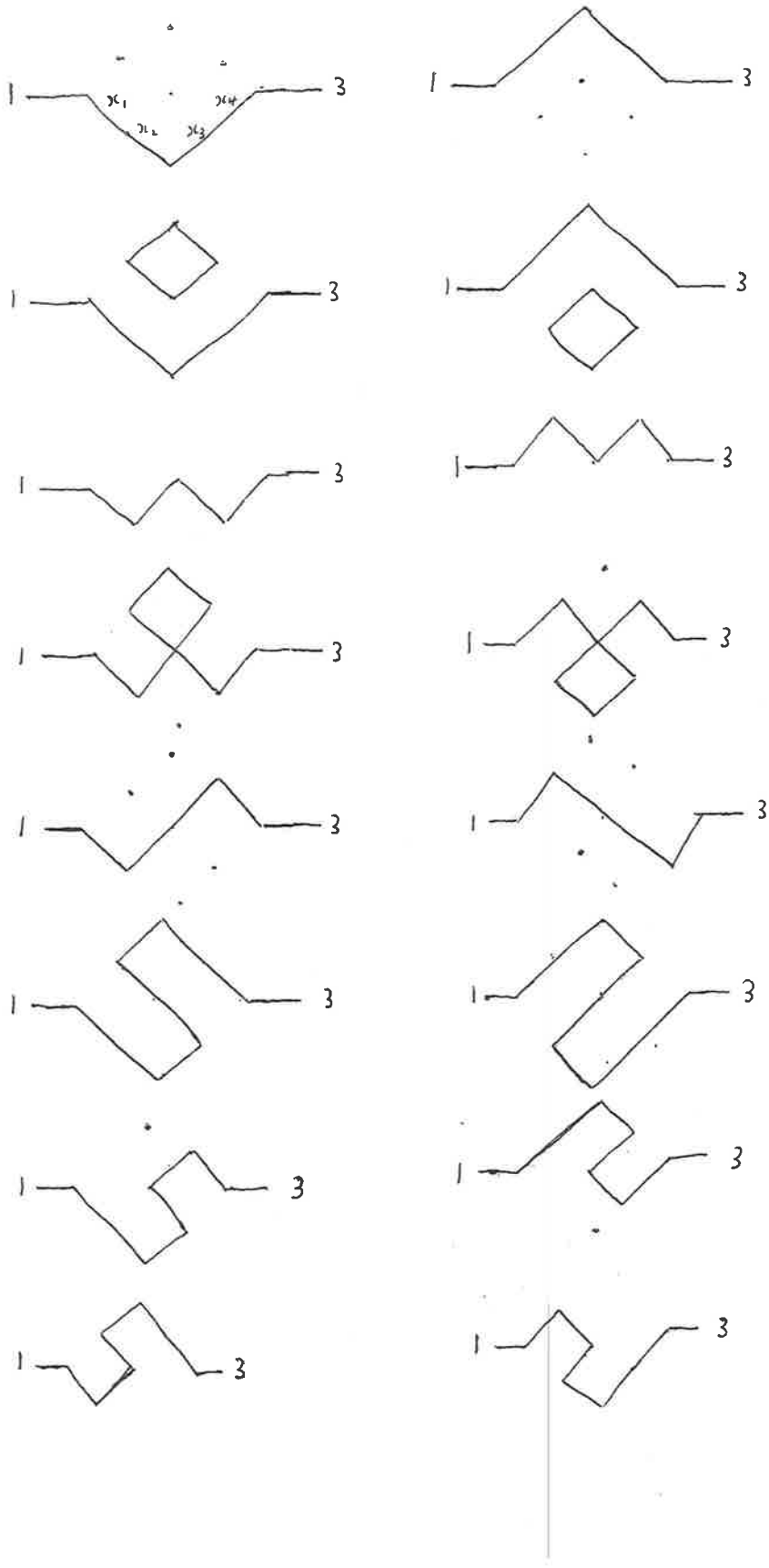


Fig. 4.5

The determinant Δ, and the critical equations for such a lattice can be found directly from the paper by Hurst[20], or by using the method of chapter 3. In terms of the original weight factors the determinant is

$$\Delta = C_0^2 + x^2 C_{13}^2 + y^2 C_{24}^2 + x^2 y^2 C_{1234}^2$$
$$- 2x \cos\theta (C_0 C_{13} - y^2 C_{24} C_{1234}) - 2y \cos\phi (C_0 C_{24} - x^2 C_{13} C_{1234})$$
$$- 2xy \cos(\theta + \phi)(C_0 C_{1234} - C_{12} C_{34})$$
$$- 2xy \cos(\theta - \phi)(C_0 C_{1234} - C_{14} C_{23}) \qquad (4.8)$$

The critical equations are given by the equation

$$C_0 - x\, C_{13} - y\, C_{24} + xy\, C_{1234} = 0 \qquad (4.9)$$

and its transformations according to equation (3.26).

The weight factors are the ways in which paths may be drawn through the cell consistant with the external bond connections and an even number of fonds to each spin of the cell. For example the weight factor C_{13} is demonstrated in Fig. 4.5.

Thus

$$C_{13} = x_1x_2x_3x_4 + x_5x_6x_7x_8 + x_1x_2x_8x_4x_6x_7x_{11}x_{12}$$
$$+ x_5x_6x_7x_8x_2x_3x_4x_{10} + x_1x_9x_{10}x_4 + x_5x_{11}x_{12}x_8$$
$$+ x_1x_9x_{10}x_4x_6x_7x_{11}x_{12} + x_5x_{11}x_{12}x_8x_2x_3x_9x_{10}$$
$$+ x_1x_9x_{11}x_5 + x_8x_{12}x_{10}x_4 + x_1x_2x_3x_{10}x_{12}x_7x_6x_5$$
$$+ x_8x_7x_6x_{11}x_9x_2x_3x_4 + x_1x_2x_3x_{10}x_{11}x_5$$
$$+ x_1x_9x_{12}x_7x_6x_5 + x_8x_7x_6x_{11}x_{10}x_4 + x_8x_{12}x_9x_2x_3x_4$$

The other weight factors can be found in the same way.

Since we wish to investigate the effect of a large number of spins in a cell and not the external bonds to a cell, we collapse the lattice by putting $x = y = 1$.

The lattice is shown in Fig. 4.6.

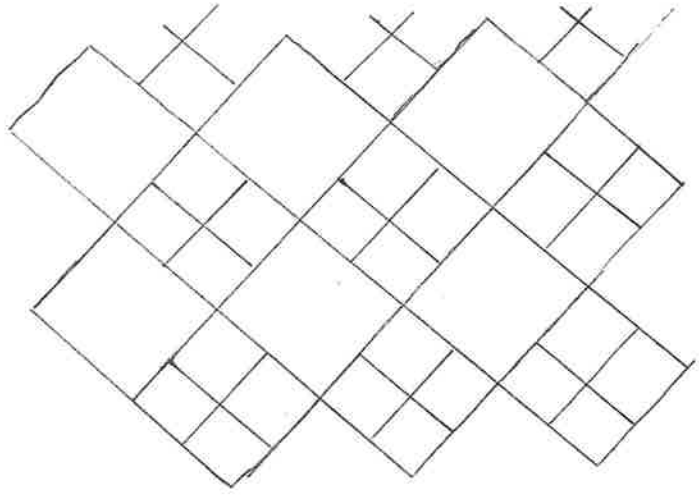


Fig. 4.6

When the weight factors are substituted in (4.9) the critical equations involve the twelve bond weights $x_1, x_2, \ldots, x_{12}$, and can only be investigated on a computer. In the following subsections we shall consider particular cases of this lattice which can be considered by analytic methods.

4.21 <u>All Bonds Equal.</u>

If $x_1 = x_2 = \ldots = x_{12} = x = \tanh \beta J$ then the critical equations obtained from (4.9) and (3.26) are

$$\begin{aligned}
&1 + 6x^4 + 16x^6 + 9x^8 = 0 && (0, 0)\\
&1 + 14x^4 + 17x^8 = 0 && (\pi, 0)\\
&1 - 10x^4 - 16x^6 - 7x^8 = 0 && (0, \pi)\\
&1 + 6x^4 + 16x^6 + 9x^8 = 0 && (\pi, \pi)
\end{aligned} \qquad (4.10)$$

Since the first, second and fourth equations consist of a sum of positive monotonic increasing functions of x, they have no real solutions. Descartes rule of sign shows that the third equation has at most one positive real solution in x^2. By considering the values of the

left hand side of the equation at 0 and 1, we see that the solution must lie in the range $0 < x^2 < 1$. Hence there is one positive solution to the equation ($x = c$ say) which gives the critical temperature as

$$\frac{1}{kT_c} = \frac{1}{J} \tanh^{-1} c.$$

As the third equation is an even function of x the same solution is obtained for the antiferromagnetic case.

4.22 Two types of Bonds.

Consider $x_1 = x_2 = x_5 = x_6 = x_{10} = x_{12} = x = \tanh \beta J$ and $x_3 = x_4 = x_7 = x_8 = x_9 = x_{11} = y = \tanh \beta J'$. The critical equations for this case are

$$1 + 4x^2y^2 + x^4 + y^4 + 8x^4y^2 + 8x^2y^4 + 9x^4y^4 = 0$$

$$1 + 16x^2y^2 - x^4 - y^4 + 2x^6y^2 + 2x^2y^6 + 13x^4y^4 = 0$$

$$1 - 8x^2y^2 - x^4 - y^4 - 8x^4y^2 - 8x^2y^4 - 2x^6y^2 - 2x^2y^6 - 3x^4y^4 = 0$$

$$1 + 4x^2y^2 + x^4 + y^4 + 8x^4y^2 + 8x^2y^4 + 9x^4y^4 = 0 \qquad (4.11)$$

Again the first and fourth equations have no real solution. The second equation can be shown to have no real solutions by using for $0 < x^2, y^2 < 1$

$$(2xy)^2 < (x^2 + y^2)^2 < (x^2y^2 + 1)^2$$

We have

$$1 + 16x^2y^2 - x^4 - y^4 + 2x^6y^2 + 2x^2y^2 + 13x^4y^4$$

$$= 1 + 18x^2y^2 - (x^2 + y^2)^2 + x^2y^2(9x^2y^2 + 2(x^2 + y^2)^2)$$

$$> 1 + 18x^2y^2 - (x^2y^2 + 1)^2 + x^2y^2(9x^2y^2 + 8x^2y^2)$$

$$> 16x^4y^4 + 16x^2y^2$$

$$> 0.$$

As above the third equation has one solution for $0 < x^2, y^2 < 1$ giving a single solution for T_c which is a function

of J and J'.

4.23 All bond equal except one centre bond.

Consider $x_{12} = y = \tanh \beta J'$ and

$x_1 = x_2 = \ldots = x_{11} = x = \tanh \beta J$. The critical equations for this case are

$$1 + 2yx^3 + 4x^4 + 8yx^5 + 8x^6 + 6yx^7 + 3x^8 = 0$$

$$1 + 6yx^3 + 8x^4 + 10yx^7 + 7x^8 = 0$$

$$1 - 2yx^3 - 8x^4 - 8yx^5 - 8x^6 - 6yx^7 - x^8 = 0$$

$$1 + 2yx^3 + 4x^4 + 8yx^5 + 8x^6 + 6yx^7 + 3x^8 = 0 \qquad (4.12)$$

These equations are linear in y and hence we can write

$$Y_1 = Y_4 = -\frac{1 + 4x^4 + 8x^6 + 3x^8}{2x^3 + 8x^5 + 6x^7}$$

$$Y_2 = -\frac{1 + 8x^4 + 7x^8}{6x^3 + 10x^7}$$

$$Y_3 = +\frac{1 - 8x - 8x - x}{2x^3 + 8x^5 + 6x^7} \qquad (4.13)$$

If we define the ratio of the bond energies by

$$\alpha = \frac{J'}{J} \qquad (4.14)$$

and use $x = \tanh \beta J$, $y = \tanh \beta J'$ we find

$$y = 1 - \frac{2}{1 + \left(\frac{1 + x}{1 - x}\right)^{\alpha}} \qquad (4.15)$$

Clearly the solution of equation (4.12) for a particular value of α will be where the curves (4.13) and (4.15) meet. Fig. 4.7 shows the graphs of Y_1, Y_2, Y_3 and the graph of y for different values of α.

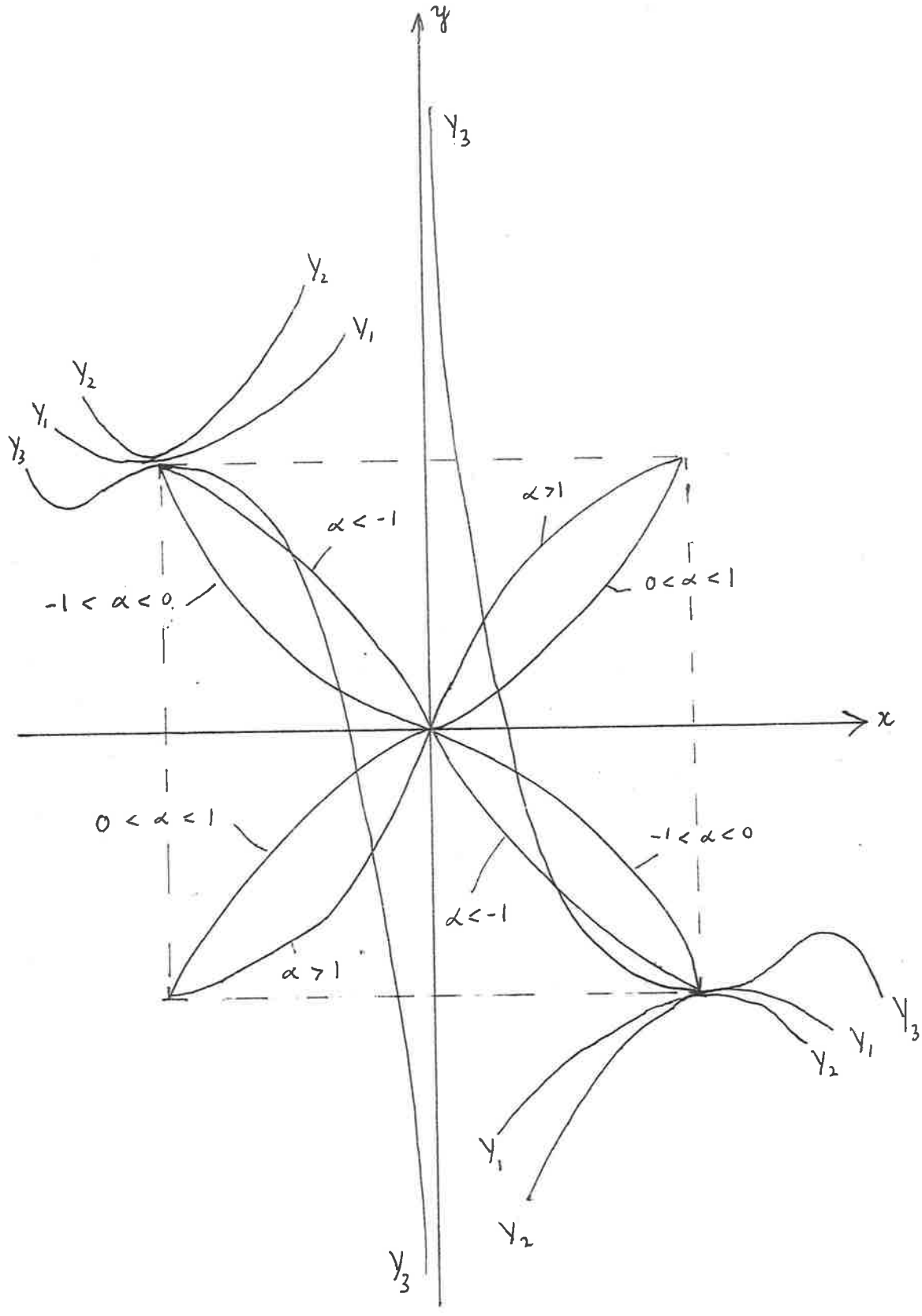

y
x
y_3
y_2
y_1
y_2
y_1
y_3
$\alpha > 1$
$\alpha < -1$
$-1 < \alpha < 0$
$0 < \alpha < 1$
$0 < \alpha < 1$
$-1 < \alpha < 0$
$\alpha < -1$
$\alpha > 1$
y_3
y_1
y_2
y_3
y_1
y_2

Fig. 4.7

It can be seen that $Y_1 = Y_4$, and Y_2 have only the degenerate solution $x = y = 1$ corresponding to $T_c = 0$. For a particular value of $\alpha > -1$ a single solution for T is given by the intersection of Y_3 and y (4.15). However, the case $\alpha < -1$ is not determined and depends upon the slope of the function Y_3 at the point (-1, 1) and (1, -1). It can be shown that (-1, 1) and (1, -1) are maximum and minimum turning points for the function Y_3 and hence Y_3 gives a solution for T for all finite values of α. However, for large negative values of α the solution approaches $x = y = -1$ or $x = -1$ $y = 1$ corresponding to $T_c = 0$.

4.24 <u>All bonds equal except one corner bond.</u>

Consider $x_1 = y = \tanh \beta J'$ and $x_2 = x_3 = \ldots = x_{12} = \tanh \beta J$. The critical equations for this case are

$$1 + 6x^4 + 8yx^5 + 8x^6 + 8yx^7 + x^8 = 0$$
$$1 + 4yx^3 + 10x^4 + 12yx^7 + 5x^8 = 0$$
$$1 - 4yx^3 - 6x^4 - 8yx^5 - 8x^6 - 4yx^7 - 3x^8 = 0$$
$$1 + 4yx^3 + 2x^4 + 8yx^5 + 8x^6 + 4yx^7 + 5x^8 = 0 \qquad (4.16)$$

For a particular value of the bond energies the solutions of these equations give the critical temperature of the lattice. The solution of these equations for different values of the ratio of the bond weights α are shown graphically in Fig. 4.8. The figure shows where the curves

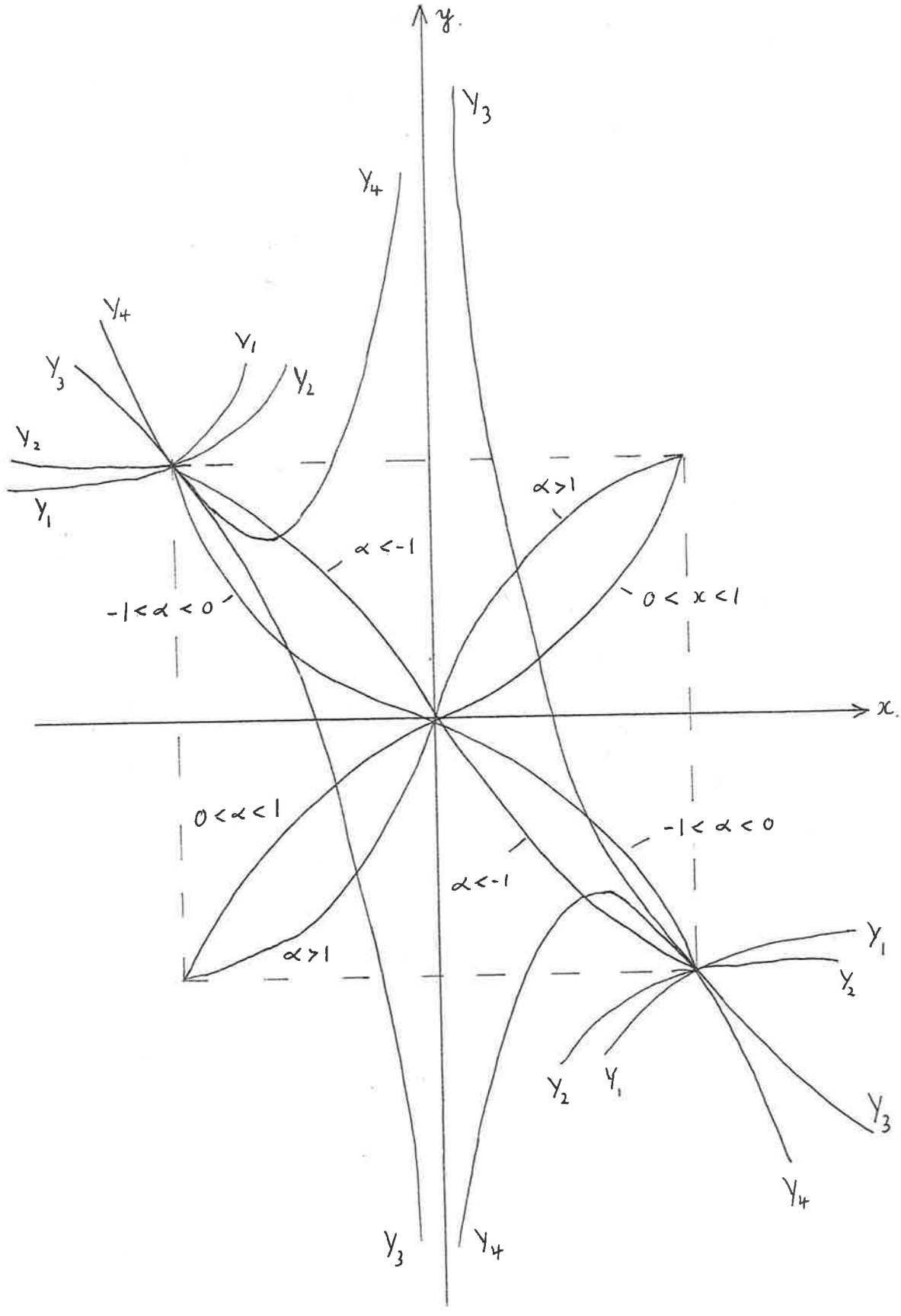

y
x
y_1
y_2
y_3
y_4
$\alpha > 1$
$\alpha < -1$
$-1 < \alpha < 0$
$0 < x < 1$
$0 < \alpha < 1$
$-1 < \alpha < 0$
$\alpha < -1$
$\alpha > 1$

Fig. 4.8

$$Y_1 = -\frac{1 + 6x^4 + 8x^6 + x^8}{8x^5 + 8x^7}$$

$$Y_2 = -\frac{1 + 10x^4 + 5x^8}{4x^3 + 12x^7}$$

$$Y_3 = +\frac{1 - 6x^4 - 8x^6 - 3x^8}{4x^3 + 8x^5 + 4x^7}$$

$$Y_4 = -\frac{1 + 2x^4 + 8x^6 + 5x^8}{4x^3 + 8x^5 + 4x^7} \qquad (4.17)$$

meet the curve (4.15) for different values of α. It can be seen that the critical temperature is given by the solution of Y_3 for $\alpha > -1$ and by Y_4 for $\alpha < -1$. The case $\alpha = -1$ requires close investigation as there are four possible situations; both Y_3 and Y_4 given non-degenerate solutions; only Y_3 gives a non-degenerate solution; only Y_4 gives a non-degenerate solution; or only the degenerate solution exists. By putting $y = -x$ in the original equations (4.16) we find that only the degenerate solution corresponding to $T_c = 0$ exists. This behaviour is similar to that of the triangular lattice in the case where all the bond energies are equal and negative[26]. It corresponds to the lattice having more than one configuration with the minimum energy. For $J > 0$ and $J' < 0$ the zero of energy for each cell is $-11J + J'$. Fig. 4.9 shows two possible configurations for each cell of the lattice, where a + signifies that the spin is in a certain state and - signifies the opposite state.

(a) (b)

Fig. 4.9

The energy associated with a cell in the configuration shown in Fig. 4.9(a) is $-11J - J'$ while that of Fig. 4.9(b) is $-9J + J'$. The condition that the cell be in the state represented by Fig. 4.9(a) is $-11J - J' < -9J + J'$ which becomes $\alpha > -1$. By similar reasoning the state represented in Fig. 4.9(b) has the lower energy when $\alpha < -1$. However, when $\alpha = -1$ both states have the same energy $-10J$, and hence either state can exist at random throughout the lattice.

Our conclusion from this discussion of a lattice with many spins to each cell is that the critical behaviour is similar to the simple triangular lattice. For a given value of the bond weights there is only one critical temperature.

4.3 Multiple Bonds between Cells.

In this section we consider the case in which there are a large number of bonds between cells. The particular lattice considered belongs to the (M, M, 0, M, M - 1) class of lattices and is shown in Fig. 4.10 for M =4. We will investigate the asymptotic behaviour of the critical temperature as M becomes large.

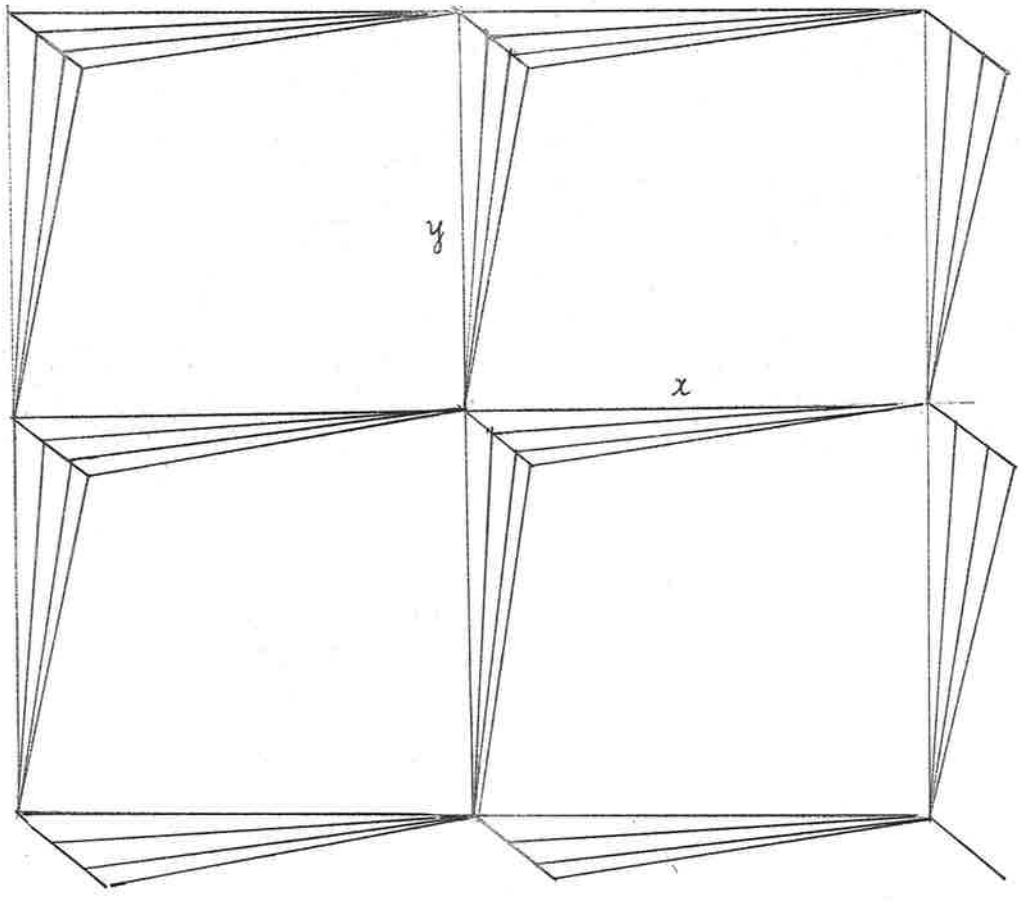


Fig. 4.10

The M horizontal, M vertical and M - 1 internal bonds are labelled by x, y and z respectively.

Such a lattice naturally arises when a cubic lattice with M^3 spins is projected onto a two dimensional plane and the M spins in the z direction are collected together into a cell. In order to solve the problem by the Pfaffian method it is necessary that the cell be planar and this means that cell connections similar to those shown in Fig. 4.11 (for M = 4) must be assumed.

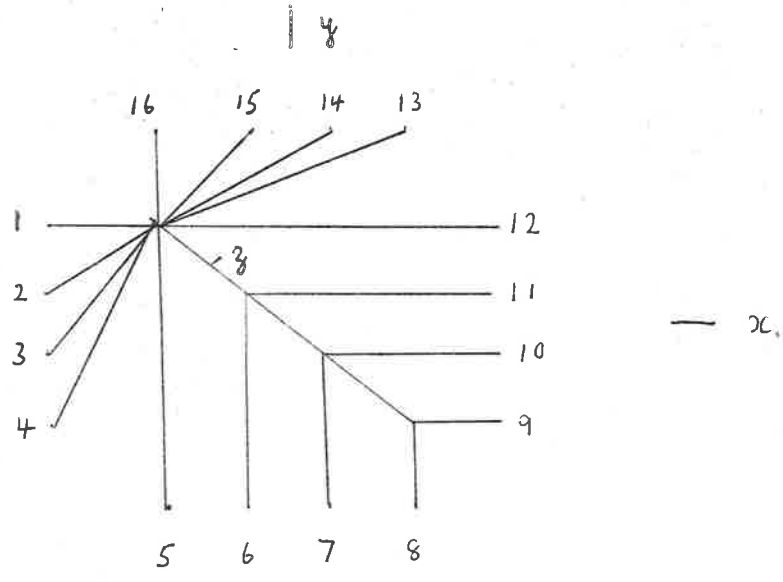


Fig. 4.11

Our model resembles the cubic lattice in that there are a large number of bonds between cells but it avoids the problem of crossed bonds which are present in the actual projection shown in Fig. 4.12.

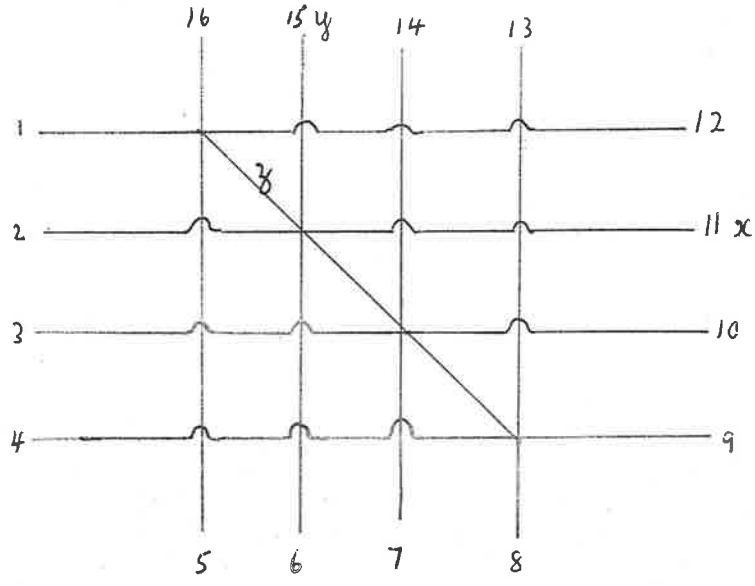


Fig. 4.12

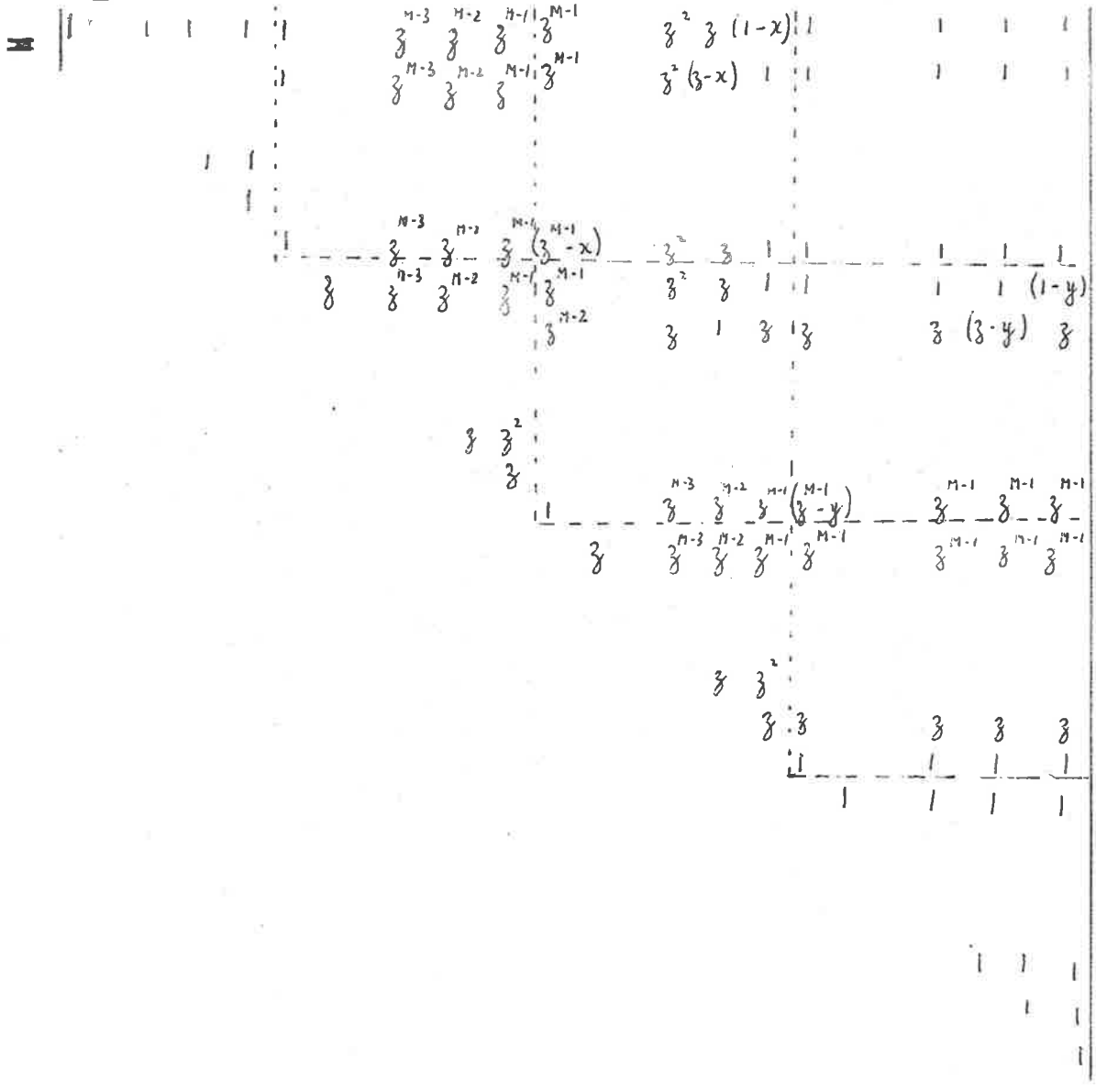
The weight factors for bond connections to the cell are found in the usual way. We have seen in Chapter 3 that the evaluation of the critical equations involves finding only the weight factors in which associated terminals are connected to the cell whereas the partition function involves more complicated weight factors. The critical equations are linear in the weight factors whereas the partition is a quadratic expression in the weight factors and involves multiple angles of θ and ϕ. For these reasons we consider only the critical equations.

For the case $\theta = \phi = 0$ the critical equation (3.22) is

$$\Delta_M^{\frac{1}{2}} \equiv G_M = 0$$

where

$G_M =$



(4.18)

In chapter 3 we have shown that this Pfaffian can be evaluated in terms of the weight factors for a cell. From (3.24) we have

$$G_M = \sum_{n_1=0}^{M} \sum_{n_2=0}^{M} \sum_{c} (-)^Q c(z)\, x^{n_1} y^{n_2} \qquad (4.19)$$

The third summation is over the weight factors $c(z)$ consistent with n_1 horizontal and n_2 vertical bonds connected to the cell. The sign $(-)^Q$ of the terms is given by (3.25). For small values of M the critical equation can be found by drawing the weight factors to each cell. We find

$$\begin{aligned} G_1 &= (1 - xy) - (x + y) \\ G_2 &= (1 - xy)^2 - (1 + z)(1 + xy)(x + y) + z(x - y)^2 \\ G_3 &= (1 - xy)^3 - (1 + z + z^2)(1 + xy)^2(x + y) \\ &\quad + z(2 + z)(1 - xy)(x - y)^2 - z(x + y)^3 \end{aligned} \qquad (4.20)$$

We can formulate G_M in terms of the lower order G's by considering the graphs which can be constructed on a cell with M spins. For the moment we consider all the weight factors with a positive sign. If no bond connects the $M-1^{th}$ spin and the M^{th} spin, either no bond or both the x and y external bonds are connected to the M^{th} spin for the M^{th} spin to have an even number of bonds connected to it: factor $(1 + xy)$. The other $M - 1$ spins can be connected as in G_{M-1} (see Fig. 4.13).

Fig. 4.13

If a bond does connect the M - 1^{th} and M^{th} spin and no bond connects the M - 2^{th} and M - 1^{th} spins, then an x^2, xy, or y^2 factor results from the last two spins (also z) and the remaining M - 2 points can be connected as in G_{M-2} (see Fig. 4.14).

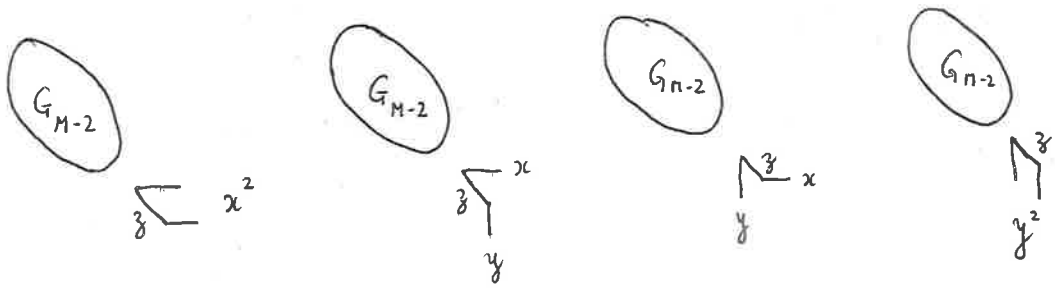


Fig. 4.14

This method can be continued until a bond z^{M-2} connects the 2nd spin to the M^{th} spin, but no bond connects the 1st and 2nd spins. From the end points of the bond we have a factor $(x + y)^2$ and the M - 3 internal points give a factor $(1 + xy)^{M-3}$. The remaining point has connections

such that there is a gap between the 1st and 2nd spin: factor 1 + xy + x + y (see Fig. 4.15).

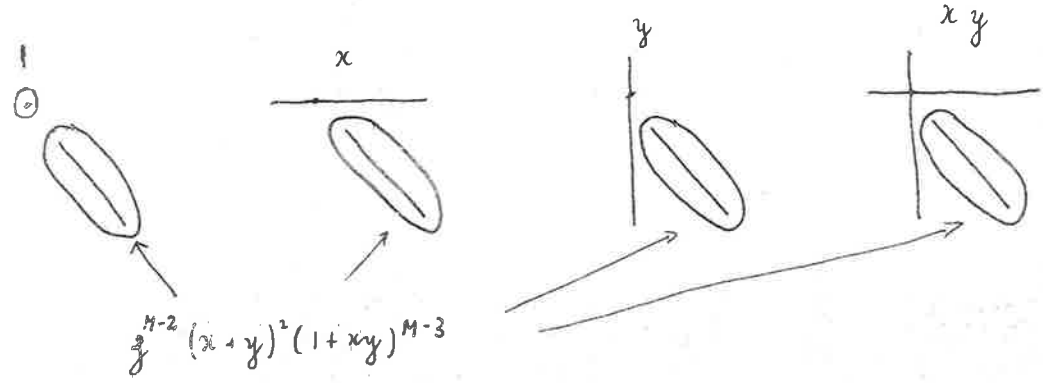
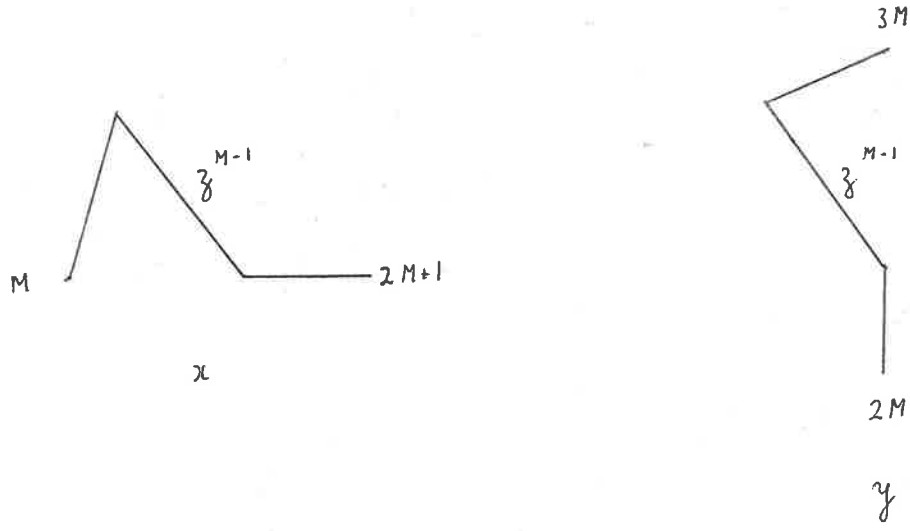
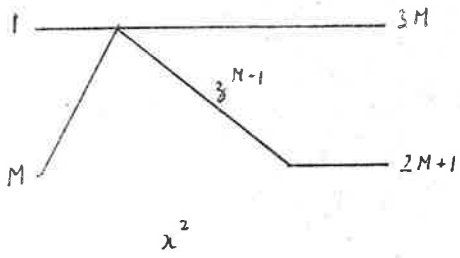


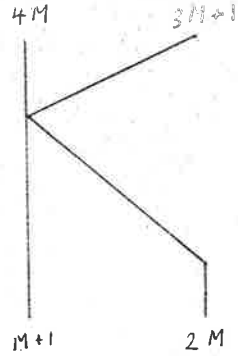
Fig. 4.15

Finally we have a bond of length z^{M-1} connecting the 1st spin to the M^{th} spin. The internal points give a factor $(1 + xy)^{M-2}$ and the end points give a factor $(x + y) + (1 + xy)(x + y)$ as shown in Fig. 4.16.

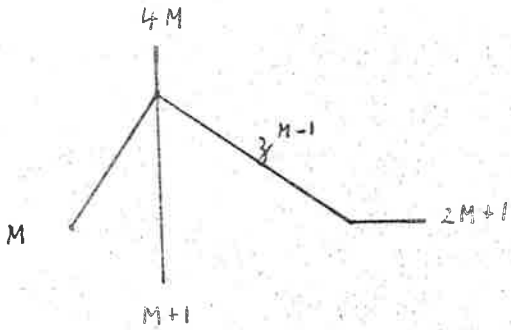




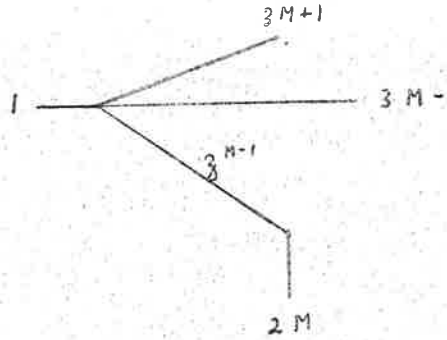
x^2



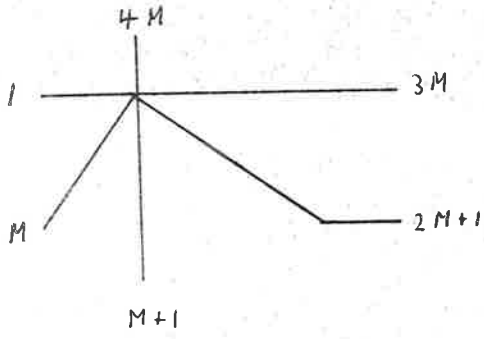
y^2



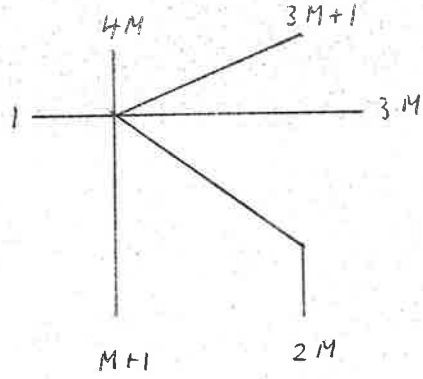
xy



yx.



x^2y



xy^2

Fig. 4.16

Thus we have formulated a difference equation for G_M in terms of the lower order G's.

$$G_M(x\ y\ z) = (1 + xy)G_{M-1}(x, y, z) + (x + y)^2 \sum_{r=2}^{M} z^{r-1}(1 + xy)^{r-2} G_{M-r}(x\ y\ z) + z^{M-1}(1 + xy)^{M-1}(x + y) \qquad M \geq 2$$

$$G_1(x, y, z) = (1 + xy)G_0 + (x + y)$$

$$G_0(x, y, z) = 1$$

Part of the term for the z^{M-1} bond has been incorporated under the summation, since it is consistent with the definition of G_0, and the remaining part has been added.

We shall now incorporate the sign factor given by (3.25) as $n + n_1n_2 = (n_1 + 1)(n_2 + 1) - 1$ in the difference equation. If $x^{n_1}y^{n_2}$ is multiplied by xy the sign is changed from $(n_1 + 1)(n_2 + 1) - 1$ to $(n_1 + 2)(n_2 + 2) - 1$ which has difference $n + 3$. Hence terms with even n are changed in sign, but those with odd n are unchanged. If $x^{n_1}y^{n_2}$ is multiplied by x^2 or y^2 there is no change in sign. In G_M the terms with even n are given by

$$G_M^{\text{even}} = \tfrac{1}{2}\{G_M(x, y, z) + G_M(-x, -y, z)\}$$

while those with odd n are given by

$$G_M^{\text{odd}} = \tfrac{1}{2}\{G_M(x, y, z) - G_M(-x, -y, z)\}$$

Thus the difference equation with the correct sign is

$$G_M(x, y, z) = G_{M-1}(x\,y\,z) + xy(-G^{even}_{M-1} + G^{odd}_{M-1})$$
$$+ (x+y)^2 \sum_{r=2}^{M} z^{r-1}(1+xy)^{r-2} G^{odd}_{M-r}$$
$$+ (x-y)^2 \sum_{r=2}^{M} z^{r-1}(1-xy)^{r-2} G^{even}_{M-r}$$
$$- z^{M-1}(1+xy)^{M-1}(x+y) \qquad M \geq 2$$

$$G_1(x, y, z) = (1-xy)G_o - (x+y)$$

$$G_o = 1 \qquad (4.21)$$

Define

$$g(v, x, y, z) = \sum_{M=0}^{\infty} v^M G_M(x, y, z) \qquad (4.22)$$

Thus

$$g(v, x, y, z) = v\,g(v, x, y, z) - v\,x\,y\,g(v, -x, -g, +z)$$
$$+ \tfrac{1}{2}\frac{(x+y)^2 v^2 z}{1 - v\,z(1+xy)}\left\{g(v,x,y,z) - g(v,-x,-y,z)\right\}$$
$$+ \tfrac{1}{2}\frac{(x-y)^2 v^2 z}{1 - v\,z(1-xy)}\left\{g(v,x,y,z) - g(v,-x,-y,z)\right\}$$
$$- \frac{v(x+y)}{1 - v\,z(1+xy)}$$
$$+ 1. \qquad (4.23)$$

$$g(v\,z\,x\,y)\left\{1 - v - \tfrac{1}{2}\frac{v^2 z(x+y)^2}{1 - v\,z(1+xy)} - \tfrac{1}{2}\frac{v^2 z(x-y)^2}{1 - v\,z(1-xy)}\right\}$$
$$+ g(v,z,-x,-y)\left\{v\,xy + \tfrac{1}{2}\frac{v\,z(x+y)}{1 - v\,z(1+xy)} - \tfrac{1}{2}\frac{v\,z(x-y)}{1 - v\,z(1-xy)}\right\}$$
$$= 1 - \frac{v(x+y)}{1 - v\,z(1+xy)}$$

We can write this as

$$h(v,z,x,y)g(v,z,x,y) + k(v,z,x,y)g(v,z,-x,-y) = l(v,z,x,y)$$

$$\therefore\ k(v,z,-x,-y)g(v,z,x,y) + h(v,z,-x,-y)g(v,z,-x,-y)$$
$$= l(v,z,-x,-y)$$

and solution is

$$g(v,z,x,y) = \frac{h(v,z,-x,-y)l(v,z,x,y) - k(v,z,x,y)l(v,z,-x,-y)}{h(v,z,x,y)h(v,z,-x,-y) - k(v,z,x,y)k(v,z,-x,-y)} \qquad (4.24)$$

Obviously

$$g(v,z,-x,-y) = \frac{h(v,z,x,y)l(v,z,-x,-y) - k(v,z,-x,-y)l(v,z,x,y)}{h(v,z,-x,-y)h(v,z,x,y) - k(v\ z\ x\ y)k(v,z,-x,-y)}$$

Here

$$h(v,z,x,y) = 1 - v - \frac{v^2z\{(1 - vz)(x^2 + y^2) + 2vz\,x^2y^2\}}{(1 - vz)^2 - v^2z^2x^2y^2}$$

$$= h(v,z,-x,-y)$$

$$\text{and } k(v,z,x,y) = \left(v\ x\ y + \frac{v^2z\{2xy(1 - vz) + v\ z\ x\ y(x^2 + y^2)\}}{(1 - vz)^2 - v^2z^2x^2y^2}\right)$$

$$= k(v,z,-x,-y)$$

$$\text{and } l(v,z,x,y) = \left(1 - \frac{v(x + y)}{1 - vz(1 + xy)}\right) \qquad (4.25)$$

Let

$$\alpha = 1 - vz(1 + xy)$$

$$\beta = 1 - vz(1 - xy)$$

$$\gamma = v^2z(x - y)^2$$

$$\delta = v^2z(x + y)^2 \qquad (4.26$$

Then after some algebraic manipulation we find that equation (4.24) can be written as

$$g(v,x,y,z) = \frac{\alpha\beta[1 - v(1 + xy)] - \beta v(x + y)[1 - v(1 - xy)] - \delta\beta + \gamma v(x + y)}{\alpha\beta[1 - 2v + v^2(1 - x^2y^2)] - \alpha\delta[1 - v(1 - xy)] - \beta\gamma[1 - v(1 + xy)] + \delta\gamma} \qquad (4.27)$$

Substituting for α, β, γ, δ in (4.27) and rearranging in powers of v we find that

$$g(v,x,y,z) = \frac{1 + Av + Bv^2 + Cv^3}{1 + Ev + Fv^2 + Gv^3 + Hv^4} \qquad (4.28)$$

Here

$$A = -(1 + x)(1 + y) - 2z$$

$$B = (x + y)(1 - xy) - z(x + 1)(y + 1)(x + y - 2) + z^2(1 - x^2y^2$$

$$C = -z(x + y)(1 - x^2)(1 - y^2) - z^2(1 - xy)(1 - x^2)(1 - y^2)$$

$$E = -2(1 + z)$$

$$F = (1 - x^2y^2) - 2z(x^2 + y^2 - 2) + z^2(1 - x^2y^2)$$

$$G = -2z(1 + z)(1 - x^2y^2) + z(x - y)^2\{1 + xy + z(1 - xy)\}$$
$$+ z(x + y)^2\{1 - xy + z(1 + xy)\}$$

$$H = z^2(1 - x^2 - y^2 - 2xy - x^2y^2)(1 - x^2 - y^2 + 2xy - x^2y^2)$$
(4.29)

If we expand out (4.28) using the binomial theorem, we find that the coefficients of v and v^2 are given by G_1 and G_2 as in (4.20). This acts as a check on our formulation and evaluation of the difference equation.

We note that the solution (4.28) to the difference equation (4.21) is a rational function in v from which a new difference equation can be derived[32]. We write

$$(1 + Ev + Fv^2 + Gv^3 + Hv^4)g(v, x, y, z) = 1 + Av + Bv^2 + Cv^3 \qquad (4.30)$$

and use the expansion (4.22) for g(v, x, y, z). Equating coefficients of v^M in (4.30) we find

$$G_M + EG_{M-1} + FG_{M-2} + GG_{M-3} + HG_{M-4} = 0 \quad M \geq 4 \qquad (4.31)$$

Thus we see that our original difference equation (4.21), which was complicated because of the sign factor $n + n_1n_2$

can be reduced to the difference equation (4.31).

We are interested in the asymptotic value for large M of $G_M(x, y, z)$ which is given by the coefficient of v^M in the expansion of (4.28). The critical equation $G_M(x, y, z) = 0$ will give the critical temperature for a large number of bonds between cells. In the following discussion we consider only the case in which all the bond weights are equal, $x = y = z (= x$ say).

The rational function (4.28) can be expanded[33] in terms of the roots of the denominator. Suppose the denominator has 4 unequal roots $\frac{1}{\beta_1}, \frac{1}{\beta_2}, \frac{1}{\beta_3}, \frac{1}{\beta_4}$ whose order of magnitude is such that

$$\left|\frac{1}{\beta_1}\right| < \left|\frac{1}{\beta_2}\right| < \left|\frac{1}{\beta_3}\right| < \left|\frac{1}{\beta_4}\right|$$

Then (4.28) can be written in partial fractions are

$$g(v, x) = \frac{\alpha_1}{1 - \beta_1 v} + \frac{\alpha_2}{1 - \beta_2 v} + \frac{\alpha_3}{1 - \beta_3 v} + \frac{\alpha_4}{1 - \beta_4 v} \qquad (4.32)$$

Expanding by the binomial theorem and selecting the coefficient of v^M we have from (4.22)

$$G_M(x) = \sum_{i=1}^{4} \alpha_i(x)\, \beta_i^M(x) \qquad (4.33)$$

where $\frac{1}{\beta_i(x)}$ are the roots of

$$1 + Ev + Fv^2 + Gv^3 + Hv^4 = 0 \qquad (4.34)$$

Alternatively $\beta_i(x)$ are the roots of the characteristic equation of the difference equation (4.31). Using equation (4.32) we find

$$\alpha_i(x) = \lim_{v \to \frac{1}{\beta_i}} \frac{(1 - \beta_i v)(1 + Av + Bv^2 + Cv^3)}{1 + Ev + Fv^2 + Gv^3 + Hv^4}$$

$$= - \left(\frac{\beta_i^3 + A\beta_i^2 + B\beta_i + C}{E\beta_i^3 + 2F\beta_i^2 + 3G\beta_i + 4H} \right) \beta_i \qquad (4.35)$$

The critical equation for determining $x = \tanh \beta J$ and hence the critical temperature is

$$\sum_{i=1}^{4} \alpha_i(x) \, \beta_i^M(x) = 0 \qquad (4.36)$$

The roots $\beta_i(x)$ are independent of M since they are just the reciprocals of the roots of (4.34) which does not depend on M. However, the solution to the critical equation (4.36) will depend on M, say $x_0(M)$. In principle the quartic equation (4.34) can be solved in terms of the coefficients and the roots $\beta_i(x)$ determined. In practice the problem would be handled best on a computer.

There are several cases for which the equation (4.36) could give a critical temperature.

(1) If $|\beta_i(x)| > 1$ for some i, then a necessary condition for (4.36) to have a solution is that

$$\lim_{M \to \infty} \alpha_i(x) = 0$$

If this condition is not satisfied the term $\alpha_i(x)\beta_i^M(x)$ will not be finite.

(2) If $|\beta_1(x)| = 1$ and $|\beta_i(x)| < 1$ for $i = 2, 3, 4$, then for large M we must have $\alpha_i(x) = 0$. From (4.35) we see that this condition is

$$1 + A + B + C = 0$$

(3) If $|\beta_i(x)| < 1$ for all i then equation (4.36) is automatically satisfied for large M. There is possibly a range of x such that $|\beta_i(x)| < 1$. This suggests that there could be a range of critical temperatures.

From equation (3.26) we find that the critical equation for the case $\theta = \phi = \pi$ is the same as the case we have considered. Theother two critical equations corresponding to $\theta = \pi$, $\phi = 0$ and $\theta = 0$, $\phi = \pi$ give the same equation which can be found using the above method with a sign factor $n - n_1 n_2$.

CHAPTER 5

COMPARISON WITH OTHER MODELS.

5.1 Domb's model with general s.

Domb[27] has suggested a model in which each cell of the lattice has one spin variable s whose z component s_z takes $(2s + 1)$ values $-s, -s + 1, \ldots, s$. The interaction energy between cells (spins) is defined as

$$E_{ij} = - \frac{J}{s^2} s_{zi} s_{zj} \qquad (5.1)$$

where the division by s^2 normalises the interaction energy i the sense that the maximum and minimum interaction energies between cells are $\pm J$. The partition function for such a model is

$$Z = \sum_{s_{zi} = -s}^{s} \prod_{i,j} \exp\{4K\, s_{zi} s_{zj}\} \qquad (5.2)$$

Here $K = \beta J/4s^2$ and the product is taken over all nearest neighbour pairs of spins on the lattice.

In order to transform the partition function to a combinatorial problem the exponential is expanded giving

$$\exp\{4K\, s_{zi} s_{zj}\} = \sum_{r=0}^{\infty} \frac{(4K)^r}{r!} (s_{zi} s_{zj})^r \qquad (5.3)$$

The general term in this expansion can be interpreted as bonds of multiplicity r between the spins s_{zi} and s_{zj}. When the product of such terms is taken as in (5.2) the general term in $(4K)^l$ will contain contributions from all possible configurations which can be drawn on a lattice with l bonds. Each configuration is represented by a product $s_{zi} s_{zj} \cdots s_{zk}$ with one $s_{zi} s_{zj}$ for each bond.

In any configuration a vertex which is the meeting point of "a" lines will give rise on summation over the values of s_{zi} to a factor

$$t_a = \sum_{s_{zi} = -s}^{s} s_{zi}^{a} \qquad (5.4)$$

Let C_l be the number of occurrences of a given configuration with l bonds on the lattice, and suppose that the bonds of the configuration have multiplicity α, β, γ, ... and the vertices have multiplicity a, b, c, ... then

$$\alpha + \beta + \gamma + \ldots\ldots = \tfrac{1}{2}(a + b + c + \ldots\ldots) = l$$

and the partition function (5.2) becomes

$$Z = t_o^N \left[1 + \sum_{l=1}^{\infty} (4K)^l \sum_{C_l} \frac{C_l \frac{t_a}{t_o} \frac{t_b}{t_o} \frac{t_c}{t_o} \ldots\ldots}{\alpha!\, \beta!\, \gamma! \ldots\ldots} \right] \qquad (5.5)$$

Since $t_a = 0$ if a is odd, only configurations all of whose vertices are even contribute. The C_l have been calculated for small values of l by Domb et al for various lattices.

In the case $s = \frac{1}{2}$ the z component takes two values of spin $s_{zi} = \frac{1}{2}\sigma_i = \pm\frac{1}{2}$ and the equation (5.3) reduces to

$$\exp(K \sigma_i \sigma_j) = \cosh K + \sigma_i \sigma_j \sinh K$$

since $\sigma_i^{\,a} = \begin{cases} 1 & \text{if a is even} \\ \sigma_i & \text{if a is odd.} \end{cases}$

This is equation (1.6) and the partition function (5.2) in this case gives rise to the problem of counting closed polygons on the lattice with single bonds between spins. Thus it corresponds to the model described in the introduction with one spin to each cell for which an exact solution can be found for the square and triangular lattices

In the case s = 1 the z component takes three values $s_{zi} = 1, 0, -1$ so the product $s_{zi}s_{zj}$ has values +1, 0, -1. The equation (5.3) gives

$$\exp\{K\, s_{zi}s_{zj}\} = 1 + 4K\, s_{zi}s_{zj} + \tfrac{1}{2}(4K\, s_{zi}s_{zj})^2 + \ldots.$$

$$= 1 + s_{zi}s_{zj} \sin 4K + (s_{zi}s_{zj})^2(\cosh 4K - 1)$$

$$= 1 + s_{zi}s_{zj}\, 2 \sinh 2K \cosh 2K + (s_{zi}s_{zj})^2\, 2 \sinh^2 2K \qquad (5.6)$$

When (5.6) is substituted in (5.3) the problem becomes that of counting the number of occurrences of polygons with an even number of bonds to each cell that can be drawn on the lattice with both single and double bonds between cells. The single bonds have a weight $2 \sinh 2K \cosh 2K$ and the double bonds a weight $2 \sinh^2 2K$. Fig. 5.1 shows some of the configurations with 6 bonds that can be drawn on a triangular lattice.

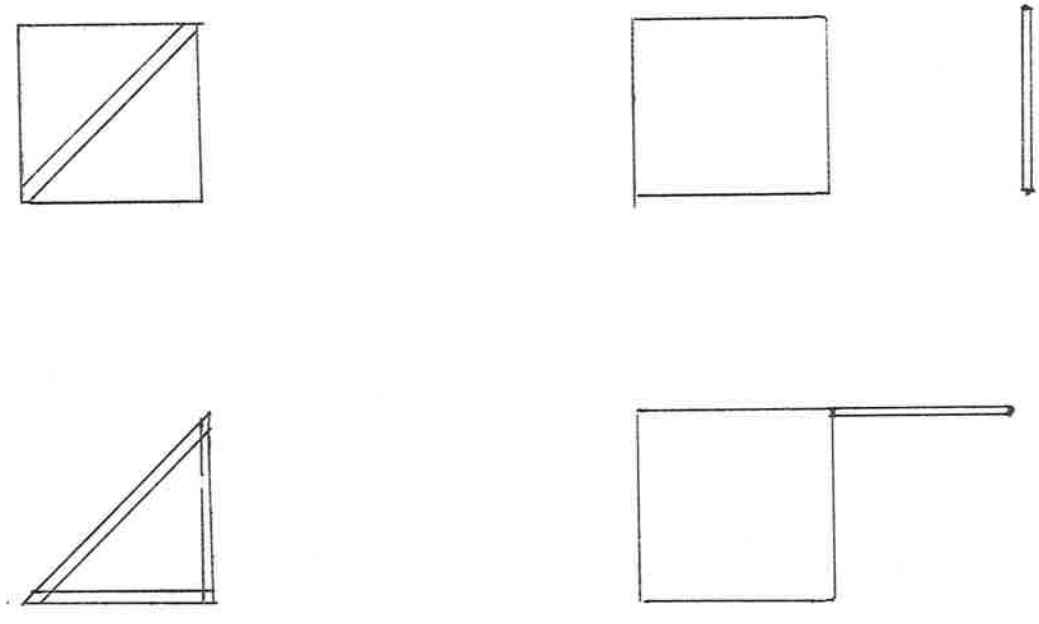


Fig. 5.1

An exact solution to this problem has not been found but the number of occurrences of polygons with a small number of bonds has been calculated.[27]

This case can be compared with the model proposed in Chapter 2 with two spins to each cell. There the z component of the spin has four values 1, 0, 0, -1 corresponding to the ++, +-, -+, and -- states of the cell respectively. We can try to obtain a 3 state model by removing one state (say +-) from the lattice. However the invariance of the states of the cell under total spin reversal, relation (2.10), means that the -+ state is also removed and we return to the two state model as shown in section 2.1. The equation (2.10) is a consequence of making the energy of interaction between cells a quadratic function of the spin variables, relation (2.9). Thus if we are to remove only the +- state from the lattice, then we have to relax the condition (2.9). Then the interaction energy between cells (2.5) will involve the multiple point interactions and does not give rise to a combinatorial problem which can be solved by the Pfaffian method. It appears therefore that Domb's model corresponds to our model with multiple point interactions. The future study of multiple point interactions may throw further light on the exact solution of Domb's model.

5.2 Green's model with f spins to a Cell.

Green[25] has considered a model similar to ours in which there are f spin half variables to each cell of the lattice. He suggests that the partition function can be expressed in

terms of the generating function

$$R(x_1, x_2, x_3, x_4) = \sum_{s} \prod_{j=1}^{N} (1 + x_1 s_j s_{j+1})(1 + x_3 s_j s_{j+m})$$

$$(1 + x_2 s_j s_{j+m+1} + x_4 s_{j+1} s_{j+m} - x_2 x_4 s_j s_{j+1} s_{j+m} s_{j+m+1}) \quad (5.7)$$

in all cases where the partition function can be found exactly. Such a generating function corresponds to the partition function of a lattice with one spin to each cell and interactions with the next nearest neighbour as shown in Fig. 5.2.

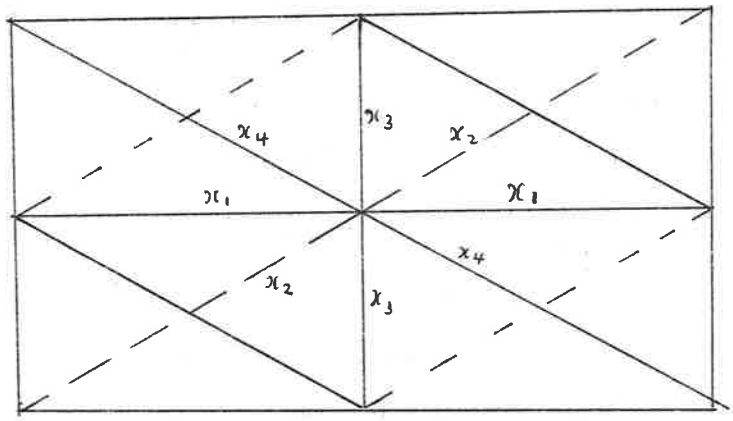


Fig. 5.2

The lattice is not a physical Ising lattice since the crossed bond term is negative. Green shows how this generating function can be evaluated by the Pfaffian method giving an 8 × 8 determinant.

The lattice can also be solved by the method developed in this work. The cell terminals are as shown in Fig. 5.3.

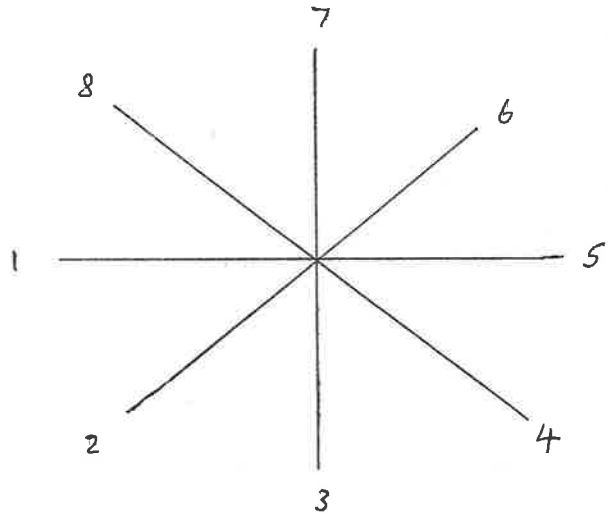


Fig. 5.3

Since there is only one spin to each cell then all the weight factors are unity. Thus the 8 × 8 determinant is given by (3.6) as

$$\Delta(e^{i\theta}, e^{i\phi}) = 1^2 \times$$

$$\begin{vmatrix} 0 & +1 & +1 & 1 & 1+x_1 e^{i\theta} & 1 & 1 & 1 \\ -1 & 0 & 1 & 1 & 1 & 1+x_2 e^{i(\theta+\phi)} & 1 & 1 \\ -1 & -1 & 0 & 1 & 1 & 1 & 1+x_3 e^{i\phi} & 1 \\ -1 & -1 & -1 & 0 & 1 & 1 & 1 & 1+x_4 e^{i(\phi-\theta)} \\ \{-1-x_1 e^{-i\theta}\} & -1 & -1 & -1 & 0 & 1 & 1 & 1 \\ -1 & \{-1-x_2 e^{-i(\theta+\phi)}\} & -1 & -1 & 1 & 0 & 1 & 1 \\ -1 & -1 & \{-1-x_3 e^{-i\phi}\} & -1 & -1 & -1 & 0 & 1 \\ -1 & -1 & -1 & \{-1-x_4 e^{-i(\phi-\theta)}\} & -1 & -1 & -1 & 0 \end{vmatrix} \qquad (5.8)$$

If the work in section 3.2 is extended to accommodate a further term (p_4, q_4), the determinant can be expanded by our method in terms of the coefficient $D(1_n;i_p;j_q;k_m)$ of $x_1^{\alpha_1} \ldots x_4^{\alpha_4} \exp i\{(p_1 + p_2 - p_4 - q_1 - q_2 + q_4)\theta + (p_2 + p_3 + p_4 - q_2 - q_3 - q_4)\phi$ by using the weight factors. The result (3.17)' is the same but the sign factor (3.18)' is

$$W = \tfrac{1}{2}\{(p_1 + q_1)(2n_1 + p_1 + q_1) + (p_2 + q_2)(2n_2 + p_2 + q_2) + (p_3 + q_3)(2n_3 + p_3 + q_3) + (p_4 + q_4)(2n_4 + p_4 + q_4) + (p + q)(2n + p + q)\} \qquad (5.9)$$

Since the selection of x_1 and x_2 from above the diagonal but not from below diagonal removes the first two rows but not the first two columns then $D(1;12i;j;k) = 0$.

Similarly

$$D(1;23i;j;k) = 0$$

$$D(1;34i;j;k) = 0$$

$$D(1;1i;4j;k) = 0.$$

The only non zero coefficients are those in which the selections $\{a, b\}$ all form an odd permutation of the set $\{i,j,i',j',\}$. This is a consequence of the weight factors being all unity and the factor $(-)^P$ where P is the parity of the permutation to rearrange the sets of indices $\{a, b\}$ and $\{a, b\}'$ in numerical order. The non zero coefficients and the terms associated with them are listed below

$$D(1_n;0;0;k_m) \rightarrow (1 + x_1^2)(1 + x_2^2)(1 + x_3^2)(1 + x_4^2)$$

$$D(1_n;1;0;k_m) \rightarrow -x_1 \cos\theta(1 - x_2^2)(1 - x_3^2)(1 - x_4^2)$$

$$D(1_n;2;0;k_m) \rightarrow -x_2 \cos(\theta + \phi)(1 - x_1^2)(1 - x_3^2)(1 - x_4^2)$$

$$D(1_n;3;0;k_m) \rightarrow -x_3 \cos\phi(1 - x_1^2)(1 - x_2^2)(1 - x_4^2)$$

$$D(l_n;4;0;k_m) \rightarrow -x_4\cos(\theta - \phi)(1 - x_1^2)(1 - x_2^2)(1 - x_3^2)$$

$$D(l_n;13;2;k_m) \rightarrow +4x_1x_2x_3 \cos 0(1 - x_4^2)$$

$$D(l_n;14;2;k_m) \rightarrow +4x_1x_2x_4 \cos \theta(1 - x_3^2)$$

$$D(l_n;14;3;k_m) \rightarrow +4x_1x_3x_4 \cos 0(1 - x_2^2)$$

$$D(l_n;24;3;k_m) \rightarrow +4x_2x_3x_4 \cos \phi(1 - x_1^2)$$

$$D(l_n;i_p;j_q;k_m) = D(l_n;j_q;i_p;k_m).$$

Summing these results gives

$$\begin{aligned}\Delta(e^{i\theta}, e^{i\phi}) &= (1 + x_1^2)(1 + x_2^2)(1 + x_3^2)(1 + x_4^2) \\ &+ 8x_1x_3\{x_2(1 - x_4^2) + x_4(1 - x_2^2)\} \\ &+ 2x_1(1 - x_3^2)\cos\theta\{4x_2x_4 - (1 - x_2^2)(1 - x_4^2)\} \\ &+ 2x_3(1 - x_1^2)\cos\phi\{4x_2x_4 - (1 - x_2^2)(1 - x_4^2)\} \\ &- 2x_2(1 - x_4^2)(1 - x_1^2)(1 - x_3^2)\cos(\theta + \phi) \\ &- 2x_4(1 - x_2^2)(1 - x_1^2)(1 - x_3^2)\cos(\theta - \phi) \qquad (5.10)\end{aligned}$$

which agrees with Green's[25] equation (30) with $\omega = e^{i\theta}$ and $\eta = e^{i\theta}$.

Green gives several examples of lattices with f spin to a cell. He shows in the examples considered that f - 1 of the spins can be summed over and the partition function expressed in terms of the generating function (5.7). Green considers the Yamamoto lattice for which the energy of interaction (2.11) is

$$E = -\sum_i\{J_1^{21}\sigma_{i_2}\sigma_{i+1_1} + J_{n+1}^{12}\sigma_{i_1}\sigma_{i+n+1_2} + J_n^{12}\sigma_{i_1}\sigma_{i+n_2} + J_0^{12}\sigma_{i_1}\sigma_{i_2}\} \qquad (5.11)$$

The partition function is

$$\begin{aligned}Z = \text{const.}\sum_\sigma \prod_i &(1 + x_1^{21}\sigma_{i_2}\sigma_{i+1_1})(1 + x_{n+1}^{12}\sigma_{i_1}\sigma_{i+n+1_2}) \\ &(1 + x_n^{12}\sigma_{i_1}\sigma_{i+n_2}) \ldots (1 + x_0^{12}\sigma_{i_1}\sigma_{i_2}) \qquad (5.12)\end{aligned}$$

Green's method is to change the factors $(1 + x_{n+1}^{12}\sigma_{i_1}\sigma_{i+n+1_2})$

$(1 + x_n^{12}\sigma_{i_1}\sigma_{i+n_2})$ to $(1 + x_{n+1}^{12}\sigma_{i-n-1_1}\sigma_{i_2})(1 + x_n^{12}\sigma_{i-n_1}\sigma_{i_2})$ under the product $\prod_i$ and then sum over the values of σ_{i_2}.

Now the partition function is expressed in term of only one spin variable σ_{i_1} as in (5.7).

Now we shall show that Green's method is not applicable to the lattices considered in this work by using the lattice Fig. 2.3(a) which has been investigated in section 4.1. The interaction energy for this (2, 3, 1, 1, 1) lattice is given by (2.11) as

$$E = -\sum_i \{ J_1^{11}\sigma_{i_1}\sigma_{i+1_1} + J_1^{12}\sigma_{i_1}\sigma_{i+1_2} + J_1^{22}\sigma_{i_2}\sigma_{i+1_2} + J_{n+1}^{21}\sigma_{i_2}\sigma_{i+n+1_1} + J_n^{21}\sigma_{i_2}\sigma_{i+n_1} + J_0^{12}\sigma_{i_1}\sigma_{i_2}\} \qquad (5.13)$$

The partition function will therefore involve the factors $(1 + x_1^{11}\sigma_{i_1}\sigma_{i+1_1})$ and $(1 + x_1^{22}\sigma_{i_2}\sigma_{i+1_2})$. These factors prevent summation over either σ_{i_1} or σ_{i_2} since it is necessary to isolate σ_{i_1} before summation with respect to that variable. We note that if $J_1^{11} = J_1^{22} = 0$ (i.e. $x_1 = x_3 = 0$ in notation of section 4.1) the expression (5.13) reduces to that of the Yamamoto lattice (5.11). We conclude therefore that Green's method is not applicable to lattices with multiple bonds between cells.

5.3 Potts' multiple state model.

Potts[28,30] has considered the critical behaviour of a square lattice in which there are r states to each cell by using the Kramers and Wannier[3] inversion formula under which the partition function is invariant when the temperature is transformed from a high to a low value. He represents the

r configurations of a cell by a vector which can point in any one of r symmetrically placed directions. Fig. 5.4 shows the vector representation for r = 2, 3 and 4.

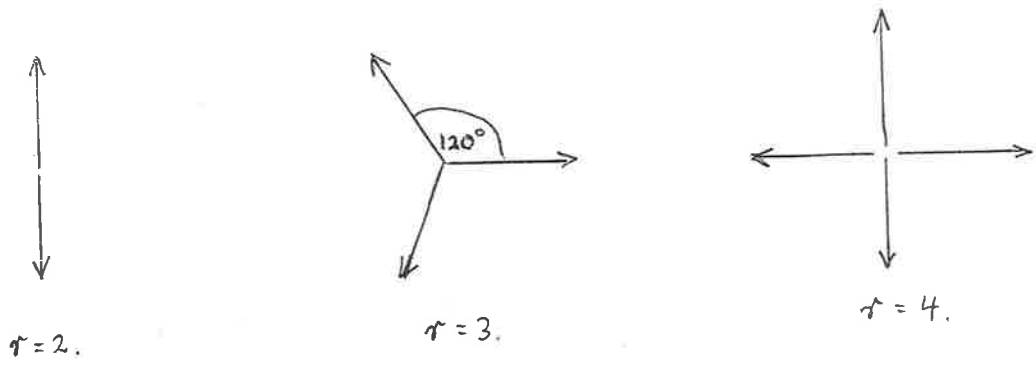


Fig. 5.4

Potts assumes that the energy of interaction between two neighbouring cells is proportional to the scalar product of the vectors representing the states of the cells. The model does not correspond to a higher value of spin like the model of Domb, but corresponds to the models suggested in this work and by Green in which the states of the cell represent physical states rather than electronic spin.

The case of two states to each cell corresponds to usual square Ising lattice with interaction energies

$-J$ between parallel vectors

$+J$ between antiparallel vectors.

The transition point of the lattice is given by

$$\frac{x_0}{x_1} = e^{2K} = (1 + \sqrt{2})$$

where $x_0 = \exp K_0 = \exp(\beta J)$ and $x_1 = \exp -K = \exp -\beta J$.

For the case of three states to each cell there are two different energies of interaction

J_0 between parallel vectors

J_1 between vectors at 120°.

Potts shows that the transition point of the lattice in this case is given by

$$\frac{x_0}{x_1} = 1 + \sqrt{3}$$

where $x_0 = \exp(-\beta J_0)$ and $x_1 = \exp(-\beta J_1)$. We have seen in section 5.1 that our model cannot be reduced from a 4 state to a 3 state model without relaxing the condition that the energy of interaction is a quadratic expression in the spin variables. The interaction energy then involves multiple point interactions and the Pfaffian method is not applicable.

For the case of four states to each cell the interaction energies are

$-J$ between parallel vectors

J between antiparallel vectors

0 between perpendicular vectors.

Potts shows that the transition temperature of the lattice for this case is

$$\frac{x_0}{x_1} = e^{2K} = 3 + \sqrt{8} \qquad (5.14)$$

where $x_0 = \exp K = \exp(\beta J)$ and $x_1 = \exp(-K) = \exp(-\beta J)$. Our model for f = 2 has the four states ++, +−, −+, and −−. Therefore our model will correspond to that of Potts if we choose

$$\begin{aligned} E^{++,++} &= E^{+-,+-} = E^{-+,-+} = E^{--,--} = -J \\ E^{++,--} &= E^{--,++} = E^{+-,-+} = E^{-+,+-} = J \\ E^{++,+-} &= E^{++,-+} = E^{--,+-} = E^{--,-+} = 0 \\ E^{+-,++} &= E^{-+,++} = E^{+-,--} = E^{-+,--} = 0 \end{aligned} \qquad (5.15)$$

The energy of interaction between the i^{th} and j^{th} cells is given by (2.5) as

$$E_{ij} = -\tfrac{1}{2}J\sigma_{i_1}\sigma_{j_1} - \tfrac{1}{2}J\sigma_{i_2}\sigma_{j_2} \qquad (5.16)$$

Thus the energy of a particular state of a square lattice is given by (2.3) as

$$E = \sum_i \{E_{ii+1} + E_{ii+n}\}$$

$$= -\sum_i \tfrac{1}{2}J\{\sigma_{i_1}\sigma_{i+1_1} + \sigma_{i_1}\sigma_{i+n_1} + \sigma_{i_2}\sigma_{i+1_2} + \sigma_{i_2}\sigma_{i+n_2}\}$$

The partition function (2.4) for $K = \beta J$ is

$$Z = \sum_{\sigma_{i_1}} \sum_{\sigma_2} \prod_{i=1}^{N} \exp\tfrac{K}{2}\{\sigma_{i_1}\sigma_{i+1_1} + \sigma_{i_1}\sigma_{i+n_1} + \sigma_{i_2}\sigma_{i+1_2} + \sigma_{i_2}\sigma_{i+n_2}\}$$

$$= \left[\sum_{\sigma_1} \prod_{i=1}^{N} \exp\tfrac{K}{2}\{\sigma_{i_1}\sigma_{i+1_1} + \sigma_{i_1}\sigma_{i+n_1}\}\right]\left[\sum_{\sigma_2} \prod_{i=1}^{N} \exp\tfrac{K}{2}\{\sigma_{i_2}\sigma_{i+1_1} + \sigma_{i_2}\sigma_{i+n_2}\}\right]$$

$$= Z_1^2$$

where Z_1 is the partition function of a square lattice with one spin to each cell. The critical point of Z will be the same as that of Z_1 with a bond energy half the usual value.

i.e. $e^K = 1 + \sqrt{2}$

$$\therefore \quad \frac{x_0}{x_1} = e^{2K} = 3 + \sqrt{8}$$

This is the value obtained by Potts, equation (5.14). It can be seen from (5.15) and (5.16) that the model considered by Potts with 4 states to a cell is a degenerate form of our model. The energies of interaction separate out and the lattice corresponds to the superposition of two non-interacting square Ising lattices similar to that shown in Fig. 2.3(c) for the triangular case. It can be seen that the interaction energy (5.16) involves only the quadratic terms and the multiple point interactions are not present.

5.4 Fisher's derived lattices.

Fisher[14] has shown how the partition function of a class of Ising lattices can be derived from that of known lattices by means of the dual, the decorating, and the star-triangle transformations. Thus the hexagonal lattice can be obtained from the triangle lattice by a dual or a star-triangle transformation, and the Kagomé lattice can be obtained from the hexagonal lattice by a decoration transformation followed by a star-triangle transformation. We shall consider these transformations in the absence of an external field as only the super-exchange lattice[29] is exactly soluble in the presence of an external field.

In the decoration transformation the centre spin, which may be an arbitrary statistical mechanical system is coupled to two cells with one spin half variable as shown in Fig. 5.5.

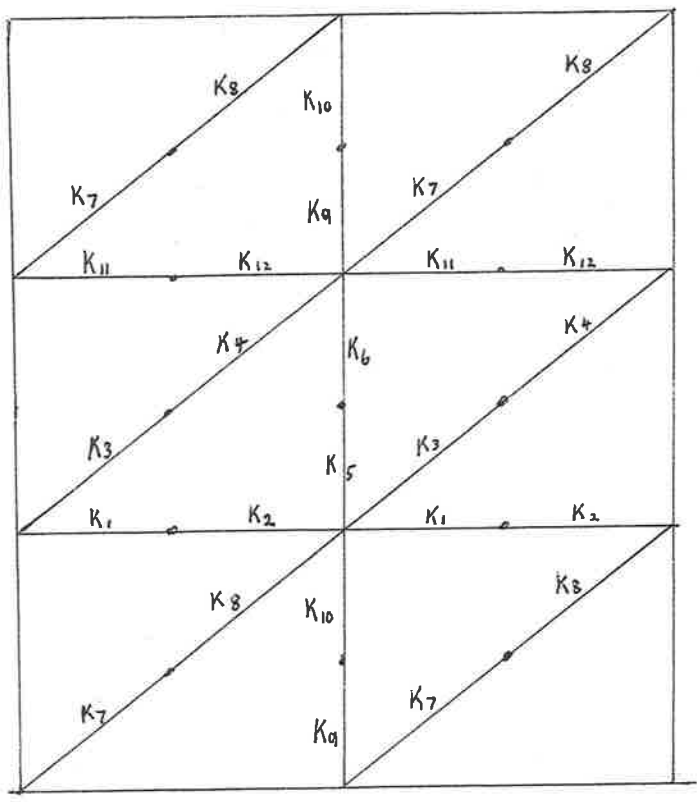
Fig. 5.5

Fisher shows that the states of the decorating spin can be summed over giving a factor f which is a function of the bond energies K_1 and K_2 and reducing the partition function of the decorating lattice to that of the known lattice with modified bond weights.

$$Z_{\text{Decorated}}(K) = f^{N_D} Z_{\text{Known}}(K') \qquad (5.17)$$

where N_D is the number of decorated bond weights. In practice

bonds must be decorated in a periodic manner so that the bonds of the known lattice are modified in a regular way. In this work we have extended the known solutions to lattices with a periodic structure of bond weights and hence we have extended the range of application of the decoration transformation. For example the partition function for a triangular lattice decorated as shown in Fig. 5.6 can be expressed in terms of the partition function whose determinant is (4.5) found in section 4.1 by using (5.17).



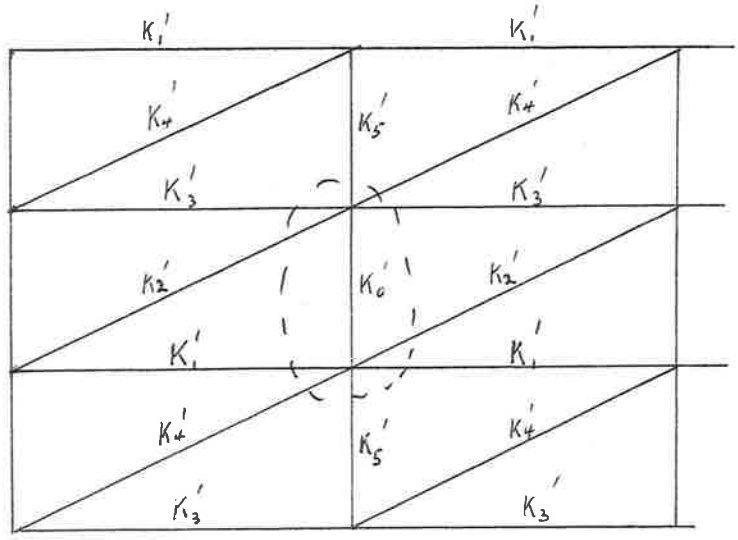


Fig. 5.6

In the star-triangle transformation the centre spin is coupled to three cells with one spin half variable as shown in Fig. 5.7.

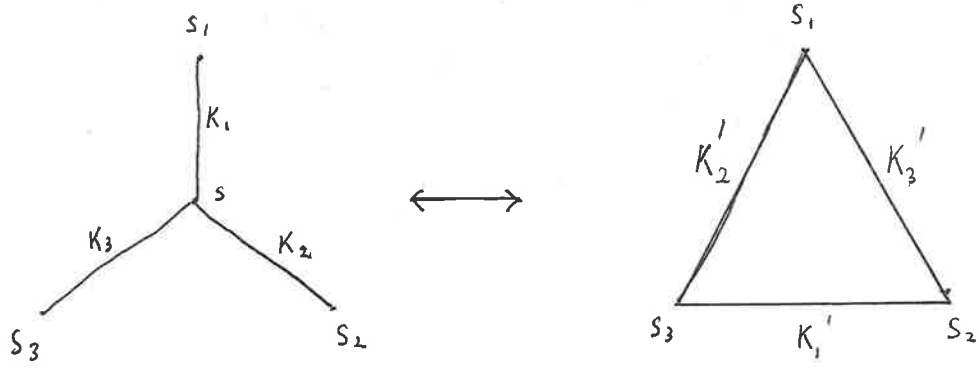


Fig. 5.7

Again Fisher shows that the states of the decorating system can be summed over given a factor f which is a function of the bond energies K_1, K_2 and K_3. Provided the states of the decorating system are invariant under

total spin reversal the partition function of the decorated (starred) lattice can be expressed in terms of the known lattice.

$$Z_{Star}(K) = f^{N_S} Z_{Known}(K')$$

where N_S is the number of star-vertices. Since we have extended the class of triangular lattices which can be solved exactly, the class of lattices which can be derived by the star-triangle transformation has been extended. For example the hexagonal lattice with a double period shown in Fig. 5.8 gives rise to the lattice shown in Fig. 2.3(a) under the star triangle transformation.

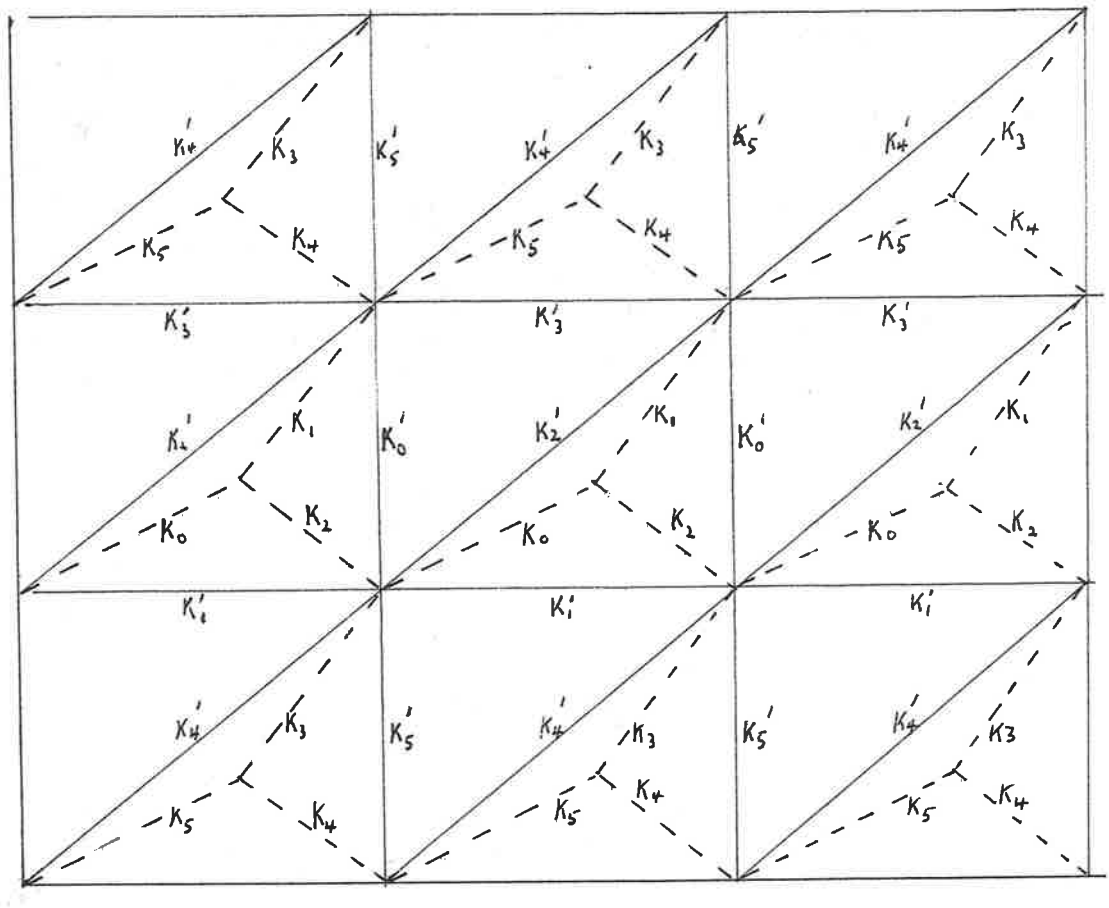


Fig. 5.8

Fisher remarks that transformations where the centre spin is attached to 4 or more spins involve considerable restrictions on the decorating system and are likely to be of little interest. However, the method used by Green[25] for the Yamamoto lattice, which was discussed in section 5.2, corresponds to the case of a centre spin attached to 4 spins as shown in Fig. 5.9.

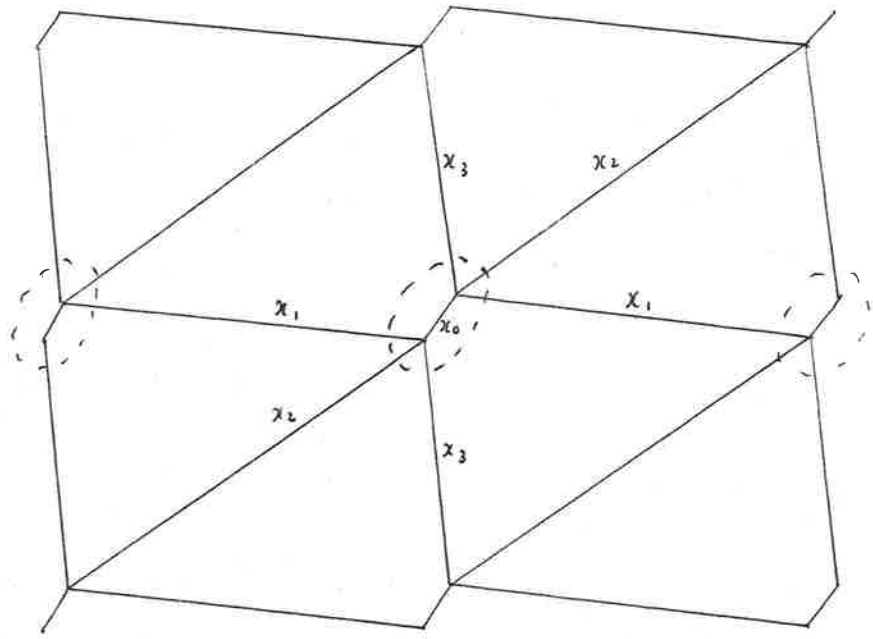


Fig. 5.9

Green sums over the top spin of the cell reducing the partition function to that of the lattice shown in Fig. 5.2 with a negative crossed bond term. Green's paper shows that the modification of the bond weights in this transformation is very involved.

Then Fisher shows how the partition function for a variety of lattices can be derived from the partition function of a known lattice by a series of decorating and star-triangle transformations. In Fisher's paper the

decorations will all be similar since the known lattice must have similar bond weights. As we have extended the class of known lattices to those whose bond weights have a periodic planar structure, then we have extended Fisher's derived lattices to those which have a periodic decorated structure. Fisher considers the case of Ising lattices which are decorated with spins of arbitrary magnitude S as shown in Fig. 5.10.

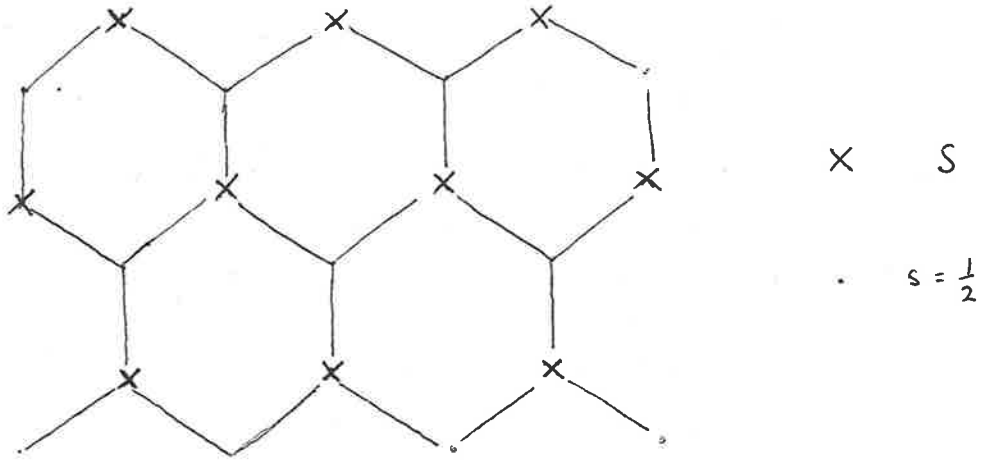


Fig. 5.10

By summing over the spins of magnitude S this reduces to a triangular lattice. Our extension to the class of known lattices enables the partition function of a lattice decorated with alternate spins S_1 and S_2 to be found as shown in Fig. 5.11.

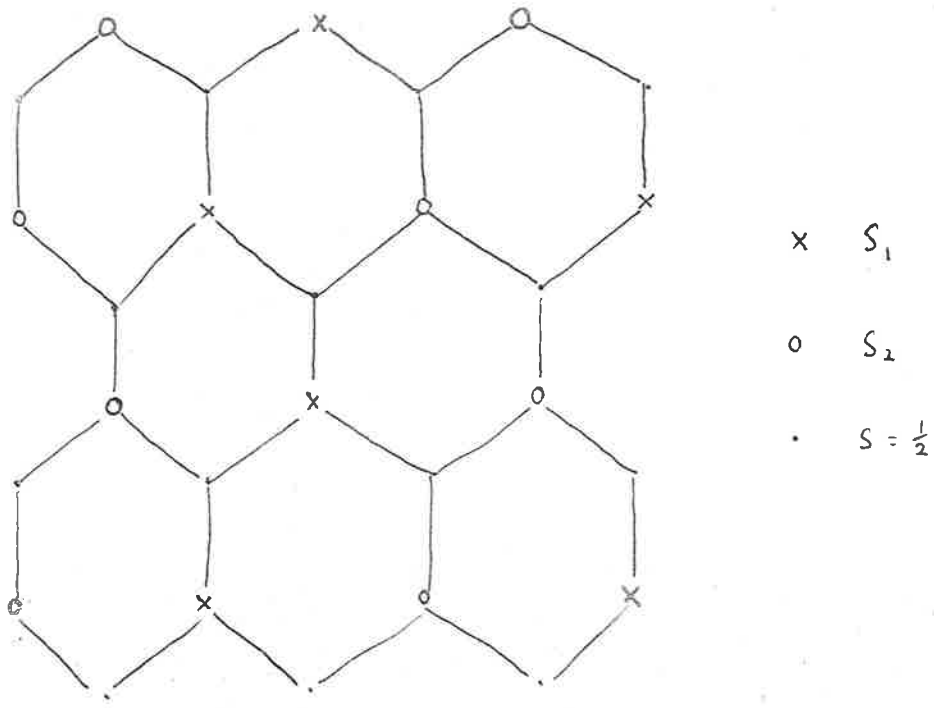


Fig. 5.11

By summing over both S_1 and S_2 the partition function of the lattice can be expressed in terms of the lattice shown in Fig. 2.3(a). Although our method does not solve Fisher's decorated lattices directly, the transformed lattices can be solved by our method and our class of exact solutions extends the range of decorated lattices with exact solutions.

Fisher also considers the "diced" lattice (his Fig. 5(a)) which can be derived from the triangular lattice by a triangle-star, a decorating, a star-triangle, and a dual transformation. The lattice is shown in Fig. 5.12.

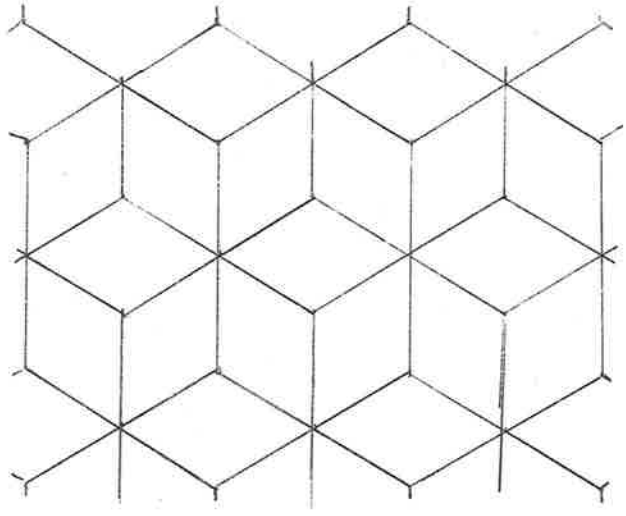


Fig. 5.12

The number of different bonds on the lattice can only be increased by the decorating transformation as shown in Fig. 5.5. Thus the partition function of the "diced" lattice with 6 different bond weights can be expressed in terms of the partition function of the known triangular lattice with 3 different bond weights.

$$Z_{\text{diced}} \sim Z_{\text{kagome}} \sim Z_{\text{decorated Hexagonal}} \sim Z_{\text{hexagonal}} \sim Z_{\text{triangular}}$$

The "diced" lattice can be classified according to the convention given in section 2.3. The cell structure of the lattice is shown in Fig. 5.13.

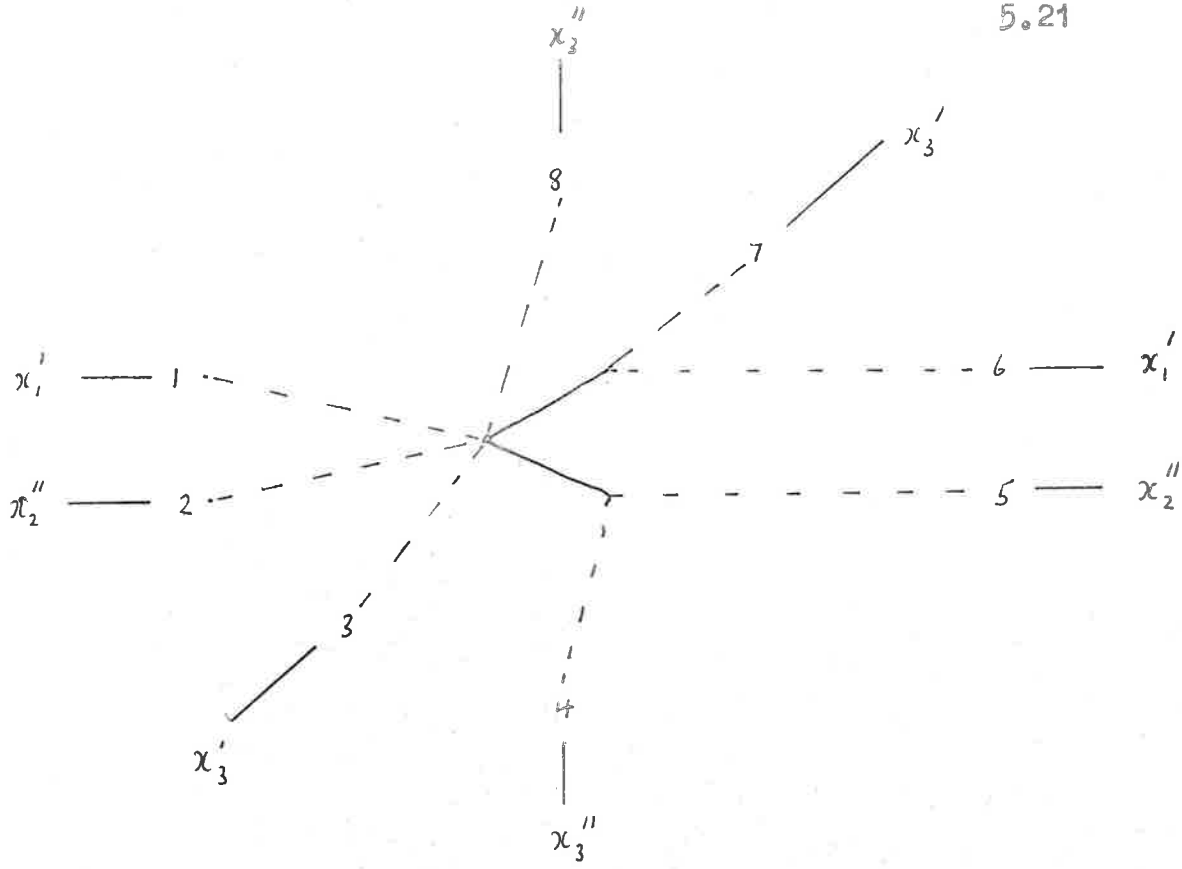


Fig. 5.13

It can be seen that it belongs to the (3, 2, 1, 1, 2) class of lattices. The bond weights x' and x" refer to the x bond of the original triangular lattice which has been doubled during the decoration process. It can be seen that Fisher's derived lattices belong to our class of multiple state lattices. If we put $x_1'' = 1$ then the lattice becomes a (2, 2, 1, 1, 1) lattice which is not as general as our (2, 3, 1, 1, 1) lattices. In both the (3, 2, 1, 1, 2) and the (2, 2, 1, 1, 1) lattices of Fisher the right hand side spins can be summed over giving a 2 state model, since all the bonds from the right hand

spins connect to left hand spins only in neighbouring cells. Fisher's decorations have the effect of producing a multiple state cell with multiple bonds between cells, but the decoration is always introduced in such a way that on summation over the states of the decorating spins the lattice reduces to a known lattice. However, we have seen in comparing our model to that of Green's, the spins of our most general lattice cannot be summed over due to the bonds between like spins in neighbouring cells. We see that our lattices are more general than those of Fisher because our lattices cannot be expressed in terms of the known 2 state lattices whereas Fisher's can.

In a recent paper Fisher[21] considers vertices (cells) which have an arbitrary number of external bonds q connected to them. He shows that a terminal lattice can be constructed at each vertex such that each spin has only 3 bonds connected to it. There is then a one to one correspondence between all polygons on the original lattice and dimers on the terminal lattice. He shows how the partition function for the original lattice can be obtained from the terminal lattice by coalescing spins. Such a model corresponds to that suggested in this thesis and the determinant (3.6) could be found by this method with the help of Kasteleyn's[17] orientation theorem. However, the evaluation of the determinant in terms of the weight factors is best done by using the consistent conditions of Hurst[19].

CHAPTER 6.

CONCLUSION.

The model considered in this work gave rise to a new class of exactly soluble Ising lattices which includes practically all previously solved lattices. A closed expression has been found for both the partition function and the critical temperature for the lattices considered. Due to the complexity of the algebra a limited number of lattices have been solved exactly, but the method of solution is in principle straightforward. It is hoped that the model can be adapted to consider the question of multiple phase transitions.

The characteristic feature of the model is that the extension of the usual model to a multiple state model gave rise to lattices with multiple bonds between cells. One can consider the lattice as a 2 state model with a variety of single bonds between spins or as a multiple state model with multiple bonds between cells. From the manner in which the model was formulated, one can see the conditions which have been applied to the interaction energy between the states of neighbouring cells. It is hoped that these conditions can be relaxed and that either exact or approximate solutions to the problem of multiple point interactions can be found.

In particular the case of 4 point interactions is of

considerable interest. We have seen that the model of Potts does not contain a 4 point interaction although there are 4 states to each cell. Our model can be made to have a 4 point interaction as well as the quadratic terms by an appropriate choice of the terms interaction energies between the states of neighbouring cells. In this case the combinatorial problem has single bonds between cells and a 4 point bond. The lattice cell polynomial is not factorizable for this case and the method developed in chapter 3 does not apply. However, it is hoped that an approximate treatment can be found using this method.

APPENDIX A

PFAFFIANS.

A Pfaffian of order 2N can be defined in terms of antisymmetric quantity $C_{ij} = -C_{ji}$ where i, j are the pairs selected from the set {1, 2, ..., 2N}. The definition is

$$P\{C_{ij}\} \equiv \backslash C_{ij}|$$

$$= \sum_{P} (-1)^{P} C_{i_1 j_1} C_{i_2 j_2} \cdots C_{i_N} C_{j_N}$$

where the summation is over all the permutations of the integers (1, 2, ..., 2N) such that

$$i_1 < i_2 < i_3 < \cdots < i_n$$

$$i_r < j_r \quad \text{(all r)} \tag{A.1}$$

and P is the parity of the permutation to arrange the integers $i_1 j_1 i_2 j_2 \cdots i_N j_N$ in numerical order 1, 2, ..., 2N. The Pfaffian of order 4 is written as

$$\backslash C_{12} \quad C_{13} \quad C_{14}|$$
$$\qquad C_{23} \quad C_{24}|$$
$$\qquad\qquad C_{34}|$$

$$= C_{12}C_{34} - C_{13}C_{24} + C_{14}C_{23}$$

An important property of a Pfaffian and one often used to define it is that the Pfaffian is the square root of the corresponding antisymmetric determinant where the integers are free to range over the set {1, 2, ..., 2N}

$$\backslash C_{ij}|^2 = |C_{ij}| \tag{A.2}$$

As a consequence many of the theorems for determinants can be modified to apply to Pfaffians. A Pfaffian can be expanded by the elements of a row and column in terms of

Pfaffian cofactors

$$\backslash C_{ij}| = \sum_j \left\{ (-)^{i+j-1} C_{ij} A_{ij} + (-)^{j+i-1} C_{ji} A_{ji} \right\} \quad (A.3)$$

where A_{ij} is the Pfaffian obtained by removing the i, j rows and columns. Thus the expansion of the above Pfaffian by the 3rd row and column is

$$\backslash \begin{vmatrix} C_{12} & C_{13} & C_{14} \\ & C_{23} & C_{24} \\ & & C_{34} \end{vmatrix}$$

$$= (-)^{1+3-1} C_{13}C_{24} + (-)^{2+3-1} C_{23}C_{14} + (-)^{3+4-1} C_{34}C_{12}$$

A Pfaffian is unchanged when the p^{th} row is added to the p'^{th} row and the p^{th} column is added to the p'^{th} column

$$\backslash C_{ij}| = \backslash C_{ij} + \delta_{ip'} C_{pj} - \delta_{p'j} C_{pi}| \qquad (i < j) \qquad (A.4)$$

A reduction of a Pfaffian to one of lower order can be established[19] by using the properties (A.3) and (A.4). All elements of the 1st row except C_{12} are made zero by using (3.4) and then the expansion by the 1st row and column using (3.3) gives

$$\backslash C_{ij}| = C_{12}^{2-N} \backslash\backslash C_{12}C_{2i}C_{ij}|| \qquad 3 < i < j$$

The process can be repeated r times giving

$$\backslash C_{ij}| = (C_{12}C_{23} \cdots C_{2r-1\,2r}|)^{2r-N} \backslash\backslash C_{12}C_{23}\cdots C_{2ri}C_{ij}|| \qquad (A.5)$$

where $2r < i < j$ and the Pfaffian on the right hand side is of order $2(N - r)$.

We now consider the reduction of partly antisymmetric determinant $|C_{ij}|$ of order $2m + r$. By partly antisymmetric we mean that the determinant has a

submatrix of order 2m whose rows and columns form an antisymmetric matrix. We select the smallest integer k such that both $C_{kk'}$ and $C_{k'k}$ are present in the determinant. To every row of the determinant other than the k'th we add a constant multiple α_p of the k' row so as to make all the elements of the k^{th} column zero except $C_{k'k}$

$$|C'_{ij}| = |C_{ij} + \sum_p \delta_{ip} \alpha_p C_{k'j}|$$

$$C'_{pk} = C_{pk} + \alpha_p C_{k'k} = 0$$

$$\therefore \quad \alpha_p = - \frac{C_{pk}}{C_{k'k}} = + \frac{C_{pk}}{C_{kk'}}$$

Then to every column of the determinant other than the k' we add a constant multiple β_p of the k' column so as to make all the elements of the k^{th} row zero except $C_{kk'}$

$$|C''_{ij}| = |C'_{ij} + \sum_p \delta_{pj} \beta_p C'_{ik'}|$$

$$\text{i.e. } |C''_{ij}| = \left| C_{ij} + \sum_p \delta_{ip} \alpha_p C_{k'j} + \sum_p \delta_{pj} \beta_p \left\{ C_{ik'} + \sum_p \delta_{ip} \alpha_p C_{k'k'} \right\} \right|$$

$$= \left| C_{ij} + \sum_p \delta_{ip} \alpha_p C_{k'j} + \sum_p \delta_{pj} \beta_p C_{ik'} \right|$$

since $C_{k'k'} = 0$. To find β_p we require $C''_{kp} = 0$, i.e.

$$C_{kp} + \beta_p C_{kk'} = 0$$

$$\beta_p = - \frac{C_{kp}}{C_{kk'}}$$

Thus

$$C''_{ij} = C_{ij} + \frac{C_{ik}}{C_{kk'}} C_{k'j} - \frac{C_{kj}}{C_{kk'}} C_{ik'}$$

$$= \frac{1}{C_{kk'}} \begin{vmatrix} C_{kk'} & C_{kj} & C_{ik} \\ & C_{k'j} & C_{ik'} \\ & & C_{ij} \end{vmatrix}$$

$$= \frac{1}{C_{kk'}} \begin{vmatrix} C_{kk'} & C_{ki} & C_{kj} \\ & C_{k'i} & C_{k'j} \\ & & C_{ij} \end{vmatrix}$$

As a check we note that $C''_{kj} = C''_{ik} = 0$. The determinant is expanded by the k^{th} row and then the k^{th} column giving

$$D = |C_{ij}| = C_{kk'}^{2 - (2m + r - 2)} \left| C_{kk'} C_{k'j} C_{ij} \right| \qquad (A.6)$$

We note the antisymmetric submatrix of the original determinant forms an antisymmetric submatrix (or order $2(m - 1)$) of the new determinant for

$$C''_{k_2k'_2} = \begin{vmatrix} C_{kk'} & C_{kk'_2} & C_{k_2k} \\ & C_{k'k'_2} & C_{k_2k'} \\ & & C_{k_2k'_2} \end{vmatrix}$$

$$= \begin{vmatrix} C_{kk'} & C_{kk_2} & -C_{k'_2k} \\ & C_{k'k_2} & -C_{k'_2k'} \\ & & -C_{k'_2k_2} \end{vmatrix}$$

$$= -C''_{k'_2k_2}$$

Therefore the reduction process can be continued until all the antisymmetric part of the original determinant has been removed.

APPENDIX B

SIGN OF EQUATION (3.6)'.

We consider only the case when $a \in \{1, 2, \ldots, h\}$ as the other possibilities can be treated by the same method. From section 2.3 the associated terminal of a is $a' = g + h - a + 1$. We wish to show $i + i' + a = k + k'$ and there are three cases to consider.

(1) If $i \in \{1, 2, \ldots, h\}$ then $i' = g + h - i + 1$.
For $i < a$ the permutation of $aa'ii'$ to numerical order $iaa'i'$ is even, while for $i > a$ the permutation $aa'ii'$ to numerical order $aii'a'$ is again even. Thus $Q = 0$ and we have $i + i' + Q = g + h + 1$. When the indices have been reordered then $k \in \{1, 2, \ldots, h - 1\}$ and $k' = (g - 1) + (h - 1) - k + 1$. Thus $k + k' = g + h - 1 = i + i' + Q \pmod 2$.

(2) If $i \in \{h + 1, \ldots, d\}$ then $i' = g + 2h + d - i + 1$ and the permutation $aa'ii'$ to numerical order $aia'i'$ is odd, $(Q = 1)$. Now $k \in \{h - 1, \ldots, h + d - 1\}$ and $k' = (g - 1) + 2(h - 1) + d - k + 1$ so again $i + i' + Q = g + d = k + k' \pmod 2$.

(3) If $i \in \{h + d + 1, \ldots, g\}$ then $i' = g + 2h + 2d + v - i + 1$ and the permutation $aa'ii'$ to numerical order $aia'i'$ is odd, $(Q = 1)$. Since $k \in \{h + d, \ldots, g - 1\}$ and $k' = (g - 1) + 2(k - 1) + 2d + v - k + 1$ then $i + i' + Q = g + v = k + k' \pmod 2$.

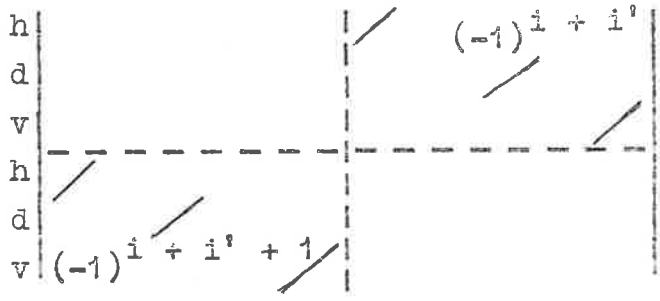
APPENDIX C

DETERMINATION OF THE SIGN OF D(1; i; j; k).

We list in this appendix the operations and their sign factors for the selection of the coefficient $D(1_n; i_p; j_q; k_m)$ from the equation (3.6), where all the C_{ij} are positive and the sign on the bond weights above and below the diagonal are $(-)^{i + i'}$ and $(-1)^{i + i' + 1}$ respectively. From equation (2.14) which relates the terminals and their associated terminals we have

$$\text{Sign}(i + i') = \text{Sign} \begin{cases} g + h + 1 & \text{if} \quad 1 \leqslant i \leqslant h \\ g + d + 1 & \text{if} \quad h < i \leqslant h + d \\ g + v + 1 & \text{if} \quad h + d < i \leqslant g \end{cases}$$

The determinant can be represented as



where the bond weights are located on the diagonals shown.

(1) Selection of $\{1_n\}$ $(n = n_1 + n_2 + n_3)$ with $\alpha_i = 2$. We select n_1 bonds from the set h above the diagonal corresponding to $1_1, \ldots, 1_{n_1}$ and n_1 bonds from the set h below the diagonal corresponding to $1', \ldots, 1'_{n_1}$. Associated with each selection is a sign from the bond weight and a sign from the position in the determinant. Due to the diagonal structure of the sets $\{h\}$, $\{d\}$, $\{v\}$ we can always assume that the n_i chosen are the n_i with the lowest row index. Thus the sign factor associated with the selection of n_1 from the set $\{h\}$ above the diagonal is

$$\text{Sign} = n_1(g + h + 1) + (1 + g + h) + (1 + g + h - 1) + \ldots\ldots + (1 + g + h - n_1 + 1)$$

$$= n_1(g + h + 1) + \tfrac{1}{2}n_1(3 + 2g + 2h - n_1)$$

$$= \tfrac{1}{2}n_1(5 - n_1).$$

We now select n_2 from the set d above the diagonal and remember that we have selected n_1 rows and columns from the set $\{h\}$.

$$\text{Sign} = n_2(g + d + 1) + (h - n_1 + 1 + g + h - n_1 + d) + \ldots\ldots + (h - n_1 + 1 + g + h - n_1 + d - n_2 + 1)$$

$$= \tfrac{1}{2}n_2(5 - n_2).$$

Similarly for the selection of n_3 from v above the diagonal

$$\text{Sign} = \tfrac{1}{2}n_3(5 - n_3).$$

When we select the same bonds from below the diagonal we remember there are now only $h - n_1 + d - n_2 + v - n_3 = g - n$ rows in the first half of the determinant. For the selection of n_1 below the diagonal

$$\text{Sign} = n_1(g + h) + (g - n + k + 1) + \ldots\ldots + (g - n + h - n_1 + 1 + 1)$$

$$= n_1(g + h) + \tfrac{1}{2}n_1(2g + 2h - 2n + 3 - n_1)$$

$$= \tfrac{1}{2}n_1(3 - 2n - n_1).$$

For the selection of n_2 below the diagonal

$$\text{Sign} = n_2(g + d) + (g - n + k - n_1 + d + h + n_1 + 1) + \ldots\ldots + (g - n + h - n_1 + d - n_2 + 1 + h - n_1 + 1)$$

$$= \tfrac{1}{2}n_2(3 - 2n - n_2).$$

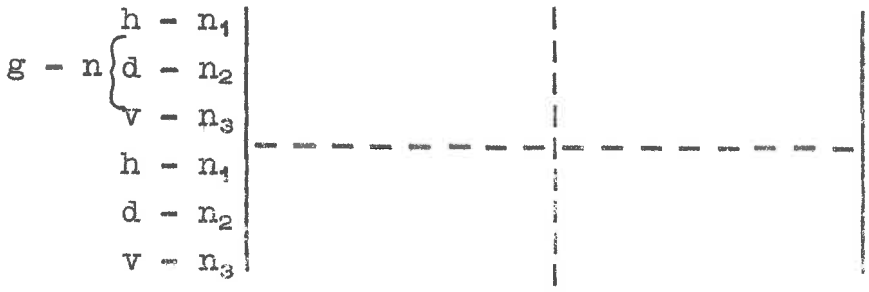
Similarly for the selection of n_3 from the set v below the diagonal

$$\text{Sign} = \tfrac{1}{2}n_3(3 - 2n - n_3).$$

Thus the total sign change on selecting out the $\{l_n\}$ bonds is

$$\tfrac{1}{2}n_1(8 - 2n - 2n_1) + \tfrac{1}{2}n_2(8 - 2n - 2n_1 - 2n_2) + \tfrac{1}{2}n_3(8 - 2n - 2n_1 - 2n_2 - 2n_3)$$
$$= n_1 n + n_1^2 + nn_2 + n_1 n_2 + n_2^2 + nn_3 + n_1 n_3 + n_2 n_3 + n_3^3$$
$$= 0. \qquad (C.1)$$

Since with regard to sign $n^2 = n = n_1^2 + n_2^2 + n_3^2$. With these rows and columns removed the form of the determinant is



(2) Selection of $\{i_p\}$ and $\{j_q\}$ with $\alpha_i = 1$.

The removal of the bonds with $\alpha_i = 1$ is done in exactly the same way as those with $\alpha_i = 2$. Both the sign factor on the bond and the sign factor for the position in the determinant contribute to the sign and again we can assume that the first p_i are chosen since the form of the bond weights is still diagonal. Sign factor on selecting p_1 from the set $\{h - n_1\}$ above the diagonal is

$$\text{Sign} = p_1(g + h + 1) + (1 + g - n + h - n_1) + \ldots\ldots + (1 + g - n + h - n_1 - p_1 + 1)$$
$$= p(g + h + 1) + \tfrac{1}{2}p_1(3 + 2g - 2n + 2h - 2n_1 - p_1)$$
$$= \tfrac{1}{2}p_1(5 - 2n - 2n_1 - p_1).$$

Similarly for the selections of p_2 from $\{d - n_2\}$ and p_3 from $\{v - n_3\}$

$$\text{Sign} = \tfrac{1}{2}p_2(5 - 2n - 2n_2 - p_2) + \tfrac{1}{2}(5 - 2n - 2n_3 - p_3).$$

For the selection of j_q we remember that the number of rows in the upper part of the determinant is $g - n - p$ so that

the sign factor on selecting q_1 from the set $\{h - n_1\}$ below the diagonal is

$$\begin{aligned}\text{Sign} &= q_1(g + h) + (g - n - p + h - n_1 + 1) + \ldots\ldots \\ &\qquad + (g - n - p + h - n_1 - q_1 + 1 + 1) \\ &= q_1(g + h) + \tfrac{1}{2}q_1(2g - 2n - 2p + 2l - 2n_1 + 3 - q_1) \\ &= \tfrac{1}{2}q_1(3 - 2n - 2p - 2n_1 - q_1).\end{aligned}$$

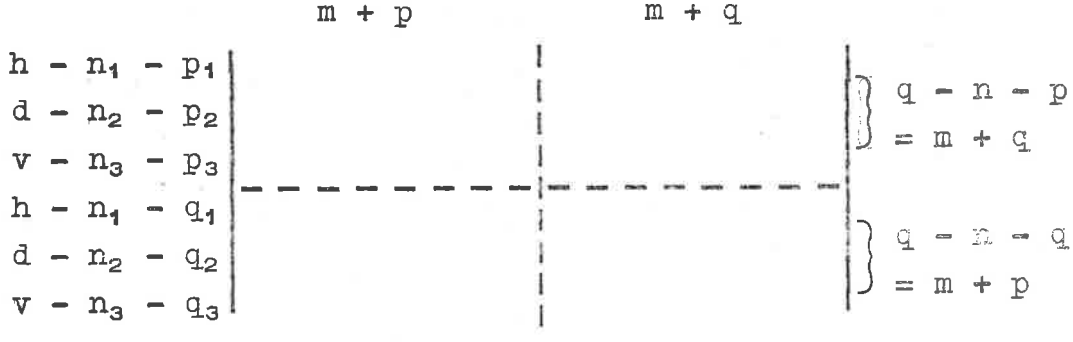
Similarly for the selection of $\{j_{q_2}\}$ and $\{j_{q_3}\}$ we have

$$\text{Sign} = \tfrac{1}{2}q_2(3 - 2n - 2p - 2n_2 - q_2) + \tfrac{1}{2}q_3(3 - 2n - 2p - 2n_3 - q$$

Thus the total sign change on selecting out the $\{i_p\}$ and $\{j_q\}$ is

$$\begin{aligned}W &= \tfrac{1}{2}p_1(1 - p_1) + \tfrac{1}{2}p_2(1 - p_2) + \tfrac{1}{2}p_3(1 - p_3) + \tfrac{1}{2}q_1(1 - q_1) \\ &\quad + \tfrac{1}{2}q_2(1 - q_2) + \tfrac{1}{2}q_3(1 - q_3) + n(p + q) + n_1(p_1 + q_1) \\ &\quad + n_2(p_2 + q_2) + n_3(p_3 + q_3) + q + pq \qquad \text{(C.2}\end{aligned}$$

The form of the determinant now is



All the remaining bonds which occur diagonally as shown are now made zero so that the determinant has only the positive elements C'_{ij}.

(3) Selection of $\{k_m\}$ with $\alpha_i = 0$.

This selection corresponds to the choice of C'_{kk}, and can be done in the same way as $\{l_n\}$, except there is no sign factor due to the bond weights. However, there is a sign factor associated with the selection of $C_{k',k}$ from below the

diagonal. Sign factor for the selection of $\{k_{m_1}\}$ from the set $\{h - n_1 - p_1\}$ is

$$\text{Sign} = (1 + m + p + h - n_1 - p_1) + \ldots\ldots + (1 + m + p + h - n_1 - p_1 - m + 1)$$
$$= \tfrac{1}{2}m_1(3 + 2m + 2p + 2h - 2n_1 - 2p_1 - m_1).$$

Similarly for the selection $\{k_{m_2}\}$ and $\{k_{m_3}\}$

$$\text{Sign} = \tfrac{1}{2}m_2(3 + 2m + 2p + 2d - 2n_2 - 2p_2 - m_2) + \tfrac{1}{2}m_3(3 + 2m + 2p + 2v - 2n_3 - 2p_3 - m_3).$$

The sign factor for the selection of $\{k_{m_1}\}$ from the set $\{h - n_1 - q_1\}$ is

$$\text{Sign} = m_1 + (m + q - m + h - n_1 - q_1 + 1) + \ldots\ldots + (q + h - n_1 - q_1 - m_1 + 1 + 1)$$
$$= \tfrac{1}{2}m_1(2q + 2h - 2n_1 - 2q_1 + 5 - m_1).$$

The sign factor for the selection of $\{k_{m_2}\}$ from the set $\{d - n_2 - q_2\}$ is

$$\text{Sign} = m_2 + (q + h - n_1 - q_1 + d - n_2 - q_2 + h - n_1 - q_1 + 1) + \ldots + (q + h - n_1 - q_1 + d - n_2 - q_2 - m_2 + 1 + h - n_1 - q_1 + 1)$$
$$= \tfrac{1}{2}m_2(2q + 2d - 2n_2 - 2q_2 + 5 - m_2).$$

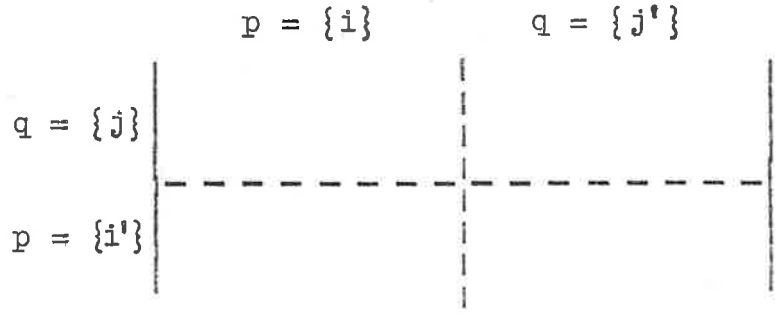
Similarly for the selection of $\{k_{m_3}\}$ from $\{v - n_3 - q_3\}$

$$\text{Sign} = \tfrac{1}{2}m_3(2q + 2v - 2n_3 - 2q_3 + 5 - m_3).$$

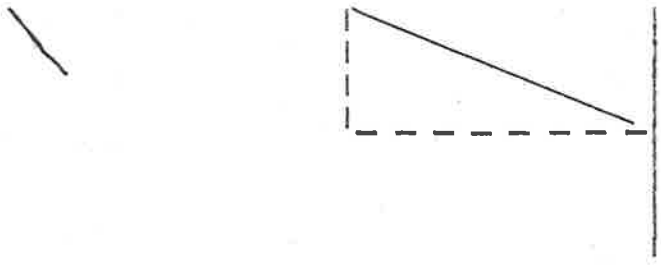
Thus the total sign factor on selecting $\{k_m\}$ is

$$U = (p + q)m + (p_1 + q_1)m_1 + (p_2 + q_2)m_2 + (p_3 + q_3)m_3 + 4m + m^2 + m_1^2 + m_2^2 + m_3^2$$
$$= (p + q)m + p_1 + q_1)m_1 + (p_2 + q_2)m_2 + (p_3 + q_3)m_3 \quad \text{(C.3)}$$

since with respect to sign $m^2 = m = m_1^2 + m_2^2 + m_3^2$. The determinant now has the form



(4) A term in the reduced determinant can be found by expanding down the principle diagonal. The corresponding term in the Pfaffian is given by expanding along the diagonal shown.



Thus the sign factor is $T = (p + q - 1)\frac{1}{2}(p + q)$ (C.4)

(5) Combining the row indices $\{j, i'\}$ and the column indices $\{i, j'\}$ in numerical order. The operations and sign factors for this task are listed below.

$$ji'ij' \rightarrow jii'j'$$

Sign $= p^2 = p$.

$$jii'j' \rightarrow \{j_{q_1}\}\{i_{p_1}\}\{j_{q_2}\}\{i_{p_2}\}\{j_{q_3}\}\{i_{p_3}\}\{i'_{p_1}\}\{j'_{q_1}\}\{i'_{p_2}\}\{j'_{q_2}\}\{i'_{p_3}\}\{j'_{q_3}\}.$$

$$\text{Sign} = p_1(q_2 + q_3) + p_2q_3 + q_1\{p_2 + p_3\} + q_2p_3$$

$$= pq + p_1q_1 + p_2q_2 + p_3q_3$$

We now consider the sets $\{j_{q_1}\}\{i_{p_1}\}$ and $\{i'_p\}\{j'_{q_1}\}$. Each set $\{\ \}$ is separately in numerical order and due to the relations (2.14) the number of interchanges to bring

$\{j_{q_1}\}\{i_{p_1}\}$ to numerical order is the same as the number to bring $\{i'_{p_1}\}\{j'_{q_1}\}$ to numerical order. Thus no further sign changes result.

$$Q = p + pq + p_1q_1 + p_2q_2 + p_3q_3 \qquad (C.5)$$

(6) Since D(l, i, j, k) is a quadratic expression in the weight factors and $\underline{k}$ occurs in both weight factors, then the sign factor resulting from bringing the k's to numerical order is

$$2 \quad V = 0 \qquad (C.6)$$

where V is the sign to rearrange $\underline{k}$ in numerical order. Thus no sign factor is necessary for this rearrangement.

(7) The sign factor for combining the numerical set $\{k_{2m}\}$ and the numerical set $\{j, i, i', j'\}$ into numerical order can be found as in (5) above.

$$\{k_{m_1}\}\{k_{m_2}\}\{k_{m_3}\}\{k'_{m_1}\}\{k'_{m_2}\}\{k'_{m_3}\}\{j_{q_1}\}\{i_{p_1}\}\ldots\{i'_{p_3}\}\{j'_{q_3}\}$$

$$\rightarrow \{k_{m_1}\}\{j_{q_1}\}\{i_{p_1}\}\ldots\{i'_{p_1}\}\{j'_{q_1}\}\{k'_{m_1}\}$$

which is the same as numerical order because of (2.14).

$$\begin{aligned} Y &= (p_1 + q_1)(m_1 + 2m_2 + 2m_3) + (p_2 + q_2)(m_1 + m_2 + 2m_3) \\ &\quad + (p_3 + q_3)(m_1 + m_2 + m_3) + (p_1 + q_1)(m_1 + m_2 + m_3) \\ &\quad + (p_2 + q_2)(m_2 + m_3) + (p_3 + q_3)m_2 \\ &= (p_1 + q_1)(m_2 + m_3) + (p_2 + q_2)(m_1 + m_3) + (p_3 + q_3)(m_1 + \text{m} \end{aligned} \qquad (C.7)$$

(8) Finally, we need to show that the sign factor on rearranging the set $\{\underline{k}, j, i, i', j'\}$ in numerical order is the same as that on arranging the sets $\{\underline{k}, a, b\}$ and $\{\underline{k}, \{a, b\}'\}$ in numerical order. We assume $1 \leqslant a, b \leqslant h$ for simplicity, but the method applies to

any selection.

$$\underline{k},\ a,\ b \rightarrow \{k_{m_1}\}ab\{k_{m_2}\}\{k_{m_3}\}\{k'_{m_1}\}\{k'_{m_2}\}\{k'_{m_3}\}$$

$$\text{Sign} = 2(m_1 + 2m_2 + 2m_3).$$

$$k,\ \{a,\ b\}' \rightarrow \{k_{m_1}\}\{j_{q_1},\ i_{p_1}\}''\{k_{m_2}\}\{j_{q_2}\}\{i_{p_2}\}\ldots\ldots$$

$$b'a'\{j'\}\{j'\}\{k'_{m_3}\}$$

where $\{j_{q_1},\ i_{p_1}\}''$ denotes that a, b are absent.

$$\text{Sign} = (p_1 + q_1 - 2)(m_1 + 2m_2 + 2m_3) + (p_2 + q_2)(m_1 + m_2 + 2m_3) + \ldots\ldots$$

$$= Y.$$

The sign factor to arrange $\{k_{m_1}\}ab$ in numerical order is compensated for by the sign factor to arrange b'a' in numerical order so the desired result follows.

If we combine the equations (C.1) to (C.7) and use the relationships

$$h = n_1 + p_1 + q_1 + m_1$$
$$d = n_2 + p_2 + q_2 + m_2$$
$$v = n_3 + p_3 + q_3 + m_3$$
$$g = n + p + q + m$$

then we obtain the sign factor for D(l; i; j; k) given in equation (3.18) and (3.18)'.

APPENDIX D

DETERMINATION OF THE SIGN OF $P(i_1 \ldots i_n)$.

The sign of the Pfaffian (3.22) after selecting out the bonds $x_1^{\alpha_1}$, $x_2^{\alpha_2}$, ..., $x_g^{\alpha_g}$ for which $\alpha_i = 1$ is the product of the sign factor $(-)^{i + i'}$ of the bond weight, and the sign factor $(-)^{i + j + 1}$ corresponding to its position in the Pfaffian. We shall list the operations and their associated sign factors for the expansion of the Pfaffian by the method of section 3.3.

(1) Selection of $i_1 \ldots i_{n_1}$ from the set $\{1, 2, \ldots, h\}$.

Here $i + i' = g + h + 1$.

$$\begin{aligned}\text{Sign} &= n_1(g + h + 1) + (1 + g + h + 1) \\ &\quad + (1 + g - 1 + h - 1 + 1) + \ldots\ldots\ldots \\ &\quad + (1 + g - n + 1 + h - n_1 + 1 + 1) \\ &= n_1(g + h + 1) + \tfrac{1}{2}n_1(8 + 4g + 4h - 2n_1) \\ &= n_1\end{aligned}$$

In finding the position of the bond weight in the Pfaffian one must remember to remove all the rows and columns containing the indices and the associated indices of the previously selected bond weights.

(2) Selection of $i_{n_1 + 1} \ldots i_{n_1 + n_2}$ such that $h < i \leqslant h + d$.

Here $i + i' = g + d + 1 \pmod 2$.

$$\begin{aligned}\text{Sign} &= n_2(g + d + 1) + (h - n_1 + 1 + g - n_1 + h - n_1 \\ &\quad + d + 1) + \ldots\ldots + (h - n_1 + 1 + g - n_1 - n_2 \\ &\quad + 1 + h - n_1 + d - n_2 + 1 + 1) \\ &= n_1 n_2 + n_2 \pmod 2\end{aligned}$$

(3) Selection of $i_{n_1 + n_2 + 1} \cdots i_n$ such that

$h + d < i \leqslant g$.

Here $i + i' = g + v + 1 \pmod 2$.

$$\begin{aligned}\text{Sign} &= n_3(g + v + 1) + (h - n_1 + d - n_2 + 1 + g \\ &\quad -n_1 - n_2 + h - n_1 + d - n_2 + v + 1) + \ldots\ldots \\ &\quad + (h - n_1 + d - n_2 + 1 + g - n_1 - n_2 - n_3 + 1 \\ &\quad + h - n_1 + d - n_2 + v - n_3 + 1 + 1) \\ &= n_1 n_3 + n_2 n_3 + n_3\end{aligned}$$

Thus the total sign factor on selecting $i_1 \ldots i_n$ is

$$Q = n + n_1 n_2 + n_2 n_3 + n_1 n_3 \qquad (D.1)$$

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