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Twenty-vertex Model on a Triangular Lattice

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Abstract

An ice-type vertex model is formulated on a triangular lattice and solved exactly for restricted values of the vertex activities. It is found to undergo an infinite-order phase transition into an ordered antiferroelectric state and a first-order phase transition into a 'frozen' ferroelectric state.

Introduction

The crystal structure of ice has prompted the study of certain lattice models in statistical mechanics. These include two-dimensional models on square lattices. In these models, each vertex is associated with an oxygen atom, and the bonds between the vertices are then given orientations corresponding to one of the two possible affinities of intermediate hydrogen atoms. The 'ice condition' imposes the requirement that each oxygen atom has exactly two hydrogen atoms close to it. Different arrangements of the hydrogens give rise to different configurations at a vertex, there being six possible types of vertices in this model. In studying lattices composed of these types of vertices, Lieb (1967*a*, 1967*b*, 1967*c*) and Sutherland (1967) have calculated partition functions for these systems. For infinite lattices, two types of phase transitions are observed.

The application of this model to real three-dimensional ice may be limited, although the solution is exact for the statement of the problem. However, the method used by Lieb (1967*a*) is perhaps instructive, and to know its limits might be helpful in developing new and broader approaches to vertex problems. It is for this reason that we investigate in this paper a somewhat artificial extension of the original ice problem. We formulate a vertex problem on a triangular lattice. This model is an extension of the square-lattice ice model in that it retains the ice condition. Each vertex has equal numbers of close and distant associates. Using a Bethe-type assumption similar to that used by Lieb, we find the partition function for a restricted class of triangular ice-type models.

Statement of Problem

We consider a triangular lattice of M rows, each row having N vertices. Instead of 'rows of vertices' we frequently refer to 'rows of vertical bonds' by which we describe the diagonal bonds joining one row of vertices to another. The labelling of vertical bonds is defined in Fig. 1. Since there are N vertices in a row there are $2N$ bonds in a row. Clearly there are M rows of bonds as well as M rows of vertices. Unless explicitly stated otherwise, the word 'row' is used here to mean 'row of vertical

bonds'. The rows have cyclic boundary conditions so that we identify the $(2N+1)$th bond with the first bond. We represent the possible affinities of intermediate atoms by placing arrows on the bonds between vertices. In keeping with the ice condition, we consider arrangements of arrows on the bonds of this lattice in which there are three arrows pointing into each vertex and three arrows pointing out. There are twenty possible such configurations at a vertex. If we identify configurations with all arrows reversed we obtain the 10 distinct configurations shown in Fig. 2. This identification simplifies computation but also introduces a degeneracy into the solution.

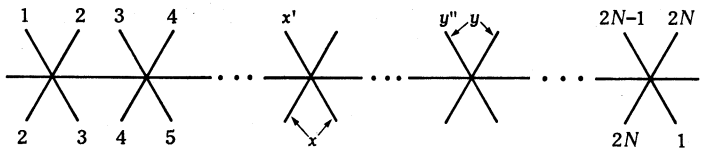

Fig. 1. Illustration of the numbering of the bonds. The bottom row is the incoming r row and the top row is the outgoing r' row. Also shown are the meanings of the prime and double-prime functions (for explicit definitions, see equations (A1) of Appendix 1), application of which gives the number of the bond on the upper left of the vertex.

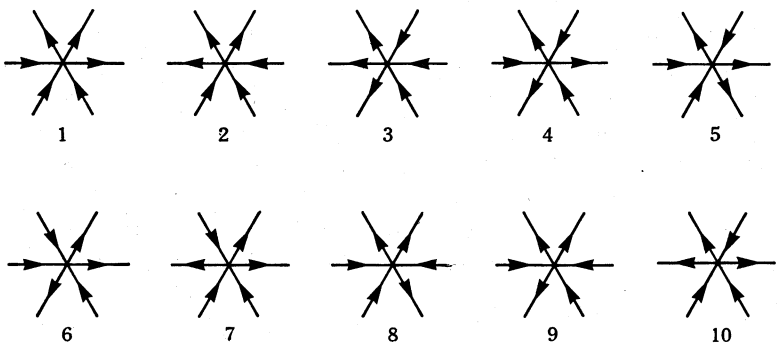

Fig. 2. Ten distinct reversal-symmetric vertex configurations.

Physically we could return to the original more-general situation by the application of an electric field, but in this paper we consider only the simple problem with no electric field. To begin with, we assign to the 10 configurations the energies $e_1, ..., e_{10}$ or, equivalently, the vertex activities $u_i = \exp(-e_i/kT)$, where $i = 1, ..., 10$.

When making a preliminary examination of this model we notice that, because of the cyclic boundary conditions, the number of down arrows in a row of vertical bonds is conserved as we pass from one row to the next. This encourages us to use the transfer matrix approach to the problem. Instead of considering overall arrangements of arrows we consider what arrangements of arrows are possible in the $(m+1)$th row given the arrangement in the mth row. To facilitate this sort of analysis we consider a new representation of the configurations. We take as a standard the entire lattice consisting of vertices of type 1, and we represent any other configuration by drawing a heavy line on a bond whose arrow is opposite to that on the standard. All allowable configurations are then represented by lattices with heavy lines propagating through them. The conservation of down arrows is now shown explicitly in the continuity of these lines. This representation is a useful device in enumerating the possible configurations with a given number of down arrows in a row.

Studying all the configurations of the lattice is equivalent to studying how down arrows propagate from one row to the next, because the lattice is homogeneous. The transfer matrix T is a $2^{2N} \times 2^{2N}$ matrix whose entries correspond to the weights given to the 2^{2N} arrangements of vertical bonds in the $(m+1)$th row, given one of the 2^{2N} arrangements of the mth row. Because of the conservation of down arrows, many of the matrix entries are zero, i.e. it is not allowable to pass from a row with n down arrows to a row with a number of down arrows different from n. Because of this, the matrix breaks up into blocks along the principal diagonal, each block corresponding to a fixed number of down arrows.

Our aim is to calculate the free energy of the system. We can do this by first calculating the partition function

$$Z = \sum \exp\left(- \sum_{i=1}^{10} p_i e_i / kT \right), \tag{1}$$

where p_i is the number of vertices with energy e_i, and the first sum is taken over all allowable configurations of the system. On identifying the first and $(M+1)$th rows of vertical bonds, we have

$$Z = \mathrm{Tr}(T^M), \tag{2}$$

where T is the transfer matrix. Equation (2) may, of course, be written as

$$Z = \sum_{i=1}^{2^{2N}} \lambda_i^M, \tag{3}$$

where the λ_i are the eigenvalues of T. In particular, we are interested in the behaviour of the partition function as the lattice gets very large. If we let the number M of rows in the lattice become large, we obtain

$$Z \simeq \{\Lambda(2N)\}^M, \tag{4}$$

where $\Lambda(2N)$ is the largest eigenvalue of the $2^{2N} \times 2^{2N}$ transfer matrix. If we also allow the number N of vertices in a row to become large, we then obtain

$$\lim_{N\to\infty} \lim_{M\to\infty} (MN)^{-1} \ln Z = \lim_{N\to\infty} N^{-1} \ln(\Lambda(2N)) = -\mathscr{F}/kT, \tag{5}$$

where $\mathscr{F}$ is the free energy per vertex.

Our objective, therefore, is to find the largest eigenvalue of the 'infinite' transfer matrix. We begin by examining the simplest entries in the transfer matrix and then proceed to the more general case, guided by a Bethe-type assumption about the eigenvectors. Ultimately we obtain a solution to a restricted class of these problems.

Simple Cases

No down arrows in a row

If r is the row configuration with no down arrows then, because of the conservation of down arrows from one row to the next, the next row configuration r' will also have no down arrows. The transfer matrix entry corresponding to this situation is the 1×1 block

$$T(r|r') = \exp(-Ne_1/kT) + \exp(-Ne_2/kT) = u_1^N + u_2^N. \tag{6}$$

The two terms represent the possibilities of having all horizontal arrows pointing to the right and to the left respectively.

One down arrow in a row

When a row configuration r has one down arrow, the next row will also have one down arrow. The position of this arrow can be on any of the $2N$ bonds in the row and, in general, each configuration will have a different weight. We can display these weights by writing the eigenvalue equation for the diagonal block of the transfer matrix for which the number of down arrows is one:

$$\Lambda_1 p(x) = \sum_{y=1}^{x'+1} u_2^{N-\frac{1}{2}(x'-y''+2)} f(x)\, c(y,x)\, p(y) + \sum_{y=x'}^{2N} u_1^{N-\frac{1}{2}(y''-x'+2)} g(y)\, d(x,y)\, p(y). \tag{7}$$

Here Λ_1 is the eigenvalue and p the eigenvector, while x and y are the numbers of the bond with the down arrow on it in configurations r and r' respectively. The functions f, g, c and d are defined so that the correct weights are given to the configurations, and the primes on x and y allow us to calculate the vertex to which the bond is connected. Exact definitions of these functions are given in equations (A1)–(A4) of Appendix 1. There are $2N+2$ terms in the sums in equation (7) revealing that, for $2N-2$ positions of the down arrow in r', there is exactly one configuration of the horizontal arrows. However, for two positions of the down arrow in r' there are two ways in which the horizontal arrows can be oriented. Fig. 3 shows a general configuration with one down arrow in the heavy line representation. Notice that the line can only propagate to the right along the horizontal bonds and up along the vertical bonds. Because of the boundary conditions, lines leaving the right of the row of vertices enter again at the left.

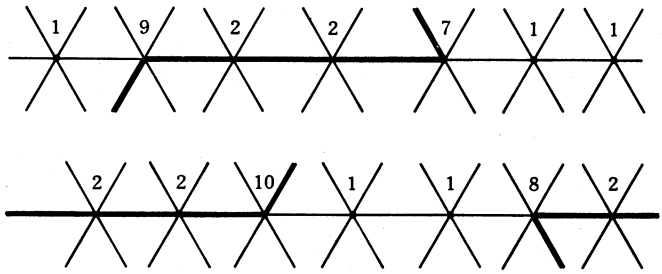

Fig. 3. Heavy line representation of two possible configurations with one down arrow. The numbers indicate the vertex types.

In Appendix 1 we transform the eigenfunction from $p(x)$ to $\bar{p}(x)$ for ease of computation. We then make the Bethe-type hypothesis

$$\left.\begin{aligned} \bar{p}(x) &= \bar{A}\exp(i\bar{k}x') \quad \text{for} \quad x \text{ odd} \\ &= \bar{B}\exp(i\bar{k}x') \qquad\quad x \text{ even}. \end{aligned}\right\} \tag{8}$$

Then, by performing the sums in equation (7) and regrouping the terms, we can write

$$\Lambda_1 \bar{p}(x) = h(x)[u_2^N\{\sigma + v(x)\exp(\mathrm{i}\bar{k}x')\} + u_1^N\{\eta(x)\exp(\mathrm{i}\bar{k}x') + \rho\}], \tag{9}$$

where the x-dependences are shown. Matching like terms in equation (9), we see that if

$$h(x)\,v(x)\exp(\mathrm{i}\bar{k}x') = \lambda\,\bar{p}(x), \qquad h(x)\,\eta(x)\exp(\mathrm{i}\bar{k}x') = \mu\,\bar{p}(x) \tag{10a, b}$$

and

$$u_2^N\sigma + u_1^N\rho = 0 \tag{11}$$

then

$$\Lambda_1 = u_2^N\lambda + u_1^N\mu. \tag{12}$$

The equations (10) can be written

$$\lambda\begin{pmatrix}\bar{A}\\ \bar{B}\end{pmatrix} = L\begin{pmatrix}\bar{A}\\ \bar{B}\end{pmatrix} \qquad \mu\begin{pmatrix}\bar{A}\\ \bar{B}\end{pmatrix} = M\begin{pmatrix}\bar{A}\\ \bar{B}\end{pmatrix}, \tag{13}$$

where L and M are certain 2×2 matrices. In order that equation (12) gives Λ_1 as an eigenvalue of the transfer matrix, λ and μ must have the same eigenvector or, equivalently, L and M must commute. We show in Appendix 1 that the condition that L and M commute imposes restrictions on the original vertex activities. In particular, relevant ratios of these activities can be expressed in terms of four arbitrary parameters. Finally, we note that equation (11) gives a method of finding $\bar{k}$, which is necessary in determining Λ_1.

Two down arrows in a row

The case of two down arrows in a row is similar to the previous case, differing only in complexity. Most of this complexity arises in attaching the correct weight to configurations in which the down arrows of r or r' are located at the same vertex.

The eigenvalue equation corresponding to equation (9) is:

$$\begin{aligned}\Lambda_2\,\bar{p}_1(x_1)\,\bar{p}_2(x_2) &= h(x_1)\,h(x_2)\\ &\times [u_2^N\{\sigma_1 + v_1(x_1)\exp(\mathrm{i}\bar{k}_1 x_1')\}\{\eta_2(x_1)\exp(\mathrm{i}\bar{k}_2 x_1') + v_2(x_2)\exp(\mathrm{i}\bar{k}_2 x_2')\}\\ &\quad + u_1^N\{\eta_1(x_1)\exp(\mathrm{i}\bar{k}_1 x_1') + v_1(x_2)\exp(\mathrm{i}\bar{k}_1 x_2')\}\{\eta_2(x_2)\exp(\mathrm{i}\bar{k}_2 x_2') + \rho_2\}]\\ &\quad + \mathrm{CT},\end{aligned} \tag{14}$$

where CT denotes correction terms. This equation is derived by a method analogous to the procedure used for one down arrow. As before we assume the eigenvectors have the form

$$\left.\begin{aligned}\bar{p}_j(x) &= \bar{A}_j\exp(\mathrm{i}\bar{k}_j x') \quad \text{for} \quad x \text{ odd}\\ &= \bar{B}_j\exp(\mathrm{i}\bar{k}_j x') \qquad\quad x \text{ even}.\end{aligned}\right\} \tag{15}$$

If we have

$$\left.\begin{aligned}h(x)\,v_j(x)\exp(\mathrm{i}\bar{k}_j x') &= \lambda_j\,\bar{p}_j(x) \quad \text{for} \quad j = 1, 2,\\ h(x)\,\eta_j(x)\exp(\mathrm{i}\bar{k}_j x') &= \mu_j\,\bar{p}_j(x) \qquad\quad j = 1, 2,\end{aligned}\right\} \tag{16}$$

and if what we call *unwanted* terms vanish, then we obtain

$$\Lambda_2 = u_2^N \lambda_1 \lambda_2 + u_1^N \mu_1 \mu_2 . \tag{17}$$

There are two kinds of unwanted terms in equation (14), and these are considered separately. First there are *internal* unwanted terms which are proportional to $\exp(\mathrm{i}(\bar{k}_1 + \bar{k}_2)x_1')$ and $\exp(\mathrm{i}(\bar{k}_1 + \bar{k}_2)x_2')$. This type of term did not occur in the single down arrow case. In order to have these terms total zero, we generalize the Bethe-type assumption to the eigenvector

$$\xi(x_1, x_2) = A_{12}\, \bar{p}_1(x_1)\, \bar{p}_2(x_2) + A_{21}\, \bar{p}_2(x_1)\, \bar{p}_1(x_2) . \tag{18}$$

In Appendix 2, we show how this leads to two equations in A_{12} and A_{21}, and we consider the case in which the two down arrows of r occur at the same vertex. In order that this configuration be given the correct weight we find two additional equations in A_{12} and A_{21}. All four of these equations involve only the ratio A_{12}/A_{21}, and we must therefore find a way to reduce them to a single equation. We find that to do this we must have further restrictions on the vertex weights and that the Bethe hypothesis is consistent with

$$u_5 = u_6 , \qquad u_7 = u_8 , \qquad u_9 = u_{10} , \tag{19a, b, c}$$

$$I = u_2 u_3 + u_1 u_5 u_9/u_7 = u_3 u_1 + u_2 u_7 u_5/u_9 = u_1 u_2 + u_3 u_7 u_9/u_5 , \tag{19d}$$

$$u_4 = I^2/u_1 u_2 u_3 - (u_1^{-1} + u_2^{-1} + u_3^{-1})I + u_1 + u_2 + u_3 . \tag{19e}$$

These conditions define a four-dimensional hypersurface S, in the ten-dimensional u-space. They are 'most general' in the sense that there is no five-dimensional surface containing S and still consistent with the Bethe hypothesis. However, there are almost certainly surfaces other than S for which the Bethe hypothesis works; in particular, the case $A_{21} = -A_{12}$ (the analogue of the square lattice free-fermion case (Fan and Wu 1969)) probably corresponds to a different surface in u-space. These conditions reduce the number of parameters specifying the vertex activities from ten to four. Since we are only interested in the ratios of the u_i's we can include an arbitrary normalization and reduce the number of effective parameters to three.

The unwanted *boundary* terms are the second kind of unwanted terms. These are the terms that involve σ and ρ. By requiring that

$$u_2^N \sigma_1 A_{12} = u_1^N \rho_1 A_{21} \qquad \text{and} \qquad u_2^N \sigma_2 A_{21} = u_1^N \rho_2 A_{12} , \tag{20}$$

these terms cancel. This gives us two equations to be solved for $\bar{k}_1$ and $\bar{k}_2$.

General Case

The generalization to the case involving n down arrows in a row is straightforward. We assume the eigenvector is of the form

$$\xi(x_1, \ldots, x_n) = \sum_{\mathscr{P}} A(\mathscr{P}) \prod_{i=1}^{n} \bar{p}_i(x_{\mathscr{P}(i)}) , \tag{21}$$

where $\mathscr{P}$ is the set of permutations of the n integers $1, \ldots, n$. The eigenvalue equation for a single wave is

$$\Lambda_n \bar{p}_1(x_1)\bar{p}_2(x_2)\ldots\bar{p}_n(x_n) = h(x_1)h(x_2)\ldots h(x_n)$$
$$\times\Big(u_2^N\{\sigma_1+v_1(x_1)\exp(\mathrm{i}\bar{k}_1x_1')\}\prod_{j=2}^{n}\{\eta_j(x_{j-1})\exp(\mathrm{i}\bar{k}_jx_{j-1}')+v_j(x_j)\exp(\mathrm{i}\bar{k}_jx_j')\}$$
$$+u_1^N\{\eta_n(x_n)\exp(\mathrm{i}\bar{k}_nx_n')+\rho_n\}\prod_{j=1}^{n-1}\{\eta_j(x_j)\exp(\mathrm{i}\bar{k}_jx_j')+v_j(x_{j+1})\exp(\mathrm{i}\bar{k}_jx_{j+1}')\}\Big)$$
$$+\mathrm{CT}. \tag{22}$$

If the conditions (19) are satisfied and if equations (15) and (16) hold for $j = 1,\ldots,n$ then we have

$$\Lambda_n = u_2^N\lambda_1\ldots\lambda_n + u_1^N\mu_1\ldots\mu_n. \tag{23}$$

The unwanted internal terms will vanish if we have

$$A(\ldots,i,j,\ldots)/A(\ldots,j,i,\ldots) = B(i,j), \tag{24}$$

where $B(i,j)$ is given by equation (A25) of Appendix 2, and the unwanted boundary terms will vanish if we have

$$(u_1/u_2)^N\exp(\mathrm{i}\bar{k}_jN) = \prod_{i=1,i\neq j}^{n}B(j,i) \qquad \text{for} \qquad j = 1,\ldots,n. \tag{25}$$

In principle, these last n equations can be solved for the n quantities $\bar{k}_i$, and with this information we can calculate the $A(\mathscr{P})$'s from equation (24) and $\bar{A}_i$ and $\bar{B}_i$ from a knowledge of the matrices L_i and M_i. At the same time we obtain λ_i and μ_i and, therefore, the eigenvalue Λ_n.

Transformation to New Set of Parameters

For equation (25) with $B(i,j)$ given by equation (A25) of Appendix 2, we find ourselves dealing with a problem similar to the ice-type problems on the square lattice. Following the methods used by Lieb (1967*a*), we search for a change of parameters under which $B(i,j)$ becomes a function of the difference of its arguments, so that in the limit of N large we have to solve an integral equation with a difference kernel. This sort of equation can sometimes be solved easily by Fourier transforms.

We first consider the effect on equation (25) of the transformation from p to $\bar{p}$ by equation (17). The use of $\bar{p}$ has made the computations neater, but if we had instead made the Bethe-type hypothesis

$$\left.\begin{aligned} p_j(x) &= A_j\exp(\mathrm{i}k_jx') \qquad \text{for} \qquad x \text{ odd} \\ &= B_j\exp(\mathrm{i}k_jx') \qquad\qquad x \text{ even}, \end{aligned}\right\} \tag{26}$$

equation (25) would have been

$$\exp(\mathrm{i}k_jN) = \prod_{i=1,i\neq j}^{n}B(j,i) \qquad \text{for} \qquad j = 1,\ldots,n, \tag{27}$$

and the problem would be to find the k_j's instead of the $\bar{k}_j$'s. We noted that, from the conditions (19), three parameters are required to specify the ratios of the ten activities $u_1,\ldots,u_{10}$. We choose these parameters to be ϕ, θ and ζ defined by

$$\cos\phi = \frac{(I-u_1u_2-u_2u_3-u_1u_3)I^{\frac{1}{2}}}{2u_1u_2u_3} \quad \text{for} \quad 0 \leqslant \mathrm{Re}(\phi) \leqslant \pi, \tag{28a}$$

$$\cos 2\theta = \frac{(u_1u_2+u_2u_3+u_1u_3)I-I^2-2u_1u_2u_3^2}{2u_1u_2u_3u_5}, \quad 0 \leqslant \mathrm{Re}(\theta) \leqslant \tfrac{1}{2}\pi, \tag{28b}$$

$$\tan\zeta = \{(u_2u_7-u_1u_9)/(u_2u_7+u_1u_9)\}\tan\theta, \quad -\tfrac{1}{2}\pi \leqslant \mathrm{Re}(\zeta) \leqslant \tfrac{1}{2}\pi. \tag{28c}$$

If we now define a new variable α_i in terms of k_j by

$$\exp(2ik_j) = \frac{\sin(\alpha_j-\phi+\theta)\sin(\alpha_j-\theta)}{\sin(\alpha_j-\theta+\phi)\sin(\alpha_j+\theta)} \quad \text{for} \quad -\tfrac{1}{2}\pi \leqslant \mathrm{Re}(\alpha_j) \leqslant \tfrac{1}{2}\pi \tag{29}$$

then we find that

$$B(i,j) = -\sin(\alpha_i-\alpha_j-\phi)/\sin(\alpha_j-\alpha_i-\phi). \tag{30}$$

Thus $B(i,j)$ depends on α_i and α_j only through their difference as required. The expressions for λ_i and μ_i are

$$\lambda_i = \frac{\sin(\alpha_i-\theta+\phi)\sin(\alpha_i+\zeta+\phi)}{\sin(\alpha_i-\theta)\sin(\alpha_i+\zeta)} \quad \text{and} \quad \mu_i = \frac{\sin(\alpha_i-\theta+\phi)\sin(\alpha_i+\zeta-\phi)}{\sin(\alpha_i-\theta)\sin(\alpha_i+\zeta)}. \tag{31, 32}$$

In terms of ϕ, θ and ζ, the relative activities are

$$u_1 \propto \sin(\theta+\zeta)\sin(\phi-\theta+\zeta)\sin 2\theta, \tag{33a}$$

$$u_2 \propto \sin(\theta-\zeta)\sin(\phi-\theta-\zeta)\sin 2\theta, \tag{33b}$$

$$u_3 \propto \sin(\phi-\theta-\zeta)\sin(\phi-\theta+\zeta)\sin(\phi-2\theta), \tag{33c}$$

$$u_4 \propto \sin(\theta-\zeta)\sin(\phi-\theta-\zeta)\sin 2\theta + \sin(\phi-\theta+\zeta)\sin(\phi+\theta-\zeta)\sin\phi, \tag{33d}$$

$$u_5 \propto \sin(\phi-\theta+\zeta)\sin(\phi-\theta-\zeta)\sin\phi, \tag{33e}$$

$$u_7 \propto \sin(\phi-\theta+\zeta)\sin\phi\sin 2\theta, \tag{33f}$$

$$u_9 \propto \sin(\phi-\theta-\zeta)\sin\phi\sin 2\theta, \tag{33g}$$

where the same proportionality constant is understood throughout.

Rotation of the lattice by $\frac{1}{3}\pi$ radians does not affect the analysis of the problem and can be represented by a permutation of the vertex activities given by

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ 2 & 3 & 1 & 4 & 7 & 8 & 9 & 10 & 6 & 5 \end{pmatrix}. \tag{34}$$

The corresponding transformations of ϕ, θ and ζ are

$$\phi \to \phi, \quad \theta \to \tfrac{1}{2}(\phi-\theta-\zeta), \quad \zeta \to \tfrac{1}{2}(3\theta-\phi-\zeta). \tag{35}$$

Antiferroelectric State $(\cos\phi > 1)$

Since our model includes the F-model on a triangular lattice discussed by Baxter (1969, 1972) we expect it to undergo at least one phase transition for certain values of the parameters. Using the F-model as a guide, we first study a regime of the parameters where the model is in an ordered F-type state. This happens when we have $\cos\phi > 1$, and ϕ, θ and ζ are all pure imaginary:

$$\phi = \mathrm{i}r, \qquad \theta = \mathrm{i}s, \qquad \zeta = \mathrm{i}v, \tag{36}$$

$$r \geqslant 2s \geqslant 2|v|. \tag{37}$$

The condition (37) ensures that $u_1, \ldots, u_{10}$ are all nonnegative.

We can write equation (27) as

$$\frac{\sin(\alpha_j - \phi + \theta)\sin(\alpha_j - \theta)}{\sin(\alpha_j - \theta + \phi)\sin(\alpha_j + \theta)} = (-1)^{n-1} \prod_{i=1}^{n} \frac{\sin(\alpha_j - \alpha_i - \phi)}{\sin(\alpha_i - \alpha_j - \phi)}. \tag{38}$$

In this regime (ϕ and θ imaginary), it is necessary that the α_j's remain real so that $k(\alpha_j) = k_j$ is real. Following Yang and Yang (1966), we define a function $\Theta(\alpha)$ by

$$\exp(\mathrm{i}\Theta(\alpha_j - a_i)) = \sin(\alpha_j - \alpha_i - \phi)/\sin(\alpha_i - \alpha_j - \phi). \tag{39}$$

Taking logs of both sides of equation (38) we have

$$N k(\alpha_j) - \sum_{i=1}^{n} \Theta(\alpha_j - \alpha_i) = \pi(2j - n - 1) \qquad \text{for} \qquad j = 1, \ldots, n. \tag{40}$$

The branches are chosen to give a symmetric distribution of k's. We now assume that, as N grows large and n/N remains fixed, the α's form a continuous distribution in the range $(-\frac{1}{2}\pi, \frac{1}{2}\pi)$. Let $N\rho(\alpha)\,\mathrm{d}\alpha$ be the number of α's in the interval $(\alpha, \alpha + \mathrm{d}\alpha)$, then equation (40) becomes

$$N k(\alpha) - \int_{-\frac{1}{2}\pi}^{\frac{1}{2}\pi} \Theta(\alpha - \alpha') N \rho(\alpha')\,\mathrm{d}\alpha' = 2\pi \int_{-\frac{1}{2}\pi}^{\alpha} N\rho(\alpha')\,\mathrm{d}\alpha' - n\pi, \tag{41}$$

with

$$n = N \int_{-\frac{1}{2}\pi}^{\frac{1}{2}\pi} \rho(\alpha)\,\mathrm{d}\alpha, \tag{42}$$

We differentiate equation (41) with respect to α in order to simplify the right-hand side, and get

$$k'(\alpha) - \int_{-\frac{1}{2}\pi}^{\frac{1}{2}\pi} \{\partial\Theta(\alpha - \alpha')/\partial\alpha\}\rho(\alpha')\,\mathrm{d}\alpha' = 2\pi\rho(\alpha). \tag{43}$$

This equation can be solved by finite Fourier transforms. From equations (29) and (39) we find

$$2\pi k'(\alpha) = 1 + 2\sum_{n=1}^{\infty} \{\exp(-2(r-s)n) + \exp(-2sn)\}\cos(2n\alpha), \tag{44a}$$

$$2\pi\{\partial\Theta(\alpha - \alpha')/\partial\alpha\} = 1 + 2\sum_{n=1}^{\infty} \exp(-2rn)\cos(2n\alpha). \tag{44b}$$

Substituting these series into equation (43), it follows that

$$2\pi\rho(\alpha) = 1 + 2\sum_{n=1}^{\infty} \{\cosh((r-2s)n)/\cosh(rn)\}\cos(2n\alpha). \tag{45}$$

From equation (42) we see that $n = N$. This is the case in which there are as many down arrows as up in a row. Following Lieb (1967*a*) and Yang and Yang (1966), we expect this to correspond to the maximum eigenvalue Λ. Using equation (5) we now calculate the partition function and free energy per vertex. We note that

$$\left|\frac{u_1\mu_i}{u_2\lambda_i}\right| = \frac{\sinh(s+v)\sinh(r-s+v)\sinh(i\alpha_i+r-s)}{\sinh(s-v)\sinh(r-s-v)\sinh(i\alpha_i-r-s)} \gtrless 1 \qquad \text{as} \qquad v \gtrless 0. \tag{46}$$

Therefore for large N and $v > 0$, we have

$$\ln \Lambda_N \approx N \ln u_1 + \sum_{i=1}^{n} \ln(\mu(\alpha_i)), \qquad \text{where} \qquad \mu(\alpha_i) = \mu_i. \tag{47}$$

In the limit as $N \to \infty$ we have

$$-\mathscr{F}/kT = \lim_{N\to\infty} \ln(\Lambda_N/N) = \ln u_1 + \int_{-\frac{1}{2}\pi}^{\frac{1}{2}\pi} \ln(\mu(\alpha))\rho(\alpha)\,d\alpha. \tag{48}$$

The integral can be evaluated to give

$$-\mathscr{F}/kT = \ln\kappa + 3r - \sum_{n=1}^{\infty} \exp(-2rn)\frac{2\cosh((r-2s)n)\cosh(2vn) + \cosh((r-4s)n)}{n\cosh(rn)}, \tag{49}$$

where κ is defined by

$$\kappa = u_1/\{8\sinh(s+v)\sinh(r-s+v)\sinh(2s)\}. \tag{50}$$

A similar development gives the same result for $v < 0$. Thus $\mathscr{F}$ is analytic at $v = 0$ and there is no phase transition here, even though the second term in the right-hand side of equation (23) dominates for $v > 0$ and the first for $v < 0$. Two forms that are equivalent to equation (49) are

$$\begin{aligned} -\mathscr{F}/kT &= \ln u_1 + 2(r-s-v) + \sum_{m=1}^{\infty} \frac{8}{m}\frac{\sinh((r-s-v)m)\cosh((s-v)m)\cosh((r-2s)m)}{\exp(2rm)+1} \\ &= \ln u_2 + 2(r-s+v) + \sum_{m=1}^{\infty} \frac{8}{m}\frac{\sinh((r-s+v)m)\cosh((s+v)m)\cosh((r-2s)m)}{\exp(2rm)+1}. \end{aligned} \tag{51}$$

Disordered State $(-1 < \cos\phi < 1)$

We now perform a similar calculation for the case in which the model is in a disordered state. Here $-1 < \cos\phi < 1$, and the parameters ϕ, θ and ζ are real. By examining the physical possibilities we see that

$$0 < \phi < \pi \qquad \text{and} \qquad \phi \geqslant 2\theta \geqslant 2|\zeta|. \tag{52}$$

In this regime the α's of equation (29) become pure imaginary. Letting M grow large as before and assuming that the α's form a continuous distribution in the interval $(-i\infty, i\infty)$, equations (43) and (42) become on setting $\alpha = i\beta$

$$k'(\beta) - \int_{-\infty}^{\infty} \{\partial\Theta(\beta-\beta')/\partial\beta\}\,\rho(\beta')\,d\beta' = 2\pi\rho(\beta) \tag{53}$$

with

$$n = N\int_{-\infty}^{\infty} \rho(\beta)\,d\beta. \tag{54}$$

We solve equation (53) by Fourier transforms to obtain

$$\rho(\beta) = (2\pi)^{-1} \int_{-\infty}^{\infty} \cosh((\phi-2\theta)m)\exp(2i\beta m)/\cosh(\phi m)\, dm, \tag{55}$$

and again we have $n = N$. We can show that

$$\left|\frac{u_1 \mu_i}{u_2 \lambda_i}\right| \gtrless 1 \quad \text{as} \quad \zeta \gtrless 0, \tag{56}$$

and therefore we arrive at an expression for the free energy

$$\begin{aligned} -\mathscr{F}/kT &= \ln u_1 + 2\int_{-\infty}^{\infty} \frac{\sinh((\pi-\phi)m)\sinh((\phi-\theta-\zeta)m)\cosh((\theta-\zeta)m)\cosh((\phi-2\theta)m)}{m\cosh(\phi m)\sinh(\pi m)}\, dm \\ &= \ln u_2 + 2\int_{-\infty}^{\infty} \frac{\sinh((\pi-\phi)m)\sinh((\phi-\theta+\zeta)m)\cosh((\theta+\zeta)m)\cosh((\phi-2\theta)m)}{m\cosh(\phi m)\sinh(\pi m)}\, dm. \end{aligned} \tag{57}$$

This integration can be performed when ϕ is in the upper half plane by integrating around the lower half m-plane to give

$$\begin{aligned} -\mathscr{F}/kT = \ln u_1 + 2(r-s-v) + \sum_{m=1}^{\infty} \frac{8}{m} \frac{\sinh((r-s-v)m)\cosh((s-v)m)\cosh((r-2s)m)}{\exp(2rm)+1} \\ -8i \sum_{m=1}^{\infty} \frac{\{\cos(\pi s(2m-1)r^{-1}) + \cos(\pi v(2m-1)r^{-1})\}\sin(\pi s(2m-1)r^{-1})}{(2m-1)\{1-\exp(\pi^2(2m-1)r^{-1})\}}. \end{aligned} \tag{58}$$

The difference between this analytic continuation and equation (51) is the singular part of the free energy at the transition. It has an essential singularity at $\phi = 0$, and the phase transition is therefore of infinite order.

Ferroelectric State $(\cos\phi < -1)$

The two states already discussed correspond to those of Baxter's (1969, 1972) F-model when $\phi = 3\theta$ and $\zeta = 0$. However, there is in this more general model a further transition when $\cos\phi = -1$, or $\phi = \pi$. As ϕ approaches π, θ approaches $\frac{1}{2}\pi$ or 0, and ζ approaches $\pm\frac{1}{2}\pi$ or 0. One of the regimes for $\cos\phi < -1$ is given by

$$\phi = \pi + ir, \qquad \theta = \tfrac{1}{2}\pi + is, \qquad \zeta = \pm\tfrac{1}{2}\pi + iv, \tag{59}$$

with the condition

$$2|v| \geqslant 2s \geqslant r \tag{60}$$

guaranteeing that all the vertex activities are nonnegative. This condition also ensures that

$$\mu_i < 1 \quad \text{and} \quad \lambda_i < 1. \tag{61}$$

Therefore Λ_n is a monotonically decreasing function of n, Λ_n has a maximum at $n = 0$, and we also have

$$\Lambda_0 = u_1^N + u_2^N \tag{62}$$

and

$$-\mathscr{F}/kT = \lim_{N\to\infty} N^{-1} \ln \Lambda_0 = \ln(\max(u_1, u_2)). \tag{63}$$

Therefore, in this region, we have a 'constant' value for the free energy, and the system is 'frozen' into a state in which all vertices are of type 1 if $u_1 > u_2$ (or type 2 if $u_1 < u_2$). It is clear from the rotational symmetry of the model that there must be a similar frozen state composed of type-3 vertices. In this regime θ and ζ are pure imaginary:

$$\phi = \pi + ir, \qquad \theta = is, \qquad \zeta = iv, \tag{64}$$

and the free energy is $\ln u_3$. In general when $\cos\phi < -1$ we have

$$-\mathscr{F}/kT = \ln(\max(u_1, u_2, u_3)). \tag{65}$$

This state is similar to the KDP state for the square lattice ice model. It is discussed in more detail by Kelland (1974), where it has been shown that the phase transition is of first order, with a latent heat at the transition.

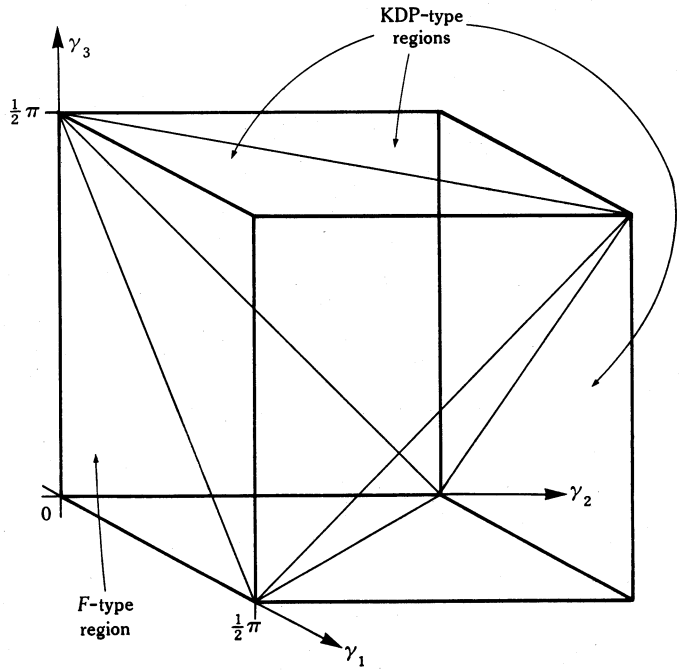

Fig. 4. Subdivision of the γ-cube by the four transition surfaces into five tetrahedrons which correspond to the five different parameter regions.

Transitions and Regions in Parameter Space Corresponding to Various States

Although we have given in terms of the parameters ϕ, θ and ζ the precise points where transitions occur, it is not always clear what is happening to the vertex activities at these points. Baxter (1969, 1972) shows that at the *F*-type transition the activities $u_4, \ldots, u_{10}$ have become considerably larger than u_1, u_2, and u_3. Kelland (1974) has shown that, at the KDP-type transition, one of u_1, u_2 or u_3 has become noticeably larger than all the other activities.

To provide a simple view of the possible states for the model, we define some new parameters γ_1, γ_2 and γ_3 by

$$\sin\gamma_1 = (u_2 u_3/I)^{\frac{1}{2}}, \qquad \sin\gamma_2 = (u_1 u_3/I)^{\frac{1}{2}}, \qquad \sin\gamma_3 = (u_1 u_2/I)^{\frac{1}{2}}, \tag{66}$$

where I is given by equation (19d), and γ_i is restricted to the range $0 \leqslant \gamma_i \leqslant \frac{1}{2}\pi$ ($i = 1, 2, 3$). The γ's are independent and can assume any value in the cube indicated. In terms of these new parameters we now have

$$\cos\phi = (1 - \sin^2\gamma_1 - \sin^2\gamma_2 - \sin^2\gamma_3)/(2\sin\gamma_1 \sin\gamma_2 \sin\gamma_3), \tag{67}$$

and the transitions occur at $\cos\phi = \pm 1$. Solutions to these equations are surfaces in the γ-cube, which is shown in Fig. 4. In particular there are four distinct solutions to the two equations:

$$\gamma_1+\gamma_2 = \gamma_3+\tfrac{1}{2}\pi, \qquad \gamma_1+\gamma_3 = \gamma_2+\tfrac{1}{2}\pi, \qquad \gamma_2+\gamma_3 = \gamma_1+\tfrac{1}{2}\pi, \qquad \gamma_1+\gamma_2+\gamma_3 = \tfrac{1}{2}\pi. \tag{68}$$

Within the cube $0 \leqslant \gamma_i \leqslant \frac{1}{2}\pi$ ($i = 1, 2, 3$) these planes describe a tetrahedron (see Fig. 4). The interior of the tetrahedron corresponds to the disordered state of the model, and the four outlying regions correspond to the three KDP-type ordered states and the one F-type ordered state. The advantages of the γ parameters is that they are symmetric with respect to each other and are fairly simply defined in terms of the vertex activities. On the other hand, the parameters ϕ, θ and ζ, although natural in terms of calculating the eigenvalue, are not so directly connected with the initial statement of the problem. Nevertheless, the γ's are not particularly helpful in working out the eigenvalue.

Summary

We have shown that the partition function and free energy for the twenty-vertex model on a triangular lattice can be calculated exactly, when certain conditions are placed on the vertex activities. These conditions involve making the ratios of the vertex activities dependent on only three parameters. The resulting free energy reveals two types of phase change. One is a first-order transition from the disordered state into one of three frozen ferroelectric states, and the other is an infinite-order transition from the disordered state into an ordered antiferroelectric state.

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Appendix 1

The definitions of the functions in equation (7) are:

$$\left.\begin{aligned} x' &= x-1 \quad \text{for} \quad x \text{ even}, & y'' &= y-1 \quad \text{for } y \text{ even}, \\ &= x-2 \qquad\ \ x \text{ odd}, & &= y \qquad\ \ y \text{ odd}; \end{aligned}\right\} \tag{A1}$$

$$\left.\begin{aligned} f(x) &= u_8 \quad \text{for} \quad x \text{ odd}, & g(y) &= u_7 \quad \text{for} \quad y \text{ odd}, \\ &= u_9 \qquad\ \ x \text{ even}, & &= u_{10} \qquad\ \ y \text{ even}; \end{aligned}\right\} \tag{A2}$$

$$\left.\begin{aligned} c(y,x) &= g(y)\,u_1^{\frac{1}{2}(x'-y''-2)} \quad \text{for} \quad y < x', \\ &= u_5/u_6 \quad \text{for} \quad y = x' \quad \text{and} \quad x \text{ even}, \\ &= u_4/u_8 \qquad\qquad\qquad\ \ x \text{ odd}, \\ &= u_3/u_9 \quad \text{for} \quad y = x'+1 \quad \text{and} \quad x \text{ even}, \\ &= u_6/u_8 \qquad\qquad\qquad\ \ x \text{ odd}; \end{aligned}\right\} \tag{A3}$$

$$\left.\begin{aligned} d(x,y) &= f(x)\,u_2^{\frac{1}{2}(y''-x'-2)} \quad \text{for} \quad y > x'+1, \\ &= u_6/u_7 \quad \text{for} \quad y = x' \quad \text{and} \quad x \text{ even}, \\ &= u_3/u_7 \qquad\qquad\qquad\ \ x \text{ odd}, \\ &= u_4/u_{10} \quad \text{for} \quad y = x'+1 \quad \text{and} \quad x \text{ even}, \\ &= u_5/u_{10} \qquad\qquad\qquad\ \ x \text{ odd}. \end{aligned}\right\} \tag{A4}$$

In transforming equation (7) into the form (9) we expand the right-hand side of (7) as

$$\begin{aligned} &\frac{u_2^{N-1}}{u_1} f(x) \left(\frac{u_2}{u_1}\right)^{-\frac{1}{2}x'} \left\{ \left(\frac{u_2}{u_1}\right)^{\frac{1}{2}} \left(u_7\, p(1) + u_{10}\, p(2)\right) + \left(\frac{u_2}{u_1}\right)^{3/2} \left(u_7\, p(3) + u_{10}\, p(4)\right) + \ldots \right. \\ &\qquad \left. + \left(\frac{u_2}{u_1}\right)^{\frac{1}{2}(x'-2)} \left(u_7\, p(x'-2) + u_{10}\, p(x'-1)\right) \right\} \\ &+ u_2^{N-1}\, c(x', x)\, f(x)\, p(x') + u_2^{N-1}\, c(x'+1, x)\, f(x)\, p(x'+1) \\ &+ u_1^{N-1}\, d(x, x')\, g(x)\, p(x') + u_1^{N-1}\, d(x, x'+1)\, g(x'+1)\, p(x'+1) \\ &+ \frac{u_1^{N-1}}{u_2} f(x) \left(\frac{u_2}{u_1}\right)^{-\frac{1}{2}x'} \left\{ \left(\frac{u_2}{u_1}\right)^{\frac{1}{2}(x'+2)} \left(u_7\, p(x'+2) + u_{10}\, p(x'+3)\right) \right. \\ &\qquad \left. + \left(\frac{u_2}{u_1}\right)^{\frac{1}{2}(x'+4)} u_7\, p(x'+4) + \ldots + \left(\frac{u_2}{u_1}\right)^{N-\frac{1}{2}} u_{10}\, p(2N) \right\}. \end{aligned} \tag{A5}$$

We then perform the sums in the braces. When terms depending on x are grouped together, equation (9) results, where

$$\left.\begin{aligned} h(x) &= u_7 u_8/u_1 u_1 \quad \text{for} \quad x \text{ odd}, \\ &= u_9 u_{10}/u_1 u_2 \quad\quad x \text{ even}; \end{aligned}\right\} \tag{A6}$$

$$\left.\begin{aligned} \eta_i(x) &= \frac{\bar{A}_i + \bar{B}_i z_i}{1-z_i} + \frac{u_6 u_2}{u_7 u_9}\frac{\bar{A}_i}{z_i} + \frac{u_4 u_2}{u_{10} u_9}\bar{B}_i \quad \text{for} \quad x \text{ even}, \\ &= \frac{\bar{A}_i + \bar{B}_i z_i}{1-z_i} + \frac{u_3 u_2}{u_7 u_8}\frac{\bar{A}_i}{z_i} + \frac{u_5 u_2}{u_{10} u_8}\bar{B}_i \quad\quad x \text{ odd}; \end{aligned}\right\} \tag{A7}$$

$$\left.\begin{aligned} v_i(x) &= \frac{u_5 u_1}{u_9 u_7}\frac{\bar{A}_i}{z_i} + \frac{u_3 u_1}{u_9 u_{10}}\bar{B}_i - \frac{\bar{A}_i/z_i + \bar{B}_i}{1-z_i} \quad \text{for} \quad x \text{ even}, \\ &= \frac{u_4 u_1}{u_8 u_7}\frac{\bar{A}_i}{z_i} + \frac{u_6 u_1}{u_8 u_{10}}\bar{B}_i - \frac{\bar{A}_i/z_i + \bar{B}_i}{1-z_i} \quad\quad x \text{ odd}; \end{aligned}\right\} \tag{A8}$$

$$\sigma_i = \frac{(\bar{A}_i/z_i + \bar{B}_i)\exp(\mathrm{i}\bar{k}_i)}{1-z_i}, \qquad \rho_i = -\frac{(\bar{A}_i/z_i + \bar{B}_i)\exp(\mathrm{i}\bar{k}_i(2N+1))}{1-z_i}, \qquad z_i = \exp(2\mathrm{i}\bar{k}_i), \tag{A9}$$

$$\bar{p}_i(y) = \prod_{y''}^{\dagger}(u_2/u_1)^{\pm y''} g(y) p_i(y). \tag{A10}$$

The elements of the matrices L and M can be determined by regarding equations (10) as four equations, two for x odd and two for x even. The resulting matrices are

$$L = \begin{bmatrix} -v_2/z(1-z) + w_4/z & v_2/(z-1) + w_7 \\ -v_1/z(1-z) + w_5/z & v_1/(z-1) + w_6 \end{bmatrix}, \tag{A11a}$$

$$M = \begin{bmatrix} v_2/(1-z) + w_2/z & v_2 z/(1-z) + w_3 \\ v_1/(1-z) + w_1/z & v_1 z/(1-z) + w_4 \end{bmatrix}, \tag{A11b}$$

where

$$\left.\begin{aligned} v_1 &= u_9 u_{10}/u_1 u_2, & v_2 &= u_7 u_8/u_1 u_1, & w_1 &= u_6 u_{10}/u_1 u_7, \\ w_2 &= u_2 u_3/u_1 u_1, & w_3 &= u_2 u_5 u_7/u_1 u_1 u_{10}, & w_4 &= u_4/u_1, \\ w_5 &= u_5 u_{10}/u_2 u_7, & w_6 &= u_3/u_2, & w_7 &= u_6 u_7/u_1 u_{10}. \end{aligned}\right\} \tag{A12}$$

The requirement that L and M commute gives rise to the five equations

$$w_1(w_7 - v_2) = w_3(w_5 - v_1), \qquad v_1(w_3 + w_7) = v_2(w_1 + w_5), \tag{A13a, b}$$

$$w_3(w_4 - v_2) = w_2(w_7 - v_2), \qquad w_6(w_3 - v_2) = w_7(w_4 - v_1), \tag{A13c, d}$$

$$v_2 w_2 + v_1(w_3 + w_7) = v_2(w_3 + w_6 + w_7). \tag{A13e}$$

The first pair of these equations offers two solutions, the first of which is

$$v_2 = w_3 + w_7 \quad \text{and} \quad v_1 = w_1 + w_5. \tag{A14}$$

This solution corresponds to the case when $L = -M$. Combined with the second

pair of equations, this solution implies the fifth equation. We have not studied this solution. Rather we have considered the solution

$$w_3 v_1 = w_1 v_2 \qquad \text{and} \qquad w_7 v_1 = w_5 v_2 . \tag{A15}$$

This solution includes the F-model already examined by Baxter (1969, 1972) and admits temperature-independent models. Having established these five relationships we now re-parameterize the model in terms of four arbitrary parameters q_1, q_2, w_1 and w_2. We then have

$$\left.\begin{aligned} w_1 &= w_3 - (1-q_1)w_2 , \qquad w_4 = q_2 w_3 + (q_1 - q_2)w_2 , \qquad w_5 = q_1 w_1 , \\ w_6 &= q_1^2 w_2 , \qquad w_7 = q_1 w_3 , \qquad v_1 = q_2 w_1 , \qquad v_2 = q_2 w_3 . \end{aligned}\right\} \tag{A16}$$

Appendix 2

The first of the internal unwanted terms that we must consider are those proportional to $\exp(\mathrm{i}(\bar{k}_i + \bar{k}_j)x_i')$. These are terms like $v_i(x)\eta_{i+1}(x)$ and correction terms which ensure the correct weight is given to configurations with two down arrows in the r' row at the same vertex. These terms are

$$S_{ij}^{(1)} = v_i(x)\eta_j(x) - \left(\frac{w_2}{v_2}\frac{\bar{A}_j}{z_j} + \frac{w_3}{v_2}\bar{B}_j\right)\left(\frac{w_4}{v_2}\frac{\bar{A}_i}{z_i} + \frac{w_7}{v_2}\bar{B}_i\right) + \frac{w_1}{w_5 v_2}\frac{u_9}{u_{10}}\frac{\bar{A}_i \bar{B}_j}{z_i}, \tag{A17a}$$

$$S_{ij}^{(2)} = v_i(x)\eta_j(x) - \left(\frac{w_1}{v_1}\frac{\bar{A}_j}{z_j} + \frac{w_4}{v_1}\bar{B}_j\right)\left(\frac{w_5}{v_1}\frac{\bar{A}_i}{z_i} + \frac{w_6}{v_1}\bar{B}_i\right) + \frac{1}{v_1}\frac{u_8}{u_7}\frac{\bar{A}_i \bar{B}_j}{z_i}, \tag{A17b}$$

where the first arises from x odd and the second from x even. Because of the generalized Bethe-type hypothesis (18), there is for each $S_{ij}^{(m)}$ an $S_{ji}^{(m)}$ ($m = 1, 2$). The condition we require for cancellation is

$$\frac{A(\ldots, i, j, \ldots)}{A(\ldots, j, i, \ldots)} = -\frac{S_{ij}^{(m)}}{S_{ji}^{(m)}} \qquad \text{for} \qquad m = 1, 2 . \tag{A18}$$

To ensure that the correct weight is given to configurations involving two down arrows at the same vertex in the r row, there are additional correction terms. These are also unwanted and must vanish if our solution for Λ_n is to be correct. These terms are of the form

$$S_{ij}^{(3)} = -\left(\frac{u_{10}}{u_9}\frac{v_1}{q_1}\frac{\bar{A}_j}{z_j} + \frac{u_{10}}{u_9}q_2 w_3 \bar{B}_j\right)\left(\frac{\bar{A}_i/z_i + \bar{B}_i}{1 - z_i}\right) + \frac{\bar{A}_i}{z_i}\bar{B}_j - \lambda_i \lambda_j \bar{B}_i \bar{A}_j , \tag{A19a}$$

$$S_{ij}^{(4)} = \left(\frac{u_{10}}{u_9}\frac{v_1}{q_1}\frac{\bar{A}_i}{z_i} + \frac{u_{10}}{u_9}q_2 w_3 \bar{B}_i\right)\left(\frac{\bar{A}_j + \bar{B}_j z_j}{1 - z_j}\right) + \frac{\bar{A}_i \bar{B}_j}{q_1^2 z_i} - \mu_i \mu_j \bar{B}_i \bar{A}_j . \tag{A19b}$$

Thus we have two more equations similar to (A18). In general these are not the same equation, but clearly we must discover under what conditions these equations become identical. To do this we rewrite the four equations in terms of the variable t_j given by

$$z_j = \frac{w(t_j - q_1 + 1) - 1}{t_j(q_1 w - t_j)}, \tag{A20}$$

where

$$w = w_2/w_3\,, \tag{A21}$$

and q_1, w_2 and w_3 are given in Appendix 1 above. This is a useful variable because it is related to the eigenvalue of L_i+M_i and therefore gives relatively simple expressions for z_j, $\bar{A}_j/\bar{B}_j$, λ_j and μ_j. The resulting forms of equation (A18) are unwieldy but by comparing similar terms we find that the condition

$$w_3^{-1} = q_1\{(q_1-q_2)w+1\} \tag{A22}$$

will make the first two equations identical. This and the further condition

$$u_9 = u_{10} \tag{A23}$$

are required to identify all four equations. This last condition is unlike the others in that it is not expressible in terms of q_1, q_2, w_1 and w_2. However, it is a condition which we have expected, since the first set of five conditions (A13) imply

$$u_5 = u_6\,. \tag{A24}$$

If we had started with a lattice rotated $\frac{1}{3}\pi$ radians clockwise, the problem would have been essentially unchanged and the condition (A23) would have been (A24). The complete set of conditions is summarized in equations (19). The resulting single equation is

$$\frac{A(\ldots,i,j,\ldots)}{A(\ldots,j,i,\ldots)} = B(i,j)$$

$$= -\frac{t_i t_j+[1-q_2+q_1\{(q_1-q_2)w+1\}]t_j-q_1 wt_i-q_1(w-q_1 w-1)}{t_i t_j+[1-q_2+q_1\{(q_1-q_2)w+1\}]t_i-q_1 wt_j-q_1(w-q_1 w-1)}. \tag{A25}$$

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