THE ICE AND POTTS MODELS IN STATISTICAL MECHANICS

A Thesis submitted to
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by

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Sections I.1 and I.2 restate the fundamental ideas of statistical mechanics originally stated by Gibbs (1902). Section III.2 is based on previously published work done in collaboration with R.J.Baxter and F.Y.Wu (Baxter et al., 1976). With these exceptions this thesis describes original work carried out by the candidate at The Australian National University.

Where it has been appropriate to relate the candidate's work to that of others, proper acknowledgement has been made in the form of specific references.
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This thesis deals with two two-dimensional lattice models in statistical mechanics. The first of these is the zero-field 20-vertex model on a triangular lattice. This model is the analogue to the ice-type, zero-field six-vertex model on a square lattice. We solve this problem exactly for a restricted set of vertex weights. The other model is the q-component Potts model on a square lattice. This model is equivalent to a staggered ice-type model on a square lattice. Using a variational method we estimate the critical exponent $\beta$ for several values of $q$.

In part I we outline the fundamental statistical mechanical ideas needed, including the definition of the partition function and its relation to the thermodynamic quantities. Mention is also made of the existence and uniqueness of the thermodynamic limit for these models.

The 20-vertex model is discussed in part II. The transfer matrix approach is adopted and a Bethe ansatz
is used for the eigenvector. Unlike the square lattice ice-type model, the triangular lattice 20-vertex model is only soluble by this method for a restricted set of vertex weights. In particular, the ten parameters determining the vertex weights must be expressed in terms of four independent parameters. This results in only one type of non-trivial temperature independent solution. This solution exhibits critical behaviour similar to the square lattice KDP model. The general solution has three states: disordered, antiferroelectric and ferroelectric. Which state the model is in is determined by one of the above four parameters. The transition from the disordered to the antiferroelectric state is of infinite-order and from the disordered to the ferroelectric state is of finite-order. We also compare our results to the free-fermion solution of the same model and note where the two methods overlap.

In part III the Potts model is considered. The model is defined and shown to be equivalent to a staggered ice-type model. A variational principle for the eigenvalues of the transfer matrix of the staggered ice model is determined. Using the zero-temperature solution as a guide a simple form for a sequence of approximations to the eigenvector, below $T_c$, is developed. By using the variational principle we arrive at a set of matrix equations determining the eigenvector at a given level of approximation. By noting some of the symmetries of the transfer matrix we are able to separate some of the dependences of the matrix elements and consequently simplify the original set of equations. We are also able to express the percolation probability (the analogue of the spontaneous magnetization for general values
of \( q \) of the Potts model as a simple function of these matrix elements. At each level of approximation there is a set of algebraic equations to solve. We have used an electronic computer to solve these equations for the first five levels of approximation, and for several values of \( q \) between zero and four. With our results we estimate the critical exponent \( \beta \) for the Potts model. These estimates agree reasonably well with previous work and indicate \( \beta = 0.145 \pm 0.017 \) for \( q = 1 \).
RELATED PUBLICATIONS

These papers, written by the candidate, or by the candidate in collaboration with others, contain some of the work appearing in this thesis.


Baxter, R.J., Kelland, S.B. and Wu, F.Y. "Equivalence of the Potts Model or Whitney Polynomial with an Ice-Type Model" (to be published in J.Phys.A. 1976)

Kelland, S.B. "Estimates of the Critical Exponent $\beta$ for the Potts Model using a Variational Approximation" (to be published in Can. J. Phys.)
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I STATISTICAL MECHANICS OF LATTICE MODELS

1) Introduction

In physics we are often faced with the formidable problem of dealing with systems containing a number of interacting particles of the order of Avagadro's number. Statistical mechanics, as formulated by Willard Gibbs (1902), attacks this problem by relating, in a probabilistic way, the many local interactions that occur between particles to the few macroscopic thermodynamic quantities. The necessity of a statistical approach becomes obvious when one considers the mathematical difficulty involved in solving the equations of motion of $10^{23}$ particles, or the experimental impossibility of determining completely the state of such a system.

During the last half of the nineteenth century
Clausius, Maxwell and Boltzmann introduced the use of probability theory while trying to develop a useful theory of gases based on microscopic properties. The important conceptual step taken by Gibbs in 1902 was to replace the time average by the "ensemble" average. This device considerably broadened the range of application of statistics to physics.

Nevertheless, even now, in the instances where statistical mechanics can be applied it can seldom be carried through to give an exact mathematical result, in closed form, for the thermodynamic quantities. Even in simple cases one is typically confronted with a very large system of integral equations to solve. It is usually necessary to make an approximation, by postulating an additional closure relation, before reasonable progress towards a solution can be achieved. There are, however, a few non-trivial instances where the application of statistics yields a precise mathematical answer. These cases are therefore of intrinsic interest.

A class of models in which statistical mechanics has had a measure of success in providing exact solutions is that of models constructed on rigid lattices. In such models the centres of interaction are assumed to be spatially arranged in a regular and immovable way. These models can represent crystalized solids or even approximate continuous substances if the lattice spacing is sufficiently small. It is with two models of this class that this thesis deals. In what follows we outline the fundamental ideas of statistical mechanics, with particular reference to lattice models.
2) Statistical Mechanics and Thermodynamics

We consider a system having a countable number of discrete configurational states. In general we can label these states with the numbers $1, 2, \ldots, i, \ldots$. With each state of the system we associate an energy $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_i, \ldots$. To develop the necessary statistics we consider a larger system, called an ensemble, consisting of $N$ identical but distinguishable such systems, each capable of occupying the same states $1, 2, \ldots, i, \ldots$. These $N$ systems interact thermally but are otherwise unable to exchange matter or energy. At any instant of time there will be $a_1$ systems in state 1, $a_2$ systems in state 2, and so on, where

$$ \sum_i a_i = N \quad (1.2.1) $$

The purpose of defining the ensemble is to consider the limit $N \rightarrow \infty$. Then the occupation numbers $a_i$ will give an indication of the probability of finding a single system in a given state. While energy is permitted to move between its parts, the ensemble itself is completely isolated from its surroundings and therefore has a constant energy $E$. It follows that

$$ \sum_i a_i \varepsilon_i = E \quad (1.2.2) $$

Because the $N$ systems are distinguishable, a state of the ensemble can be specified by giving the states of the $N$ constituent systems. We now make the basic assumption that all states of the ensemble leading to the same energy $E$ are equally likely. This assumption is
equivalent to the "ergodic hypothesis" (Ehrenfest, 1959, p.21) and by no means rigorously provable. Nevertheless the empirical success of this assumption recommends it highly. This allows us to proceed with a simple probability argument.

The total number of states available to the ensemble is

\[ \sum_{\{a_i\}} \frac{N!}{a_1! \, a_2! \ldots} = \sum_{\{a_i\}} P(a_1, a_2, \ldots) \]  

where the sums are over all sets of non-negative integers \( a_i \) satisfying equations (I.2.1-2). We can then write the average value of \( a_i \) as

\[ \langle a_i \rangle = \frac{\sum_{\{a_i\}} a_i \, P(a_1, a_2, \ldots)}{\sum_{\{a_i\}} P(a_1, a_2, \ldots)} \]  

It is a theorem (Schrödinger, 1948, p.27) that, in the limit \( N \to \infty \), the r.h.s. of equation (I.2.4) approaches the value obtained by replacing each sum with the term corresponding to the maximum of \( P(a_1, a_2, \ldots) \) with the restraints (I.2.1-2). (The proof of the theorem is not simple and will not be given here.)

To obtain the required maximum of \( P \), or equivalently \( \ln P \), we use the undetermined Lagrangian multipliers \( \alpha \) and \( \beta \).

\[ \frac{\partial}{\partial a_i} \left( \ln P + \alpha \left( \sum_i a_i - N \right) - \beta \left( \sum_i a_i \varepsilon_i - E \right) \right) = 0 \] 

(I.2.5)
By the use of Stirling's formula

\[
\lim_{N \to \infty} \frac{\ln(N!)}{N(N\ln N - 1)} = 1
\]  

(I.2.6)

we can replace the factorials in the expression for \( \ln P \).

This gives

\[
\frac{\partial}{\partial a_i} \left[ N(\ln N - 1) - \sum_i a_i (\ln a_i - 1) + \alpha \left( \sum_i a_i - N \right) - \beta \left( \sum_i a_i \epsilon_i - E \right) \right]
\]

\[
= -\ln a_i + \alpha - \beta \epsilon_i
\]

\[
= 0
\]  

(I.2.7)

and therefore the maximizing \( a_i \) is \( a_i^* \)

\[
a_i^* = e^{\alpha - \beta \epsilon_i}
\]  

(I.2.8)

From equation (I.2.4) and the subsequent theorem we have

\[
\langle a_i \rangle = e^{\alpha - \beta \epsilon_i}
\]  

(I.2.9)

We can now use our basic assumption to give a probability interpretation to \( \langle a_i \rangle \). In particular we have the probability that a system is in state \( i \) given by

\[
p_i = \frac{\langle a_i \rangle}{N}
\]  

(I.2.10)

By normalizing these probabilities we can eliminate the parameter \( \alpha \) from equation (I.2.9).

\[
\sum_i p_i = \sum_i N^{-1} e^{\alpha - \beta \epsilon_i} = 1
\]  

(I.2.11)
This implies

\[ N^{-1} e^{\alpha} = \left\{ \sum_i e^{-\beta \varepsilon_i} \right\} \]  
(I.2.12)

and therefore

\[ p_i = \frac{e^{-\beta \varepsilon_i}}{\sum_i e^{-\beta \varepsilon_i}} \]

\[ = Z^{-1} e^{-\beta \varepsilon_i} \]  
(I.2.13)

The factor \( Z \) in the denominator of \( p_i \) contains a good deal of thermodynamic information as we shall see. It is called the partition function. We notice immediately that

\[ -\beta \frac{1}{\beta} \ln Z = \sum_i p_i \varepsilon_i \]

\[ = \langle \varepsilon_i \rangle \]  
(I.2.14)

The quantity \( \langle \varepsilon_i \rangle \) is the expected value of the energy of the system and is naturally identified with the thermodynamic internal energy \( U \).

\[ U \equiv \langle \varepsilon_i \rangle \]  
(I.2.15)

So far we have said nothing about the structure of the system in question. This thesis concerns models constructed on incompressible lattices. The thermodynamic variables pressure and volume are therefore not applicable. We do, however, deal with magnetic and electric fields and their conjugate variables. In this brief exposition then, we will consider a magnetic system subject to an external
field \( \vec{H} \), and having a magnetic moment \( \vec{M} \). We define

\[ H \equiv |\vec{H}| \]  
(I.2.16)

and the magnetization

\[ M \equiv |\vec{M}| \cos \theta \]  
(I.2.17)

where \( \theta \) is the angle between \( \vec{H} \) and \( \vec{M} \).

In order to interpret \( \beta \) in equation (I.2.13) we must consider a process which changes the internal energy of the system. The first law of thermodynamics

\[ dU = dQ + dW \]  
(I.2.18)

indicates there are two ways of doing this, by adding heat \( dQ \) to the system, and by doing work \( dW \) on the system. From equations (I.2.14-15)

\[ dU = \sum_i \epsilon_i dp_i + \sum_i p_i d\epsilon_i \]  
(I.2.19)

In general the division of \( dU \) into the parts \( dQ \) and \( dW \) depends on the process involved in changing the internal energy. In the case of a magnetic system we can do work on the system by taking the field \( \vec{H} \) to be fixed and altering \( M \). If \( M \) is increased by a small amount \( dM \) the work done is

\[ dW = -HdM \]  
(I.2.20)

Heat can be added to the system by placing it in a heat bath of very nearly the same temperature.

From the statistical point of view we can do work on the ensemble of systems by altering each of the
\( \varepsilon_i \) by the small amount \( d\varepsilon_i \). The resulting average amount of work done on each system is

\[
dW = \sum_i p_i d\varepsilon_i \quad (I.2.21)
\]

This explains the correspondence between equations (I.2.18) and (I.2.19), and allows us to write

\[
\sum_i p_i d\varepsilon_i = dU - dQ \quad (I.2.22)
\]

We are now able to derive the second law of thermodynamics. From equations (I.2.13), (I.2.14) and (I.2.21)

\[
d(lnZ) = \sum_i \frac{\partial lnZ}{\partial \beta} d\beta + \sum_i \frac{\partial lnZ}{\partial \varepsilon_i} d\varepsilon_i
\]

\[
= -Ud\beta - \beta dU + \beta dQ \quad (I.2.23)
\]

and therefore

\[
d(lnZ + \beta U) = \beta dQ \quad (I.2.24)
\]

The left hand side, and therefore the right hand side, of equation (I.2.24) is an exact differential and therefore \( \beta \) is an integrating factor for \( dQ \). From thermodynamics \( \beta \) must be proportional to \( T^{-1} \). We therefore have

\[
\beta = \frac{1}{kT} \quad (I.2.25)
\]

where \( k \) is Boltzmann's constant. Defining the entropy \( S \) by

\[
TdS = dQ \quad (I.2.26)
\]
and integrating both sides of equation (I.2.24) we have, to within an additive constant

\[ k(\ln Z + U \beta) = S \]  \hspace{1cm} \text{(I.2.27)}

If we define the Helmholtz free energy \( F \) by

\[ F = U - ST \]  \hspace{1cm} \text{(I.2.28)}

it follows from equation (I.2.27) that

\[ F = -kT \ln Z \]  \hspace{1cm} \text{(I.2.29)}

Further, we have from equations (I.2.18), (I.2.20) and (I.2.24)

\[ dF = -SdT + HdM \]  \hspace{1cm} \text{(I.2.30)}

which is a statement of the second law of thermodynamics.

We can now express the magnetic field as a derivative of the partition function

\[ H = -\beta^{-1} \frac{\partial \ln Z}{\partial M} \]  \hspace{1cm} \text{(I.2.31)}

In practice it is the field which can be varied by the experimenter and the magnetization which is the quantity to be calculated. In this case we can define a modified partition function, or equivalently change the boundary between the system and its surroundings. We define a new state energy to include the effect of the field by

\[ \epsilon_i^* = \epsilon_i + HM_i \]  \hspace{1cm} \text{(I.2.32)}

where \( H \) is the magnetic field, constant throughout the ensemble, and \( M_i \) is the magnetization of the \( i \)th state.
We then have

\[ Z^* = \sum_i e^{-\beta \epsilon_i^*} \]  \hspace{1cm} (I.2.33)

and

\[ -\beta^{-1} \frac{\partial \ln Z^*}{\partial H} \bigg|_T = \langle M_i \rangle \equiv M \]  \hspace{1cm} (I.2.34)

3) Phase Transitions and the Thermodynamic Limit

Those lattice models which have been exactly solved, or hold promise of solution in the near future, are very simple in construction. For this reason they cannot be expected to model accurately the much more complex real situation. Nevertheless, mathematical elegance is not the only reason for studying these models. In the region of a phase transition the doctrine of universality claims that the nature of the singularities depends only on the dimension and symmetries of the system, and not on the detailed form of the interactions. The extent to which this is true is an important question. The theory of scaling also suggests that the critical exponents associated with all phase transitions obey certain common relations (Fisher, 1967; Stanley, 1971). In the light of these ideas it may be the case that the critical behaviour of these simple lattice models does have some bearing on more complicated systems.
To obtain a system which displays a phase transition it is necessary to consider a special limit. In developing the ensemble average we have allowed the size of the ensemble to become infinite. The systems making up the ensemble, however, have remained of fixed size. The lattice models with which this thesis deals have a finite number of configurational possibilities when defined on a lattice of finite size. The partition function for such a finite lattice model is a sum, over a finite number of states, of functions analytic in $\beta$. Therefore the sum and all its derivatives will be analytic in $\beta$. In view of equation (1.2.14) this precludes the possibility of a phase transition. In this situation the only way we can achieve non-analytic behaviour in the partition function is by allowing the lattice to become infinitely large and so include an infinite number of terms in the sum. We then have the possibility of modelling a phase transition, and in fact, in this thermodynamic limit we do sometimes obtain singularities in the derivatives of $Z$. A more detailed account of this behaviour is given by Ruelle (1969).

Having established the need for taking the thermodynamic limit we must ensure that this limit of the partition function exists. This is a very difficult problem in general but the existence has been established for a large class of lattice models by Ruelle (1969). Lieb and Wu (1972) have extended this result to include the existence of the thermodynamic limit for ice-type models with either free or periodic boundary conditions. Free boundary conditions are physically more acceptable; however,
periodic boundary conditions seem to be necessary in order to solve these problems. The question of whether or not the thermodynamic limit is the same in both cases is an important one. For the 20-vertex model on a triangular lattice the answer can be given in the affirmative. Brascamp, Kunz and Wu (1973) have shown that this is the case for the six-vertex model on a square lattice. Their method of weak graph expansions can be applied to the triangular lattice with the result that the soluble cases of the 20-vertex model can be transformed into 32-vertex models with positive vertex weights. It then follows that free and periodic boundary conditions lead to the same thermodynamic limit. The equivalence of these two types of boundary conditions for the staggered ice model used in section III has not been established and is still an open question. However, our results in this case compare favourably with results obtained by methods which do not depend on boundary conditions.
II TWENTY-VERTEX MODEL ON A TRIANGULAR LATTICE

1) Introduction

In the statistical mechanics of critical phenomena there have been few models which have yielded exact results. As mentioned in the first part of this thesis, success in this field has mainly been confined to models constructed on two-dimensional lattices. Essentially there are three different types of models which have been solved. The first is the Ising model in zero field, solved by Onsager (1944). The second is the ice-type model, solved by Lieb (1967a,b,c) and Sutherland (1967), and the most recent is the eight-vertex model solved by Baxter (1972). In addition to increasing our understanding of phase transitions these solutions are of intrinsic mathematical interest. Some of the models can be solved by various methods, while others require very special techniques.
Because it is useful to know the scope of these methods, we have attempted the solution of an ice-type model on a triangular lattice. We begin by taking quite general vertex weights but find that restrictions must be imposed if we are to solve the model by known methods. Under certain conditions the Bethe ansatz method, used in solving the square lattice ice-type models, gives the required result, while under different conditions the free-fermion method, used by Hurst and Green (1960) to solve the Ising model, is successful. Included in the solutions is a temperature independent case which is analogous to the square lattice KDP model of Slater (1941).

The ice-type model originated as a model of hydrogen bonded crystals. In real ice the crystal lattice forms a wurtzite structure. The oxygen atoms are localized about the vertices of the lattice, while the hydrogen nuclei are confined between the oxygen pairs. The most stable situation is for a hydrogen nucleus to be closer to one of its oxygen neighbours than the other. To preserve local electrical neutrality exactly two hydrogens should be close to each oxygen. At zero temperature the residual entropy of ice is determined by the number of ways the hydrogen nuclei can be arranged so as to comply with this restriction. In two dimensions the square lattice has the same coordination number as the wurtzite lattice. In this case the topological considerations are easier and Lieb (1967a) has solved the problem. Pauling (1935) suggested a simple method for approximating the degeneracy of the zero temperature solution. A vertex configuration can be specified by indicating which of the four possible hydrogen
nuclei are near to the oxygen. The condition that there are exactly two means there are six possible vertex configurations. If there were no such restriction there would be 16 possibilities. A square lattice of N sites has 2N edges, and on each edge is a hydrogen nucleus which can be close to one of two oxygens. Ignoring the interaction of adjacent vertices, the number of configurations is approximately

\[ 2^{2N} \left( \frac{6}{16} \right)^N = \left( \frac{3}{2} \right)^N \]  

(II.1.1)

Lieb's result is

\[ \left( \frac{4}{3} \right)^{3N/2} = \left( 1.5396... \right)^N \]  

(II.1.2)

in the limit as N becomes large. The model can be generalized and made temperature dependent by giving the six allowable vertex configurations different weights. The most general model with all six vertex weights different was solved by Sutherland et al. (1967).

We consider an ice-type model on a triangular lattice. As in the square lattice model we place "hydrogen nuclei" on the edges of the lattice so that at each lattice vertex there are equal numbers of close and distant hydrogens. This gives 20 different vertex configurations. Baxter (1969) has solved this problem for a restricted set of vertex weights, corresponding to the square lattice F-model, solved by Lieb (1967b). The more general solution we find includes this as a special case.
2) Statement of the Problem

The model is constructed on a triangular lattice of $M$ rows of $N$ vertices each. Between successive rows of vertices there is a row of diagonal edges joining the vertices of one row to the vertices of the next. Unless explicitly stated otherwise the word "row" will refer to such a row of diagonal edges. Clearly there are $2N$ edges in a row. The labelling of successive rows is given in figure (II.1). The rows have cyclic boundary conditions so that we identify the $(2N+1)$th edge with the first edge. We represent possible positions of intermediate hydrogen nuclei by placing arrows on the edges between vertices. We therefore consider arrangements of arrows on the edges of this lattice, in which there are three arrows pointing into each vertex, and three arrows pointing out. There are 20 possible arrow configurations at a vertex. If we treat as identical pairs of configurations which can be obtained from each other by reversing all arrows, we obtain the ten distinct configurations shown in figure (II.2). This identification introduces a degeneracy into the solution which could be removed by application of an electric field. However, we have considered only the simple problem without an electric field. To begin with, we assign to the ten configurations the energies $e_1, e_2, \ldots, e_{10}$ or equivalently, the vertex weights $u_i = \exp(-e_i/kT)$ where $i=1,2,\ldots,10$.

Because of the cyclic boundary conditions the number of down arrows in a row is conserved as we move from one row to the next. This suggests using the transfer matrix approach to the problem. Instead of considering
Figure II.1  The numbering of the diagonal edges in two successive rows. Below is the $r$ row and above the $r'$ row.

Figure II.2  The ten distinct reversal-symmetric vertex configurations.
overall arrangements of arrows, we consider what arrangements of arrows are possible in the \((m+1)\)th row given the arrangement in the \(m\)th 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 (figure II.2), and we represent any other configuration by drawing heavy lines on edges whose arrows are 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 on the lattice is equivalent to studying how the down arrows propagate from one row to the next, because the lattice is homogeneous. To define the transfer matrix \(T\), we let \(r\) and \(r'\) represent arrow configurations on two successive rows of diagonal edges. The elements of \(T\) are given by

\[
T(r,r') = \sum_{\text{allowable horizontal arrow configurations}} \prod (\text{vertex weights})
\]

(II.2.1)

where the sum is over the permitted arrow configurations on the intermediate horizontal edges and the product is of the resulting vertex weights. \(T\) is a \(2^N \times 2^N\) matrix. Because it is not allowable to pass from a row with \(n\) down arrows to a row with a number of down arrows different from \(n\), many of the matrix entries are zero. Therefore the
transfer matrix breaks up into blocks along the principle diagonal, each block corresponding to a fixed number of down arrows.

In order to calculate the free energy of the system we use the partition function

\[ Z = \sum \exp \left\{-\sum_{i=1}^{10} p_i e_i / kT\right\} \]  \hspace{1cm} (II.2.2)

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

\[ Z = \operatorname{Tr}(T^M) \]

\[ = \sum_{i=1}^{2^{2N}} \lambda_i^M \]  \hspace{1cm} (II.2.3)

where the \( \lambda_i \) 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 \( M \), the number of rows in the lattice, become large we obtain

\[ Z = \left( \lambda(2N) \right)^M \]  \hspace{1cm} (II.2.4)

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

\[ \lim_{N \to \infty} \lim_{M \to \infty} (MN)^{-1} \ln Z = \lim_{N \to \infty} N^{-1} \ln \left( \lambda(2N) \right) \]

\[ = -\mathcal{F}/kT \]  \hspace{1cm} (II.2.5)
where $\mathcal{F}$ is the free energy per vertex.

To find the largest eigenvalue of the "infinite" transfer matrix we first consider the simple cases of few down arrows in a row. We are then able to generalize to n down arrows in a row, and ultimately obtain an expression for this eigenvalue.

3) Simple Cases

(a) No down arrows in a row

If $\mathbf{r}$ 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 $\mathbf{r}'$ will also have no down arrows. The part of the transfer matrix corresponding to this situation is the $1 \times 1$ block

$$T(\mathbf{r}, \mathbf{r}') = \exp(-N\epsilon_1/kT) + \exp(-N\epsilon_2/kT)$$

$$= u_1^N + u_2^N \quad (\text{II.3.1})$$

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

(b) One down arrow in a row

When a row configuration $\mathbf{r}$ has one down arrow, the next row $\mathbf{r}'$ will also have one down arrow. The position of this down arrow can be on any of the $2N$ edges 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,
\[ \Lambda_1 p(x) = \sum_{y=1}^{x'+1} u_2^{N-(x'-y''+2)/2} f(x) c(y,x) p(y) + \sum_{y=x'}^{2N} u_1^{N-(y''-x'+2)/2} g(y) d(x,y) p(y) \]

where \( x \) and \( y \) are the numbers of the edges with down arrows in configurations \( r \) and \( r' \) respectively, \( \Lambda_1 \) is the eigenvalue and \( p(x) \) is the component of the eigenvector for the state with a down arrow on edge \( x \). The functions \( c, d, f, \) and \( g \) give the correct weights to the configurations and the primes on \( x \) and \( y \) relate these edges to their respective vertices. The definitions of these functions are

\[ c(y,x) = g(y) u_1^{(x'-y''-2)/2} \quad \text{for } y<x' \]
\[ = u_5/u_9 \quad \text{for } y=x' \quad \text{and } x \text{ even} \]
\[ = u_4/u_8 \quad \text{for } x \text{ odd} \]
\[ = u_3/u_9 \quad \text{for } y=x'+1 \quad \text{and } x \text{ even} \]
\[ = u_6/u_8 \quad \text{for } x \text{ odd} \]

\[ (II.3.3) \]

\[ d(x,y) = f(x) u_2^{(y''-x'+2)/2} \quad \text{for } y>x'+1 \]
\[ = u_6/u_7 \quad \text{for } y=x' \quad \text{and } x \text{ even} \]
\[ = u_3/u_7 \quad \text{for } x \text{ odd} \]
\[ = u_6/u_10 \quad \text{for } y=x'+1 \quad \text{and } x \text{ even} \]
\[ = u_6/u_10 \quad \text{for } x \text{ odd} \]

\[ (II.3.4) \]

\[ f(x) = u_8 \quad \text{for } x \text{ odd} \]
\[ = u_9 \quad \text{x even} \]

\[ (II.3.5) \]
\[ g(x) = \begin{cases} u_7 & \text{for } x \text{ odd} \\ u_{10} & \text{for } x \text{ even} \end{cases} \quad (\text{II.3.6}) \]

\[ x' = \begin{cases} x - 1 & \text{for } x \text{ even} \\ x - 2 & \text{for } x \text{ odd} \end{cases} \quad (\text{II.3.7}) \]

\[ y'' = \begin{cases} y - 1 & \text{for } y \text{ even} \\ y & \text{for } y \text{ odd} \end{cases} \quad (\text{II.3.8}) \]

There are $2N+2$ terms in the sums in equation (II.3.2). 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. Figure (II.3) shows a general configuration, with one down arrow, in the heavy line representation. The heavy line can only propagate to the right along horizontal edges and upwards along diagonal edges. Because of the boundary conditions lines leaving the right of the row of vertices enter again at the left.

Expanding the right-hand side of equation (II.3.2) we have

\[ A_1 p(x) = \frac{u_2}{u_1} f(x) \left( \frac{u_2}{u_1} \right)^{-x'/2} \left[ \left( \frac{u_2}{u_1} \right)^{\frac{1}{2}} \left( u_{7p(1)} + u_{10p(2)} \right) + \left( \frac{u_2}{u_1} \right)^{3/2} \left( u_{7p(3)} + u_{10p(4)} \right) + \ldots + \left( \frac{u_2}{u_1} \right)^{(x'-2)/2} \left( u_{7p(x'-2)} + u_{10p(x'-1)} \right) \right] \]
Figure II.3  Heavy line representation of two possible configurations with one down arrow. The numbers indicate the vertex types.
To simplify the algebra we make the transformation

\[ \overline{p}(y) = \left( \frac{u_2}{u_1} \right)^{y''/2} g(y) p(y) \quad (II.3.10) \]

Following Lieb (1967a,b,c) we assume the Bethe ansatz form of the eigenvector

\[ \overline{p}(x) = A \exp(ikx') \quad \text{for } x \text{ odd} \]
\[ = \overline{B} \exp(ikx') \quad \text{x even} \quad (II.3.11) \]

Then by performing the sums within the large brackets of equation (II.3.9) we can write

\[ \Lambda_1 \overline{p}(x) = h(x) \left( u_2^N \left( \sigma + v(x) \exp(ikx') \right) + u_1^N \eta(x) \exp(ikx') + \tau \right) \]

(II.3.12)

In writing the expressions for \( h(x) \), \( v(x) \), \( \eta(x) \), \( \sigma \) and \( \tau \) it is useful to define the following nine parameters
\[ v_1 = \frac{u_9 u_{10}}{u_1 u_2} \quad w_3 = \frac{u_2 u_5 u_7}{u_1^2 u_{10}} \]
\[ v_2 = \frac{u_7 u_8}{u_1^2} \quad w_4 = \frac{u_8}{u_1} \]
\[ w_5 = \frac{u_5 u_{10}}{u_2 u_7} \]
\[ w_1 = \frac{u_6 u_7}{u_1 u_7} \quad w_6 = \frac{u_3}{u_2} \]
\[ w_2 = \frac{u_2 u_3}{u_1^2} \quad w_7 = \frac{u_6 u_7}{u_1 u_{10}} \]

(II.3.13)

The functions in equation (II.3.12) can now be written as

\[ h(x) = v_1 \quad \text{for } x \text{ even} \]
\[ = v_2 \quad x \text{ odd} \] (II.3.14)

\[ \eta(x) = \frac{\bar{A} + \bar{B} z}{1-z} + \frac{w_1 A}{v_1 z} + \frac{w_5 B}{v_1} \quad \text{for } x \text{ even} \]
\[ = \frac{\bar{A} + \bar{B} z}{1-z} + \frac{w_2 A}{v_2 z} + \frac{w_3 B}{v_2} \quad x \text{ odd} \] (II.3.15)

\[ \nu(x) = \frac{w_5 A}{v_1 z} + \frac{w_6 B}{v_1} - \frac{\bar{A}/z + \bar{B}}{1-z} \quad \text{for } x \text{ even} \]
\[ = \frac{w_4 A}{v_2 z} + \frac{w_7 B}{v_2} - \frac{\bar{A}/z + \bar{B}}{1-z} \quad x \text{ odd} \] (II.3.16)

\[ \sigma = (\bar{A}/z + \bar{B}) \exp(i\bar{k})/(1-z) \] (II.3.17)

\[ \tau = -(\bar{A}/z + \bar{B}) \exp \left[ i\bar{k}(2N+1) \right] / (1-z) \] (II.3.18)

\[ z = \exp(2i\bar{k}) \] (II.3.19)

Matching like terms in equation (II.3.12) we see that if

\[ h(x) \nu(x) \exp(i\bar{k}x') = \lambda \tilde{p}(x) \]
\[ h(x) \eta(x) \exp(i\bar{k}x') = \mu \tilde{p}(x) \] (II.3.20)
and
\[ u_2^N \sigma + u_1^N \tau = 0 \]  \hspace{1cm} (II.3.21)
then
\[ \Lambda_1 = u_2^N \lambda + u_1^N \mu \]  \hspace{1cm} (II.3.22)

The equations (II.3.20) can be written as
\[ L \begin{pmatrix} \frac{\lambda}{B} \\ \frac{\bar{\lambda}}{B} \end{pmatrix} = \lambda \begin{pmatrix} \frac{\lambda}{B} \\ \frac{\bar{\lambda}}{B} \end{pmatrix} \]
\[ M \begin{pmatrix} \frac{\lambda}{B} \\ \frac{\bar{\lambda}}{B} \end{pmatrix} = \mu \begin{pmatrix} \frac{\lambda}{B} \\ \frac{\bar{\lambda}}{B} \end{pmatrix} \]  \hspace{1cm} (II.3.23)

where \( L \) and \( M \) are the 2 x 2 matrices.
\[ L = \begin{pmatrix} v_2/z(z-1) + w_4/z & v_2/(z-1) + w_7 \\ v_1/z(z-1) + w_5/z & v_1/(z-1) + w_6 \end{pmatrix} \]
\[ M = \begin{pmatrix} v_2/(1-z) + w_2/z & v_2z/(1-z) + w_3 \\ v_1/(1-z) + w_1/z & v_1z/(1-z) + w_4 \end{pmatrix} \]  \hspace{1cm} (II.3.24)

In order that equation (II.3.22) gives \( \Lambda_1 \) as an eigenvalue of the transfer matrix, \( \lambda \) and \( \mu \) must have the same eigenvector, or equivalently, \( L \) and \( M \) must commute. Further, since we expect \( z \) to be determined by the boundary conditions (II.3.21), and not by any requirement at this stage, \( L \) and \( M \) must commute for all complex numbers \( z \).
This imposes restrictions on the \( v_i \)'s and the \( w_i \)'s, and therefore on the vertex weights. The equations that result
from this requirement are

\[ v_1 (w_3 + w_7) = v_2 (w_1 + w_5) \]
\[ w_1 (w_7 - v_2) = w_3 (w_5 - v_1) \]
\[ w_3 (w_4 - v_2) = w_2 (w_7 - v_2) \]
\[ w_6 (w_3 - v_2) = w_7 (w_4 - v_1) \]
\[ v_2 w_2 + v_1 (w_3 + w_7) = v_2 (w_3 + w_6 + w_7) \]  

(II.3.25)

The first pair of equations has two solutions. One of these is

\[ v_2 = w_3 + w_7 , \quad v_1 = w_1 + w_5 \]  

(II.3.26)

This solution corresponds to the case when \( L = -M \). It turns out that this case is more easily solved, not using the Bethe ansatz approach, but rather the fermion operator method (Green and Hurst, 1964). Therefore we will leave this case for the moment and return to it later.

The second solution of equations (II.3.25a,b) is

\[ w_3 v_1 = w_1 v_2 , \quad w_7 v_1 = w_5 v_2 \]  

(II.3.27)

This solution includes the F-model already examined by Baxter (1969), and admits temperature-independent solutions (i.e. solvable for all temperatures).

Using equations (II.3.27) and (II.3.25c,d,e) we now re-parameterize the model in terms of four arbitrary parameters \( q_1, q_2, w_2, \) and \( w_3 \). We therefore have

\[ w_1 = w_3 - (1-q_1) w_2 , \quad w_7 = q_1 w_3 \]
\[ w_4 = q_2 w_3 + (q_1-q_2) w_2 , \quad v_1 = q_2 w_1 \]
\[ w_5 = q_1 w_1 \quad , \quad v_2 = q_2 w_3 \]

\[ w_6 = q_6 w_2 \]  \hspace{1cm} \text{(II.3.28)}

To summarize, equations (II.3.20) have introduced some restrictions on the original ten vertex weights. Equation (II.3.21) can, in principle, be solved for \( \vec{k} \), and equation (II.3.22) then gives the eigenvalue \( \lambda_1 \).

(c) 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 giving the correct weight to configurations in which the down arrows of \( \tau \) and \( \tau' \) are located at the same vertex. The eigenvalue equation corresponding to equation (II.3.12) is

\[ \lambda_1 \vec{p}_1(x_1)\vec{p}_2(x_2) = h(x_1)h(x_2) \]

\[ \cdot \left[ u_2^N \left( \sigma_1 + v_1(x_1)\exp(i\vec{k}_1 x_1) \right) \left( \eta_2(x_1)\exp(i\vec{k}_2 x_1) + v_2(x_2)\exp(i\vec{k}_2 x_2) \right) \right] \]

\[ + \ u_1^N \left( \eta_1(x_1)\exp(i\vec{k}_1 x_1) + v_1(x_2)\exp(i\vec{k}_1 x_2) \right) \left( \eta_2(x_2)\exp(i\vec{k}_2 x_2) + \tau_2 \right) \]

\[ + \ C_2 \]  \hspace{1cm} \text{(II.3.29)}

where \( C_2 \) denotes correction terms which specifically give the correct weight to configurations with more than one down arrow at a vertex. The exact form of these terms is given below in equations (II.3.32-35). We have, for the moment, made the assumption that the component of the eigenvector for the state with down arrows at \( x_1 \) and \( x_2 \)
is simply the product of one down arrow components. Thus the subscripts on $\eta, \nu, \tau,$ and $\sigma$ refer to a generalization of $\overline{p}(x)$ to $\overline{p}_i(x)$, where

$$
\overline{p}_i(x) = \overline{A}_i \exp(iK_i x') \quad \text{for } x \text{ odd, } i=1,2
$$

$$
\overline{p}_i(x) = \overline{B}_i \exp(iK_i x') \quad \text{x even, } i=1,2
$$

(II.3.30)

Similarly the generalizations of equations (II.3.20) are

$$
h(x)\nu_i(x)\exp(iK_i x') = \lambda_i \overline{p}_i(x)
$$

$$
h(x)\eta_i(x)\exp(iK_i x') = \mu_i \overline{p}_i(x) \quad , \quad i=1,2
$$

(II.3.31)

There are terms in equation (II.3.29) of a type that did not occur in equation (II.3.12). These terms must also be considered if we are to generalize equation (II.3.22). Terms proportional to $\exp[i(k_1+k_2)x_1]$ and $\exp[i(k_1+k_2)x_2]$ are the first type of unwanted internal terms. They are terms with coefficients like $\nu_1(x_1)\eta_2(x_1).$ Some also occur in the correction terms which ensure the correct weight is given to configurations with two down arrows at the same vertex in the $\tau'$ row. The complete coefficient for these terms can be written as

$$
S_{12}^{(1)} = \nu_1(x)\eta_2(x) - \nu_2^2(w_2\overline{A}_2/z_2 + w_3\overline{B}_2)(w_4\overline{A}_1/z_1 + w_7\overline{B}_1)
$$

$$
+ \frac{w_1 w_9 \overline{A}_1 \overline{B}_2}{w_5 v_2 u_1 z_1}
$$

(II.3.32)

when $x$ is odd, and
\[ S_{12}^{(2)} = v_1(x) \eta_2(x) - v_1^2(w_1 \overline{A}_2/z_2 + w_6 \overline{B}_2) (w_5 \overline{A}_1/z_1 + w_6 \overline{B}_1) \]

\[ + \frac{u_9 \overline{A}_1 \overline{B}_2}{v_1 u_7 z_1} \]  

(II.3.33)

when \( x \) is even. The second type of unwanted internal term occurs in \( C_2 \) to give the correct weight to configurations involving two down arrows at a vertex in the \( r \) row. The coefficients of these terms are of the form

\[ S_{12}^{(3)} = -\frac{u_{10}}{u_9} \left( \frac{v_1 \overline{A}_2}{q_1 z_2} + q_2 w_3 \overline{B}_2 \right) \left( \frac{\overline{A}_1/z + \overline{B}_1}{1 - z_1} \right) + \frac{\overline{A}_1 \overline{B}_2}{z_1} - \lambda_1 \lambda_2 \overline{B}_1 \overline{A}_2 \]  

(II.3.34)

\[ S_{12}^{(4)} = \frac{u_{10}}{u_9} \left( \frac{v_1 \overline{A}_1}{q_1 z_1} + q_2 w_3 \overline{B}_1 \right) \left( \frac{\overline{A}_2 + \overline{B}_2 z_2}{1-z_2} \right) + \frac{\overline{A}_1 \overline{B}_2}{q_1 z_1} - \mu_1 \mu_2 \overline{B}_1 \overline{A}_2 \]  

(II.3.35)

In order to have these terms total zero we assume that the component of the eigenvector for two down arrows is not simply a product of one down arrow components, but rather a linear combination of such products. We therefore take the new component of the eigenvector, for down arrows at \( x_1 \) and \( x_2 \), to be \( \xi(x_1, x_2) \) defined by

\[ \xi(x_1, x_2) = A_{12} \overline{p}_1(x_1) \overline{p}_2(x_2) + A_{21} \overline{p}_2(x_1) \overline{p}_1(x_2) \]  

(II.3.36)

This results in additional unwanted terms with coefficients \( S_{21}^{m} \), \( m=1,2,3,4 \). The conditions required for the cancellation of these terms are
\[ \frac{A_{12}}{A_{21}} = -\frac{S_{12}^{(m)}}{S_{21}^{(m)}}, \quad m=1,2,3,4 \]  

(II.3.37)

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 variables \( t_i \), given by

\[ z_i = \frac{w(t_i - q_i + 1) - 1}{t_i(q_1 w - t_i)} \quad i=1,2 \]  

(II.3.38)

where

\[ w = \frac{w_2}{w_3} \]  

(II.3.39)

The variable \( t_i \) is related to the eigenvalue of \( L_i + M_i \) and gives relatively simple expressions for \( z_i, \bar{A}_i/\bar{B}_i, \lambda_i, \) and \( u_i \). The resulting forms of equation (II.3.37) are unwieldy, but by comparing similar terms we find that the condition

\[ w_3^{-1} = q_1 \left( (q_1 - q_2)w + 1 \right) \]  

(II.3.40)

will make the first two equations identical. The further condition

\[ u_9 = u_{10} \]  

(II.3.41)

makes all four equations the same. This last condition is unlike the others in that it is not expressible in terms of \( q_1, q_2, w_2, \) and \( w_3 \); however, it is a condition which we have expected. The conditions (II.3.25) imply

\[ u_5 = u_6 \]  

(II.3.42)
If we had started with a lattice rotated $\frac{\pi}{3}$ radians clockwise, the problem would have been essentially unchanged and condition (II.3.41) would have been (II.3.42). Combining the conditions (II.3.25), (II.3.27), and (II.3.40-41) we can summarize the restrictions on the vertex weights as

$$u_5 = u_6 \quad , \quad u_7 = u_8 \quad , \quad u_9 = u_{10}$$

$$I = u_2 u_3 + u_1 u_5 u_9 / u_7$$
$$= u_3 u_1 + u_2 u_7 u_5 / u_9$$
$$= u_1 u_2 + u_4 u_7 u_9 / u_5$$

$$u_4 = I^2 / u_1 u_2 u_3 - (u_1^{-1} + u_2^{-1} + u_3^{-1}) I + u_1 + u_2 + u_3$$

(II.3.43)

These equations define a four-dimensional hypersurface in ten-dimensional $u$-space. The surface is maximal with respect to the Bethe ansatz, in the sense that there is no five-dimensional surface containing it and still consistent with the Bethe ansatz. 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.

In addition to unwanted internal terms there are unwanted boundary terms. These are terms that involve $\sigma_i$ and $\tau_i$. In a manner similar to equation (II.3.21) we require

$$u_2^N \sigma_1 A_{12} = u_1^N \tau_1 A_{21}$$

$$u_2^N \sigma_2 A_{21} = u_1^N \tau_2 A_{12}$$

(II.3.44)
These two equations determine $\bar{K}_1$ and $\bar{K}_2$. Finally we can write the eigenvalue $\Lambda_2$ as

$$\Lambda_2 = u_2^N \lambda_1 \lambda_2 + u_1^N \mu_1 \mu_2 \quad (II.3.45)$$

4) General Case

The generalization to the case involving $n$ down arrows in a row is straightforward. The Bethe ansatz for the component of the eigenvector with down arrows at $x_1, x_2, \ldots, x_n$ is

$$\xi(x_1, \ldots, x_n) = \sum_{\mathcal{P}} A(\mathcal{P}) \prod_{i=1}^{n} \bar{P}_i \left[ x_{\mathcal{P}(i)} \right] \quad (II.4.1)$$

where the form of the $\bar{P}_i$'s is given by equation (II.3.30), $i=1, 2, \ldots, n$. $\mathcal{P}$ is the set of permutations of the $n$ integers $1, 2, \ldots, n$. The eigenvalue equation for a single wave is

$$\Lambda_n \bar{P}_1(x_1) \bar{P}_2(x_2) \ldots \bar{P}_n(x_n) = h(x_1)h(x_2)\ldots h(x_n)$$

$$\cdot \left[ u_2^N \left( \sigma_1 + \nu_1(x_i) \exp(i\bar{K}_1 x_i) \right) \prod_{j=2}^{n} \left( n_j(x_{j-1}) \exp(i\bar{K}_j x_{j-1}) + \nu_j(x_j) \exp(i\bar{K}_j x_j) \right) \right]$$

$$+ u_1^N \left[ n_n(x_n) \exp(i\bar{K}_n x_n) + \prod_{j=1}^{n-1} \left( n_j(x_{j+1}) \exp(i\bar{K}_j x_{j+1}) + \nu_j(x_{j+1}) \exp(i\bar{K}_j x_{j+1}) \right) \right]$$

$$+ \mathcal{C}_n \quad (II.4.2)$$
If equations (II.3.43) are satisfied, and if equations (II.3.31) hold for \( i = 1, 2, \ldots, n \), then

\[
\Lambda_n = u_2^N \lambda_1 \ldots \lambda_n + u_1^N \mu_1 \ldots \mu_n \quad (II.4.3)
\]

The unwanted internal terms will vanish if

\[
A(...,i,j,...)/A(...,j,i,...) = B(i,j) \quad (II.4.4)
\]

where \( B(i,j) \) is the unique left hand side of equations (II.3.37) obtained by imposing restrictions (II.3.40-41).

In terms of the variables \( t_i \) and \( t_j \), defined by equation (II.3.38), \( i = 1, 2, \ldots, n \), we have

\[
B(i,j) = \frac{t_i t_j + \left[ 1 - q_2 + q_1 \left( (q_1 - q_2) w + 1 \right) \right] t_j - q_1 w t_i - q_1 (w - q_1 w - 1)}{t_i t_j + \left[ 1 - q_2 + q_1 \left( (q_1 - q_2) w + 1 \right) \right] t_i - q_1 w t_j - q_1 (w - q_1 w - 1)} \quad (II.4.5)
\]

The unwanted boundary terms will vanish if we have

\[
(u_1/u_2)^N \exp(2i \bar{k}_i N) = \prod_{j=1}^{n} B(i,j) \quad \text{for } i = 1, 2, \ldots, n \quad (II.4.6)
\]

In principle, these last \( n \) equations can be solved for the \( n \) quantities \( \bar{k}_i \). Using

\[
\lambda_i = \frac{(q_1 w - t_i)(t_i(q_1 - q_2) + q_1)}{(t_i + 1)q_1(q_1 - q_2)w + 1} \quad (II.4.7a)
\]

\[
\mu_i = \frac{(q_1 w - t_i)(t_i + 1 - q_2)}{(t_i + 1)q_1(q_1 - q_2)w + 1} \quad (II.4.7b)
\]
and equations (II.3.19), (II.3.38) and (II.4.3), we can find the eigenvalue $\Lambda_n$.

5) Transformation to New Set of Parameters

Equation (II.4.6) is similar to equation (3.12) of Lieb (1967a). Following his method we require a change of variable which makes $B(i,j)$ a function of the difference of its arguments. Then, in the limit of $N$ large, we will have to solve an integral equation with a difference kernel. This sort of equation can sometimes be solved easily by Fourier transforms.

We first simplify equation (II.4.6) by reverting from $p_1(x)$ to the original eigenvector $p_i(x)$, where

$$p_i(x) = A_i \exp(ik_i x') \quad \text{for} \ x \ \text{odd}$$

$$= B_i \exp(ik_i x') \quad \text{for} \ x \ \text{even}$$

(II.5.1)

Equation (II.4.6) then becomes

$$\exp(2ik_i N) = \prod_{\substack{j=1 \atop j \neq i}}^n B(i,j)$$

(II.5.2)

in terms of $k_i$ instead of $\tilde{k}_i$. We noted from the conditions (II.4.43) that three parameters are required to specify the ratios of the ten vertex weights. We choose these parameters to be $\phi$, $\theta$ and $\zeta$, defined by
\[ \cos \phi = \frac{(I - u_1u_2 - u_2u_3 - u_1u_3)I_3}{2u_1u_2u_3}, \quad 0 \leq \text{Re}(\phi) < \pi \]  
 \text{(II.5.3a)}

\[ \cos 2\theta = \frac{(u_1u_2 + u_2u_3 + u_1u_3)I - I^2 - 2u_1u_2u_3}{2u_1u_2u_3u_5}, \quad 0 \leq \text{Re}(\theta) < \frac{\pi}{2} \]  
 \text{(II.5.3b)}

\[ \tan \zeta = \left( \frac{u_1u_2 - u_2u_3}{u_1u_3 + u_2u_3} \right) \tan \theta, \quad -\frac{\pi}{2} \leq \text{Re}(\zeta) \leq \frac{\pi}{2} \]  
 \text{(II.5.3c)}

We now define a new variable \( \alpha_i \) in terms of \( k_i \) by

\[ \exp(2ik_i) = \frac{\sin(\alpha_i - \phi + \theta) \sin(\alpha_i - \theta)}{\sin(\alpha_i - \theta + \phi) \sin(\alpha_i + \theta)}, \quad -\frac{\pi}{2} \leq \text{Re}(\alpha_i) \leq \frac{\pi}{2} \]  
 \text{(II.5.4)}

It then follows that

\[ B(i,j) = -\frac{\sin(\alpha_i - \alpha_j - \phi)}{\sin(\alpha_j - \alpha_i - \phi)} \]  
 \text{(II.5.5)}

Thus \( B(i,j) \) depends on \( \alpha_i \) and \( \alpha_j \) only through their difference as required. The expressions for \( \lambda_i \) and \( \mu_i \) are

\[ \lambda_i = \frac{\sin(\alpha_i - \theta + \phi) \sin(\alpha_i + \zeta + \phi)}{\sin(\alpha_i - \theta) \sin(\alpha_i + \zeta)} \]  
 \text{(II.5.6a)}

\[ \mu_i = \frac{\sin(\alpha_i - \theta + \phi) \sin(\alpha_i + \zeta - \phi)}{\sin(\alpha_i - \theta) \sin(\alpha_i + \zeta)} \]  
 \text{(II.5.6b)}
In terms of $\phi$, $\theta$ and $\zeta$ the vertex weights are

\[ u_1 = \rho \sin(\theta + \zeta) \sin(\phi - \theta + \zeta) \sin 2\theta \]
\[ u_2 = \rho \sin(\theta - \zeta) \sin(\phi - \theta - \zeta) \sin 2\theta \]
\[ u_3 = \rho \sin(\phi - \theta + \zeta) \sin(\phi - \theta + \zeta) \sin(\phi - 2\theta) \]
\[ u_4 = \rho \sin(\phi - \theta - \zeta) \sin(\phi - \theta - \zeta) \sin 2\theta \]
\[ + \sin(\phi - \theta + \zeta) \sin(\phi + \theta - \zeta) \sin \phi \]
\[ u_5 = \rho \sin(\phi - \theta + \zeta) \sin(\phi - \theta - \zeta) \sin \phi \]
\[ u_7 = \rho \sin(\phi - \theta + \zeta) \sin \phi \sin 2\theta \]
\[ u_9 = \rho \sin(\phi - \theta - \zeta) \sin \phi \sin 2\theta \] \hspace{1cm} (II.5.7)

where $\rho$ is an arbitrary normalization factor.

A fundamental symmetry of this problem is that the analysis is unaffected by rotating the lattice through $\frac{\pi}{3}$ radians. While this symmetry is implicitly contained in the equations developed so far, it can also be expressed explicitly in terms of a permutation of the vertex weights. A counterclockwise rotation of $\frac{\pi}{3}$ radians results in a permutation given by

\[
\begin{bmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
2 & 3 & 1 & 4 & 7 & 8 & 9 & 10 & 6 & 5
\end{bmatrix}
\] \hspace{1cm} (II.5.8)

The corresponding transformations of $\phi$, $\theta$ and $\zeta$ are

\[ \phi \rightarrow \phi \]
\[ \theta \rightarrow (\phi - \theta - \zeta)/2 \]
\[ \zeta \rightarrow (3\theta - \phi - \zeta)/2 \] \hspace{1cm} (II.5.9)
6) Antiferroelectric State \((\cos \phi > 1)\)

This model includes the triangular lattice F-model discussed by Baxter (1969). It therefore undergoes a phase transition for at least one set of 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 antiferroelectric state. This happens when

\[ \cos \phi > 1 \]  
\text{(II.6.1)}

and \(\phi, \theta\) and \(\zeta\) are pure imaginary

\[ \phi = ir, \quad \theta = is, \quad \zeta = iv \]  
\text{(II.6.2)}

\[ r > 2s > 2|v| \]  
\text{(II.6.3)}

Condition (II.6.3) ensures that all the vertex weights are real and positive.

Equation (II.5.2) can be written as

\[ \exp(2ik_i N) = (-1)^{n-1} \prod_{j=1}^{n} \frac{\sin(\alpha_i - \alpha_j - \phi)}{\sin(\alpha_j - \alpha_i - \phi)} \]  
\text{(II.6.4)}

In this regime equation (II.5.4) implies that the \(\alpha_i\)'s must remain real for the \(k_i\)'s to be real. Following Yang and Yang (1966) we define a function \(\Theta(\alpha)\) by

\[ \exp\left(i \ \Theta(\alpha_i - \alpha_j)\right) = \frac{\sin(\alpha_i - \alpha_j - \phi)}{\sin(\alpha_j - \alpha_i - \phi)} \]  
\text{(II.6.5)}

Taking logarithms of both sides of equation (II.6.4), and choosing the branches to give a symmetric distribution of
the $k_i$'s, we have

$$2Nk(\alpha_i) - \sum_{j=1}^{n} \Theta(\alpha_i - \alpha_j) = \pi(2i-n-1) \quad i=1,2,\ldots,n$$  \hfill (II.6.6)

Following Lieb (1967a) we now assume that as we let $N$ become large, keeping $n/N$ fixed, the $\alpha_i$'s continuously fill the range $(-\pi/2, \pi/2)$. Let $2N\rho(\alpha)d\alpha$ be the number of $\alpha$'s in the interval $(\alpha, \alpha+d\alpha)$. Then equation (II.6.6) becomes

$$k(\alpha) - \int_{-\pi/2}^{\pi/2} \Theta(\alpha-\alpha') \rho(\alpha')d\alpha' = 2\pi \int_{-\pi/2}^{\pi/2} \rho(\alpha')d\alpha' - n\pi$$  \hfill (II.6.7a)

with

$$\frac{n}{N} = 2 \int_{-\pi/2}^{\pi/2} \rho(\alpha)d\alpha$$  \hfill (II.6.7b)

We differentiate equation (II.6.7a) with respect to $\alpha$ in order to simplify the right hand side and get

$$k'(\alpha) - \int_{-\pi/2}^{\pi/2} \left( \Theta(\alpha-\alpha')/3\alpha \right) \rho(\alpha')d\alpha' = 2\pi\rho(\alpha)$$  \hfill (II.6.8)

This equation can be solved by finite Fourier transforms. From equations (II.5.4) and (II.6.5) we find

$$2k'(\alpha) = 1 + 2 \sum_{n=1}^{\infty} \left[ \exp\left(2(s-r)n\right) + \exp(-2sn) \right] \cos(2n\alpha)$$  \hfill (II.6.9)
\[ 2\pi \left( \partial \Theta(\alpha - \alpha') / \partial \alpha \right) = 1 + 2 \sum_{n=1}^{\infty} \exp(-2rn) \cos(2n\alpha) \]  

(II.6.10)

Substituting these series into equation (II.6.8), it follows that

\[ 2\pi \rho(\alpha) = 1 + 2 \sum_{n=1}^{\infty} \left( \frac{\cosh((r-2s)n)}{\cosh(rn)} \right) \cos(2n\alpha) \]  

(II.6.11)

Using this expression for \( \rho(\alpha) \) we see from equation (II.6.7b) that \( n = N \). This is the case in which there are as many down arrows as up arrows in a row. As is the case with the square lattice model we expect this to correspond to the maximum eigenvalue \( \Lambda \). To calculate the free energy we first note that

\[ \begin{vmatrix} u_1 & v_1 \\ u_2 & v_2 \end{vmatrix} = \frac{\sinh(s+v) \sinh(r-s+v) \sinh(ia_i+r-s)}{\sinh(s-v) \sinh(r-s-v) \sinh(ia_i-r-s)} \]

\[ < 1 \text{ for } v < 0 \]
\[ > 1 \text{ for } v > 0 \]  

(II.6.12)

Therefore, from equation (II.2.5), for large \( N \) and \( v > 0 \) we have

\[ \ln \Lambda_N = N \ln u_1 + \sum_{i=1}^{n} \ln \left( \mu(\alpha_i) \right) \]  

(II.6.13a)

where

\[ \mu(\alpha_i) = \mu_i \]  

(II.6.13b)

In the limit, as \( N \rightarrow \infty \), the summation becomes an integral.
and we have

\[
-\frac{\mathcal{F}}{kT} = \lim_{N \to \infty} N^{-1} \ln \Lambda_N
\]

\[
= \ln u_1 + 2 \int_{-\pi/2}^{\pi/2} \ln \left[ \mu(\alpha) \right] \rho(\alpha) d\alpha
\]

(II.6.14)

The integral can be evaluated to give

\[
-\frac{\mathcal{F}}{kT} = \ln \kappa + 3r - \sum_{n=1}^{\infty} \exp(-2rn)
\]

\[
2 \cosh[(r-s)n] \cosh(2vn) + \cosh[(r-2s)n]
\]

\[
\frac{n \cosh(rn)}{n \cosh(rn)}
\]

(II.6.15)

where \( \kappa \) is defined by

\[
\kappa = \frac{u_1}{8 \sinh(s+v) \sinh(r-s+v) \sinh(2s)}
\]

(II.6.16)

Comparing (II.6.16) with the equations (II.5.7) shows that \( \kappa \) is in fact a constant. A similar development gives the same result for \( v < 0 \). Thus \( \mathcal{F}/kT \) is symmetric in \( v \), as would be expected, and analytic at \( v = 0 \). Two forms that are equivalent to equation (II.6.15) are

\[
-\frac{\mathcal{F}}{kT} = \ln u_1 + 2(r-s-v)
\]

\[
+ 8 \sum_{m=1}^{\infty} \frac{\sinh[(r-s-v)m] \cosh[(s-v)m] \cosh[(r-2s)m]}{m \left( \exp(2rm) + 1 \right)}
\]
\[-\mathcal{F}/kT = \ln u_2 + 2(r-s+v)\]
\[
+ 8 \sum_{m=1}^{\infty} \frac{\sinh((r-s+v)m) \cosh((s+v)m) \cosh((r-2s)m)}{m \left( \exp(2rm)+1 \right)}
\]

\[(\text{II.6.17})\]

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

We now evaluate the free energy when

\[-1 < \cos \phi < 1\]

\[(\text{II.7.1})\]

In this regime the parameters \(\phi, \theta\) and \(\zeta\) are real. The requirement that the vertex weights be positive implies

\[\pi > \phi > 2\theta > 2|\zeta|\]

\[(\text{II.7.2})\]

and it follows from equation (II.5.4) that the \(\alpha_i\)'s are pure imaginary. Letting \(N\) become large, as before, and assuming that the \(\alpha\)'s form a continuous distribution in the interval \((-i\infty, i\infty)\), equations (II.6.8) and (II.6.7b) become

\[k'(\beta) - \int_{-\infty}^{\infty} \left( \frac{\partial (\beta-\beta')}{\partial \beta} \right) \rho(\beta') d\beta' = 2\pi \rho(\beta)\]

\[(\text{II.7.3a})\]

\[
\frac{n}{N} = 2 \int_{-\infty}^{\infty} \rho(\beta) d\beta
\]

\[(\text{II.7.3b})\]

where \(\alpha=i\beta\). Equation (II.7.3a) can be solved by Fourier
transforms to obtain

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

(II.7.4)

and again we have n=N. It can be shown that

$$\left| \frac{u_1\mu_i}{u_2\lambda_i} \right| > 1 \quad \text{for } \zeta > 0$$

$$\left| \frac{u_1\mu_i}{u_2\lambda_i} \right| < 1 \quad \text{for } \zeta < 0$$

(II.7.5)

and therefore we arrive at the following expressions for the free energy

$$-\mathcal{F}/kT = \ln u_1$$

$$+ 2 \int_{-\infty}^{\infty} \frac{\sinh((\pi - \phi)m) \sinh((\phi - \Theta)m) \cosh(\Theta - \zeta)m \cosh((\phi - 2\Theta)m) }{m \cosh(\phi m) \sinh(\pi m)} \, dm$$

$$= \ln u_2$$

$$+ 2 \int_{-\infty}^{\infty} \frac{\sinh((\pi - \phi)m) \sinh((\phi + \Theta + \zeta)m) \cosh(\Theta + \zeta)m \cosh((\phi - 2\Theta)m) }{m \cosh(\phi m) \sinh(\pi m)} \, dm$$

(II.7.6)

This integration can be performed when \(\phi\) is in the upper half plane, to obtain the analytic continuation of this function in the regime where \(\phi\) is pure imaginary. The result is
\[-\mathcal{G}/kT = \ln u_1 + 2(r-s-v)\]

\[+ 8 \sum_{m=1}^{\infty} \frac{\sinh[(r-s-v)m] \cosh[(s-v)m] \cosh[(r-2s)m]}{m \exp(2rm)+1}\]

\[\cos[\pi s(2m-1)r^{-1}] + \cos[\pi v(2m-1)r^{-1}] \sin[\pi s(2m-1)r^{-1}]\]

\[-8i \sum_{m=1}^{\infty} \frac{(2m-1) \left[1 - \exp(\pi^2(2m-1)r^{-1})\right]}{(2m-1)\left[1 - \exp(\pi^2(2m-1)r^{-1})\right]}\]

The difference between this and equation (II.6.17) is the singular part of the free energy. This difference has an essential singularity at the transition point \(\phi=0\), similar to the square lattice F-model.

The two states already discussed correspond to those of Baxter's (1969) triangular lattice F-model when \(\phi=3\theta\) and \(\zeta=0\). His parameter \(\phi\) corresponds to \(2\theta\) in this model.

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

To complete the range of possibilities we now consider a parameter regime in which

\[\cos \phi < -1\]

(II.8.1)

An example of this case occurs when

\[\phi = \pi + ir\ , \ \theta = \pi/2 + is\ , \ \zeta = \pi/2 + iv\]

(II.8.2)
with \( 2v > 2s > r > 0 \) \quad \text{(II.8.3)}

These conditions ensure that all the vertex weights are positive and also imply that \( u_1 \) is the largest vertex weight. In \( rsv \)-space this regime occupies a convex region. Any point in the region lies on a ray which is completely within the region and has as its end point the origin. Such rays are characterized by

\[
\begin{align*}
  v &= ar \\
  s &= br \\
  a &> b > r/2 \\
  r &> 0
\end{align*} \quad \text{(II.8.4)}
\]

For any \( a \) and \( b \) satisfying (II.8.4) the ratios \( u_i/u_1 \), \( i=2,3,\ldots,10 \), are all less than one and approach zero monotonically as \( r \) approaches infinity. For finite \( M \) and \( N \) the partition function \( Z \) is a continuous, monotonically decreasing function of \( r \). Therefore, in the thermodynamic limit, \( Z \) is a non-increasing function of \( r \). Using specific vertex configurations we can show that

\[
\lim_{N \to \infty} \lim_{M \to \infty} Z^{1/MN} > u_1
\quad \text{(II.8.5)}
\]

independent of \( r \). At \( r=0 \) equation (II.7.6) gives

\[
\lim_{N \to \infty} \lim_{M \to \infty} Z^{1/MN} = u_1 \quad \text{(II.8.6)}
\]

It follows, using the continuity of the free energy, that (II.8.6) is valid for all \( r \geq 0 \). Every point in the region lies on a ray for some \( a \) and \( b \) and therefore the free energy is unchanged throughout the region. Similarly, in the regime where \( \phi \) and \( \theta \) are given by (II.8.2) and

\[
\zeta = -\pi/2 - iv
\quad \text{(II.8.7)}
\]
$u_2$ is the largest vertex weight and

$$\lim_{N \to \infty} \lim_{M \to \infty} Z^{1/MN} = u_2$$  \hspace{1cm} (II.8.8)$$

Because of the rotational symmetry of the model there must also be a regime dominated by the vertex with weight $u_3$. The appropriate ranges of the parameters can be determined from the relations (II.5.9). The resulting regime is

$$\phi = \pi + ir \quad , \quad \theta = is \quad , \quad \zeta = iv$$  \hspace{1cm} (II.8.9)$$

with

$$|v| < |s| , \quad s < 0 , \quad r > 0$$  \hspace{1cm} (II.8.10)$$

We can therefore write the general form of the free energy, for $\cos \varphi < -1$, as

$$-\mathcal{F}/kT = \ln \left( \max(u_1, u_2, u_3) \right)$$  \hspace{1cm} (II.8.11)$$

In each of these three cases the model is "frozen" into a state in which essentially all the vertices are of the same type. This is similar to the KDP ordered state for the square lattice ice model.

9) Temperature Independent Solution

In the disordered state and the ferroelectric state it is possible to define a model which can be solved by the Bethe ansatz for all temperatures. To do this in the regime specified by the conditions (II.7.2), we set
\[ 2\phi - \pi = 2\theta = \zeta + \pi/2 \]  \hspace{1cm} \text{(II.9.1)}

In the ordered state specified by the conditions (II.8.2-3), we set

\[ 2r = 2s = v \]  \hspace{1cm} \text{(II.9.2)}

Then, by normalizing the weights we have

\[ u_1 = 1 \]
\[ u_2 = u_3 = u_4 = u_5 = u_7 = u_9 = u < 1 \]  \hspace{1cm} \text{(II.9.3)}

Recalling that

\[ u = \exp(-e/kT) \]  \hspace{1cm} \text{(II.9.4)}

where \( e \) is the energy associated with the vertex, and \( k \) is Boltzmann's constant, we see that the temperature \( T \) can be varied and the model still remains soluble. In fact, as the temperature is lowered from infinity, the model passes from the disordered state into the ordered ferroelectric state, consisting only of vertices with weight \( u_1 \). This transition occurs at

\[ \cos \phi = -1 \]  \hspace{1cm} \text{(II.9.5)}

or equivalently

\[ u = 1/3 \]  \hspace{1cm} \text{(II.9.6)}

The transition temperature is given by

\[ T_c = \frac{e}{k \ln 3} \]  \hspace{1cm} \text{(II.9.7)}
When $T<T_c$ the free energy is zero. When $T>T_c$ the free energy is given by equation (II.7.6). This integral can be expanded at the transition temperature to give

$$-\mathcal{F}/kT = \frac{3}{4} \frac{\ln 3}{T_c} \left( T - T_c \right) + \frac{\sqrt{3}}{4\pi} (\ln 3)^{3/2} \left( T - T_c \right)^{3/2} + \ldots$$

(II.9.8)

Therefore the internal energy at the transition is $\frac{3}{4} e$, and the leading behaviour of the specific heat is

$$C_v = \frac{3\sqrt{3}}{16\pi} (\ln 3)^{3/2} \left( T - T_c \right)^{-\frac{1}{2}}$$

(II.9.9)

The critical exponent $\alpha$, describing the singular behaviour of $C_v$, is $\frac{1}{2}$.

There are two other similar temperature independent solutions, one for $u_2$, and one for $u_3$. These, however, are the only such solutions obtainable by the Bethe ansatz.

10) Free-Fermion Solution

In section (II.3) we put aside the case when $L=-M$, mentioning that it was not an instance of the problem which was most easily solved by a Bethe ansatz. We now return to this case using the fermion operator method of Green and Hurst (1964). This method has been applied to several models, including the Ising model (Hurst and Green, 1960), the free-fermion approximation to the eight-vertex model (Fan and Wu, 1969), and recently
the triangular 32-vertex model (Sacco and Wu, 1975). The 20-vertex model we are dealing with is contained in this last application. It is interesting to note how the solution of Sacco and Wu (1975) relates to the Bethe ansatz solution already developed.

The method is straightforward and well outlined by Hurst (1966). The restriction that we have a system of non-interacting, or free, fermions gives the following conditions on the vertex weights.

\[
\begin{align*}
    u_1u_2 &= u_5u_6 - u_3u_4 \\
    u_1u_2 &= u_9u_{10} - u_2u_4 \\
    u_1u_4 &= u_7u_8 - u_2u_3 \\
    u_1u_5 &= u_7u_9 - u_2u_6 \\
    u_1u_6 &= u_8u_{10} - u_2u_5 \\
    u_1u_7 &= u_4u_8 - u_5u_9 \\
    u_1u_8 &= u_4u_7 - u_6u_{10} \\
    u_1u_9 &= u_5u_7 - u_3u_{10} \\
    u_1u_{10} &= u_6u_8 - u_3u_9 \\
    u_1^2 + u_5^2 &= u_3^2 + u_8^2 \quad (II.10.1)
\end{align*}
\]

It is a simple matter to show that these equations imply equations (II.3.26).

It turns out that the vertex weights can be parameterized in terms of \( x, y \) and \( z \) where

\[
u_6 = u_5 \cos x
\]
\[ u_7 = u_8 \cos y \]
\[ u_{10} = u_9 \cos z \]  \hspace{1cm} (II.10.2)

Equations (II.10.1) and the requirement that all the weights have the same sign implies that \( x, y \) and \( z \) must all be real and in the interval \( (0, \pi/2) \), or all be pure imaginary. In the case where they are all real

\[ u_6 \geq u_5 \]
\[ u_7 \geq u_6 \]
\[ u_{10} \geq u_9 \]  \hspace{1cm} (II.10.3)

and the complete parameterization is

\[ u_1 = \rho (\cos y - \cos x \cos z) \]
\[ u_2 = \rho (\cos z - \cos x \cos y) \]
\[ u_3 = \rho (\cos x - \cos y \cos z) \]
\[ u_4 = \rho (1 - \cos x \cos y \cos z) \]
\[ u_5 = \rho \cos x \sin y \sin z \]
\[ u_6 = \rho \sin y \sin z \]
\[ u_7 = \rho \sin x \sin z \]
\[ u_8 = \rho \cos y \sin x \sin z \]
\[ u_9 = \rho \cos z \sin x \sin y \]
\[ u_{10} = \rho \sin x \sin y \]  \hspace{1cm} (II.10.4)

The case where \( x, y \) and \( z \) are pure imaginary can be parameterized by replacing \( \cos x \) by \( \sec x' \), and similarly
with \( y \) and \( z \), in equations (II.10.2). \( x', y' \) and \( z' \) are then real. The resulting parameterization is the same as (II.10.4) with \( u_5 \) and \( u_6 \), \( u_7 \) and \( u_8 \), and \( u_9 \) and \( u_{10} \) interchanged. Therefore both cases are essentially the same. The only restrictions on the parameters are

\[
\cos x \geq \cos y \cos z
\]

\[
\cos y \geq \cos x \cos z
\]

\[
\cos z \geq \cos x \cos y
\]

(II.10.5)

These ensure that all the weights are positive. An immediate consequence of (II.10.4) and (II.10.5) is

\[
u_4 \geq u_1 + u_2 + u_3
\]

(II.10.6)

The three parameters \( x, y \) and \( z \) give us three degrees of freedom in determining the ratios of the vertex weights. For convenience we can choose \( \rho \) so that \( u_1 = 1 \). The free energy is then given by (Green and Hurst, 1964)

\[
\frac{-\mathcal{F}}{kT} = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \ln \left[ 2u_4 - 2\cos(\theta + \phi) + 2u_2 \cos \theta + 2u_3 \cos \phi \right] d\theta d\phi
\]

(II.10.7)

This integral has an Ising-like singularity on the boundary of the physical regime

\[
u_4 = 1 + u_2 + u_3
\]

(II.10.8)

To determine the domain of the overlap of the free-fermion and Bethe ansatz methods we add to the conditions (II.10.1)
the further requirements, that must hold for the Bethe ansatz to work,

\[ u_5 = u_6 = a \]
\[ u_7 = u_8 = b \]
\[ u_9 = u_{10} = c \quad (II.10.9) \]

With \( u_1 = 1 \), the other weights are given by

\[ u_2 = \frac{bc}{a} - 1 \]
\[ u_3 = \frac{ab}{c} - 1 \]
\[ u_4 = \frac{ac}{b} + 1 \quad (II.10.10) \]

with the condition

\[ a^2b^2 + b^2c^2 - a^2c^2 - 2abc = 0 \quad (II.10.11) \]

It can be shown that this model is identical to the one obtained by setting \( \phi = \pi/2 \) in expressions (II.5.7) of the Bethe ansatz solution. Moreover, the same model results if we take the critical case of the free-fermion solution determined by equation (II.10.8). It therefore follows that the two methods coincide in a two dimensional space which is entirely within the disordered state of the Bethe ansatz solution and is a critical surface in the free-fermion solution.

11) Simple Parameter Space

To clarify the arrangement of the various
regimes discussed in the previous sections we now consider a description of the 20-vertex model in terms of a new set of symmetric parameters.

Define $\gamma_1$, $\gamma_2$ and $\gamma_3$ by

$$
\sin \gamma_1 = (u_2 u_3 / I)^{1/2}
$$

$$
\sin \gamma_2 = (u_1 u_3 / I)^{1/2}
$$

$$
\sin \gamma_3 = (u_1 u_2 / I)^{1/2}
$$

where $I$ is given by equation (II.3.43), and $0 < \gamma_i < \pi/2$, $i=1,2,3$. The $\gamma_i$'s are independent and can assume any value in the cube indicated. In terms of these new parameters equation (II.5.3a) can be written as

$$
\cos \phi = \frac{(1 - \sin^2 \gamma_1 - \sin^2 \gamma_2 - \sin^2 \gamma_3)}{(2 \sin \gamma_1 \sin \gamma_2 \sin \gamma_3)}
$$

(II.11.2)

In the Bethe ansatz solution the transitions occur at

$$
\cos \phi = \pm 1.
$$

(II.11.3)

The equations (II.11.3) define four distinct surfaces in the $\gamma$-cube (see figure II.4). The equations of the surfaces are

$$
\gamma_1 + \gamma_2 = \gamma_3 + \pi/2
$$

$$
\gamma_2 + \gamma_3 = \gamma_1 + \pi/2
$$

$$
\gamma_1 + \gamma_3 = \gamma_2 + \pi/2
$$

$$
\gamma_1 + \gamma_2 + \gamma_3 = \pi/2
$$

(II.11.4)
Within the $\gamma$-cube these triangular planes describe five tetrahedra. The central tetrahedron corresponds to the disordered state of the model. The tetrahedron, one of whose vertices is the origin, corresponds to the ordered antiferroelectric state, and the other three tetrahedra correspond to the ordered ferroelectric states. Phase transitions occur on passing through the planes (II.11.4). The temperature independent models are represented by straight lines joining the points

\[(0, 0, \pi/2) \text{ and } (\pi/2, \pi/2, 0)\]
\[(0, \pi/2, 0) \text{ and } (\pi/2, 0, \pi/2)\]
\[(\pi/2, 0, 0) \text{ and } (0, \pi/2, \pi/2)\]

Baxter's (1969) F-model solution is represented by a straight line joining

\[(0, 0, 0) \text{ and } (\pi/2, \pi/2, \pi/2)\]

The solution common to the free-fermion and Bethe ansatz methods is represented by a curved surface, whose edges coincide with those of the triangular plane closest to the origin, but which otherwise lies entirely within the central tetrahedron.

The equation of the surface is

\[\sin^2\gamma_1 + \sin^2\gamma_2 + \sin^2\gamma_3 = 1 \quad (\text{II.11.5})\]

12) Summary

We have shown that the partition function and
Figure II.4 Subdivision of the γ-cube by the four transition surfaces into five tetrahedra. The four exterior tetrahedra are labelled as ferroelectric or antiferroelectric. The interior tetrahedron corresponds to the disordered state of the model.
free energy for the 20-vertex model on a triangular lattice can be calculated exactly, by means of a Bethe ansatz, 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 from the disordered state into one of three frozen ferroelectric states. The other is an infinite-order transition from the disordered state into an ordered antiferroelectric state. Within this framework we find three equivalent, temperature independent solutions. These are similar to the square lattice KDP model and undergo a first-order phase transition.

We have compared our results to the free-fermion solution of Sacco and Wu (1975) and determined the relationship between these two methods. The free-fermion method, when restricted to this ice-type model, also results in a three-dimensional parameter space which intersects the Bethe ansatz parameter space in a two-dimensional surface.
1) Introduction

Potts (1952) suggested an extension of the nearest neighbour Ising model which, instead of having just two possible states at each lattice site, allowed for an arbitrary number of states, \( q \), at each site. The model was similar to the Ising model in that if two neighbouring sites were in the same state they contributed an energy \(-\varepsilon\), and if they were in different states they contributed an energy zero to the total energy of the system. For the square lattice, Potts showed, by means of the transformation between high and low temperatures (Kramers and Wannier, 1941), where the transition from ordered to disordered state would occur.

Since its first introduction interest in the Potts model has continued although no exact solution
has yet been found for any value of \( q \) other than 2. There are a number of reasons for this interest. The Potts model can provide a simple model of a many component alloy in the same way as the Ising model can be used as a crude model for a binary alloy. It has also been shown that other unsolved models of critical phenomena can be related to the Potts model. By writing the Potts model partition function as a Whitney (1932) colouring polynomial it can be seen that for \( q=1 \) it is equivalent to the bond percolation problem (Frisch and Hammersley, 1963; Kasteleyn and Fortuin, 1969) on the same lattice. In the limit \( c->\infty \) no two neighbours can be in the same state. Hence for \( q=4 \) we have the famous four colour problem. More generally for \( q=4 \) we have a special case of the Ashkin-Teller (1943) model. In two dimensions Temperley and Lieb (1971) and more recently Baxter et al. (1976) have shown that the partition functions of certain ice-type models (Lieb, 1967) are also expressible as Whitney polynomials and can be equated to corresponding Potts model partition functions. A solution of the Potts model would therefore shed light on several outstanding problems.

The most recent interest in this model has been in connection with its critical exponents. Since Baxter's (1972) discovery that the critical exponents of the eight-vertex model vary continuously with the parameters of the model other examples of this behaviour have been looked for. It appears, from series expansion work (Enting, 1974-5; Straley and Fisher, 1973; Sykes et al., 1974) and the known Ising model result, that the
critical exponents of the Potts model also vary, in particular with the parameter q. This aspect has especially interested us and we make some estimate of this dependence in what follows.

Previous work on the Potts model has not been without success. Kihara et al. (1954), apparently independently of Potts, began the series expansion work by restating the relationship between high and low temperature regions of the model and then developing the low temperature series for the free energy to sixteen terms. As already mentioned Temperley and Lieb first showed the relation between the Potts model and staggered ice model. Using this relationship Baxter (1973) was able to solve the Potts model on a square lattice at the transition temperature. This was useful because it revealed that for q>4 the transition was first order and for q<4 the transition was of higher order. The order of the transition in three dimensions is still an open question. Refined methods of series analysis have given estimates of some of the exponents α', β, δ and γ for q=1, 3 and 4 (Enting, 1974-5; Kim and Joseph, 1975). These techniques have worked for both two and three dimensions. Renormalization group methods have also been used (on a continuous version of the Potts model) in an attempt to find the order of the transition as a function of dimension (Golner, 1973; Young and Stinchcombe, 1975).

This present work deals only with the two dimensional Potts model on a square lattice below the transition temperature. It does, however, use the transformation to the ice-type model which allows a
generalized definition of the model to non-integer values of q. Using a variational method we have formed successive approximations to the free energy and spontaneous order by systematically enlarging the trial function space. The approximations are indexed by the parameter p. In the limit of large p we derive an infinite hierarchy of equations, the solution to which would give the free energy and spontaneous order exactly. By this method we have been able to compute estimates of the critical exponent $\beta$ for values of q between zero and four.

The results obtained by this method are consistent with previous work as well as providing new estimates for intermediate values of q. In addition to these results the method also poses some questions of its own. Not the least of these is how the hierarchy is to be solved in the case $q=2$. Here we have an exact solution to the problem by other means and should therefore be able to solve the infinite system obtained by this method exactly. It is not yet clear how this is to be done.

ALGEBRAIC FORMULATION

2) Potts Model and Staggered Ice Model

We begin by defining the Potts model. Let L be a square lattice with N sites. At each site place a spin $\sigma=1,2,...,q$. Associate an interaction energy $-\varepsilon$ with two nearest neighbour sites that have the same spin state, and zero if they are different. The partition function can then be written as
\[ Z = \sum_{\{\sigma\}} \exp\left( \beta \varepsilon \sum_{\text{n.n.}} \delta_{\sigma, \sigma'} \right) \]  

(III.2.1)

where the sum inside the brackets is over nearest neighbours and the first sum is over all spin states of the lattice. \( \beta = 1/kT \) where \( k \) is Boltzmann's constant. If we let

\[ v = \exp(\beta \varepsilon) - 1 \]  

(III.2.2)

this can be written as

\[ Z = \sum_{\{\sigma\}} \prod_{\text{n.n.}} \left( 1 + v \delta_{\sigma, \sigma'} \right) \]  

(III.2.3)

The product over nearest neighbours has a factor for each edge of the lattice \( L \). Each factor is the sum of two terms. The product can therefore be expanded into a sum of \( 2^N \) terms. Moreover, each term can be characterized by a bond-graph on the lattice \( L \). We place a bond on an edge of the lattice if we take the \( v \delta_{\sigma, \sigma'} \) term in the corresponding factor or leave the edge empty if we take the unit term. We can therefore write the partition function as a sum over graphs in the following way

\[ Z = \sum_{\mathcal{G}} q^C v^L \]  

(III.2.4)

where \( C \) is the number of connected components in the graph (counting isolated sites as components), \( L \) is the number of bonds in the graph and the sum is over all bond-graphs on the lattice. This sum is a Whitney polynomial (Whitney, 1932).

We now define an ice-type model on another lattice and show that its partition function is simply
related to that of the Potts model. We associate with $L$ a new lattice $L'$ by placing sites at the midpoints of the edges of $L$ (including the boundary edges) as shown in figure (III.1). There will be two types of sites on this lattice: the A sites lying on horizontal edges, and the B sites lying on vertical edges. On the lattice $L'$ we define the staggered ice model by the following rules:

(a) Place arrows on each edge of the lattice so that at each site there are as many arrows pointing in as out.

(b) Give the following weights to the interior (those not lying on boundary edges of $L$) sites according to their type as shown in figure (III.2).

<table>
<thead>
<tr>
<th>vertex type</th>
<th>A sites</th>
<th>B sites</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>$x$</td>
<td>$x^{-1}$</td>
</tr>
<tr>
<td>4</td>
<td>$x$</td>
<td>$x^{-1}$</td>
</tr>
<tr>
<td>5</td>
<td>$s^2 + xs^{-2}$</td>
<td>$s^2 + x^{-1}s^{-2}$</td>
</tr>
<tr>
<td>6</td>
<td>$s^{-2} + xs^2$</td>
<td>$s^{-2} + x^{-1}s^2$</td>
</tr>
</tbody>
</table>

(c) At the boundary sites the two arrows must follow each other through the site. If moving in the direction of the arrows a right (left) turn is made, give the site weight $s$ ($s^{-1}$). These rules define allowable states for the model and prescribe the weights to be attached to each state. The partition function for this model can be written as

$$Z_{SI} = \sum_{\text{states}} \prod_{\text{sites}} \text{(weights)} \quad \text{(III.2.6)}$$
Figure III.1 The lattices $L$ and $L'$. The A sites of the $L'$ lattice are those on the horizontal edges of the $L$ lattice. The B sites are on the vertical edges.
Figure III.2  The six types of arrow configurations allowed at an interior site of L'.

Figure III.3  Labelling of the edges around an interior site of L' and the pairing effect of the Kronecker deltas in equation (III.2.7)
Label the edges around each interior site with the variables $\alpha, \beta, \lambda$ and $\mu$ as shown in figure (III.3). Let $\alpha, \beta, \lambda, \mu = \frac{1}{2}, \frac{-1}{2}$ if the arrow on the respective edge has a component pointing to the right (left). The partition function can then be written as

$$Z_{SI} = \sum_{\text{states}} s^{R-L} \prod_{\text{interior sites}} \left[ s^{2(\beta-\alpha)} \delta_{\lambda}^{\alpha} \delta_{\mu}^{\beta} + x_i s^{2(\alpha-\beta)} \delta_{\mu}^{\alpha} \delta_{\lambda}^{\beta} \right]$$

(III.2.7)

where $R-L$ is the difference between the number of right and left turns at the boundary sites and $x_i = x$ for $A$ sites and $x_i = x^{-1}$ for $B$ sites. $\delta_{\alpha'}^{\alpha}$ is the Kronecker delta equal to 1 if $\alpha = \alpha'$ and equal to zero otherwise. The expression in the brackets gives the correct weight to each interior site. Graphically, the effect of the delta functions is to split each site into two parts (see figure (III.3)). The left hand pair of delta functions requires that the $\lambda$ and $\alpha$ arrows follow each other through the site and similarly the $\beta$ and $\mu$ arrows. The site has been split into an upper part and a lower part. In a similar way the right hand pair of delta functions splits the site into a right part and a left part. The same method of expanding this binomial product as was used for the Potts model partition function can be used here. The expansion will have $2^M$ additive terms where $M$ is the number of interior sites of the lattice $L'$. A term in the expansion corresponds to choosing, at each site, the right or left term in equation (III.2.7). We can, therefore, graphically represent each term by a configuration of polygons on the lattice $L'$ by splitting
each site in the manner just described. The boundary sites need not be split since they have only two edges entering them, but their presence ensures that all polygons will be closed. An example of such a polygon graph is given in figure (III.4). The delta functions in (III.2.7) require that the arrows on the perimeter of each polygon will follow each other in the same direction. The decomposition of the lattice into disjoint polygons implies that each term in the expansion can be written as a product over polygons. The following rule gives the correct s-weight to each term:

Moving around the perimeter of a polygon in the direction of the arrows, give each right (left) turn weight \( s \) (\( s^{-1} \)).

Each polygon can be traversed in a clockwise or counterclockwise direction. Because the polygons are simple and closed there will be in the one case an excess of four right turns, and in the other four left turns. The correct s-weight for each polygon is therefore \( s^4 + s^{-4} \). Let

\[
s = e^{\theta/4}
\]

then the weight given to each polygon is \( 2\cosh \theta \). The complete partition function can be written as

\[
Z_{\text{SI}} = \sum_{\text{polygon configurations}} (2\cosh \theta)^p x^{n-m}
\]

where \( p \) is the number of polygons, \( n \) is the number of right-left splittings on A sites, and \( m \) the number of right-left splittings on B sites.

The configurations of polygons on \( L' \) can be related in a one-to-one way with bond-graphs on the
Figure III.4  A polygon configuration on L' with the corresponding bond-graph on L. There is a polygon surrounding each component of the bond-graph and a polygon within each circuit of the bond-graph.
lattice \( L \). Each interior site of \( L' \) lies on an edge of \( L \). Use the following rule to identify bond-graphs with polygon configurations:

Only place bonds on horizontal (vertical) edges of \( L \) for which the corresponding site of \( L' \) is split into upper and lower (right and left) parts.

By superimposing bond-graphs on the corresponding polygon configurations it can be seen that there are two types of polygon: those surrounding a component of the bond-graph and those surrounded by a component of the bond-graph. The number of the former is \( C \), the number of components of the bond-graph, and the latter is \( S \), the number of circuits. Therefore

\[
\text{\( p = C + S \) (III.2.10)}
\]

Euler's relation gives

\[
\text{\( S = C + \lambda - N \) (III.2.11)}
\]

where \( \lambda \) is the number of bonds in the graph. The \( n \) of equation (III.2.9) is just the number of empty horizontal edges, and \( m \) is the number of vertical bonds. We therefore have

\[
\text{\( n - m = N - \lambda \) (III.2.12)}
\]

It follows that we can write the partition function as

\[
Z_{SI} = \sum_{G} (2\cosh\theta)^{2C-\lambda-N} x^{N-\lambda}
= \sum_{G} (2\cosh\theta)^{2C-\lambda-N} x^{\lambda-N}
= (2x \cosh\theta)^{-N} \sum_{G} (2\cosh\theta)^{2C} (2x \cosh\theta)^{\lambda}
\]

which is also a Whitney polynomial. By comparison with (III.2.4) the Potts model partition function is
\[ Z = (2x \cosh \theta)^N Z_{SI} \quad (\text{III.2.14}) \]

with

\[ q = 4 \cosh^2 \theta \quad (\text{III.2.15a}) \]

\[ v = 2x \cosh \theta \quad (\text{III.2.15b}) \]

Since the staggered ice model is defined for all values of $\theta$, equation (III.2.15a) allows us to define an analogue to the Potts model for continuous values of $q$. It is interesting to note that as $q$ passes through the value 4, $\theta$ changes from being real to pure imaginary (up to a multiple of $2\pi i$). At $q=4$ Baxter (1973) predicts there is a change from a first order phase transition for $q>4$ to a higher order transition for $q<4$. In the latter case the critical exponent $\beta$ can be defined by

\[ M_\sigma = (1 - T/T_C)^\beta, \quad T \to T_C \quad (\text{III.2.16}) \]

measuring the rapidity with which the spontaneous magnetization vanishes as the transition temperature is approached from below. Since this is the quantity we are most interested in, we will be dealing with staggered ice models in which $\theta$ is pure imaginary.

Having established the relationships (III.2.14-15) for finite lattices, we will assume in what follows that they hold in the limit of large lattices independent of boundary conditions. In particular we will work with a staggered ice model rotated through 45° so that the edges of the lattice $L'$ are horizontal and vertical, and with toroidal boundary conditions.
3) Spontaneous Magnetization and Percolation Probability

In the introduction we mentioned that the usual order parameter for the Potts model in zero field is the spontaneous magnetization. In transforming to the staggered ice model formulation we constructed a model which is equivalent to the q-state Potts model for integer q, and also defined for non-integer values of q. As a generalized order parameter we are able to use the percolation probability (Frisch and Hammersley, 1963). The percolation probability is defined for general values of q and we will show that it agrees with the spontaneous magnetization at those values of q for which this quantity is defined.

For a model which has a partition function which, in the thermodynamic limit, is a sum over graphs,

$$Z = \sum_{\text{Graphs}} w(\text{graph}) \quad (\text{III.3.1})$$

we can define a percolation probability $\mathcal{P}$ for a site P on the graph by

$$\mathcal{P} = \frac{Z^*}{Z} \quad (\text{III.3.2})$$

where

$$Z^* = \sum_{\text{Graphs}} w(\text{graph}) \delta(\text{graph}) \quad (\text{III.3.3})$$

$$\delta(\text{graph}) = \begin{cases} 1 & \text{if P belongs to an infinite component of the graph} \\ 0 & \text{otherwise.} \end{cases}$$

The percolation probability is, then, the probability that a site is connected to infinitely many other sites by bonds of the graph. Since the Potts model lattice is
homogeneous we expect this probability to be identical for all sites P.

The partition function for the Potts model of N sites in a field which favours the "1" state can be written as

$$Z_N(h) = \sum_{\{\sigma\}} \exp \left( \frac{\beta \epsilon}{\text{n.n.}} \sum_{\sigma, \sigma'} \delta_{\sigma, \sigma'} + h \sum_{i=1}^{N} \delta_{\sigma_i, 1} \right)$$  \hspace{1cm} (III.3.4)

where h is the coupling to the magnetic field. Setting

$$e^{\beta \epsilon} = 1 + \nu$$ \hspace{1cm} (III.3.5)

we can write

$$Z_N(h) = \sum_{\{\sigma\}} \prod_{\text{n.n.}} \left( 1 + \nu \delta_{\sigma, \sigma'} \right) \prod_{i=1}^{N} \exp \left( h \delta_{\sigma_i, 1} \right)$$  \hspace{1cm} (III.3.6)

As noted previously, this expression can be expanded as a sum over graphs giving

$$Z_N(h) = \sum_{\text{Graphs}} \nu^l \prod_{i=1}^{m_i} \left( q - 1 + e^{hi} \right)^{m_i}$$ \hspace{1cm} (III.3.7)

As before, \(l\) is the number of bonds on the graph and \(m_i\) is the number of components of \(i\) sites. In the low temperature region, where we expect spontaneous magnetization, \(\nu\) is large and the most significant terms in this series are those graphs with many bonds and therefore few components. In the zero temperature limit only the complete graph of one component is important.
Deviations from this case consist of graphs with one large component and some small isolated components. In this case we can write asymptotically

$$Z_N(h) \sim \sum_{\text{Graphs}} \prod_i \left( q^{-1} + e^{h_i} \right)^{m_i} \left( q^{-1} + e^{hN} \right)$$

(III.3.8a)

where $N = N - \sum_j m_j$  

(III.3.8b)

The product over $i$ and sum over $j$ include ranges of $i$ and $j$ which are small compared to $N$. Taking the logarithmic derivative w.r.t. $h$ gives

$$\frac{\partial}{\partial h} \ln Z_N(h) = \left\langle \sum_i \frac{i m_i e^{h_i}}{q^{-1} + e^{h_i}} \right\rangle + \left\langle \frac{N e^{hN}}{q^{-1} + e^{hN}} \right\rangle$$

(III.3.9)

where $\langle \cdot \rangle$ is the expectation. We now take the thermodynamic limit, $N \to \infty$, which gives

$$\lim_{N \to \infty} \frac{\partial}{\partial h} N^{-1} \ln Z_N(h) = \lim_{N \to \infty} \left\{ N^+ \left\langle \sum_i \frac{i m_i e^{h_i}}{q^{-1} + e^{h_i}} \right\rangle - \left\langle \sum_j m_j \right\rangle \right\}$$

(III.3.10)

Setting $h=0$, we therefore have

$$\lim_{N \to \infty} \frac{\partial}{\partial h} N^{-1} \ln Z_N(h) \bigg|_{h=0} = 1 - \frac{q^{-1}}{q} \lim_{N \to \infty} \left\langle N^{-1} \sum_i m_i \right\rangle$$

(III.3.11)
The final limit in equation (III.3.11) is just the probability that a site on the Potts model lattice belongs to a finite component of the graph in the thermodynamic limit. Therefore

\[
\lim_{N \to \infty} \left\langle N^{-1} \sum_{i} \right\rangle = 1 - \mathcal{P} \quad (\text{III.3.12})
\]

where \( \mathcal{P} \) is the percolation probability (i.e. the probability that a site belongs to an infinite component). Defining the free energy per site \( f(h) \) by

\[
-\beta f(h) = \lim_{N \to \infty} N^{-1} \ln Z_N(h) \quad (\text{III.3.13})
\]

we have

\[
\frac{\partial}{\partial h} \left[ -\beta f(h) \right]\bigg|_{h=0} = q^{-1} \left[ 1 + (q-1) \mathcal{P} \right] \quad (\text{III.3.14})
\]

On the other hand, from equation (III.3.4)

\[
\frac{\partial}{\partial h} Z_N(h) = \sum_{\{ \sigma \}} \exp \left\{ \beta c \sum_{\text{n.n.}} \delta_{\sigma, \sigma'} + h \sum_{i=1}^{N} \delta_{\sigma_{i,1}, 1} \right\} \sum_{i=1}^{N} \delta_{\sigma_{i,1}, 1} \nonumber
\]

\[
= \left\langle \sum_{i=1}^{N} \delta_{\sigma_{i,1}, 1} \right\rangle_N Z_N(h) \quad (\text{III.3.15})
\]

Letting \( N \to \infty \) and \( h \to 0 \) gives

\[
\frac{\partial}{\partial h} \left[ -\beta f(0) \right] = \lim_{N \to \infty} N^{-1} \left\langle \sum_{i=1}^{N} \delta_{\sigma_{i,1}, 1} \right\rangle_N = n_1 \quad (\text{III.3.16})
\]
where \( n_1 \) is the fraction of sites in state "1" in the thermodynamic limit. We take as our definition of spontaneous magnetization

\[
M_0 = \frac{q n_1 - 1}{q - 1}
\]  

(III.3.17)

\( M_0 \) ranges from 0 to 1 as \( n_1 \) goes from \( q^{-1} \) to 1. From equations (III.3.16 - 17)

\[
\frac{\partial}{\partial h} (-\beta f(0)) = q^{-1} \left( 1 + (q-1)M_0 \right)
\]  

(III.3.18)

and we see from equations (III.3.14) and (III.3.18) that \( M_0 \) and \( \phi \) are identical. Since the meaning of \( M_0 \) is not clear when \( q \) is non-integral, we shall use \( \phi \) exclusively as the order parameter for the Potts model.

4) Transfer Matrix

To put the problem in a form to which the variational method can be applied, we first set up the transfer matrix for the staggered ice model. The vertex weight for the staggered ice model can be written as

\[
t^{\alpha\beta}_{\lambda\mu}(x,\theta) = e^{\theta(\beta-\alpha)/2} \delta^\alpha_\lambda \delta^\beta_\mu + xe^{\theta(\alpha-\beta)/2} \delta^\alpha_{-\mu} \delta^\beta_{-\lambda}
\]  

(III.4.1)

where \( \alpha, \beta, \lambda \) and \( \mu \) are associated with the bonds shown in figure (III.5), and can take the values \( \pm \frac{1}{2} \). There are 16 quantities \( t^{\alpha\beta}_{\lambda\mu} \) in all. By suppression of the upper or lower indices, indicated by a dot, these quantities
Figure III.5  Labelling of the edges around a site of the staggered ice model defined in section III.4

Figure III.6  Positions of P and Q, and the intervening vertical edges of the staggered ice lattice: $a_{2i+1}$ to $a_{2j}$. By altering the weight given to these edges, configurations with polygons surrounding only P can be made to have zero weight, while configurations without such polygons have their weights unaffected.
can be written as four $2 \times 2$ matrices.

\[
t_{+\frac{1}{2}, \frac{1}{2}} = \begin{pmatrix} 1 & 0 \\ 0 & x \end{pmatrix}, \quad t_{+\frac{1}{2}, -\frac{1}{2}} = \begin{pmatrix} 0 & e^{-\theta/2 + xe^{\theta/2}} \\ 0 & 0 \end{pmatrix}
\]

\[
t_{-\frac{1}{2}, \frac{1}{2}} = \begin{pmatrix} 0 & e^{\theta/2 + xe^{-\theta/2}} \\ e^{\theta/2 + xe^{-\theta/2}} & 0 \end{pmatrix}, \quad t_{-\frac{1}{2}, -\frac{1}{2}} = \begin{pmatrix} x & 0 \\ 0 & 1 \end{pmatrix}
\]

(III.4.2)

This is a useful way of writing these quantities because, by multiplying these matrices together, the weight given to a row of vertices can be expressed.

The matrices with the lower indices suppressed will be called $\rho$-matrices. In a similar way, the upper indices can be suppressed resulting in another class of $2 \times 2$ matrices which will be called $\sigma$-matrices. With these simple matrices we will construct expressions for the elements of the transfer matrix.

In the case of ice-type problems, the transfer matrix method arrives at an expression for the partition function by building up the lattice a row at a time.

If the lattice has $N$ sites in a row, the dimension of the transfer matrix is $2N \times 2N$. The weight given to a row of vertices is the product of its constituent vertex weights. An element of the transfer matrix is the sum of those row weights which correspond to allowable arrangements of arrows on horizontal edges between specified arrangements of vertical arrows. If the lattice is homogeneous, has $M$ rows, and is wrapped on a torus, then the partition function can simply be written as
a trace over the M'th power of the transfer matrix.

In the staggered ice model there are two types of rows. We first consider a row with an even number of sites beginning with an A site. If \( t_{\lambda \mu}^{\alpha \beta}(x, \theta) \) is the vertex function for A sites, then \( t_{\lambda \mu}^{\alpha \beta}(x^{-1}, \theta) \) is the vertex function for B sites. We form the matrix element

\[
T_1(\alpha, \beta) = \text{Tr}\left[ t_{1}^{\alpha_1 \beta_1}(x, \theta) t_{2}^{\alpha_2 \beta_2}(x^{-1}, \theta) \ldots t_{N}^{\alpha_N \beta_N}(x^{-1}, \theta) \right]
\]

where matrix multiplication is understood between the t's, \( \alpha = (\alpha_1, \alpha_2, \ldots, \alpha_N) \) and \( \beta = (\beta_1, \beta_2, \ldots, \beta_N) \). This element is the sum of the weights of the allowable configurations on a row of vertices when \( \alpha \) and \( \beta \) are specified, and \( \nu_N = \lambda_1 \). In a similar way we form

\[
T_2(\alpha, \beta) = \text{Tr}\left[ t_{1}^{\alpha_1 \beta_1}(x^{-1}, \theta) t_{2}^{\alpha_2 \beta_2}(x, \theta) \ldots t_{N}^{\alpha_N \beta_N}(x, \theta) \right]
\]

which represents the same quantity for a row beginning with a B site. If there are M rows altogether on the staggered ice lattice, and if we assume the last row of vertical bonds corresponds to the first, then we can write the partition function as

\[
Z_{SI} = \text{Tr}(T_2 T_1)^{M/2}
\]

\[
= \sum_{i} \lambda_i^{M/2}
\]

(III.4.5)

where \( \lambda_i \) are the eigenvalues of \( T_2 T_1 \). In the limit of a large lattice \( Z_{SI} \approx \lambda^{M/2} \) where \( \lambda \) is the largest eigenvalue.
From equation (III.2.14) it is clear that the dependence of $Z_{SI}$ on $\theta$ is only through $\cosh \theta$. Therefore for $\theta$ either real or pure imaginary, $Z_{SI}$ is a real quantity. Consequently, the largest eigenvalue of $T_2 T_1$ should be real for these values of $\theta$.

It is useful to introduce some transformation properties of the $T_i$'s. Define two numerically equivalent $2 \times 2$ matrices $u_\phi$ and $u^\phi$, that operate on $\rho$- and $\sigma$-matrices respectively, by

$$u_\phi = \begin{pmatrix} e^\phi & 0 \\ 0 & e^{-\phi} \end{pmatrix} \quad u^\phi = \begin{pmatrix} e^\phi & 0 \\ 0 & e^{-\phi} \end{pmatrix}$$  \hspace{1cm} (III.4.6)

where $\phi$ is some number. Define the transformation

$$t_\phi \to \hat{t}_\phi \text{ by}$$

$$\hat{t}_\phi = u_\phi^{-1} t_\phi u_\phi = u^\phi^{-1} t_\phi u^\phi$$  \hspace{1cm} (III.4.7)

This equation represents the four equations that could be written either by not suppressing the $\sigma$-indices or by not suppressing the $\rho$-indices of the $t$'s. This similarity transformation can be effected equally well in the $\rho$- or the $\sigma$-space. Replacing $t$ by $\hat{t}$ in $T_1$ and $T_2$ leaves the matrices unchanged. We further define $U$ by

$$U = u^\phi \otimes u^\phi \otimes \cdots \otimes u^\phi$$  \hspace{1cm} (III.4.8)

the $N$-fold $\sigma$-tensor product of $u^\phi$. The invariance of $T_1$ and $T_2$ under the above replacement can be written as
\[ U^{-1} T_i U = T_i \quad i = 1,2 \quad (III.4.9) \]

It follows that \( U \) commutes with \( T_i \) and therefore a set of common eigenvectors can be found.

Two further useful properties are

\[ t_{\lambda \mu}^{\alpha \beta}(x,\theta) = t_{-\mu,-\lambda}^{-\beta,-\alpha}(x,\theta) \quad (III.4.10a) \]

\[ t_{\lambda \mu}^{\alpha \beta}(x^{-1},\theta) = x^{-1}t_{-\lambda,-\mu}^{\beta \alpha}(x,\theta) \quad (III.4.10b) \]

Using (III.4.9 - 10) we have

\[ T_2(\alpha,\beta) = \text{Tr} \left[ t_{\alpha_1 \beta_1}(x^{-1},\theta) t_{\alpha_2 \beta_2}(x,\theta) \ldots t_{\alpha_N \beta_N}(x,\theta) \right] \]

\[ = \text{Tr} \left[ t_{\beta_1 \alpha_1}(x,\theta) t_{\beta_2 \alpha_2}(x^{-1},\theta) \ldots t_{\beta_N \alpha_N}(x^{-1},\theta) \right] \]

\[ = T_1(\beta,\alpha) \quad (III.4.11) \]

Therefore

\[ T_2 = T_1^T \quad (III.4.12) \]

where the superscript \( T \) means transpose.

Define

\[ T \equiv T_2T_1 = T_1^T T_1 \quad (III.4.13) \]

and it follows that \( T \) is symmetric.
5) Variational Principle

The eigenvalues of the symmetric matrix $T$ can be characterized by a variational principle. Let $T_{ij}$ be the elements of $T$, and $\psi_i$ the components of a vector $\psi$ whose dimension matches $T$ ($\psi^T \psi \neq 0$). Set

$$I = \frac{\sum_{ij} \psi_i T_{ij} \psi_j}{\sum_i \psi_i^2}$$

(III.5.1)

and differentiate w.r.t. $\psi_k$

$$\frac{\partial I}{\partial \psi_k} = \sum_j \left( T_{kj} + T_{jk} \right) \psi_j - 2 \psi_k \frac{\sum_{ij} \psi_i T_{ij} \psi_j}{\left( \sum_i \psi_i^2 \right)^2}$$

(III.5.2)

Since $T$ is symmetric this can be written as

$$\frac{\partial I}{\partial \psi} = \frac{2T\psi}{\psi^T \psi} - \frac{2\psi^T T \psi}{\psi^T \psi} \psi$$

$$= \frac{2}{\psi^T \psi} (T\psi - I\psi)$$

(III.5.3)

Therefore

$$T\psi = \lambda_i \psi$$

(III.5.4)

if and only if $I$ is stationary. The largest eigenvalue, $\lambda$, is characterized by

$$\lambda = \max \left\{ \text{stat} - \frac{\psi^T T \psi}{\psi^T \psi} \right\}$$

(III.5.5)

where "stat" means the set of stationary values.
6) Transfer Matrix for the Percolation Probability

The percolation probability is the probability that a site on the Potts model lattice will belong to a component of the graph with an infinite number of sites in it. Let P and Q be two sites on the Potts model lattice. Define

$$Z_{PQ}^* = (2x \cosh \theta)^{-N/2} \sum_{\text{Graphs}} x^\ell (2 \cosh \theta)^{\ell + 2} \delta(\text{graph})$$

(III.6.1)

where $\delta(\text{graph}) = 1$ if P and Q are in the same component, $= 0$ otherwise.

In this model where in the low temperature limit a single infinite component is present we have the following expression for the percolation probability

$$P^2 = \lim_{|P-Q| \to \infty} \lim_{N \to \infty} \frac{Z_{PQ}^*}{Z_{SI}}$$

(III.6.2)

where $|P-Q|$ is the distance between P and Q.

In fact, we can construct a transfer matrix which allows $Z_{PQ}^*$ to be written in a form analogous to $Z_{SI}$. We take the sites P and Q to be between the same two rows on the staggered ice lattice. We make the reasonable assumption that (III.6.2) holds regardless of the absolute positions of P and Q, as long as the distance between them becomes infinite. Let P be at position i, and Q at position j, as shown in figure (III.6). Define

$$D_{ij}(\alpha, \beta) = e^{2\lambda(\alpha_{2i+1} + \alpha_{2i+2} + \ldots + \alpha_{2j})} \delta_{\alpha, \beta}$$

(III.6.3)
Then let

\[ Z_{PQ}^* = \text{Tr}\left( (T_1T_2)^m D_{ij} (T_1T_2)^n \right), \quad m+n = \frac{M}{2} \]

(III.6.4)

In terms of the staggered ice lattice, the effect of \( D_{ij} \) is to leave unchanged the weights of polygons surrounding both, or neither of, \( P \) and \( Q \). However, the weight given to polygons surrounding only \( P \) is altered to \( 2\cosh(\theta - \lambda) \). If we set \( \lambda = \frac{\pi}{2} + \theta \), then this term vanishes. Since the configurations in which \( P \) and \( Q \) are not connected are exactly those in which \( P \) is surrounded by a polygon not surrounding \( Q \), we have the required formulation for \( Z_{PQ}^* \). Letting \( M \) become large, and using (III.6.2) and (III.6.4), we have

\[ \mathcal{P}^2 = \lim_{|P-Q| \to \infty} \frac{\psi_2^T D_{ij} \psi_2}{\psi_2^T \psi_2} \]

(III.6.5)

where \( \psi_2 \) is defined below in equations (III.7.1).

7) Eigenvectors

We want to find the largest eigenvalue of \( T = T_2T_1 \) where \( T_1 \) and \( T_2 \) are given by equations (III.4.3) and (III.4.4). We can write this eigenvalue problem as

\[ T_1 \psi_1 = \Lambda \psi_2 \]

\[ T_2 \psi_2 = \Lambda \psi_1 \]

(III.7.1)

or, with
\( \mathcal{J} = \begin{pmatrix} 0 & T_2 \\ T_1 & 0 \end{pmatrix} \) and \( \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \) \hspace{1cm} (III.7.2)

in a more compact form

\( \mathcal{J} \psi = \Lambda \psi \) \hspace{1cm} (III.7.3)

If we let

\[
U = \begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix}
\] \hspace{1cm} (III.7.4)

where \( U \) is given by (III.4.8), then it follows that

\( \mathcal{J} U = U \mathcal{J} \) \hspace{1cm} (III.7.5)

and we can choose a suitable \( \psi \) belonging to the largest \( \Lambda \) such that

\( U \psi = \alpha \psi \) \hspace{1cm} (III.7.6)

This implies \( U \psi_1 = \alpha \psi_1 \) and \( U \psi_2 = \alpha \psi_2 \). Since \( U \) is diagonal

\[
(U \psi)(\alpha) = \exp \left( \sum_1^\infty \alpha_i \right) \psi(\alpha)
\] \hspace{1cm} (III.7.7)

Following Yang and Yang (1966) we expect the largest eigenvalue of equation (III.7.3) to arise from the space in which \( \sum \alpha_i = 0 \), so that there are as many up arrows as down arrows in each row of the staggered ice lattice. We would therefore expect the required \( \psi \)'s to be invariant under \( U \)

\( U \psi_1 = \psi_1 \) and \( U \psi_2 = \psi_2 \) \hspace{1cm} (III.7.8)
In the limit of \( x \to \infty \), or from equation (III.2.15b) the zero temperature limit, the solution is straightforward. From equations (III.4.1) and (III.2.8)

\[
x^{-1} t_{\lambda \mu}^{\alpha \beta}(x, \theta) = e^{(2\alpha - \beta)/2} \delta_{\alpha} \delta_{\beta}^{\lambda \mu} = \phi_{\alpha}^{\lambda} \phi_{\beta}^{\mu}
\]

\[
t_{\lambda \mu}^{\alpha \beta}(x^{-1}, \theta) = e^{(2\beta - \alpha)/2} \delta_{\alpha}^{\lambda} \delta_{\beta}^{\mu} = \phi_{-\beta}^{\lambda} \phi_{-\alpha}^{\mu}
\]

where

\[
\phi_{\mu}^{\alpha} = e^{\theta \alpha /2} \delta_{\alpha}^{\mu}
\]

Then

\[
T_1(\alpha, \beta) = x^{N/2} \sum_{\mu} \phi_{-\mu_1}^{\alpha_1} \phi_{-\mu_2}^{\beta_1} \phi_{-\mu_3}^{\alpha_2} \phi_{-\mu_2}^{\beta_2} \phi_{-\mu_3}^{\alpha_3} \phi_{-\mu_4}^{\beta_3} \ldots
\]

\[
= x^{N/2} \left\{ \sum_{\mu_1, \mu_3, \mu_5} \phi_{-\mu_1}^{\alpha_1} \phi_{-\mu_3}^{\alpha_2} \phi_{-\mu_5}^{\alpha_3} \phi_{-\mu_5}^{\alpha_4} \phi_{-\mu_5}^{\alpha_5} \ldots \right\}^{+1/2}
\]

\[
+ \left\{ \sum_{\mu_2, \mu_4, \mu_6} \phi_{-\mu_2}^{\beta_1} \phi_{-\mu_4}^{\beta_2} \phi_{-\mu_4}^{\beta_3} \phi_{-\mu_6}^{\beta_4} \ldots \right\}^{+1/2}
\]

\[
= x^{N/2} \phi_{2}(\alpha) \phi_{1}(\beta)
\]

(III.7.11)
where

$$
\phi_1(\beta) = \text{Tr} \left[ \phi_{12}^{\beta_1} \left( \phi_{12}^{\beta_2} \right)^T \phi_{12}^{\beta_3} \left( \phi_{12}^{\beta_4} \right)^T \ldots \left( \phi_{12}^{\beta_N} \right)^T \right]
$$

$$
\phi_2(\alpha) = \text{Tr} \left[ \left( \phi_{12}^{-\alpha_1} \right)^T \phi_{12}^{\alpha_2} \left( \phi_{12}^{-\alpha_3} \right)^T \ldots \left( \phi_{12}^{-\alpha_{N-1}} \right)^T \phi_{12}^{\alpha_N} \right]
$$

$$
\phi_{\alpha} = \left( \phi_{\frac{1}{2}}, \phi_{-\frac{1}{2}} \right) \quad (\text{III.7.12})
$$

Therefore

$$
T_1 \phi_1 = \phi_2 \left[ x^{N/2} \sum_{\beta} \phi_1^2 (\beta) \right]
$$

$$
T_2 \phi_2 = \phi_1 \left[ x^{N/2} \sum_{\beta} \phi_2^2 (\beta) \right] \quad (\text{III.7.13})
$$

With suitable normalization $\phi_1$ and $\phi_2$ are the only non-trivial solutions to equations (III.7.1) for zero temperature.

This solution can be used as a basis for an iterative procedure to compute solutions at higher temperatures. If $\phi$ is a vector not orthogonal to the required eigenvector of $\mathcal{J}$, then repeated application of $\mathcal{J}$ to $\phi$ will asymptotically tend to $\Lambda^N \psi$ where $\Lambda$ is the largest eigenvalue and $\psi$ is the corresponding eigenvector. Since $\phi_1$ satisfies $T_2 T_1 \phi_1 = \Lambda^2 \phi_1$ at zero temperature, we do not expect it to be orthogonal to the solution at low temperatures. We therefore consider the action of $T_1$ and $T_2$ on vectors of the form
\[
\psi_1(\alpha) = \text{Tr} \left[ F_{\alpha_1} \left( F^{-\alpha_2} \right)^T \ldots \left( F^{-\alpha_N} \right)^T \right] \quad (III.7.14a)
\]
\[
\psi_2(\alpha) = \text{Tr} \left[ \left( F^{-\alpha_1} \right)^T F_{\alpha_2} \ldots F_{\alpha_N} \right] \quad (III.7.14b)
\]

where \( F_{\alpha} \) is a matrix of dimension \( m \) by \( n \). Writing the traces out in full we have

\[
\psi_1(\alpha) = \sum_{\lambda} \sum_{\mu} \frac{\alpha_{1\lambda}}{\mu_1 \mu_2} \frac{\alpha_{2\lambda}}{\mu_2 \mu_3} \ldots \frac{\alpha_{N\lambda}}{\mu_N \mu_1} \quad (III.7.15a)
\]
\[
\psi_2(\alpha) = \sum_{\lambda} \sum_{\mu} \frac{-\alpha_{1\lambda}}{\lambda_1 \lambda_2} \frac{\alpha_{2\lambda}}{\lambda_2 \lambda_3} \ldots \frac{\alpha_{N\lambda}}{\lambda_N \lambda_1} \quad (III.7.15b)
\]

\( T_1 \) operating on \( \psi_1 \) is

\[
(T_1 \psi_1)(\alpha) = \sum_{\beta} T(\alpha, \beta) \psi_1(\beta)
\]
\[
= \sum_{\beta} \sum_{\mu} \frac{\alpha_{1\mu}}{\mu_1 \mu_2} \frac{\alpha_{2\mu}}{\mu_2 \mu_3} \ldots \frac{\alpha_{N\mu}}{\mu_N \mu_1} \quad (III.7.15a)
\]
\[
= \sum_{\beta} \sum_{\mu} \frac{\alpha_{1\mu}}{\mu_1 \mu_2} \frac{\alpha_{2\mu}}{\mu_2 \mu_3} \ldots \frac{\alpha_{N\mu}}{\mu_N \mu_1} \quad (III.7.15b)
\]

\[
= \sum_{\beta} \sum_{\mu} \frac{\alpha_{1\mu}}{\mu_1 \mu_2} \frac{\alpha_{2\mu}}{\mu_2 \mu_3} \ldots \frac{\alpha_{N\mu}}{\mu_N \mu_1} \quad (III.7.15b)
\]
\[
\sum_{\mu \lambda} \mathcal{F}^{\alpha_1}_{\mu_2 \lambda_2, \mu_1 \lambda_1} \mathcal{F}^{\alpha_2}_{\mu_2 \lambda_2, \mu_3 \lambda_3} \cdots \mathcal{F}^{\alpha_N}_{\mu_N \lambda_N, \mu_1 \lambda_1}
\]
\[
= \text{Tr} \left( \left( \mathcal{F}^{-\alpha_1}_I \right)^T \mathcal{F}^{\alpha_2}_I \cdots \mathcal{F}^{\alpha_N}_I \right)
\]

where

\[
\mathcal{F}^{\alpha}_{\mu' \lambda'}, \mu \lambda = x^{\frac{1}{2}} \sum_{\beta} t^{\alpha \beta}_{\mu' \mu} (x^{-1}, \theta) F^{-\beta}_{\lambda \lambda'}
\]

Since \( \mu \) and \( \mu' = \pm \frac{1}{2} \), the dimension of \( \mathcal{F}^{\alpha}_I \) is 2n by 2m.

The last line of equation (III.7.16) is the same sort of vector as \( \psi_2 \). Application of \( T_2 \) to this vector produces a vector of the same type as \( \psi_1 \) with \( \mathcal{F}^{\alpha}_I \)-matrices having dimension 4m by 4n. Since \( \phi_1 \) is of the same form as \( \psi_1 \) we expect the iteration procedure to approach a vector which is the eigenvector of the largest eigenvalue of \( T \) having the same form as \( \psi_1 \). In this limit the matrices \( \mathcal{F}^{\alpha}_I \) become infinite in size.

We have already seen that it is no restriction to assume that the eigenvectors of \( T \) are also eigenvectors of \( U \) (equation III.4.9). We will now investigate the consequences of this property on the \( \mathcal{F}^{\alpha}_I \)-matrices. For ease of notation we will rewrite equation (III.7.14a) in terms of tensor products of matrices.

\[
\psi_1 = \text{Tr}_\rho \left( \mathcal{F}^*_I \otimes \mathcal{F}^*_I \otimes \cdots \otimes \mathcal{F}^*_I \right)
\]

where
\[ F^* = \begin{pmatrix} F_{1}^* \\ F_{2}^* \end{pmatrix} \text{ and } \tilde{F}^* = \begin{pmatrix} F_{1}^* \\ F_{2}^* \end{pmatrix}^T \quad (III.7.19) \]

\( F^* \) is a two component vector in the \( \sigma \)-space and an \( m \) by \( n \) matrix in \( \rho \)-space. We have immediately that

\[ U \psi_1 = \text{Tr}_\rho \left( u^* F^* \tilde{\otimes} u^* \tilde{F}^* \tilde{\otimes} \ldots \tilde{\otimes} u^* \tilde{F}^* \right) \quad (III.7.20) \]

In the case of \( t^* \) transformations in the \( \sigma \)-space by \( u^* \) could be brought about by transformations in the \( \rho \)-space as in equation (III.4.7). If \( \psi_1 \) is to be invariant under \( U \)

\[ u^* F^* = U_1 F^* U_2^{-1} \]

\[ u^* \tilde{F}^* = U_2 \tilde{F}^* U_1^{-1} \quad (III.7.21) \]

must hold where \( U_i \) are \( \rho \)-matrices matching the dimension of \( F^* \). The simplest case and the nature of the iteration procedure indicate that \( U_i \) are tensor products of \( u \) in \( \rho \)-space.

Label the levels in the iteration procedure with index \( p \). Let \( p=0 \) correspond to the first level where the dimension of the \( F^* \)-matrices is given by \( m=1, n=2 \). At the next level, \( p=1, m=4, n=2 \), and so on.

In general

\[ m = 2^p \quad n = 2^{p+1} \quad p \text{ even} \]

\[ m = 2^{p+1} \quad n = 2^p \quad p \text{ odd} \quad (III.7.22) \]
At level $p$, $p$ even, we require $U_1$ to be a $p$-fold tensor product of $u_\phi$, and $U_2$ to be a $p+1$-fold product of $u_\phi$ in order to match the dimension of $F^\alpha$. When $p$ is odd the requirements on $U_1$ and $U_2$ are reversed.

The matrices $u_\phi$, for general $\phi$, form a representation of the subgroup of "principle" transformations of the unitary group (Weyl, 1931, p.137) of transformations in two dimensions. All of the irreducible representations of this group are of the form

$$U_{m,m'}^{(j)} = e^{im\phi} \delta_{m,m'} \quad (\text{III.7.23})$$

where

$$j = 0, \frac{1}{2}, 1, 3/2, \ldots$$

$$m = j, j-1, j-2, \ldots , -(j-1), -j \quad (\text{III.7.24})$$

therefore

$$u_\phi = U_{\frac{1}{2}} \quad (\text{III.7.25})$$

A tensor product of $U_{\frac{1}{2}}$ representations can be expressed as a direct sum of irreducible representations. For a $p$-fold tensor product of $U_{\frac{1}{2}}$ representations the representation $U^{(j)}$ occurs with frequency $d^p_j$ in the direct sum (Brinkman, 1956, p.43), where

$$d^p_j = \frac{p! (2j + 1)}{(p/2 + j + 1)! (p/2 - j)!} \quad (\text{III.7.26})$$
Since it is true that

\[ \sum_{j=0}^{p/2} d_j^P (2j + 1) = 2^P \]

or \( \frac{p}{2} \)

we can relabel the \( F_{\lambda_1, \lambda_2}^\alpha \) as \( F_{n_1 j_1 m_1, n_2 j_2 m_2}^\alpha \)

where

\[ n_1 = 1, 2, \ldots d_j^{p_1}, \quad n_2 = 1, 2, \ldots d_j^{p_2} \]

(III.7.27)

\[ p_1 = p + 1, \quad p_2 = p, \quad p \text{ even} \]

(III.7.28)

\[ j_i = p_i/2, (p_i/2) - 1, \ldots 0 \text{ or } \frac{1}{2} \]

(III.7.29)

\[ m_i = j_i, j_i - 1, j_i - 2, \ldots -j_i + 1, -j_i \]

We also have

\[ U = \delta_{m, m'} \delta_{j, j'} \delta_{n, n'} e^{\phi m} \]

(III.7.30)

where \((n, j, m)\) and \((n', j', m')\) are different sets of indices belonging to the same \(p\), the multiplicity of the tensor product in \(U\). This diagonal form is also true for the \(p\)-matrices \(U_1\) and \(U_2\).

From equations (III.7.21) and (III.7.30) we have

\[ F_{n_1 j_1 m_1, n_2 j_2 m_2}^\alpha = e^{\phi (m_1 - m_2 - \alpha)} F_{n_1 j_1 m_1, n_2 j_2 m_2}^\alpha \]

(III.7.31)
for arbitrary $\phi$. From this it follows that

$$F_{n_1j_1m_1,n_2j_2m_2}^\alpha = 0 \quad \text{if} \quad m_1-m_2 \neq \alpha \quad \text{or} \quad |j_1-j_2| \neq \frac{1}{2}$$

(III.7.32)

The last condition is necessary to ensure the ranges of $m_1$ and $m_2$ are compatible. By using this transformation property of the $F^\alpha$-matrix the number of variational parameters can be considerably reduced.

To this point we have defined the transfer matrix $T$, and noted that its largest eigenvalue $\Lambda^2$ can be expressed as a stationary variational principle. Beginning with the zero temperature solution we have developed a sequence of trial functions $\psi_1$ and $\psi_2$ which can be written in terms of the matrices $F^\alpha$. At successively increasing levels of the sequence, indexed by $p$, the matrices $F^\alpha$ are of larger dimensions and therefore the trial function space is larger. As $p$ increases the variational principle should give increasingly accurate values for $\Lambda$. In the limit of infinite dimensional $F^\alpha$ we expect the trial function space to include the eigenvector corresponding to the eigenvalue $\Lambda^2$. Using some of the symmetries of $T$ it has been possible to place restrictions on the $F^\alpha$, thus reducing the number of variational parameters.

8) Matrix Equations

By using equations (III.7.14a,b) the variational principle (III.5.5) can be written as
Expressions, in terms of traces over products of matrices have been developed for \( \psi_1, \psi_2, \) and \( T_1 \).
Substituting these expressions into equation (III.8.1), and using its stationary property, equations involving the matrices appearing in the expressions for \( \psi_1 \) and \( \psi_2 \) will be derived.

The numerator on the right hand side of equation (III.8.1) can itself be written as the eigenvalue of a certain equation. Substituting equations (III.7.14a,b) and (III.4.3) into equation (III.8.1) gives

\[
\psi_2^T T_1 \psi_1 = \sum_{\alpha \beta} \psi_2 (\alpha) T_1 (\alpha, \beta) \psi_1 (\beta)
\]

\[
= \sum_{\alpha \beta} \sum_{\mu} F_{\mu_1}^{-\alpha_1} F_{\mu_2}^{\alpha_2} F_{\mu_3}^{-\alpha_3} \cdots F_{\mu_N}^{\alpha_N} \\
\times \left( \sum_{\lambda} t_{\lambda_1 \lambda_2}^{\alpha_1 \beta_1}(x, \theta) \cdot t_{\lambda_2 \lambda_3}^{\alpha_2 \beta_2}(x^{-1}, \theta) \cdots t_{\lambda_N \lambda_1}^{\alpha_N \beta_N} \right) \\
\times \left( \sum_{\rho} G_{\rho_1 \rho_2}^{\beta_1} G_{\rho_2 \rho_3}^{\beta_2} G_{\rho_3 \rho_4}^{\beta_3} \cdots G_{\rho_1 \rho_N}^{\beta_N} \right)
\]

\[
= \sum_{\mu} \sum_{\lambda} \sum_{\rho} \mathcal{G}_{\mu_1 \lambda_1 \rho_1, \mu_2 \lambda_2 \rho_2} \mathcal{K}_{\mu_2 \lambda_2 \rho_2, \mu_3 \lambda_3 \rho_3} \cdots \mathcal{K}_{\mu_N \lambda_N \rho_N, \mu_1 \lambda_1 \rho_1}
\]

\[
= \text{Tr}(g \mathcal{K} g \mathcal{K} \cdots \mathcal{K}) \quad \text{(III.8.2)}
\]

where
\[ J_{\mu\lambda, \mu'\lambda'} = \sum_{\alpha\beta} F^{-\alpha}_{\mu \mu'} t^{\alpha\beta}_{\lambda \lambda'} (x, \theta) F^\beta_{\rho \rho'} \]  

\text{(III.8.3a)}

\[ K_{\mu\lambda, \mu'\lambda'} = \sum_{\alpha\beta} F^\alpha_{\mu \mu'} t^{\alpha\beta}_{\lambda \lambda'} (x^{-1}, \theta) F^{-\beta}_{\rho \rho'} \]  

\text{(III.8.3b)}

As \( N \), the number of vertices in a row, becomes large, the trace in equation (III.8.2) behaves as \( \eta^N \) where \( \eta^2 \) is the largest eigenvalue of \( J'K' \). Introducing the vectors \( P \) and \( Q \) this can be written as

\[ \sum_{\mu_2 \lambda_2 \rho_2} J_{\mu_1 \lambda_1 \rho_1, \mu_2 \lambda_2 \rho_2} P_{\mu_2 \lambda_2 \rho_2} = \eta Q_{\mu_1 \lambda_1 \rho_1} \]  

\text{(III.8.4a)}

\[ \sum_{\mu_1 \lambda_1 \rho_1} K_{\mu_2 \lambda_2 \rho_2, \mu_1 \lambda_1 \rho_1} Q_{\mu_1 \lambda_1 \rho_1} = \eta P_{\mu_2 \lambda_2 \rho_2} \]  

\text{(III.8.4b)}

Using definitions (III.8.3a,b) these equations can be written as

\[ \sum_{\alpha\beta\lambda_2} t^{\alpha\beta}_{\lambda_1 \lambda_2} (x, \theta) \left[ F^{-\alpha}_{\lambda} \right]^T P_{\lambda_2} \left[ F^\beta_{\lambda} \right]^T = \eta Q_{\lambda_1} \]  

\text{(III.8.5a)}

\[ \sum_{\alpha\beta\lambda_1} t^{\alpha\beta}_{\lambda_2 \lambda_1} (x^{-1}, \theta) F^\alpha_{\lambda_1} F^{-\beta} = \eta P_{\lambda_2} \]  

\text{(III.8.5b)}

where \( F^\alpha_{\lambda} = F^\alpha_{\lambda} \) and \( P_{\lambda} \) is the matrix \( \left[ P_{\mu\lambda \rho} \right] \) with indices \( \mu \) and \( \rho \), and similarly \( Q_{\lambda} \). Matrix multiplication is
understood in these equations. By using relations (III.4.10a,b) it can be shown that equation (III.8.5a) is the same as equation (III.8.5b) if

\[ Q_\lambda = \frac{x^{\frac{1}{2}}}{\lambda} p^T_{\lambda} \]  \hspace{1cm} (III.8.6)

From the definition of \( f \) and \( \lambda \) we see that \( \lambda \) is a simple index taking the values \( \pm \frac{1}{2} \). While equation (III.8.6) may not hold for all solutions of (III.8.5), the largest value of \( n \) is expected to correspond to this most symmetric case. We therefore write the equation for \( P \) and \( n \) as

\[ \sum_{\alpha \beta \lambda_2}^{\frac{1}{2}} t^{\alpha \beta}_{\lambda_1 \lambda_2} (x, \theta) \left[ F^{-\alpha} \right]_{\lambda_2} \left[ F^{\beta} \right]_{\lambda_1} = n x^{\frac{1}{2}} p^T_{\lambda_1} \]  \hspace{1cm} (III.8.7)

Substituting (III.7.14a) into the denominator of equation (III.8.1) leads to a similar eigenvalue equation

\[ T \psi_1 \psi_1 = \sum_{\alpha} \psi_1(\alpha) \psi_1(\alpha) \]

\[ = \sum_{\alpha} \left( \sum_{\mu} F_1^{\alpha_1 \mu_1 \mu_2} F_{\mu_3 \mu_4}^{-\alpha_2} \ldots F_{\mu_1 \mu_N}^{-\alpha_N} \right) \left( \sum_{\lambda} F_1^{\lambda_1 \lambda_2} F_{\lambda_3 \lambda_2}^{-\alpha_2} \ldots F_{\lambda_1 \lambda_N}^{-\alpha_N} \right) \]

\[ = \sum_{\alpha} \left( \sum_{\mu} F_1^{\alpha_1 \mu_1 \mu_2} F_{\lambda_1 \lambda_2}^{\alpha_1} \right) \left( \sum_{\alpha} F_{\mu_3 \mu_4}^{-\alpha_2} F_{\lambda_3 \lambda_2}^{-\alpha_2} \right) \ldots \left( \sum_{\lambda} F_{\mu_1 \mu_N}^{-\alpha_N} F_{\lambda_1 \lambda_N}^{-\alpha_N} \right) \]

\[ = \sum_{\alpha} \left( \sum_{\mu} W_{\mu_1 \lambda_1, \mu_2 \lambda_2} \ldots W_{\mu_1 \lambda_1, \mu_N \lambda_N} \right) \]

\[ = \text{Tr} \left[ \sum_{W} W^T W^T \ldots W^T \right] \]  \hspace{1cm} (III.8.8)
\[ \mathcal{W}_{\mu \lambda, \nu \lambda'} = \sum_{\alpha} F_{\mu \mu}^{\alpha}, F_{\lambda \lambda'}^{\alpha} \]  

(III.8.9)

It is also useful to note that \( \mathcal{W} \) can be written as a tensor product

\[ \mathcal{W} = \left( F^\ast \right)^T \otimes F^\ast \]  

(III.8.10a)

\[ \mathcal{W}^T = \tilde{F}^\ast \otimes \left( \tilde{F}^\ast \right)^T \]  

(III.8.10b)

where the transpose of \( F^\ast \) is in the \( \sigma \)-space and the usual inner product is taken in this space. As \( N \) becomes large the trace in equation (III.8.8) tends to \( \xi^N \) where \( \xi^2 \) is the largest eigenvalue of \( \mathcal{W} \mathcal{W}^T \). Introducing the eigenvectors \( X \) and \( Y \) we can write this as

\[ \sum_{\mu_2 \lambda_2} \mathcal{W} \cdot \mu_1 \lambda_1, \mu_2 \lambda_2 X_{\mu_2 \lambda_2} = \xi Y_{\mu_1 \lambda_1} \]  

(III.8.11a)

\[ \sum_{\mu_1 \lambda_1} \mathcal{W} \cdot \mu_1 \lambda_1, \mu_2 \lambda_2 Y_{\mu_1 \lambda_1} = \xi X_{\mu_2 \lambda_2} \]  

(III.8.11b)

Using the definitions (III.8.9) these equations become

\[ \sum_{\alpha} F_{\alpha}^\ast X \cdot \left( F_{\alpha}^\ast \right)^T = \xi Y \]  

(III.8.12a)

\[ \sum_{\alpha} \left( F_{\alpha}^\ast \right)^T Y \cdot F_{\alpha} = \xi Y \]  

(III.8.12b)

where \( X \) and \( Y \) are understood to be matrices. Equations
(III.8.12a,b) are consistent with $X = X^T$ and $Y = Y^T$. We will choose the solutions with this symmetry.

By means of the transformation property (III.7.21) of $F^*$ we are able to derive transformation properties of $X$ and $Y$ under $U_1$ and $U_2$. Let

$$S_i = U_i \otimes U_i^{-1} \quad (III.8.13)$$

$$S_1 \mathcal{W} S_2^{-1} = \left[ U_1 \otimes U_1^{-1} \right] \left[ (F^*)^T \otimes F^* \right] \left[ U_2^{-1} \otimes U_2 \right]$$

$$= U_1 \left[ (F^*)^T \otimes F^* \right] U_2^{-1} \otimes U_1^{-1} F^* U_2$$

$$= U_1 (u_1^H (u_i^* F^*) U_2) U_2^{-1} \otimes U_1^{-1} (u_1 (u_i^* F^*) U_2) U_2$$

$$= (F^*)^T \otimes F^*$$

$$= \mathcal{W} \quad (III.8.14)$$

and similarly

$$S_2 \mathcal{W}^T S_1^{-1} = \mathcal{W}^T \quad (III.8.15)$$

from which it follows that

$$S_1^{-1} Y = U_1^{-1} Y U_1 \quad (III.8.16a)$$

$$= Y$$

$$S_2^{-1} X = U_2^{-1} X U_2 \quad (III.8.16b)$$

$$= X$$
where, on the left hand side of the equation, \( X \) and \( Y \) are understood to be vectors, and on the right hand side matrices.

To this point we have four equations (III.8.7) and (III.8.12a,b) in the unknowns \( F^\alpha, P_\lambda, X, Y, \eta \) and \( \xi \). We have not yet used the stationary property of the variational principle in equation (III.8.1). By means of this property some of the unknowns can be eliminated.

Since \( \eta \) in equation (III.8.7) is an eigenvalue we ought to be able to represent it alone as a variational principle. If \( P_{\pm \frac{1}{2}} \) are solutions to equation (III.8.7) then they must also satisfy

\[
V(P) \equiv \sum_{\lambda', \lambda} t^{\alpha \beta}_{\lambda', \lambda} (x, \theta) P_{\rho'} \gamma_{\lambda', \mu'} F^\alpha_{\lambda, \lambda'} P_{\mu \lambda \rho} F^\beta_{\rho', \rho} \\
= \eta x_{\frac{1}{2}} \tag{III.8.17}
\]

It is sufficient for our purposes to show that \( V(P) \) is stationary with respect to small changes in the components of \( P \) when \( P \) is a solution of equation (III.8.7). Let

\[
P^*_{\mu \lambda \rho} = P_{\mu \lambda \rho} + \epsilon \text{ for } \mu=i, \ \lambda=j, \ \rho=k \\
= P_{\mu \lambda \rho} \text{ otherwise} \tag{III.8.18}
\]

then
\[ \frac{\partial}{\partial \varepsilon} V(P^*) \bigg|_{\varepsilon=0} \]

\[ \sum_{\alpha \beta} \left( \sum_{\mu \lambda \rho} t_{\mu \lambda \rho}^\alpha \chi_{\mu \lambda \rho} \right) F_{\mu \lambda}^\alpha \rho_{\lambda \rho} + \sum_{\mu' \lambda' \rho'} t_{\lambda' \rho'}^\alpha \chi_{\mu' \lambda' \rho'} \rho'_{\lambda' \mu'} F_{\lambda' \rho'}^\alpha \rho'_{\lambda' \mu'} \]

\[ \sum_{\rho'_{\lambda' \mu'}} \rho'_{\lambda' \mu'}^2 \]

\[ \frac{2P_{ijk}}{\sum_{\mu' \lambda' \rho'}} \rho'_{\lambda' \mu'} \cdot \frac{\eta x^2}{P_{\rho'_{\lambda' \mu'}}} \]

\[ \left( \sum_{\rho'_{\lambda' \mu'}} \rho'_{\lambda' \mu'}^2 \right)^2 \]

\[ \eta x^2 P_{ijk} \sum_{\mu' \lambda' \rho'} t_{\mu \lambda}^\alpha (x, \theta) \rho'_{\lambda' \mu'} \rho'_{\lambda' \mu'} F_{\mu \lambda}^\alpha \rho'_{\lambda' \mu'} \]

\[ = \frac{\eta x^2}{2P_{ijk}} \rho'_{\lambda' \mu'} \rho'_{\lambda' \mu'} \]

\[ = 0 \quad (III.8.19) \]

This is true for all \( i, j, \) and \( k, \) and therefore \( V(P) \) is stationary with respect to \( P \) as required.

In a similar fashion \( \xi \) can be expressed as a variational principle. We can write equation (III.8.11) as

\[ \mathcal{W}^T \mathcal{W} \chi = \xi^2 \chi \quad (III.8.20) \]

where \( \chi \) is regarded as a vector. Since \( \mathcal{W}^T \mathcal{W} \) is symmetric, a variational principle for \( \xi^2 \) is
where again the transpose of $X$ is in the vector sense. Using equations (III.8.11) this reduces to

\[ \xi^2 = \max_{\text{stat}} \left\{ \frac{X^T \omega \omega X}{X^T X} \right\} \quad (\text{III.8.21}) \]

\[= \max_{\text{stat}} \left\{ \frac{\text{Tr} \left[ \sum_{\alpha} Y^T F^\alpha X \left( F^\alpha \right)^T \right]}{\text{Tr} X^T X} \right\} \quad (\text{III.8.22}) \]

where the transposes in the last expression are in the matrix sense. When $X$ and $Y$ are solutions of equations (III.8.11) then the left hand side of equation (III.8.22) is stationary with respect to small variations in $X$ and $Y$. Equations (III.8.17) and (III.8.22) can be combined to give a detailed expression for the variational principle given in equation (III.8.1).

\[\Lambda = \max_{\text{stat}} \left[ \frac{\eta}{\xi} \right]^N \]

\[= \max_{\text{stat}} \left\{ \frac{x^{-N/2} \text{Tr} \left[ X^T X \right]}{\text{Tr} \left[ \sum_{\alpha \beta} \alpha \beta \lambda \lambda', (x, \theta) P_{-\lambda', (x, \theta) P_{\lambda}} \left( F^{-\alpha} \right)^T P_{\lambda} \left( F^{\beta} \right)^T \right]} \right\} \]

\[= \max_{\text{stat}} \left\{ \frac{\text{Tr} \left[ \sum_{\alpha} Y^T F^\alpha X \left( F^\alpha \right)^T \right]}{\text{Tr} \left[ \sum_{\lambda} P^T \lambda P_{\lambda} \right]} \right\} \]

\[\equiv V' \left[ F^* \right] \quad (\text{III.8.23}) \]

This expression is already stationary with respect to
X, Y and P because its separate parts have these properties. Therefore, treating X, Y and P as constants this principle must be stationary with respect to small changes in the components of $F^{\alpha}$, when these $F^{\alpha}$ are such that $\psi_1$ and $\psi_2$ are solutions to the original equations (III.7.1). Let

$$F^{\alpha}_{\mu\lambda} = F^{\alpha}_{\mu\lambda} + \epsilon , \quad \text{for } \alpha = i, \mu = j, \lambda = k$$

$$= F^{\alpha}_{\mu\lambda} \quad \text{otherwise} \quad \text{(III.8.24)}$$

then

$$\frac{\partial}{\partial \epsilon} V' \left[ F^* \right] \bigg|_{\epsilon = 0} = \sum_{\beta\lambda'\lambda} t^{\beta i}_{\lambda'\lambda} (x, \theta) P^\rho_{\beta',\lambda'k} P_{j\lambda\rho} F^{\beta}_{\rho'\rho}$$

$$+ \sum_{\alpha\lambda'\lambda, \mu'\mu} t^{\alpha i}_{\lambda'\lambda} (x, \theta) P_{j-\lambda'\mu', \mu'\mu} F^{\alpha}_{\mu'\mu} P_{\mu\lambda k}$$

$$- \left( \sum_{\mu'\lambda'} Y_{j\mu'}, X_{\lambda\lambda}, F^i_{\mu'\lambda'}, + \sum_{\mu\lambda} Y_{j\mu} F^i_{\mu\lambda} X_{\lambda k} \right) \kappa x^2 \zeta$$

$$= 0 \quad \text{(III.8.25)}$$

where

$$\zeta = \frac{\sum_{\rho'\lambda'\mu', \rho'\mu'\lambda'} P^2_{\rho'\lambda'\mu'}}{\sum_{\mu'\mu, \lambda'\lambda, \lambda'\alpha} X_{\mu\mu}, F^{\alpha}_{\mu\lambda}, Y_{\lambda\lambda}, F^{\alpha}_{\mu'\lambda'}}$$

Equation (III.8.25) is the condition that $V' \left[ F^* \right]$ is
stationary. It is equivalent to equation (III.8.7) if

$$P_\lambda = Y^\frac{1}{2} F\lambda X^\frac{1}{2}$$  \hspace{1cm} (III.8.27)

We use this relation to eliminate $P_\lambda$ from the equations. Taking

$$A^2 = Y, \quad B^2 = X$$  \hspace{1cm} (III.8.28)

the following equations result from (III.8.7), (III.8.12a,b) and (III.8.27)

$$\sum_\alpha F^\alpha B^2 \left(F^\alpha\right)^T = \xi A^2$$  \hspace{1cm} (III.8.29a)

$$\sum_\alpha \left(F^\alpha\right)^T A^2 F^\alpha = \xi B^2$$  \hspace{1cm} (III.8.29b)

$$\sum_{\alpha\beta\lambda_2} t^{\alpha\beta}_{\lambda_1\lambda_2} \left(x,0\right) F^\beta B \left(F^\lambda_2\right)^T A F^{-\alpha} = \eta x^\frac{1}{2} A F^{-\lambda_1} B$$  \hspace{1cm} (III.8.30)

Since $X$ and $Y$ are symmetric we are also able to choose $A$ and $B$ symmetric. The replacements $A \rightarrow LAL^{-1}, \quad B \rightarrow MBM^{-1}$ and $F^\alpha \rightarrow LF^\alpha M^{-1}$, where $L$ and $M$ are orthogonal matrices, leave the equations (III.8.29) and (III.8.30) unaltered. In general, therefore, we can take $A$ and $B$ to be diagonal matrices. Since, however, for imaginary $\theta$, $A$ and $B$ will be complex matrices, they may not always be diagonalizable by orthogonal $L$ and $M$. In fact, for special values of $\theta$ this assumption fails and either $A$ or $B$ has repeated eigenvalues as we shall mention later.

Finally, the partition function of the Potts model, from equations (III.2.14), (III.4.5), (III.7.1),
can be written as

\[ Z^{1/N} = \nu Z_{SI}^{2/N'} \]

\[ = \nu \frac{\eta^2}{\xi^2} \quad \text{(III.8.31)} \]

where \( N \) is the number of sites on the Potts model lattice and \( N' \) is the number of sites on the staggered ice lattice.

9) Percolation Probability and the Matrix Equation

Variables

From equation (III.6.5) we see that to calculate the percolation probability we must evaluate the two terms \( \psi_T^T \psi_T \) and \( \psi_T^D_{ij} \psi_T \). The first of these has been done

\[ \psi_T^T \psi_T = \psi_T^T \psi_1 \sim \xi^N \quad \text{N large (III.9.1)} \]

where \( \xi \) satisfies equations (III.8.29a,b). Let

\[ U_{\lambda\lambda',\mu\mu'} = \sum_{\alpha} e^{(\theta + i\pi/2)\alpha} F_{\lambda\mu}^{\alpha} F_{\lambda'\mu'}^{\alpha} \]

\[ U^*_{\lambda\lambda',\mu\mu'} = \sum_{\alpha} e^{-(\theta + i\pi/2)\alpha} F_{\mu\lambda}^{\alpha} F_{\mu'\lambda'}^{\alpha} \quad \text{(III.9.2)} \]

then

\[ \psi_T^D_{ij} \psi_T = \text{Tr} \left[ (W^T W)^i (U^* U)^j-i [W^T W]^{N/2-j} \right] \]

\[ \text{(III.9.3)} \]
where $\mathcal{W}$ is defined in equation (III.8.9). It is useful to introduce tensor product notation for the $\mathcal{V}$'s.

$$\mathcal{V} = \left( u^* \cdot \bar{F}^* \right)^T \otimes u^* \cdot F^*$$

$$= \left( U_1 \otimes U_1 \right) \mathcal{W} \left( U_2^{-1} \otimes U_2^{-1} \right)$$

$$\mathcal{V}^* = u^* \cdot \bar{F}^* \otimes \left( u^* \cdot \bar{F}^* \right)^T$$

$$= \left( U_2 \otimes U_2 \right) \mathcal{W}^T \left( U_1^{-1} \otimes U_1^{-1} \right)$$

(III.9.4)

where again the transpose of $F^*$ is in the $\sigma$-space and the usual inner product is taken in $\sigma$-space as well as the tensor product in $\rho$-space. The $u^*$ and $U_1$ are understood to have $\phi=\theta+\frac{i\pi}{2}$. As $N$ becomes large the trace in equation (III.9.3) will approach a limit which is a function of the largest eigenvalues and corresponding eigenvectors of $\mathcal{W}^T \mathcal{W}$ and $\mathcal{V}^* \mathcal{V}$. Define $\xi'$, $X'$ and $Y'$ by

$$\sum_{\mu\mu'} \mathcal{V}_{\lambda\lambda',\mu\mu'} X'_{\mu\mu'} = \xi' Y'_{\lambda\lambda'}$$

$$\sum_{\lambda\lambda'} \mathcal{V}^*_{\mu\mu',\lambda\lambda'} Y'_{\lambda\lambda'} = \xi' X'_{\mu\mu'}$$

(III.9.5)

Then, as $N$ and $i-j$ become large
\[ \psi_2^T D_{ij} \psi_2 = \xi^N \left( \frac{\xi'}{\xi} \right)^2 (i-j) \frac{T_{X'}^{T} X}{(\text{Tr} X'X)(\text{Tr} X'TX')} \]  

(III.9.6)

Equations (III.9.5) can be written as

\[ \begin{pmatrix} 0 & \mathbf{V}^* \\ \mathbf{V} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{X}' \\ \mathbf{Y}' \end{pmatrix} = \begin{pmatrix} \mathbf{U}_2 \mathbf{X} \mathbf{U}_2 & 0 \\ 0 & \mathbf{U}_1 \mathbf{X} \mathbf{U}_1 \end{pmatrix} \begin{pmatrix} 0 & \mathbf{W} \mathbf{X} \\ \mathbf{W} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{U}_2^{-1} \mathbf{X} \mathbf{U}_2^{-1} & 0 \\ 0 & \mathbf{U}_1^{-1} \mathbf{X} \mathbf{U}_1^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{X}' \\ \mathbf{Y}' \end{pmatrix} \]

= \xi' \begin{pmatrix} \mathbf{X}' \\ \mathbf{Y}' \end{pmatrix} \]  

(III.9.7)

where \( \mathbf{X}' \) and \( \mathbf{Y}' \) are regarded as vectors. We can also write equations (III.8.11) as

\[ \begin{pmatrix} 0 & \mathbf{W} \\ \mathbf{W} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix} = \xi \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix} \]  

(III.9.8)

from which it follows that \( \xi = \xi' \) and

\[ \mathbf{U}_2 \mathbf{X} \mathbf{U}_2 = \mathbf{X}' \]

\[ \mathbf{U}_1 \mathbf{Y} \mathbf{U}_1 = \mathbf{Y}' \]  

(III.9.9)

where here \( \mathbf{X}, \mathbf{Y}, \mathbf{X}', \) and \( \mathbf{Y}' \) are matrices. We therefore have for the percolation probability

\[ \mathcal{P} = \frac{\text{Tr} X'^T X}{\sqrt{\text{Tr} X^T X \cdot \text{Tr} X'^T X'}} \]

\[ = \frac{\text{Tr}(\mathbf{U}_2 \mathbf{X} \mathbf{U}_2 \mathbf{X})}{\sqrt{\text{Tr}(XX) \cdot \text{Tr}(\mathbf{U}_2 \mathbf{X} \mathbf{U}_2 \mathbf{X} \mathbf{U}_2 \mathbf{X})}} \]  

(III.9.10)
using the symmetry of $X$.

10) The Reduced Equations

Equations (III.8.29a,b) and (III.8.30), with a suitable normalization condition, could, in principle, be solved for the quantity $\eta/\xi$, for matrices $F^{\alpha}$ of an arbitrary size. In equations (III.7.21) and (III.8.16a,b) we do, however, have some additional information about $F^{\alpha}$, $X$ and $Y$ that allows equations (III.8.29a,b) and (III.8.30) to be written more economically. These transformation properties indicate that the $m$-dependence of $F^{\alpha}$, $X$ and $Y$ is separable from the $j$-, $n$-dependence. We therefore write the components of $F^{\alpha}$ as

$$ F^{\alpha}_{m_1j_1n_1,m_2j_2n_2} = \delta^{\alpha}_{m_1-m_2} \tau(m_1,m_2) f^{j_1n_1,j_2n_2} $$

$$ = \delta^{\alpha}_{m_1-m_2} \tau(m_1,m_2) f^{j_1,j_2} $$

(iii.10.1)

where

$$ f^{j_1n_1,j_2n_2} = 0 \quad \text{if} \quad |j_1-j_2| \neq \frac{1}{2} $$

(iii.10.2)

and $f^{j_1,j_2}$ is a matrix with indices $n_1$ and $n_2$.

Recalling that we can take $A$ and $B$ to be diagonal, we similarly write the components of $A$ and $B$ as

$$ A_{m_1j_1n_1} = \zeta(m_1) a^{j_1n_1} $$
\[ C(m) \alpha_j \quad j = \frac{1}{2}, 3/2, 5/2, \ldots \]

\[ B_{m_2 j_2 n_2} = \zeta(m_2) \alpha_j \]

\[ = \zeta(m_2) \alpha_j \quad j = 0, 1, 2, \ldots \]

A and B are distinguished as belonging to distinct values of j and \( \alpha_j \) is a diagonal matrix with index n. To this point \( \tau \) and \( \zeta \) are quite general functions of the m's. In these functions there is an implicit dependence on the corresponding j's, so that \( \tau \) for different j's might be a different function of the m's.

Using (III.10.1), (III.10.3) and (III.10.4) we rewrite equations (III.8.29) and (III.8.30).

\[ \sum_{\alpha m_2 j_2} \delta_{m_1-m_2}^{\alpha} \tau(m_1, m_2) \frac{\xi^{j_1 j_2}}{2} \zeta^2(m_2) \left[ \alpha_j \right]^2 \delta_{m_1-m_2}^{\alpha} \tau(m_1, m_2) \frac{\xi^{j_1 j_2}}{2} \]

\[ = \sum_{\alpha m_2 j_2} \delta_{m_1-m_2}^{\alpha} \tau(m_1, m_2) \xi^{j_1 j_2} \zeta^2(m_2) \frac{\xi^{j_1 j_2}}{2} \left[ \alpha_j \right]^2 \frac{\xi^{j_1 j_2}}{2} \]

\[ = \xi \zeta^2(m_1) \left[ \alpha_j \right]^2 \]

\[ \sum_{m_1 j_1} \delta_{m_2-m_1}^{\alpha} \tau^2(m_2, m_1) \zeta^2(m_1) \frac{\xi^{j_2 j_1}}{2} \left[ \alpha_j \right]^2 \frac{\xi^{j_1 j_2}}{2} \]

\[ = \xi \zeta^2(m_2) \left[ \alpha_j \right]^2 \]
\[ \sum_{\alpha\beta\lambda_2} t^{\alpha\beta}_{\lambda_1\lambda_2} (x, \theta) \mathcal{F}^\beta_{\lambda_2} \mathcal{F}^\lambda_{\lambda_2} = \sum_{\alpha\beta\lambda_2} \left( z^{(\beta-\alpha)} \delta^{\alpha}_{\lambda_1} \delta^{\beta}_{\lambda_2} + xz^{(\alpha-\beta)} \delta^{\alpha}_{\lambda_2} \delta^{\beta}_{\lambda_1} \right) \mathcal{F}^\beta_{\lambda_2} \mathcal{F}^\lambda_{\lambda_2} \]

\[ = \sum_{\alpha\beta\lambda_2} z^{(\beta-\alpha)} \delta^{\alpha}_{\lambda_1} \delta^{\beta}_{\lambda_2} \delta^{\lambda}_{\lambda_1} \delta^{\lambda}_{\lambda_2} \delta^{\alpha}_{m_1-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ + \sum_{\alpha\beta\lambda_2} xz^{(\alpha-\beta)} \delta^{\alpha}_{-\lambda_1} \delta^{\beta}_{-\lambda_2} \delta^{\lambda}_{-\lambda_1} \delta^{\lambda}_{-\lambda_2} \delta^{\alpha}_{m_1-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ + \sum_{\beta m_2 j_2 m_3 j_3} z^{(\beta+m_3-m_4)} \delta^{\lambda}_{m_3-m_4} \delta^{m_3}_{m_1} \delta^{\beta}_{m_1-1} \delta^{\lambda}_{m_2} \delta^{\lambda}_{m_2} \delta^{\lambda}_{m_3} \delta^{\lambda}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ + \sum_{\alpha m_2 j_2 m_3 j_3} xz^{(\alpha-m_1+m_2)} \delta^{\lambda}_{m_1-1} \delta^{m_2}_{m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\lambda}_{m_3} \delta^{\lambda}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ = \sum_{j_2} \tau(m_1 m_4) \zeta(m_1) z^{m_1-m_4} \delta^{m_1-m_4} + \sum_{\beta m_2} z^{m_2-m_1} \delta^{\beta}_{m_1-1} \delta^{\lambda}_{m_2} \delta^{\lambda}_{m_2} \delta^{\lambda}_{m_3} \delta^{\lambda}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ + \sum_{j_3} x\tau(m_1 m_4) \zeta(m_4) z^{m_4-m_1} \delta^{m_4-m_1} + \sum_{\alpha m_3} z^{m_3-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ = \tau^{(j_2)} \zeta(m_1) \tau(m_1 m_4) \zeta(m_4) \delta^{m_1-m_4} + \sum_{j_4} z^{m_1-m_4} \delta^{m_1-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ + \sum_{j_4} x\tau(m_1 m_4) \zeta(m_4) z^{m_4-m_1} \delta^{m_4-m_1} + \sum_{\alpha m_3} z^{m_3-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ = \tau^{(j_2)} \zeta(m_1) \tau(m_1 m_4) \zeta(m_4) \delta^{m_1-m_4} + \sum_{j_4} z^{m_1-m_4} \delta^{m_1-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ + \sum_{j_4} x\tau(m_1 m_4) \zeta(m_4) z^{m_4-m_1} \delta^{m_4-m_1} + \sum_{\alpha m_3} z^{m_3-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ = \tau^{(j_2)} \zeta(m_1) \tau(m_1 m_4) \zeta(m_4) \delta^{m_1-m_4} + \sum_{j_4} z^{m_1-m_4} \delta^{m_1-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ + \sum_{j_4} x\tau(m_1 m_4) \zeta(m_4) z^{m_4-m_1} \delta^{m_4-m_1} + \sum_{\alpha m_3} z^{m_3-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ = \tau^{(j_2)} \zeta(m_1) \tau(m_1 m_4) \zeta(m_4) \delta^{m_1-m_4} + \sum_{j_4} z^{m_1-m_4} \delta^{m_1-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ + \sum_{j_4} x\tau(m_1 m_4) \zeta(m_4) z^{m_4-m_1} \delta^{m_4-m_1} + \sum_{\alpha m_3} z^{m_3-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ = \tau^{(j_2)} \zeta(m_1) \tau(m_1 m_4) \zeta(m_4) \delta^{m_1-m_4} + \sum_{j_4} z^{m_1-m_4} \delta^{m_1-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ + \sum_{j_4} x\tau(m_1 m_4) \zeta(m_4) z^{m_4-m_1} \delta^{m_4-m_1} + \sum_{\alpha m_3} z^{m_3-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ = \tau^{(j_2)} \zeta(m_1) \tau(m_1 m_4) \zeta(m_4) \delta^{m_1-m_4} + \sum_{j_4} z^{m_1-m_4} \delta^{m_1-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]

\[ + \sum_{j_4} x\tau(m_1 m_4) \zeta(m_4) z^{m_4-m_1} \delta^{m_4-m_1} + \sum_{\alpha m_3} z^{m_3-m_4} \delta^{\alpha}_{m_4} \delta^{\alpha}_{m_3-m_4} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3} \delta^{\alpha}_{m_3-m_2} \delta^{\beta}_{m_3-m_2} \delta^{\alpha}_{m_3-m_4} \]
\[ j_1 = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots \quad \text{and} \quad j_4 = 0, 1, 2, \ldots \quad (\text{III.10.7}) \]

where

\[ z = e^{i\theta/2} \quad (\text{III.10.8}) \]

It is possible to separate the \( m \)-dependence of equations (III.10.5) and (III.10.6) giving

\[ \sum_{j_2} f^{j_1 j_2} (a^{j_2})^2 f^{j_2 j_1} = \xi (a^{j_1})^2 \quad (\text{III.10.9a}) \]

\[ \sum_{j_1} f^{j_2 j_1} (a^{j_1})^2 f^{j_1 j_2} = \xi (a^{j_2})^2 \quad (\text{III.10.9b}) \]

\[ \sum_{m_2 \alpha} \delta_{m_1 - m_2} \tau^2(m_1 m_2) \zeta^2(m_2) = \zeta^2(m_1) \quad (\text{III.10.10a}) \]

\[ \sum_{m_1 \alpha} \delta_{m_1 - m_2} \tau^2(m_1 m_2) \zeta^2(m_1) = \zeta^2(m_2) \quad (\text{III.10.10b}) \]

The following summations appear in equation (III.10.7)

\[ \sum_{\beta m_2} z^{-m_2} \delta_{m_1 - m_2} \tau^2(m_1 m_2) \zeta(m_2) \]

\[ \sum_{\alpha m_3} z^{-m_3} \delta_{m_3 - m_4} \tau^2(m_3 m_4) \zeta(m_3) \]

If \( \tau \) is a symmetric function of its two arguments, and if \( \zeta(m) \) is of the form
\[ \zeta(m) = r_j z^{-m} \quad (III.10.11) \]

where \( r_j \) is a function of the corresponding \( j \), then the four sums in equations (III.10.10a,b) and (III.10.7) have the same form

\[ \tau^2(m,m-\frac{1}{2}) r_j^2, z^{-2m+1} + \tau^2(m,m+\frac{1}{2}) r_j^2, z^{-2m-1} = r_j^2 z^{-2m} \quad (III.10.12) \]

from which it follows that

\[ \left( \frac{r_j}{r_{j'}} \right)^2 = \tau^2(m,m-\frac{1}{2}) z + \tau^2(m,m+\frac{1}{2}) z^{-1} \quad (III.10.13) \]

where \( j \) is related to the first argument of \( \tau \) and \( j' \) to the second. For a given pair \( (j,j') \) with \( j-j'=\frac{1}{2} \) there are \( 2j+1 \) equations derivable from (III.10.13) for different values of \( m \). By interchanging \( j \) and \( j' \) a further \( 2j \) equations are possible. The resulting equations are

\[ \tau^2(j,j-\frac{1}{2}) z = \left( \frac{r_j}{r_{j-\frac{1}{2}}} \right)^2 \]

\[ \tau^2(j-\frac{1}{2},j) z^{-1} + \tau^2(j-\frac{1}{2},j-1) z = \left( \frac{r_{j-\frac{1}{2}}}{r_j} \right)^2 \]

\[ \tau^2(j-1,j-\frac{1}{2}) z^{-1} + \tau^2(j-1,j-3/2) z = \left( \frac{r_j}{r_{j-\frac{1}{2}}} \right)^2 \]

\[ \vdots \]

\[ \tau^2(-j+\frac{1}{2},-j+1) z^{-1} + \tau^2(-j+\frac{1}{2},-j) z = \left( \frac{r_{-j+\frac{1}{2}}}{r_{-j}} \right)^2 \]

\[ \tau^2(-j,-j+\frac{1}{2}) z^{-1} = \left( \frac{r_j}{r_{j-\frac{1}{2}}} \right)^2 \quad (III.10.14) \]
Repeated elimination gives

\[ 0 = \left( \frac{r_j}{r_{j-L}} \right)^2 - z^2 \left( \frac{r_{j-2}}{r_j} \right)^2 + z^{-4} \left( \frac{r_{j-4}}{r_j} \right)^2 - \ldots - z^{-8j+2} \left( \frac{r_{j-8j}}{r_j} \right)^2 + z^{-8j} \left( \frac{r_j}{r_{j-8j}} \right)^2 \]

(III.10.15)

A simple rearrangement leads to the result

\[ \left( \frac{r_j}{r_{j-L}} \right)^4 = \frac{z^{4j-2} + z^{4j-6} + \ldots + z^{-4j+2}}{z^{4j} + z^{4j-4} + \ldots + z^{-4j}} \]

(III.10.16)

This is satisfied by

\[ r_j^{-4} = z^{4j} + z^{4j-4} + \ldots + z^{-4j} \]  

(III.10.17)

In equation (III.10.7) we must evaluate two sums and we will use equation (III.10.17) for this purpose.

\[ \zeta^{-1}(m_4) z^{2m_1-m_4} \sum_{\beta m_2} z^{-m_2} \delta_{m_1-m_2} \tau^2(m_1m_2) \zeta(m_2) \]

\[ = \frac{r_j^{-1} z^{2m_1} r_{j-1}^{-1}}{r_j^2} \sum_{\beta m_2} \delta_{m_1-m_2} \tau^2(m_1m_2) \zeta^2(m_2) \]

\[ = \frac{r_{j-1}^2}{r_{j-2} r_j} \]

(III.10.18)

and similarly

\[ \zeta^{-1}(m_1) z^{2m_4-m_1} \sum_{\alpha m_3} z^{-m_3} \delta_{m_3-m_4} \tau^2(m_3m_4) \zeta(m_3) \]

\[ = \frac{r_{j-1}^2}{r_{j-3} r_j} \]

(III.10.19)
Equations (III.10.9a,b) are valid for $j_1 = \frac{3}{2}, 3/2, 5/2, \ldots$ and $j_2 = 0, 1, 2, \ldots$ respectively. They can be combined to form a single equation

$$f^{j,j+\frac{1}{2}}_{\pm} \left( a^j \pm \frac{1}{2} \right)^2 f^{j+\frac{1}{2},j}_{\pm} + f^{j,j-\frac{1}{2}}_{\pm} \left( a^j \pm \frac{1}{2} \right)^2 f^{j-\frac{1}{2},j}_{\pm} = \xi \left( a^j \right)^2$$

for $j = 0, \frac{1}{2}, 1, \ldots$ (III.10.20)

There are two types of equations (III.10.7) for $j_1 - j_2 = \frac{1}{2}$. These can be combined into

$$v_j f^{j,j-\frac{1}{2}} \left( a^j - \frac{1}{2} \right) f^{j-\frac{1}{2},j}_{\pm} a^j f^{j,j+\frac{1}{2}}_{\pm}$$

$$+ u_j f^{j,j+\frac{1}{2}} \left( a^j + \frac{1}{2} \right) f^{j+\frac{1}{2},j}_{\pm} a^j f^{j,j+\frac{1}{2}}_{\pm}$$

$$+ v_{j+\frac{1}{2}} f^{j,j+\frac{1}{2}} \left( a^{j+\frac{1}{2}} - \frac{1}{2} \right) f^{j+1,j+\frac{1}{2}}_{\pm} a^{j+1} f^{j+1,j+\frac{1}{2}}_{\pm}$$

$$= n \left( a^j f^{j,j+\frac{1}{2}} \right) a^{j+\frac{1}{2}}_{\pm}$$

for $j = 0, \frac{1}{2}, 1, \ldots$ (III.10.21)

where

$$v_j = x^{-\frac{1}{2}} r_j^2 r_{\frac{j-1}{2}} r_{\frac{j+1}{2}}^{-1} \quad j = \frac{3}{2}, 3/2, 5/2, \ldots$$

$$= x^{\frac{1}{2}} r_j^2 r_{\frac{j-1}{2}}^{-1} r_{\frac{j+1}{2}}^{-1} \quad j = 0, 1, 2, \ldots$$

$$u_j = x^{-\frac{1}{2}} r_j^2 r_{\frac{j+1}{2}}^{-2} + x^{\frac{1}{2}} r_j^2 r_{\frac{j+1}{2}} r_{\frac{j+2}{2}}^{-1} \quad j = \frac{3}{2}, 3/2, 5/2, \ldots$$

$$= x^{\frac{1}{2}} r_j^2 r_{\frac{j+1}{2}}^{-2} + x^{-\frac{1}{2}} r_j^2 r_{\frac{j+1}{2}} r_{\frac{j+2}{2}}^{-2} \quad j = 0, 1, 2, \ldots$$

(III.10.22)
and \( r_j \) is given by equation (III.10.17). This completes the reduction of the equations.

For a given size of the F-matrices in equation (III.7.14a,b), or equivalently for a certain value of \( p \) in equations (III.7.27) and (III.7.28), the range of \( j \) is bounded. In particular, the \( j \) of equation (III.10.20) is not greater than \((p+1)/2\) and the \( j \) of equation (III.10.21) is not greater than \( p/2 \). In this case equations (III.10.20) and (III.10.21) form a finite set which can be solved for \( \eta/\xi \). In terms of the elements of the \( f \)- and \( a \)-matrices these are algebraic equations. However, even for quite small values of \( p \) the number of variables is large.

11) Reduced Expression for the Percolation Probability

Since we have taken \( A \) and \( B \) to be diagonal we can write the percolation probability, from equation (III.9.10), as

\[
\mathcal{P} = \frac{\text{Tr}(U^2 B^4)}{\sqrt{\text{Tr} B^4 \text{Tr}(U^b B^b)}} \tag{III.11.1}
\]

where

\[
B = a^j \delta_{jj}, \delta_{mm}, r_j z^{-m} \quad j=0,1,2,... \tag{III.11.2}
\]

\[
U = \delta_{nn}, \delta_{jj}, \delta_{mm}, z^m e^{im\pi/2} \tag{III.11.3}
\]

Then
\[
B^4 = \left( a_j^4 \right)^4 \delta_{jj} \delta_{mm} r_j^4 z^{-4m}
\]
\[
U^2 B^4 = \left( a_j^4 \right)^4 \delta_{jj} \delta_{mm} r_j^4 e^{4im\pi}
\]
\[
U^4 B^4 = \left( a_j^4 \right)^4 \delta_{jj} \delta_{mm} r_j^4 z^{4m} e^{2mim}
\]

(III.11.4)

Let
\[
s_j^4 = \text{Tr} \left( a_j^4 \right)^4
\]

(III.11.5)

then
\[
\text{Tr} B^4 = \sum_{j=0}^{\infty} s_j^4
\]

(III.11.6a)

\[
\text{Tr} U^2 B^4 = \sum_{j=0}^{\infty} (-1)^j s_j^4 r_j^4
\]

(III.11.6b)

\[
\text{Tr} U^4 B^4 = \sum_{j=0}^{\infty} s_j^4
\]

(III.11.6c)

We therefore have
\[
\varphi = \frac{s_0^4 - s_1^4 r_1^4 + s_2^4 r_2^4 - \ldots}{s_0^4 + s_1^4 + s_2^4 + \ldots}
\]

(III.11.7)

**NUMERICAL SOLUTION**

12) Method of Approximation

The equations (III.10.20) and (III.10.21) have been obtained by a variational calculation using (III.7.14) as a trial function for the eigenvector of the transfer matrix \( T \). In principle this trial function can be made exact by allowing the matrices \( F_\alpha \) to be infinitely large.
The equations (III.10.20) and (III.10.21) then form an infinite system, the solution to which will give the free energy and percolation probability of the q-state Potts model exactly. However, there appears to be no immediate way of finding this solution. We therefore content ourselves with taking the $F^a$ to be finite, and expect that if we take successively larger matrices, the resulting approximations for the free energy and percolation probability will converge to the exact values. For example, when $p=0$ there are three equations, when $p=1$ there are five equations, when $p=2$ there are ten equations, etc. In each successive case we would expect the values of $Z^{1/N}=v\eta^2\xi^{-2}$ and $\mathcal{P}$ would more closely approximate the exact solution. The equations which result are algebraic in $\eta$, $\xi$ and the elements of the matrices $f^{j,k}_{i,j}$ and $a^j$. It is not a difficult matter to program an electronic computer to find a solution to such a system of equations, providing a solution exists and a sufficiently good guess at the solution is available. Limitations of computer time and size have allowed us to compute solutions up to $p=4$. At this level there are 58 equations.

In the next few sections we will outline how a useful starting guess at the solution can be obtained, some of the numerical problems posed by the equation, including a transformation to a less symmetric form, and the basic structure of the program used to solve the system of equations.
13) The Initial Guess

At each level, or value of $p$, an initial guess at the solution is required. This is not only because the program needs a starting point close to the desired solution, but also because it allows us to compare the solution obtained by the computer to what we might reasonably expect. In the case of $p=0$ or $p=1$ there are only a few equations and all the possible solutions can be enumerated; however, for $p=4$ there are $58$ non-homogeneous quintic equations which can be expected to have many solutions. If we do not have a clear idea of what the solution we are looking for should be, the results would be meaningless. We are able to obtain the necessary guess by solving the equations to leading order at each level in terms of the temperature dependent variable

$$ y = v^{-1} = \left( e^{\beta \xi} - 1 \right)^{-1} \quad (III.13.1) $$

First take the case $p=0$. All the matrices in this case are scalars. We can normalize $\xi = a^0 = 1 \quad (III.13.2)$

without affecting the value of $\eta/\xi$. Let

$$ f^{0,j}_{0,k} = f \quad (III.13.3) $$

then the equations are

$$ f^2 a^2 = 1 \quad (III.13.4a) $$
\[ f^2 = a^2 \quad (\text{III.13.4b}) \]
\[ u_0 f^3 a = \eta f a \quad (\text{III.13.4c}) \]

A solution is

\[ f = a = 1 \]
\[ \eta = u_0 = y^{-\frac{1}{2}} + y^\frac{1}{2} \quad (\text{III.13.5}) \]

From equation (III.11.7) the percolation probability is

\[ \mathcal{P} = 1 \quad (\text{III.13.6}) \]

From equation (III.8.31)

\[ z^{1/N} = y^{-1} \eta^2 = (y^{-1} + 1)^2 = e^{2\beta\epsilon} \quad (\text{III.13.7}) \]

This is clearly the zero temperature solution.

The second case is \( p=1 \). Again all the matrices are scalars, and we use the notation

\[ f^0, x = f \quad f^x, 1 = g \]
\[ a^{x} = a \quad a^1 = b \]

The equations at this level are

\[ f^2 a^2 = 1 \quad (\text{III.13.8a}) \]
\[ g^2 b^2 + f^2 = a^2 \quad (\text{III.13.8b}) \]
\[ g^2 a^2 = b^2 \quad (\text{III.13.8c}) \]
\[ u_0 f^3 a + v_2 f g^2 a b = \eta f a \quad (\text{III.13.8d}) \]
\[ v_2 f^2 g a + u_2 g^3 a b = \eta g a b \quad (\text{III.13.8e}) \]
Some of the equations at this level are similar to those of the previous level. Some have refinements to them. Since the p=0 case gives the correct answer for zero temperature, these changes will be corrections for a non-zero temperature. If the temperature is not too high the changes should be small and therefore we expect terms like $g^2b^2$ to be small when compared to $f^2$. The reordering of relative sizes allows us to determine the leading order behaviour, in $y$, of the new variables. From equation (III.13.8e)

$$b = \frac{V_{\frac{1}{2}}f^2}{\eta} = \frac{y^{\frac{3}{2}(q-1)^{\frac{1}{4}}}}{y^{\frac{1}{2}} + y^{-\frac{1}{2}}} \approx y(q-1)^{\frac{1}{4}} \quad (III.13.9)$$

and from equation (III.13.8c)

$$g \approx b \approx y(q-1)^{\frac{1}{4}} \quad (III.13.10)$$

Therefore, to leading order in $y$, for $p=1$

$$a \approx 1, \quad f \approx 1, \quad b \approx y(q-1)^{\frac{1}{4}} \quad (III.13.11)$$

In fact, the system of equations (III.13.8a-e) can be reduced to the single quartic equation

$$V_{\frac{1}{2}}(b^4 - 1) - u_{\frac{1}{2}}b^3 + u_0b = 0 \quad (III.13.12)$$

and an exact solution found at this level. The resulting expression for the partition function in powers of $y$ is

$$z^{1/N} = \left(y^{-1} + 1\right)^2 \left[1 + (q-1)(y^4 - 4y^5 + 12y^6 + [2q-36]y^7 + [113-16q]y^8 + O[y^9])\right] \quad (III.13.13)$$
This differs from the exact expression to this order, given by Kihara et al. (1954), only in the coefficient of $y^8$ where 113 is replaced by 114. Even at this low level of approximation the results are quite good.

The same procedure, to obtain the leading order behaviour of the variables can be used at subsequent levels $p=2,3$ and 4. In some cases it is necessary to find the second order behaviour of some of the variables before being able to find the leading order of all the variables. This is not a serious complication, however, and the calculation is straightforward.

14) Rescaling

A more apparent difficulty at this stage is that in each of these levels some of the coefficients in the equations become infinite for certain values of $q$. This is somewhat unnecessary since, judging from the leading order calculations, corresponding variables appear to vanish at an equal rate. Part of the problem can be overcome by a change of variables. We therefore make the following replacements.

$$a_j^i \rightarrow q^{1/8} r_{j+1}^{-1} a_j^i \quad j=0,1,2,...$$

$$+ r_{j+1}^{-1} a_j^i \quad j=\frac{1}{2}, \frac{3}{2}, \frac{5}{2},...$$

$$f_{j^i,j+\frac{1}{2}} \rightarrow q^{-1/8} r_{j^i} r_{j^i+\frac{1}{2}}^{-1} f_{j^i,j+\frac{1}{2}} \quad j=0,1,2,...$$
This gives the following set of equations

\[ \sigma_j f^{j,j+\frac{1}{2}} \left( a^{j+\frac{1}{2}} \right)^2 f^{j+\frac{1}{2},j} + f^{j,j-\frac{1}{2}} \left( a^{j-\frac{1}{2}} \right)^2 f^{j-\frac{1}{2},j} = \xi \left( a^j \right)^2 \]

(III.14.2a)

\[ \rho_j f^{j,j-\frac{1}{2}} a^{j-\frac{1}{2}} f^{j-\frac{1}{2},j} a^j f^{j,j+\frac{1}{2}} \]

\[ + \left( \sigma_j \rho_j^{j+\frac{1}{2}} + \rho_j \right) f^{j,j+\frac{1}{2}} a^{j+\frac{1}{2}} f^{j+\frac{1}{2},j} a^j f^{j,j+\frac{1}{2}} \]

\[ + \sigma_j a^{j+\frac{1}{2}} \rho_j^{j+\frac{1}{2}} f^{j,j+\frac{1}{2}} a^{j+\frac{1}{2}} f^{j+\frac{1}{2},j+1} a^{j+1} f^{j+1,j+\frac{1}{2}} \]

\[ = \eta^1 a^j f^{j,j+\frac{1}{2}} a^{j+\frac{1}{2}} \]

(III.14.2b)

where

\[ \sigma_j = q^{\frac{1}{2}} \left( r_j r_j^{-1} \right)^4 \]

\[ = q^{-\frac{1}{2}} \left( r_j r_j^{-1} \right)^4 \]

\[ \rho_j = 1 \]

\[ \eta^1 = \eta y^{\frac{1}{2}} \]

(III.14.3)

In this way the divergences of the coefficients are deferred by one level (i.e. \( \sigma_1 \) diverges at \( q=1 \) but it does not appear until \( p=2 \) rather than \( p=1 \)). The remaining divergences present a more difficult problem. They cannot be removed by a simple rescaling of the variables,
due to a violation of the assumption at the end of section III.8 that A and B can be diagonalized by a similarity transformation. Rather than develop appropriate representations of these matrix equations for these special cases, we have avoided the problem by solving the system at values of \( q \) slightly larger and slightly less than that required and interpolating to get an intermediate result. A further complication which arises is that for some values of \( q \) some of the variables will be pure imaginary to leading order in \( y \). Fortunately, however, the distribution of these variables is such that no complete term in any of the equations becomes imaginary without all of the others becoming imaginary. We are therefore able to do all computations using real arithmetic as long as we keep track of which variables are in fact imaginary and make any necessary changes in sign in terms containing squares of these numbers. Because the program converges to a solution in these cases we can be sure that these variables are indeed pure imaginary to higher orders in \( y \).

15) Correspondence with Bethe Approximation

After the rescaling outlined in the previous section, equation (III.13.12) can be written as

\[
b^4(q-1) - (v+q-1)b^3 + (v+1)b - 1 = 0
\]  

(III.15.1)

Noticing that \( b=1 \) is a non-physical solution, this can immediately be reduced to
\[ b^3(q-1) - v(b^2+b) + 1 = 0 \quad (III.15.2) \]

In terms of the solution to this equation the free energy and percolation probability at this level are given by

\[ e^{-\beta f} = \frac{Z^{1/N}}{b^2 (1+b)^2 (1+(q-1)b^4)} \quad (III.15.3) \]

\[ \phi = \frac{1 - b^4}{1 + (q-1)b^4} \quad (III.15.4) \]

where \( f \) is the free energy per site of the Potts model.

Bethe (1935) suggested an approximation to the Ising model which was a slight improvement over the mean field or Bragg-Williams (1934,5) approximation. The Bethe approximation counted the interactions of a small cluster of spins in the middle of the lattice exactly and considered the average effect of the rest of the lattice spins on the cluster. This method can easily be generalized to the Potts model on a square lattice and be shown to agree exactly with the \( p=1 \) result above.

Consider a cluster of five sites somewhere in the middle of a large lattice: a central site with four nearest neighbours. Because this is a square lattice, the outer sites are not themselves nearest neighbours and the calculation is simpler. Approximate the Potts model by the following interactions:

(a) allow an energy \(-\epsilon\) for like pairs of nearest neighbours in the cluster;

(b) an energy of interaction with an external
field of \(-h\) for all spins in the cluster of type "1";
(c) an additional interaction energy of \(-g_\sigma\)
for each spin in the outside shell representing
the effect of the rest of the spins in the
lattice on that spin. (\(\sigma=1,2,3,\ldots,q\))

Because the states 2,3,\ldots,q are equivalent, \(g_2=g_3=\ldots=g_q\) and we normalize the energy so that \(g_1=g\) and \(g_2=g_3=\ldots=g_q=0\). Let \(w(1,Z_1)\) be the probability that the central site is in state "1" and there are \(Z_1\) sites in state "1" in the shell. Similarly, \(w(\#1,Z_1)\) is the same probability for the central spin not in state "1". It is a simple matter to show

\[
w(1,Z_1) = C \left(\frac{4}{Z_1}\right) e^{\beta(\epsilon Z_1 + [Z_1+1]h + Z_1g)} (q-1)^{4-Z_1}
\]

\[
w(\#1,Z_1) = C (q-1) \sum_{n=0}^{4-Z_1} \left(4-Z_1\right) \left(\frac{4-Z_1}{n}\right) e^{\beta(\epsilon n + Z_1 h + Z_1 g)} (q-2)^{4-Z_1-n}
\]

(III.15.5)

where \(C\) is a normalization constant ensuring that the total probability is 1. The probabilities \(p_1\) and \(p_\#1\) that the central spin is "1" or not "1" are simply

\[
p_1 = \sum_{Z_1=0}^{4} w(1,Z_1) = C y(q-1+xy\zeta)^n
\]

(III.15.6)

\[
p_\#1 = \sum_{Z_1=0}^{4} w(\#1,Z_1) = C (q-1)(q-2+x+y\zeta)^n
\]

(III.15.7)

where
The average number of spins in state "1" in the shell $\bar{Z}_1$ can be written as

$$\bar{Z}_1 = \frac{4}{\sum Z_1 = 0} Z_1 \left[ w(1,Z_1) + w(\#1,Z_1) \right]$$

(III.15.9)

This can be quickly evaluated if we notice that the factor $Z_1$ in front of $w$ can be replaced by $\frac{\partial}{\partial \zeta}$. This yields

$$\frac{\bar{Z}_1}{4} = C \left[ \gamma(q-1+xy\zeta)^3 xy\zeta + (q-1)(q-2+x+y\zeta)^3 y\zeta \right]$$

(III.15.10)

Since all sites are equivalent $p_{l} = \bar{Z}_1/4$, which gives the required equation for $\zeta$. Letting $\zeta^{1/3} = \gamma^{-1}$, and setting $y=1$ for zero field, we have

$$(q-1)\gamma^4 - (q-2+x)\gamma^3 + xy - 1 = 0$$

(III.15.11)

Dividing by the solution $\gamma=1$ gives

$$(q-1)\gamma^3 - v(\gamma^2 + \gamma) + 1 = 0$$

(III.15.12)

where $v = e^{\beta \epsilon} - 1$. The spontaneous magnetization is given by

$$M_o = \frac{qp_{l}(p_{l} + p_{\#l})^{-1} - 1}{q-1}$$

$$= \frac{1 - \gamma^4}{1 - (q-1) \gamma^4}$$

(III.15.13)
In fact, from equation (III.15.10) we can derive an expression for the magnetization $M$ for general values of $\gamma$. From the definition of the partition function (III.3.4) the free energy can be written as an integral over the magnetic field $h$,

$$\beta f = 2\beta \varepsilon + \beta h - \frac{\beta}{2} \int_{h}^{\infty} (M-1)dh' \quad (III.15.14)$$

When evaluated at $h=0$ this agrees exactly with equation (III.15.3). Therefore the Bethe approximation in zero field coincides precisely with our $p=1$ approximation.

16) The Program

As can be seen from the flow chart in figure (III.7) the computer program is a slightly modified Newton's Method. The input consists of the level $p$, the number of components $q$ of the Potts model, the Boltzmann factor $e^{\varepsilon/kT}$, and a guess at the solution. The equations (III.14.2a,b) can be expressed as functions $h_j=0$. The vector of function values $H=(h_1, h_2, \ldots h_n)$ is evaluated at the guess $X=(x_1, x_2, \ldots x_n)$ and the Jacobian matrix of derivatives $J$ is evaluated at the same point. Using Gaussian elimination the Jacobian is inverted and the iteration formula

$$X_{i+1} = X_i - J^{-1} H \quad (III.16.1)$$

is applied. If the relative change in all the variables is less than $10^{-15}$ the procedure is assumed to have
Figure III.7. Flow chart for program to solve the equations $h_j = 0$, $j=1,2,...,n$. 
converged. If it has not converged but the relative change in all variables is less than $10^{-2}$ then $H$ is recalculated and on every fifth iteration $J$ is recalculated. Otherwise both $J$ and $H$ are recalculated on each iteration. If the procedure does not converge after ten iterations it is assumed that a satisfactory solution will not be found by this method with this initial guess and the attempt is halted.

Once a solution is found it can be used as an initial guess for a slightly different value of the Boltzmann factor or $q$. When a few solutions are obtained simple extrapolation procedures can be used to provide quite good guesses at other solutions and thus reduce the number of iterations required.

The output consists of the computed solution to the equations and the corresponding values of $z^{1/N}$ and $\rho$. In addition the relative tolerance achieved in solving the equations is computed. That is the magnitude of the difference between the left and the right hand sides of the equations divided by the sum of the absolute values of the additive terms in the equation. This gives an indication of how well the equations have been satisfied.

The computing was done on a Univac 1108 computer in double precision floating point arithmetic having 18 significant digits.

RESULTS AND CONCLUSIONS

17) Estimates of the Critical Exponent $\beta$

The aim of this work is to obtain estimates
of the critical exponent $\beta$ (see equation III.2.16). The immediate result of the calculations is a series of approximations to the percolation probability as a function of temperature for a fixed value of $q$. Figure (III.8) shows such approximations for $q=3$. How best to go from the data produced by these approximate solutions to an estimate of the exact value of $\beta$ is not clear. We have tried two methods and will describe both of them.

It is instructive to plot $\ln P$ against $\ln(1-T/T_c)$ as in figure (III.9). The exact value for $T_c$ can be obtained from

$$q^k = \exp(\varepsilon/kT_c) - 1 \quad (III.17.1)$$

In the case of the exact percolation probability the curve will begin at the origin and descend in the lower left quadrant approaching a straight line with slope equal to $\beta$. From the graph in figure (III.8) it is clear that the percolation probabilities of the approximations have their zeros at higher temperatures than the exact $T_c$. The resulting log graph descends but then levels off, having a finite negative value at $-\infty$. Successive approximations have steeper and more extended declines. To estimate $\beta$ we have taken successive maximum slopes of the approximate curves and plotted them against $p^{-1}$, $p=1,2,3$, and 4, where $p$ is the level of approximation (see figure III.9). We have then fitted a straight line to these points and noted where the line crosses $p^{-1}=0$. For the known case $q=2$ the result is remarkably good. The results for several values of $q$ are given below.
Figure III.8  Plot of $p=1, 2, 3$ and 4 approximations to $\mathcal{P}$ against $e^{-\epsilon/kT}$ for $q=3$. 
Figure III.9  Plot of approximations to \( \ln \varphi \) against \( \ln \left( 1 - \frac{T}{T_c} \right) \). The dashed line is obtained by geometric extrapolation from the last three approximations.
\[ \beta = \begin{align*}  &0.133 & q=1 \\  &0.123 & q=2 \\  &0.112 & q=3 \\  &0.095 & q=4 \end{align*} \]

No error bars are given at this point because this method of estimation is very rough and only intended as a guide to how successful our results are.

A more precise method of interpreting the data is to extrapolate the approximate curves for the percolation probability to an estimation of the exact curve and then assuming \( \ln \mathcal{P} \) has an expansion of the form

\[ \ln \mathcal{P} = \beta \log(1-T/T_c) + C_0 + C_1(1-T/T_c) + C_2(1-T/T_c)^2 + \ldots \]

fit a curve of this type to give an estimate of \( \beta \). Examining table I seems to justify a geometric extrapolation of the percolation probability. The change from level to level decreases by a fairly constant factor. We performed a pointwise geometric extrapolation from the last three levels of approximation and fitted series of the above form of varying lengths (3, 4 and 5 parameters). In general the results (table II) give consistent values of \( \beta \). Error bars are determined by assuming the estimation of the exact curve is no further from the exact curve than it is from the \( p=4 \) approximation.

Some difficulty with the \( q=1 \) case may be due to deficiencies in interpolating the percolation probability values between \( q=.8,.9,1.1 \) and 1.2. The values of \( \beta \) at these surrounding values of \( q \) do not indicate a sudden change in the behaviour of \( \beta \) at \( q=1 \).
Table I Approximations to the percolation probability for $p=1,2,3$ and 4. The $p=0$ approximation is identically 1. The rate of convergence of the approximations justifies the use of geometric extrapolation. These extrapolations are given in the last column. ($q=3$).
<table>
<thead>
<tr>
<th>q</th>
<th>3 parameter fit</th>
<th>4 parameter fit</th>
<th>5 parameter fit</th>
<th>last fitted</th>
<th>$e^{-\varepsilon/kT}$</th>
<th>$e^{-\varepsilon/kT_c}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.8</td>
<td>0.156 ± 0.010</td>
<td>0.154 ± 0.022</td>
<td>0.151 ± 0.038</td>
<td>0.51</td>
<td>0.528</td>
<td></td>
</tr>
<tr>
<td>0.9</td>
<td>0.150 ± 0.010</td>
<td>0.148 ± 0.023</td>
<td>0.152 ± 0.041</td>
<td>0.49</td>
<td>0.513</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>0.149 ± 0.001</td>
<td>0.140 ± 0.004</td>
<td>0.131 ± 0.008</td>
<td>0.46</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.146 ± 0.002</td>
<td>0.133 ± 0.005</td>
<td>0.118 ± 0.009</td>
<td>0.47</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.133 ± 0.001</td>
<td>0.105 ± 0.001</td>
<td>0.066 ± 0.004</td>
<td>0.48</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>1.1</td>
<td>0.145 ± 0.005</td>
<td>0.142 ± 0.012</td>
<td>0.144 ± 0.022</td>
<td>0.46</td>
<td>0.488</td>
<td></td>
</tr>
<tr>
<td>1.2</td>
<td>0.143 ± 0.004</td>
<td>0.140 ± 0.010</td>
<td>0.141 ± 0.018</td>
<td>0.45</td>
<td>0.477</td>
<td></td>
</tr>
<tr>
<td>2.0</td>
<td>0.126 ± 0.001</td>
<td>0.126 ± 0.002</td>
<td>0.124 ± 0.003</td>
<td>0.39</td>
<td>0.414</td>
<td></td>
</tr>
<tr>
<td>3.0</td>
<td>0.107 ± 0.002</td>
<td>0.110 ± 0.004</td>
<td>0.110 ± 0.006</td>
<td>0.36</td>
<td>0.366</td>
<td></td>
</tr>
<tr>
<td>3.99</td>
<td>0.093 ± 0.004</td>
<td>0.094 ± 0.006</td>
<td>0.094 ± 0.008</td>
<td>0.33</td>
<td>0.333</td>
<td></td>
</tr>
</tbody>
</table>

Table II  Estimates of $\beta$ for several values of $q$. The estimates are obtained by fitting a curve as outlined in the text. We have tried fits with three, four and five parameters. Error bars are difficult to establish but we believe those given by the four parameter fit are realistic. Also indicated is the proximity of the last point fitted to the exact transition point. With the exception of $q=1$ (obtained by interpolating the percolation probability for $q=0.8,0.9,1.1$, and 1.2, and then fitting as in the other cases) the results are quite consistent. However if $\beta$ is a continuous function of $q$ at $q=1$, then we expect $\beta=0.145 ± 0.017$ at $q=1$. 
18) Conclusions

A staggered ice model, equivalent to the Potts model on a square lattice, has been formulated. Using a variational method a hierarchy of equations, determining the largest eigenvalue of the transfer matrix of the model, has been constructed. Successive approximations to this hierarchy have been formed, and these approximate systems solved numerically. In addition to the free energy, approximations to the order parameter (percolation probability) have been computed and estimates of the critical exponent $\beta$ have been made.

The estimates of $\beta$ are in good agreement with those obtained by the series method.

\[
\begin{align*}
\beta &= 0.089 \pm 0.003 \quad q=4 & \text{(Enting, 1975)} \\
\beta &= 0.105 \pm 0.005 \quad q=3 & \text{(Enting, 1974b)} \\
\beta &= 0.103 \pm 0.010 \quad q=3 & \text{(Straley and Fisher, 1973)} \\
\beta &= 0.14 \pm 0.03 \quad q=1 & \text{on triangular lattice (Sykes et al., 1974)}
\end{align*}
\]

The variational method has shown itself to be useful in this type of problem. Reasonable estimates of the critical behaviour have been achieved by the solution of only a moderate number of algebraic equations. Moreover, the method casts the problem into a form which may shed more light on the nature of the exact solution.
REFERENCES

Baxter, R.J., Kelland, S.B. and Wu, F.Y. 1976 "Equivalence of the Potts Model or Whitney Polynomial with an Ice-Type Model" to be published.


Green, H.S. and Hurst, C.A. 1964 Order-Disorder Phenomena Wiley London.


