CORNER TRANSFER MATRICES
OF
THE ISING MODEL
IN
STATISTICAL MECHANICS

by

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Except where acknowledgments in the form of specified references are made in the text, this dissertation is an account of my own original work carried out from May,1976 to February,1979 at the Department of Theoretical Physics, Research School of Physical Sciences, Australian National University for the degree of Doctor of Philosophy.

Tsang Shiu Kuen

S. K. Tsang

To K. B.

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ABSTRACT

The work of this thesis is mainly on an investigation of the "corner transfer matrices" (CTM) of the Ising model in statistical mechanics. The thesis starts with a review on the Ising model and is followed by a brief discussion of various methods for investigating the Ising model. In particular, new techniques and approaches developed by Baxter form the basis for further research described in this thesis. Thus in Section I, the review is introduced first.

In Section II, the new technique for investigating the zero field, eight-vertex model on the squ are lattice using the CTM suggested by Baxter (1976) is applied to the anisotropic, ferromagnetic, triangular Ising lattice in zero field below its critical temperature. The diagonal form of the CTM of the triangular lattice shows essentially the same structure as that for the square Ising lattice. The spontaneous magnetization can be obtained easily from this method. It is hoped that this technique will give illuminating insights into the problems of critical phenomena.

In Section III, the variational approximation approach for the square lattice Ising model developed by Baxter (1978) is studied. The accuracy and rate of

convergence of this approach is tested by applying the method to the zero field Ising model on the square lattice. The problem is simplified to that of solving a relatively small system of non-linear equations. The estimates to the spontaneous magnetization and the critical temperature from the sequence of variational approximations are obtained. The results converge rapidly to the exact ones. They exhibit a cross-over phenomenon and satisfy a scaling relationship for the spontaneous magnetization. Since this method can be applied to many systems such as the square lattice Ising model with a magnetic field, where the exact solution is not available yet, one may expect to obtain good approximations to the thermodynamic functions of these models by using this method.

The work described in this thesis has been reported in the following papers :

(i) Tsang, S. K., (1977) J. Stat. Phys. 17:137-152.
'Corner Transfer Matrices of the Triangular Ising Model'

(ii) Tsang, S. K., (1979) J. Stat. Phys. 20:95-114.
'Square Lattice Variational Approximations Applied to the Ising Model'

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SECTION I

statistical mechanics of phase transitions

1 Phase Transitions and Critical Phenomena

Statistical mechanics is the study of the equilibrium properties of macroscopic systems in terms of their microscopic properties. It was only in 1902 that a comprehensive formulation of statistical mechanics was given by Gibbs (1902). Since then, a better understanding of the relations between the macroscopic description of many physical phenomena through thermodynamics and the underlying atomic theory has been established.

One of the oldest problems in equilibrium statistical mechanics is the theory of phase transitions. In particular, a great deal of attention has been given to the theoretical and experimental investigation of critical phenomena in phase transitions (Stanley, 1971).

A wide variety of physical systems exhibit critical phenomena, for example, fluid systems, magnetic systems, ferroelectric systems, metallic alloy systems. Since this is a fairly general physical phenomenon, using equilibrium statistical mechanics alone, one expects to be able to find the existence of the critical phenomena and the thermodynamic behaviour near the critical region of such systems.

Consider, for example, a system of magnetic spins, in the presence of a strong magnetic field H parallel to the magnetic axis of the system. At sufficiently low temperature, if we decrease the magnetic field to zero, a spontaneous magnetization of the system remains. Fig. 1.1 shows the change of this spontaneous magnetization with the temperature of the system. Above a certain temperature known as the critical temperature of the system, the spontaneous magnetization vanishes completely. The point at which the spontaneous magnetization of the system vanishes is known as the critical point of the system.

In the study of such critical phenomena, we are interested in the thermodynamic behaviour of functions like the magnetization, the specific heat, the susceptibility

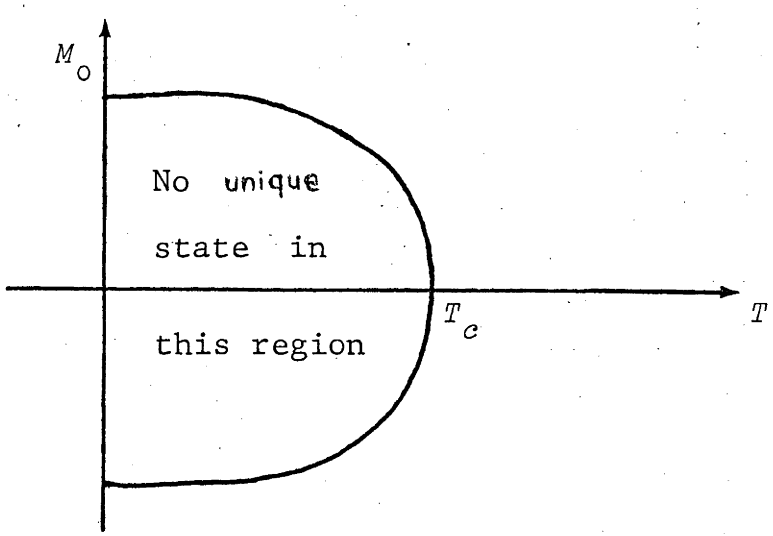


Fig. 1.1 The spontaneous magnetization M_0 as a function of temperature T, T_c being the critical temperature.

and the correlation function. Obviously, the spontaneous magnetization of the system is singular at this point. It is customary to consider the singularity at the critical point as a power law singularity. That is, we expect that near the critical point, the spontaneous magnetization behaves as

$$M_0 \propto (T_c - T)^{\beta} , \quad T \to T_c^- \tag{1.1.1}$$

where β is known as the critical exponent for M_0. Other commonly considered critical exponents are

(i) δ for the critical isotherm,

$$H \sim | M |^{\delta} , \tag{1.1.2}$$

where H is the magnetic field and M the magnetization;

(ii) α , α' for the specific heat C_H at constant magnetic field,

$$\begin{aligned} C_H &\sim (T_c - T)^{-\alpha'} , \quad T \to T_c^- \\ C_H &\sim (T - T_c)^{-\alpha} , \quad T \to T_c^+ \end{aligned} \tag{1.1.3}$$

(iii) γ , γ' for the zero field isothermal susceptibility,

$$\begin{aligned} \chi_T &\sim (T_c - T)^{-\gamma'} , \quad T \to T_c^- \\ \chi_T &\sim (T - T_c)^{-\gamma} , \quad T \to T_c^+ \end{aligned} \tag{1.1.4}$$

(iv) ν , ν' for the correlation length,

$$\xi \sim (T_c - T)^{-\nu'} , \quad T \to T_c^- \qquad (1.1.5)$$

$$\xi \sim (T - T_c)^{-\nu} , \quad T \to T_c^+$$

(Stanley, 1971).

Consequently, a problem of central interest in the theory of critical phenomena is the determination of the critical exponents governing the approach of the system to the critical point.

Using standard statistical mechanics, for a molecular system with general intermolecular forces, the relative statistical weight of a state s of the system with energy $E(s)$ is given by $\exp (- E(s)/k_B T)$ where k_B is the Boltzmann's constant and T the temperature of the system. By forming the partition function of the system

$$Z = \sum_{(s)} \exp (- E(s)/k_B T) \qquad (1.1.6)$$

where the summation is over all allowable states s of the system, we can then derive all the thermodynamic functions of the system by the usual procedures of statistical mechanics and in particular, one can find out whether the system undergoes a phase transition in the thermodynamic limit.

However, the interactions between the molecules in a real macroscopic system are far too complicated for the sum over states in (1.1.6) to be tractable. So, some kind of

approximation or idealization of the system is necessary. In general, a model of some kind, simplifying the interactions and the Hamiltonian of the system is introduced. Amongst these, we have the Ising model, the spherical model, the Heisenberg model, the ferroelectric model, the eight-vertex model, the Potts model etc. In particular, the Ising model undoubtedly has received the most attention.

2 THE ISING MODEL

An ideal model in statistical mechanics should describe the characteristics of a realistic system which is important for the phenomenon under study and at the same time be tractable mathematically. The Ising model provides such a model in the study of ferromagnetism.

The system considered in the model is an array of N fixed points in a d-dimensional periodic lattice. Associated with each lattice site j is a spin variable σ_j which may take up values $+1$ or -1. A particular set of values of all the spins constitutes a configuration of the lattice and one may assume particular interactions between spins such as nearest-neighbour or next nearest-neighbour interactions or even other two-body or many body interactions. However, in general, to resemble the realistic situation, it is usually assumed that there are only short range forces between the molecules, in particular, that there are only nearest-neighbour interactions.

The model was first considered by Ising (1925) as a model for ferromagnetism. He studied the one-dimensional Ising chain with nearest-neighbour interaction and found no phase transition. There was not much development on the

model until 1936 when Peierls (1936b) showed that the Ising model in two and three dimensions did exhibit spontaneous magnetization at sufficiently low temperatures. Unfortunately, his proof was not rigorous and was corrected by Griffiths (1964). In 1941, Kramers and Wannier (1941a,b) investigated, on the square lattice, an Ising model with nearest-neighbour interactions only and were able to locate the transition temperature of the system using a dual transformation relating the low and high temperature expansions of the partition function. Approximations for the free energy of the system were obtained using a variational method (Kramers and Wannier, 1941b). A major breakthrough in the development came in 1944 when Onsager (1944), using the transfer matrix formulation of the model (Kramers and Wannier, 1941a; Montroll, 1941), obtained the exact solution of the two-dimensional square Ising model in the absence of a magnetic field. In 1949, a simplified version of his solution was given by Kaufman using spinor algebra (Kaufman, 1949; Kaufman and Onsager, 1949). Although the result for the spontaneous magnetization of the system was announced by Onsager (1949), the derivation was given only in 1952 by Yang (Yang, 1952; Chang, 1952). Exact results for many other lattice systems such as the triangular lattice (Newell, 1950; Wannier, 1950), the honeycomb lattice (Husimi and Syozi, 1950; Syozi, 1950; Houtappel, 1950) and the Kgomé lattice (Syozi, 1951) were put forward almost simultaneously. Unfortunately all these results are for zero magnetic field. Further advances in our

mathematical and physical understanding of the model was provided by Yang and Lee (1952a,b) in their description of the model as a lattice gas and their theorem on the roots of the partition function of the system. In the 1960 s, many different methods for obtaining the exact results were developed. Examples are the combinatorial method (Kac and Ward, 1952; Potts and Ward, 1955; Potts, 1955); the Pfaffian approach (Hurst and Green, 1960; Fisher, 1961, 1966; Kasteleyn, 1961,1963; Montroll, Potts and Ward, 1963); the field theory approach (Schultz, Mattis and Lieb, 1964; Hurst, 1966; Gibberd and Hurst, 1967); using perturbation theory (Herman and Dorfman, 1968) and recently, using star-triangle relations (Baxter and Enting, 1978; Hilhorst, Schick and van Leeuwen, 1978). However, all these methods merely re-derived the original results: no new results were produced. The two-dimensional Ising model in the presence of a magnetic field and the three dimensional problem has yet remained unsolved.

It is therefore necessary to investigate these problems using other approximation methods. Some of the better known approximation methods studied are :

(i) Closed form approximation methods including the cluster variation method (Peierls, 1936a; Li, 1949; Kikuchi, 1951; Kikuchi and Brush, 1967); the constant coupling approximation (Kasteleyn, 1956; Danielian, 1963); and the matrix and variational methods (Kramers and Wannier, 1941b; Woodbury, 1969).

However, these methods, although they give reasonably good description of the system away from the critical point, fail to account for the correct thermodynamic behaviour of the system near the critical region. Recently, a special approximation method using the variational principle was developed (Baxter, 1978). The method is interesting as it is possible to obtain reasonably good estimates of the critical temperature as well as many other thermodynamic properties of the system with only moderate amount of computational efforts.

(ii) Series expansions in powers of some appropriate variable (Domb, 1949; Sykes, Essam and Gaunt, 1965; Sykes *et al.*, 1973a,b,c; Domb, 1974). If sufficient terms in the expansions can be derived, it is possible to estimate the critical temperature and the critical exponents of the system from the series. In particular, they provide the best estimates of the critical temperature and critical exponents of the three-dimensional Ising model. However, using the conventional combinatorial technique, enormous amount of computation work is required to obtain the series. Hence, it may be more efficient to obtain the series using algebraic techniques like the variational method (Baxter, 1978; Baxter and Enting, 1979).

(iii) Renormalization group method (Kadanoff, 1966; Wilson, 1971a,b). In this method, one focusses attention on the critical region directly, by means of a sequence of transformations. [footnote 1] Though very good estimates of the thermodynamic functions of the systems considered may be obtained using simple approximation methods (Kadanoff, 1975; Southern, 1978), no exact result has yet been arrived through this approach, with the exception of the recent derivation of the critical exponent α of the two-dimensional Ising model by Hilhorst, Schick and van Leeuwen (1978).

Despite all the intensive studies on the model, exact results have only been obtained in the two-dimensional case in the absence of a magnetic field. It is therefore interesting to further investigate the properties of the model. It is hoped that such investigation may bring illuminating insights to various unsolved problems of the model as well as problems arising from other models for phase transition.

Recently, a new technique for investigating the zero field, eight-vertex model on the square lattice using "corner transfer matrices" was suggested by Baxter (1976). The following sections of the work will be devoted to the corner transfer matrices of the triangular Ising model as well as the investigation of the convergence of the variational approximation when applied to the square lattice Ising model.

SECTION II

corner transfer matrices of the triangular Ising model

INTRODUCTION 1

The "transfer matrix" technique has proved to be very useful in solving many models of statistical mechanics. The idea was first applied by Kramers and Wannier (1941a), and Montroll(1941) to the Ising problem. It was shown that the partition function of a two-dimensional square Ising lattice can be written as the trace of a product of row (or column) transfer matrices. In the thermodynamic limit, this is proportional to the largest eigenvalue of the transfer matrix involved.

From the time Onsager (1944) solved the two-dimensional Ising model on the square lattice, papers began to flow forth on the subject and the "transfer matrix" technique was used to solve many models of phase transitions (e.g. the Ising model, the eight-vertex model, etc.). In 1976, a new form of transfer matrix was suggested by Baxter (1976): namely, the "corner transfer matrix" (denoted by CTM). Baxter used this technique to investigate the zero field, eight-vertex model on the square lattice. In the special case when the eight-vertex model reduces to two independent and identical Ising models, an exact solution of the CTM can be obtained (Baxter, 1977). This method is interesting because the diagonal form of the

CTM has a very simple direct product structure. So, it is encouraging to see whether other models also have similar properties.

The following work aims at applying these ideas to the anisotropic, ferromagnetic, triangular Ising model. One of the advantages of this approach is that it provides a relatively simple derivation of the spontaneous magnetization of the system.

The triangular Ising lattice has been of great interest to many authors. Since Onsager's celebrated result of the square lattice Ising model was produced, the thermodynamic properties of the triangular lattice have been studied independently by various authors (Husimi and Syozi, 1950; Wannier, 1950; Newell, 1950; Temperley, 1950). The spontaneous magnetization of the lattice was obtained in 1952 by Potts (1952) after Yang (1952) gave the derivation of the spontaneous magnetization for the square lattice. A thorough investigation on its spin correlations both in the ferromagnetic case and the antiferromagnetic case was carried out by Stephenson (1964, 1966, 1970a,b).

It is the purpose of this work to evaluate the CTM of this model. We will define the CTM for the triangular Ising lattice in Section II.2. We are able to diagonalize the CTM and obtain its eigenvalues by using spinor representatives, which were first developed by Kaufman (1949). The essential procedures in the derivation and the results of our analysis of the representatives of the CTM are

presented in Section II.3 to II.5. In Section II.6, we conclude by giving the diagonal form of the CTM and obtain the expression for the spontaneous magnetization of the ferromagnetic triangular Ising model.

THE CTM OF THE TRIANGULAR LATTICE 2

§ 2.1 THE CORNER TRANSFER MATRIX

As the starting point of our formulation, we define the corner transfer matrix for a general anisotropic triangular Ising lattice in zero magnetic field.

Consider a hexagonal-shaped lattice plane with $(2n + 1)$ spins sites along the major diagonals of the hexagonal as shown in Fig. 2.1. We impose the condition that the boundary spins of the lattice are all $+1$. Label the three principal directions of the lattice as $\vec{a}$, $\vec{b}$ and $\vec{c}$, and assume only nearest-neighbour interactions with energies J_1 , J_2 and J_3 along these three directions $\vec{a}$, $\vec{b}$ and $\vec{c}$ respectively.
Let $\sigma_i = \pm 1$ be the spin of the i th site, then, the Hamiltonian of the system is given by

$$H = - \sum_{\text{n.n.}} J_{ij} \sigma_i \sigma_j \qquad (2.2.1)$$

where the summation is over all nearest neighbours and $J_{ij} = J_1$, J_2 or J_3 depending on whether the bond between the spins σ_i and σ_j is in the direction $\vec{a}$, $\vec{b}$ or $\vec{c}$ respectively. The partition function is given by

$$Z_n = \sum \exp (- H/k_B T) \qquad (2.2.2)$$

where k_B is the Boltzmann's constant and T the temperature. The summation here is over all possible spin configurations of the lattice.

In a similar way to Baxter (1976), we divide the lattice into six "corners" (A to F) with three cuts along the major diagonals of the hexagon. The partition is such that each corner contains all the bonds between the spins inside the corner but only bonds on the left cut, as seen from the centre spin of the lattice (see Fig. 2.2 for corner A).

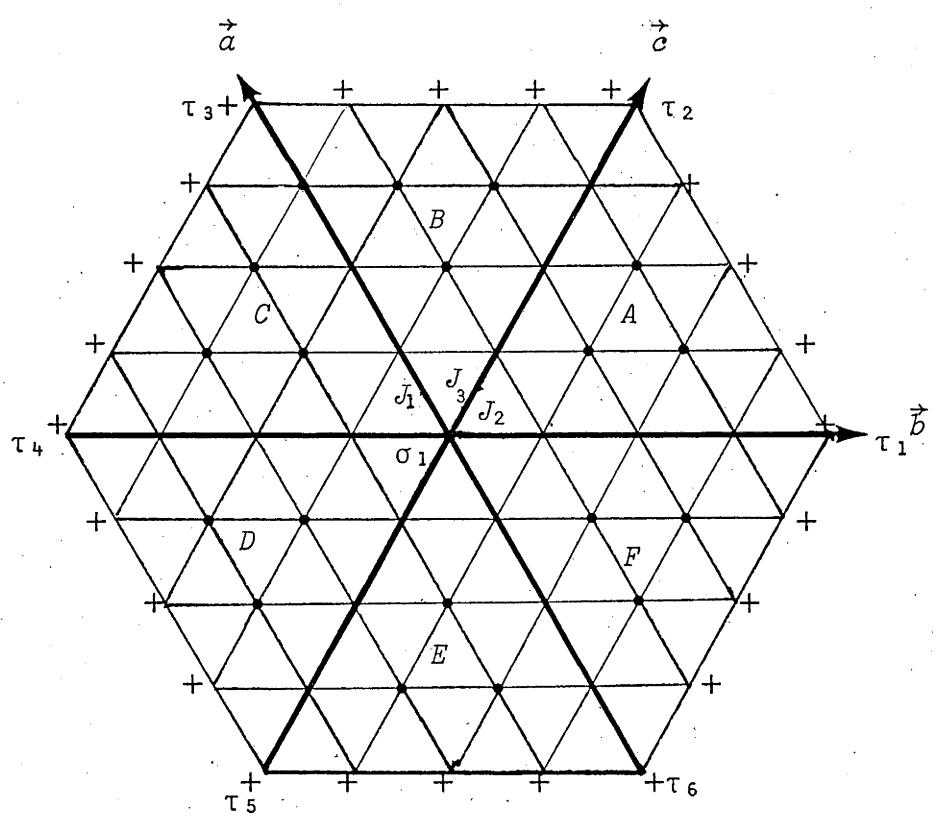


Fig. 2.1 A triangular lattice with hexagonal boundary and $2n + 1$ ($n = 4$) spins along each diagonal.

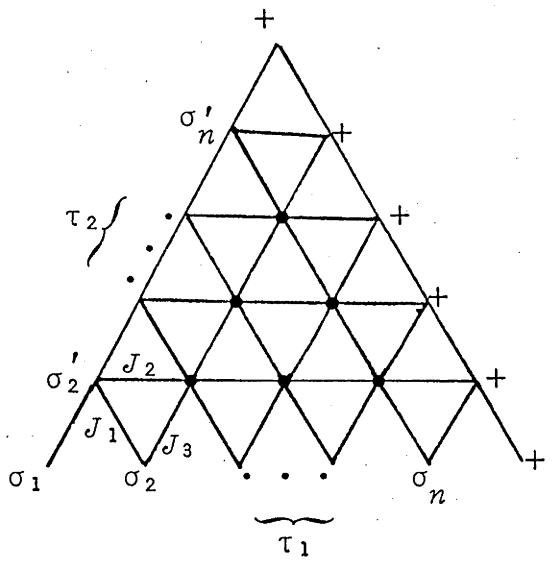


Fig. 2.2 Corner A of the lattice corresponding to CTM A. The summation in (2.2.4) is over all dotted spins.

Let the centre spin of the lattice be σ_1 and denote the six half-cuts of the lattice by τ_1, τ_2, ..., τ_6 as in Fig. 2.1. Clearly, if all the spins on τ_1 to τ_6 are held fixed, the summation in (2.2.2) can be factorized into six parts and Z_n can be written as

$$Z_n = \sum_{\tau_1} \cdots \sum_{\tau_6} A(\tau_1|\tau_2)\, B(\tau_2|\tau_3) \ldots F(\tau_6|\tau_1) \qquad (2.2.3)$$

where $A(\tau_1|\tau_2)$, $B(\tau_2|\tau_3)$, ..., $F(\tau_6|\tau_1)$ are the corner transfer matrices that account for the contributions to Z_n from bonds in the respective corners. More explicitly, if we denote the spins of τ_1 by σ_1, σ_2, ..., σ_n and τ_2 by σ_1', σ_2', ..., σ_n', we have, for example, that the matrix A is given by

$$A(\tau_1|\tau_2) = \delta_{\sigma_1,\sigma_1'} \sum \exp\left(-H_{\mu\gamma}/k_B T\right) \qquad (2.2.4)$$

where $H_{\mu\gamma}$ is the interaction Hamiltonian involving all the bonds of the corner and the summation is over all interior spins of the corner as shown in Fig. 2.2.

Furthermore, it can be seen readily that the matrix D is the same as A, E as B, and F as C. Hence (2.2.3) can be written as

$$Z_n = \text{Trace } (ABC)^2 \quad . \tag{2.2.5}$$

We further note that B is obtained from A by replacing J_1 by J_2, J_2 by J_3 and J_3 by J_1. Similarly C is obtained from A by replacing J_1 by J_3, J_3 by J_2 and J_2 by J_1.

In the thermodynamic limit, the partition function per site is given by

$$Z = \lim_{n\to\infty} Z_n^{1/N} \tag{2.2.6}$$

where N is the total number of sites in the lattice and the free energy per site f is

$$f = - \lim_{n\to\infty} \frac{k_B T}{N} \ln Z_n \tag{2.2.7}$$

Also, the spontaneous magnetization M is just

$$M = \langle \sigma_1 \rangle = \frac{\text{Trace } \{ S(ABC)^2 \}}{\text{Trace } \{ (ABC)^2 \}} \tag{2.2.8}$$

where

$$S(\sigma_1,\ldots,\sigma_n \mid \sigma_1',\ldots,\sigma_n') = \sigma_1 \delta_{\sigma_1,\sigma_1'} \delta_{\sigma_2,\sigma_2'} \ldots \delta_{\sigma_n,\sigma_n'} \tag{2.2.9}$$

is the diagonal centre-spin operator. Since the matrices A , B and C all break into two diagonal blocks corresponding to $\sigma_1 = +1$ or -1 , they commute with the diagonal matrix S .

The trace of a matrix is simply given by the sum of all its eigenvalues and therefore by (2.2.5) , the problem of evaluating the partition function reduces to finding the eigenvalues of the product of the corner transfer matrices ABC .

The following arguments will be mainly focussed on the analysis of the CTM A . Those for B and C may be obtained similarly by making the necessary changes of the parameters involved.

§ 2.2 HALF-ROW MATRICES

To further simplify the corner transfer matrices, we would like to decompose them into row matrices in a similar way as for the square lattice (Baxter, 1976).

We consider a more symmetric corner which includes the bonds on both of the cuts and denote it by A' for corner A and similarly B' and C' for corners B and C respectively. Denote

$$K_j = J_j / k_B T \quad , \quad j = 1, 2, 3 \quad . \qquad (2.2.10)$$

Obviously, the new corner transfer matrix A' is related to CTM A through

$$A = L_A A' \tag{2.2.11}$$

where L_A is the matrix which cancels the effect of the added bonds, or, more explicitly

$$L_A(\sigma_1,\sigma_2,\ldots,\sigma_n \mid \sigma_1',\sigma_2',\ldots,\sigma_n') = \{\exp[-K_2(\sigma_1\sigma_2+\sigma_2\sigma_3+\ldots+\sigma_n\sigma_{n+1})]\}\,\delta_{\sigma_1,\sigma_1'}\delta_{\sigma_2,\sigma_2'}\ldots\delta_{\sigma_n,\sigma_n'} \tag{2.2.12}$$

with $\sigma_{n+1} = 1$.

The corner A' can be built up by rows of triangles as shown in Fig. 2.3. If we define $2^n \times 2^n$ matrices G_j ($j = 1, 2, \ldots, n$) by

$$G_j(\sigma_1,\sigma_2,\ldots,\sigma_n \mid \sigma_1',\sigma_2',\ldots,\sigma_n') = \delta_{\sigma_1,\sigma_1'}\delta_{\sigma_2,\sigma_2'}\ldots\delta_{\sigma_j,\sigma_j'} \exp\{\sum_{\ell=j}^{n} K_1\sigma_{\ell+1}\sigma_{\ell+1}' + K_2\sigma_\ell\sigma_{\ell+1} + K_3\sigma_\ell'\sigma_{\ell+1}'\} \tag{2.2.13}$$

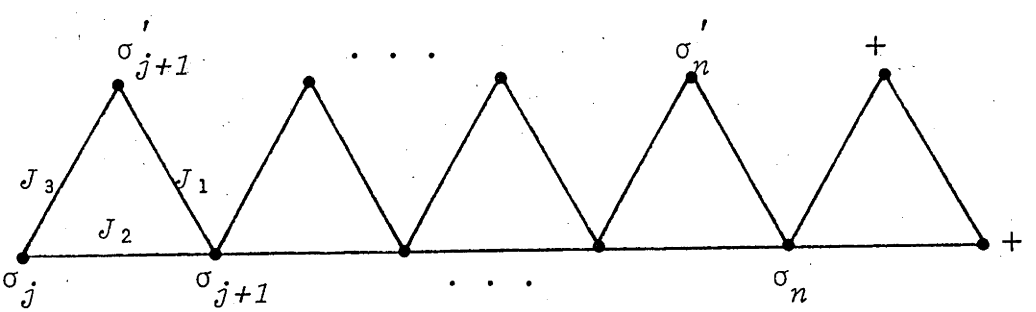


Fig. 2.3 The j th row of the corner A' , which corresponds to the matrix G_j .

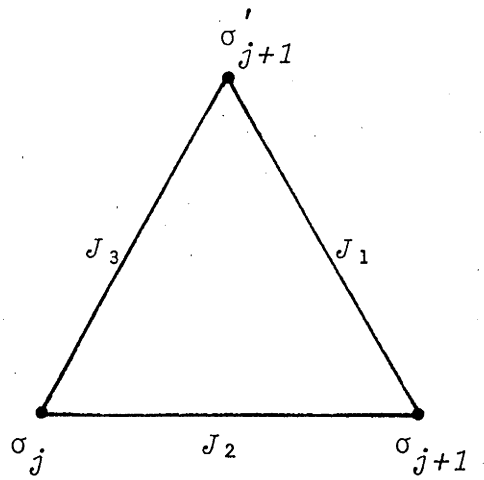


Fig. 2.4 The spin interactions correspond to matrix V_j .

with $\sigma_{n+1} = \sigma'_{n+1} = 1$, it can be easily seen that

$$A' = G_1 G_2 \ldots G_n \quad . \tag{2.2.14}$$

Furthermore, each row can be regarded as building up by triangles of spins one at a time (see Fig. 2.4).
So each G_j can be written as

$$G_j = V_n V_{n-1} \ldots V_j \tag{2.2.15}$$

where V_j is given by

$$V_j(\sigma_1,\sigma_2,\ldots,\sigma_n \mid \sigma'_1,\sigma'_2,\ldots,\sigma'_n) =$$
$$\delta_{\sigma_1,\sigma'_1}\,\delta_{\sigma_2,\sigma'_2}\ldots\delta_{\sigma_j,\sigma'_j}\,\delta_{\sigma_{j+2},\sigma'_{j+2}}\ldots\delta_{\sigma_n,\sigma'_n}$$
$$\times \exp\left[K_1\sigma_{j+1}\sigma'_{j+1} + K_2\sigma_j\sigma_{j+1} + K_3\sigma'_j\sigma'_{j+1}\right] \quad . \tag{2.2.16}$$

§ 2.3 SPIN MATRICES

We introduce a set of Pauli spin operators in terms of which all the V_j s can be conveniently expressed.

Denote the three familiar anticommuting 2×2 Pauli spin matrices by

$$s \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \quad c \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad d \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{2.2.17}$$

(where $i = \sqrt{-1}$)

and define three corresponding sets of $2^n \times 2^n$ matrices, s_j , c_j and d_j ($j = 1, 2, \ldots, n$) as follows

$$\begin{aligned} s_j &\equiv I_2 \otimes I_2 \otimes \ldots \otimes s \otimes \ldots \otimes I_2 \quad (n \text{ factors}) \\ c_j &\equiv I_2 \otimes I_2 \otimes \ldots \otimes c \otimes \ldots \otimes I_2 \quad (n \text{ factors}) \\ d_j &\equiv I_2 \otimes I_2 \otimes \ldots \otimes \underset{\substack{\uparrow \\ j\text{th factor}}}{d} \otimes \ldots \otimes I_2 \quad (n \text{ factors}) \end{aligned} \tag{2.2.18}$$

where I_m is the $m \times m$ identity matrix and $\otimes$ denotes the direct product of the matrices.

One can easily verify that s_j , c_j and d_j for a given j ($j = 1, 2, \ldots, n$)

(i) are anticommuting with each other, i.e.

$$\begin{aligned} s_j c_j + c_j s_j &= 0 \\ c_j d_j + d_j c_j &= 0 \\ d_j s_j + s_j d_j &= 0 \end{aligned} \tag{2.2.19}$$

whereas they commute with any other matrix of the sets of operators;

(ii) satisfy the following relations

$$s_j^2 = c_j^2 = d_j^2 = I_{2^n} \tag{2.2.20}$$

$$s_j\, c_j = i\, d_j \; ; \quad c_j\, d_j = i\, s_j \; ; \quad d_j\, s_j = i\, c_j \; . \tag{2.2.21}$$

§ 2.4 THE MATRICES AS A PRODUCT OF SPIN OPERATORS

In order to express the matrices in terms of the spin operators defined in Section II.2.3, we further decompose V_j into a product of three matrices. From (2.2.16), we have

$$V_j = R_j^{(2)}\, Y_j^{(1)}\, R_j^{(3)} \tag{2.2.22}$$

where

$$R_j^{(\ell)}(\sigma_1,\sigma_2,\ldots,\sigma_n \mid \sigma_1',\sigma_2',\ldots,\sigma_n') = \delta_{\sigma_1,\sigma_1'}\,\delta_{\sigma_2,\sigma_2'}\cdots\delta_{\sigma_n,\sigma_n'}\,\exp\,(K_\ell \sigma_j \sigma_{j+1})$$

and

$$Y_j^{(\ell)}(\sigma_1,\sigma_2,\ldots,\sigma_n \mid \sigma_1',\sigma_2',\ldots,\sigma_n') = \delta_{\sigma_1,\sigma_1'}\delta_{\sigma_2,\sigma_2'}\cdots\delta_{\sigma_j,\sigma_j'}\delta_{\sigma_{j+2},\sigma_{j+2}'}\cdots\delta_{\sigma_n,\sigma_n'}\exp\,(K_\ell \sigma_{j+1}\sigma_{j+1}')$$

$$\ell = 1,\ 2,\ 3$$

$$j = 1,\ 2,\ \ldots,\ n-1 \; . \tag{2.2.23}$$

It may be noted that for any matrix X whose square is the unit matrix, the following identity holds :

$$\exp (\theta X) = \cosh \theta + X \sinh \theta \qquad (2.2.24)$$

for any scalar θ . Hence, it is obvious that

$$R_j^{(\ell)} = \exp (K_\ell \, s_j \, s_{j+1}) \qquad (2.2.25)$$

and by equating elements, we have

$$Y_j^{(\ell)} = (2 \sinh 2K_\ell)^{\frac{1}{2}} \exp (K_\ell^* \, c_{j+1}) \qquad \ell = 1, 2, 3 \qquad j = 1, 2, \ldots, n-1 \qquad (2.2.26)$$

where

$$\tanh K_\ell^* = \exp (- 2 K_\ell) , \quad \ell = 1, 2, 3 . \qquad (2.2.27)$$

Hence, we may write

$$V_j = (2 \sinh 2K_1)^{\frac{1}{2}} \exp(K_2 s_j s_{j+1}) \exp(K_1^* c_{j+1}) \exp(K_3 s_j s_{j+1}) \qquad j = 1, 2, \ldots, n-1 \qquad (2.2.28a)$$

and also

$$V_n = \exp (K_2 \, s_n) \exp (K_3 \, s_n) . \qquad (2.2.28b)$$

Similarly, L_A can be written as

$$L_A = \prod_{j=1}^{n} \exp (- K_2 \, s_j \, s_{j+1}) , \qquad s_{n+1} = 1 . \qquad (2.2.29)$$

In view of (2.2.24), V_j can also be written in the

form

$$V_j = \tfrac{1}{2}\left[(f+g) + (f-g)s_j s_{j+1} + (h+r)c_{j+1} + (h-r)s_j s_{j+1} c_{j+1}\right] \tag{2.2.30}$$

where

$$\begin{aligned} f &= \exp\,(\,K_1 + K_2 + K_3\,) \\ g &= \exp\,(\,K_1 - K_2 - K_3\,) \\ h &= \exp\,(\,-K_1 + K_2 - K_3\,) \\ r &= \exp\,(\,-K_1 - K_2 + K_3\,) \end{aligned} \tag{2.2.31}$$

The form is similar to that obtained for the square lattice Ising model (Baxter, 1977).

Hence, all the corner transfer matrices can be written as a product of matrices of the type $\exp\,(\,x s_j s_{j+1}\,)$ and $\exp\,(\,y c_j\,)$. In fact, it is one of the delightful properties of the Ising model that in the absence of the magnetic field, all the $2^n \times 2^n$ matrices that occur have this structure. As will be shown in the next section, this means that they belong to the group of spinor representations.

3 THE REPRESENTATIVES OF THE CTM

The problem now is to diagonalize the CTMs A , B and C . In Section II.2, we have shown that, in the absence of a magnetic field, all the matrices that occur in the model are of the type $\exp (x s_j s_{j+1})$, $\exp (y c_j)$ and their products. It was illustrated by Kaufman (1949) that all such matrices form a 2^n-dimensional representation of the group of rotations in $2n$-dimensions and hence they can be represented by $2n \times 2n$ matrices. As a result, we may equivalently work on the representation of the CTMs in this $2n$-dimensional rotational space.

§ 3.1 THE SPINOR REPRESENTATIONS

We study here the relations between the $2n$-dimensional rotation (i.e. orthogonal matrix) and the corresponding 2^n-dimensional matrix in the spin representation.

Given a set of μ operators, Γ_j of dimensions $2^n \times 2^n$ with ($j = 1, 2, \ldots, \mu$; $\mu \geq 2n$) satisfying the anticommutation rule

$$\Gamma_j \Gamma_\ell + \Gamma_\ell \Gamma_j = 2 \delta_{\ell,j} , \qquad (2.3.1)$$

$$\ell, j = 1, 2, \ldots, \mu ,$$

the set of all non-singular $2^n \times 2^n$ matrices X such that

$$X \Gamma_\ell X^{-1} = \sum_{j=1}^{2n} \hat{x}_{j,\ell} \Gamma_j , \quad \ell = 1, 2, \ldots, \mu . \qquad (2.3.2)$$

for some $\hat{x}_{j,\ell}$, forms a group $\mathcal{G}$. The $\mu \times \mu$ matrix with elements $\hat{x}_{j,\ell}$ is called the representative of X and is denoted by $\hat{X}$. The representatives have the following properties

(i) From the anticommuting properties of the Γ_j, each representative of the group is orthogonal. Furthermore, each representative determines its parent matrix to within a multiplicative constant.

(ii) If $X_1, X_2, \ldots, X_j, Y$ are members of the group $\mathcal{G}$ such that $X_1 X_2 \ldots X_j = Y$ then the corresponding representatives $\hat{X}_1, \hat{X}_2, \ldots, \hat{X}_j, \hat{Y}$ satisfy the same relationship, i.e. $\hat{X}_1 \hat{X}_2 \ldots \hat{X}_j = \hat{Y}$.

In order to formulate our problem in this spin representations, we define a set of $2n$ anticommuting operators by

$$\Gamma_1 = d_1 ; \quad \Gamma_2 = c_1 s_2 ;$$

$$\Gamma_{2j-1} = c_1 c_2 \ldots c_{j-1} d_j ; \quad \Gamma_{2j} = c_1 c_2 \ldots c_j s_{j+1} ,$$

$$j = 1, 2, \ldots, n . \qquad (2.3.3)$$

where s_j, c_j and d_j are the Pauli spin operators acting

on the j th spin as defined in (2.2.18), and s_{n+1} is the identity matrix.

With this set of operators, for any X in the group formed by the transformation in (2.3.2), we may further establish the following properties on the representatives :

(iii) If X is real and symmetric, then $\hat{X}$ is Hermitian and

$$\hat{X}^* = \mathcal{L}\hat{X}\mathcal{L} \tag{2.3.5}$$

where $*$ here denotes the complex conjugate of the matrix and $\mathcal{L}$ is a $2n \times 2n$ diagonal matrix with elements

$$\mathcal{L}_{j,j} = (-1)^j, \quad j = 1, 2, \ldots, 2n . \tag{2.3.6}$$

(iv) If X is real and orthogonal, then $\hat{X}$ is real and

$$\hat{X} = \mathcal{L}\hat{X}\mathcal{L} . \tag{2.3.7}$$

This implies that $\hat{X}$ is built up of 2×2 diagonal subblocks.

(v) If X is diagonal, it must be of the form

$$X = \text{const.} \times \prod_{j=1}^{n} \tfrac{1}{2}\left[(1+\rho_j) + (1-\rho_j)s_j s_{j+1}\right] \tag{2.3.8}$$

for some scalars ρ_j ($j = 1, 2, \ldots, n$) and $\hat{X}$ is block diagonal in the form

$$\hat{X} = \begin{pmatrix} \lambda_1 & & & & \\ & \lambda_2 & & & \\ & & \ddots & & \\ & & & \lambda_j & \\ & & & & \ddots \\ & & & & & \lambda_n \end{pmatrix} \qquad (2.3.9)$$

where λ_j are 2×2 orthogonal matrices and can be written as

$$\lambda_j = \tfrac{1}{2} \begin{pmatrix} \rho_j + \rho_j^{-1} & i\,(\rho_j^{-1} - \rho_j) \\ -i\,(\rho_j^{-1} - \rho_j) & \rho_j + \rho_j^{-1} \end{pmatrix} \qquad (2.3.10)$$

$$j = 1, 2, \ldots, n . \quad (i = \sqrt{-1}).$$

§ 3.2 THE REPRESENTATIVES OF THE V_j

We are now ready to express the corner transfer matrices in terms of spin representation.

It can be verified that all the matrices V_j and L_A defined in (2.2.16) and (2.2.12) belong to the group $\mathcal{G}$ mentioned above. Using the set of operators defined in (2.3.3), we find that

(i) $$R_j^{(2)} \Gamma_\ell R_j^{(2)-1} = \alpha \Gamma_{2j-1} - i\beta \Gamma_{2j}, \quad \text{if } \ell = 2j-1$$
$$= i\beta \Gamma_{2j-1} + \alpha \Gamma_{2j}, \quad \text{if } \ell = 2j$$
$$= \Gamma_\ell, \quad \text{otherwise .} \qquad (2.3.11a)$$

$$\text{(ii)}\quad R_j^{(3)}\,\Gamma_\ell\,R_j^{(3)-1} = \alpha'\Gamma_{2j-1} - i\beta'\Gamma_{2j}\ ,\ \text{if}\ \ell = 2j-1$$

$$= i\beta'\Gamma_{2j-1} + \alpha'\Gamma_{2j}\ ,\ \text{if}\ \ell = 2j$$

$$= \Gamma_\ell\ ,\ \text{otherwise}\ . \qquad (2.3.11b)$$

and

$$\text{(iii)}\quad Y_j^{(1)}\,\Gamma_\ell\,Y_j^{(1)-1} = \gamma\ \Gamma_{2j} - i\delta\ \Gamma_{2j+1},\ \text{if}\ \ell = 2j$$

$$= i\delta\ \Gamma_{2j} + \gamma\ \Gamma_{2j+1}\ ,\ \text{if}\ \ell = 2j+1$$

$$= \Gamma_\ell\ ,\ \text{otherwise}\ . \qquad (2.3.11c)$$

where

$$\gamma = \coth 2K_1\ ,\quad \delta = \operatorname{cosech} 2K_1$$

$$\alpha = \cosh 2K_2\ ,\quad \beta = \sinh 2K_2 \qquad (2.3.12)$$

$$\alpha' = \cosh 2K_3\ ,\quad \beta' = \sinh 2K_3$$

Hence, from (2.2.22), $\hat{V}_j$ is simply given by

$$\hat{V}_j = \begin{array}{c} \\ 2j-1 \\ 2j \\ 2j+1 \\ \\ \\ \\ \end{array} \begin{array}{c} \begin{array}{ccc} \qquad 2j-1 & \qquad 2j & \qquad 2j+1 \end{array} \\ \begin{pmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & 1 & & & & \\ & & & \ddots & & & \\ & & & & \alpha\alpha'+\beta\beta'\gamma & i(\alpha\beta'+\alpha'\beta\gamma) & -\beta\delta \\ & & & & -i(\alpha'\beta+\alpha\beta'\gamma) & \beta\beta'+\alpha\alpha'\gamma & i\alpha\delta \\ & & & & -\delta\beta' & -i\alpha'\delta & \gamma \\ & & & & & & & 1 & \\ & & & & & & & & \ddots \end{pmatrix} \end{array} \qquad (2.3.13)$$

and from (2.2.29) ,

$$\hat{L}_A = \begin{pmatrix} \alpha & -i\beta & 0 & 0 & & \\ i\beta & \alpha & 0 & 0 & & \\ 0 & 0 & \alpha & -i\beta & & \\ 0 & 0 & i\beta & \alpha & & \\ & & & & \ddots & \\ & & & & & \ddots \end{pmatrix} . \qquad (2.3.14)$$

Hence the CTMs A , B and C are also members of the group (i.e. their representatives under Γ_j exist).

4 THE DIAGONALIZATION OF $\hat{A}\ \hat{B}\ \hat{C}$

§ 4.1 THE CTMS AND THEIR REPRESENTATIVES

Before we continue our analysis, we observe that the CTMs A , B and C (hence their representatives) do not necessary commute with each other for arbitrary J_1 , J_2 and J_3 . However, our aim is to diagonalize the matrix

$$\mathcal{D} = A\ B\ C \tag{2.4.1}$$

i.e. to look for a matrix, say P_2 , such that

$$P_2^{-1}\ \mathcal{D}\ P_2 = \mathcal{D}_d \tag{2.4.2}$$

where $\mathcal{D}_d$ is a diagonal matrix. From property (v) of the representatives (Section II.3.1), this is equivalent to finding a similarity transformation which brings $\hat{\mathcal{D}}$ to a block diagonal form. We have

$$\hat{\mathcal{D}}_d = \hat{P}_2^{-1}\ \hat{\mathcal{D}}\ \hat{P}_2 = \begin{pmatrix} \lambda_1 & & & & \\ & \lambda_2 & & & \\ & & \ddots & & \\ & & & \lambda_j & \\ & & & & \ddots \end{pmatrix} \tag{2.4.3}$$

where λ_j are 2×2 orthogonal matrices.

Since $\hat{\mathcal{D}}$ and $\hat{\mathcal{D}}_d$ are orthogonal matrices, one can choose $\hat{P}_2$ to be orthogonal also. As $\hat{A}$, $\hat{B}$ and $\hat{C}$ are all orthogonal matrices, we may define orthogonal matrices $\hat{P}_1$ and $\hat{P}_3$ such that

$$\hat{P}_2^{-1}\,\hat{A}\,\hat{P}_3 = \hat{A}_d \tag{2.4.4a}$$

$$\hat{P}_3^{-1}\,\hat{B}\,\hat{P}_1 = \hat{B}_d \tag{2.4.4b}$$

$$\hat{P}_1^{-1}\,\hat{C}\,\hat{P}_2 = \hat{C}_d \tag{2.4.4c}$$

and require that $\hat{A}_d$, $\hat{B}_d$ and $\hat{C}_d$ are all orthogonal and of block diagonal form. For example, $\hat{A}_d$ is given by

$$\hat{A}_d = \begin{pmatrix} \lambda_1^{(1)} & & & & & \\ & \lambda_2^{(1)} & & & & \\ & & \ddots & & & \\ & & & \lambda_j^{(1)} & & \\ & & & & \ddots & \\ & & & & & \ddots \end{pmatrix} \tag{2.4.5}$$

where $\lambda_j^{(1)}$ are 2×2 orthogonal matrices, similarly for $\hat{B}_d$ and $\hat{C}_d$ with $\lambda_j^{(1)}$ replaced by $\lambda_j^{(2)}$ and $\lambda_j^{(3)}$ respectively. Obviously, we then have

$$\hat{A}_d\,\hat{B}_d\,\hat{C}_d = \hat{\mathcal{D}}_d \quad . \tag{2.4.6}$$

Note that from the set of equations (2.4.4a-c), $\hat{P}_1$ is a matrix which diagonalizes the matrix $\hat{C}\hat{A}\hat{B}$ and $\hat{P}_3$ a matrix which diagonalizes $\hat{B}\hat{C}\hat{A}$ to block diagonal form.

From prpperties (i) and (ii) of the representatives, the corresponding matrices in $\mathcal{G}$ of the representatives $\hat{A}_d$, $\hat{B}_d$, $\hat{C}_d$ and $\hat{P}_\ell$ can be chosen to satisfy the set of equations (2.4.4a-c) also, i.e. we can find $2^n \times 2^n$ matrices A_d , B_d , C_d and P_ℓ , $\ell = 1, 2, 3$ in $\mathcal{G}$ satisfying

$$P_2^{-1} A P_3 = A_d \; ; \; P_3^{-1} B P_1 = B_d \; ; \; P_1^{-1} C P_2 = C_d \; . \tag{2.4.7}$$

Also

$$A_d B_d C_d = \mathcal{D}_d \quad . \tag{2.4.8}$$

Hence, if we can solve (2.4.3) or equivalently (2.4.4a-c), we shall have obtained the diagonal form of $\mathcal{D}$.

We now perform the analysis on the representatives. It is convenient to group the elements of the matrices $\hat{A}$, $\hat{B}$, $\hat{C}$ and $\hat{P}_\ell$ ($\ell = 1, 2, 3$) into 2×2 blocks and write

$$\hat{A} = (a_{ij}) \; ; \; \hat{B} = (b_{ij}) \text{ and } \hat{C} = (c_{ij}) \tag{2.4.9}$$

and

$$\hat{P}_\ell = (p_{ij}^{(\ell)}), \quad \ell = 1, 2, 3 \quad . \tag{2.4.10}$$

$$i, j = 1, 2, \ldots, n \quad .$$

where a_{ij} , b_{ij} , c_{ij} and $p_{ij}^{(\ell)}$ are all 2×2 matrices. In the limit of n large, each element tends to a limit. These limiting values are conveniently expressed in terms of generating functions defined by

$$\mathcal{A}(y,z) = \sum_{i,j=1}^{\infty} a_{i,j}\, y^{i-1}\, z^{j-1} \qquad (2.4.11a)$$

$$\mathcal{B}(z,x) = \sum_{i,j=1}^{\infty} b_{i,j}\, z^{i-1}\, x^{j-1} \qquad (2.4.11b)$$

$$\mathcal{C}(x,y) = \sum_{i,j=1}^{\infty} c_{i,j}\, x^{i-1}\, y^{j-1} \qquad (2.4.11c)$$

and

$$p_m^{(\ell)}(x) = \sum_{j=1}^{\infty} p_{j,m}^{(\ell)}\, x^{j-1}\,, \quad \ell = 1, 2, 3 \quad m = 1, 2, \ldots \quad . \qquad (2.4.12)$$

From (2.4.12) we have

$$p_{j,m}^{(\ell)} = (2\pi i)^{-1} \int_{c_\ell} y^{-j}\, p_m^{(\ell)}(y)\, dy\,, \quad \ell = 1, 2, 3 \quad j, m = 1, 2, \ldots \quad . \qquad (2.4.13)$$

where the contour of integration c_ℓ is a simple closed curve surrounding the origin in the y plane within and on which $p_j^{(\ell)}(y)$ is analytic.

In view of equations (2.4.9) and (2.4.10), the set of equations (2.4.4a-c) can be expressed in the form

$$\sum_{\ell=1}^{\infty} a_{i,\ell}\, p_{\ell,j}^{(3)} = p_{i,j}^{(2)}\, \lambda_j^{(1)} \qquad (2.4.14a)$$

$$\sum_{\ell=1}^{\infty} b_{i,\ell}\, p_{\ell,j}^{(1)} = p_{i,j}^{(3)}\, \lambda_j^{(2)} \qquad (2.4.14b)$$

$$\sum_{\ell=1}^{\infty} c_{i,\ell}\, p_{\ell,j}^{(2)} = p_{i,j}^{(1)}\, \lambda_j^{(3)} \qquad (2.4.14c)$$

$$i, j = 1, 2, \ldots \quad .$$

Hence, from (2.4.11a-c), (2.4.13) and (2.4.14a-c) , one can easily arrive at the coupled integral equations

$$(2\pi i)^{-1} \int_{c_3} \mathcal{A}(y, z^{-1})\, p_j^{(3)}(z)\, dz/z = p_j^{(2)}(y)\, \lambda_j^{(1)} \qquad (2.4.15a)$$

$$(2\pi i)^{-1} \int_{c_1} \mathcal{B}(z, x^{-1})\, p_j^{(1)}(x)\, dx/x = p_j^{(3)}(z)\, \lambda_j^{(2)} \qquad (2.4.15b)$$

$$(2\pi i)^{-1} \int_{c_2} \mathcal{C}(x, y^{-1})\, p_j^{(2)}(y)\, dy/y = p_j^{(1)}(x)\, \lambda_j^{(3)} \qquad (2.4.15c)$$

The main task reduces to solving these set of coupled integral equations.

§ 4.2 THE GENERATING FUNCTION $\mathcal{A}(y, z)$

It is possible to evaluate the generating function $\mathcal{A}(y, z)$ (and similarly $\mathcal{B}(z, x)$, $\mathcal{C}(x, y)$) explicitly.

Define matrices $\hat{H}_r$ ($r = 1, 2, \ldots, n$) by

$$\hat{H}_r = \hat{V}_r \hat{V}_{r-1} \ldots \hat{V}_1 . \qquad (2.4.16)$$

We can evaluate $\hat{H}_r$ directly from (2.3.13) .

With w_j , $j = 0, 1, 2$ and h_j , g_j , $j = 0, 1, 2, \ldots, n$ being 2×2 blocks defined as follows :

$$w_0 = \begin{pmatrix} -\beta\delta & 0 \\ i\alpha\delta & 0 \end{pmatrix}$$

$$w_1 = \begin{pmatrix} -\delta\beta' & -i\alpha'\delta \\ 0 & 0 \end{pmatrix}$$

$$w_2 = \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix} \qquad (2.4.17)$$

$$h_o = \begin{pmatrix} \alpha\alpha'+\beta\beta'\gamma & i(\alpha\beta'+\alpha'\beta\gamma) \\ -i(\alpha'\beta+\alpha\beta'\gamma) & \beta\beta'+\alpha\alpha'\gamma \end{pmatrix}$$

$$h_1 = h_o w_1 = \begin{pmatrix} -\delta\beta'(\alpha\alpha'+\beta\beta'\gamma) & -i\alpha'\delta(\alpha\alpha'+\beta\beta'\gamma) \\ i\delta\beta'(\alpha'\beta+\alpha\beta'\gamma) & -\alpha'\delta(\alpha'\beta+\alpha\beta'\gamma) \end{pmatrix}$$

$$h_j = (-\delta\beta')^{j-1} h_1 , \quad j = 1, 2, \ldots, n . \qquad (2.4.18)$$

and

$$g_o = h_o w_2 = \begin{pmatrix} \gamma(\alpha\alpha'+\beta\beta'\gamma) & i(\alpha\beta'+\alpha'\beta\gamma) \\ -i\gamma(\alpha'\beta+\alpha\beta'\gamma) & \beta\beta'+\alpha\alpha'\gamma \end{pmatrix}$$

$$g_1 = h_1 w_2 = \begin{pmatrix} -\delta\beta'\gamma(\alpha\alpha'+\beta\beta'\gamma) & -i\alpha'\delta(\alpha\alpha'+\beta\beta'\gamma) \\ i\delta\beta'\gamma(\alpha'\beta+\alpha\beta'\gamma) & -\alpha'\delta(\alpha'\beta+\alpha\beta'\gamma) \end{pmatrix}$$

$$g_j = (-\delta\beta')^{j-1} g_1 , \quad j = 1, 2, \ldots, n ,$$

(2.4.19)

we have,

$$\hat{H}_r = \begin{pmatrix}
h_0 & w_0 & 0 & 0 & \cdots & 0 & 0 & \\
h_1 & g_0 & w_0 & 0 & & 0 & 0 & \\
h_2 & g_1 & g_0 & w_0 & & 0 & 0 & \\
h_3 & g_2 & g_1 & g_0 & \ddots & 0 & 0 & \\
\vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \\
h_{r-1} & g_{r-2} & g_{r-3} & g_{r-4} & \cdots\ g_0 & w_0 & 0 & \cdots \\
(-\delta\beta')^{r-1} w_1 & (-\delta\beta')^{r-2} w_1 w_2 & (-\delta\beta')^{r-3} w_1 w_2 & (-\delta\beta')^{r-4} w_1 w_2 & \cdots\ w_1 w_2 & w_2 & 0 & \\
0 & 0 & 0 & 0 & \cdots\ 0 & 0 & I_2 & \\
\vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \ddots
\end{pmatrix}$$

(r th block)

$$r = 1, 2, \ldots, n \quad . \tag{2.4.20}$$

Hence the matrices $\hat{H}_r$, $\hat{H}_{r+1}$, $\hat{H}_{r+2}$, ..., have their first $2(r-1)$ rows in common and so we expect each element (ℓ,m) of $\hat{H}_r$ tends to a limit as r and n tend towards infinity.

In view of (2.2.15), we have

$$\hat{G}_1 = \hat{H}_n \quad , \tag{2.4.21}$$

so, in the thermodynamic limit ($n\to\infty$) , we expect

$$\hat{G} = \lim_{n\to\infty} \hat{G}_1 = \lim_{n,r\to\infty} \hat{H}_r \quad . \tag{2.4.22}$$

Also, noting the structure of $\hat{V}_j$ from (2.3.13), we observe that for $n = \infty$,

$$\hat{G}_2 = \begin{pmatrix} I_2 & \vdots \\ \cdots\cdots & \cdots \\ & \vdots\ \hat{G}_1 \end{pmatrix} \tag{2.4.23}$$

or equivalently using (2.2.14), we may write

$$\hat{A}' = \hat{G} \begin{pmatrix} I_2 \\ \hline \hat{A}' \end{pmatrix} . \qquad (2.4.24)$$

To calculate the generating functions of the CTMs , we define a matrix $\mathcal{M}$ by

$$\mathcal{M} = \begin{pmatrix} I_2 & 0 & & & \\ \delta\beta' I_2 & I_2 & 0 & & \\ 0 & \delta\beta' I_2 & I_2 & \ddots & \\ & 0 & \delta\beta' I_2 & \ddots & \ddots \\ & & 0 & \ddots & \ddots \\ & & & \ddots & \ddots \\ & & & & \ddots \end{pmatrix} \qquad (2.4.25)$$

and write (2.4.24) as

$$\mathcal{M}\,\hat{A}' = \mathcal{M}\,\hat{G} \begin{pmatrix} I_2 \\ \hline \hat{A}' \end{pmatrix} \qquad (2.4.26)$$

Note that

$$\mathcal{M}\,\hat{G} = \begin{pmatrix} h_0 & w_0 & 0 & 0 & \cdots \\ m_0 & m_1 & w_0 & 0 & \cdots \\ 0 & m_0 & m_1 & w_0 & \\ 0 & 0 & m_0 & m_1 & \ddots \\ \vdots & & \ddots & \ddots & \ddots \\ \vdots & & & \ddots & \ddots \\ \vdots & & & & \ddots \end{pmatrix} \qquad (2.4.27)$$

where

$$m_0 = \delta\beta' h_0 + h_1 = \begin{pmatrix} 0 & -i\delta\alpha \\ 0 & -\delta\beta \end{pmatrix}$$

$$m_1 = \delta\beta' w_0 + g_0 = \begin{pmatrix} \beta\beta'+\alpha\alpha'\gamma & i(\alpha\beta'+\alpha'\beta\gamma) \\ -i(\alpha\beta'+\alpha'\beta\gamma) & \beta\beta'+\alpha\alpha'\gamma \end{pmatrix}$$

(2.4.28)

In a similar way to $\mathcal{A}(y,z)$, we define

$$\mathcal{A}'(y,z) = \sum_{\ell,j=1}^{\infty} a'_{\ell j}\, y^{\ell-1}\, z^{j-1} \qquad (2.4.29)$$

where $(a'_{\ell j})$ are 2×2 block elements of $\hat{A}'$. Equating elements in (2.4.26) , we have the following set of equations :

$$\begin{aligned} a'_{1,1} &= h_0 \\ a'_{1,j} &= w_0\, a'_{1,j-1} \quad , \qquad j = 2, 3, \ldots \\ \delta\beta'\, a'_{1,1} + a'_{2,1} &= m_0 \\ \delta\beta'\, a'_{\ell-1,1} + a'_{\ell,1} &= 0 \qquad , \qquad \ell = 3, 4, \ldots \end{aligned}$$

(2.4.30)

and

$$\delta\beta'\, a'_{\ell-1,j} + a'_{\ell,j} = m_0\, a'_{\ell-2,j-1} + m_1\, a'_{\ell-1,j-1} + w_0\, a'_{\ell,j-1}$$

$$\ell, j \geq 2 \quad . \qquad (2.4.31)$$

Multiplying (2.4.31) by $y^{\ell-1}\, z^{j-1}$ and summing over ℓ , $j = 2, 3, \ldots$ gives

$$\sum_{\ell,j=2}^{\infty} (a'_{\ell,j} + \delta\beta' a'_{\ell-1,j}) y^{\ell-1} z^{j-1} =$$

$$\sum_{\ell,j=2}^{\infty} (m_0 a'_{\ell-2,j-1} + m_1 a'_{\ell-1,j-1} + w_0 a'_{\ell,j-1}) y^{\ell-1} z^{j-1}$$

(2.4.32)

On simplification and using (2.4.30) also, this gives the generating function $\mathcal{A}'(y,z)$ as

$$\mathcal{A}'(y,z) = (1 + \delta\beta' y - m_0 y^2 z - m_1 yz - w_0 z)^{-1} (h_0 + m_0 y)$$

(2.4.33)

It can be easily verified that

$$(1 + \delta\beta' y - m_0 y^2 z - m_1 yz - w_0 z)^{-1} =$$

$$\frac{1}{(1+\delta\beta' y)\ \Delta(y,z)} \begin{pmatrix} 1+\delta\beta' y-(\beta\beta'+\alpha\alpha'\gamma)yz+\delta\beta y^2 z & iyz(\alpha\beta'+\alpha'\beta\gamma-\alpha\delta y) \\ -i[(\alpha\beta'+\alpha'\beta\gamma)y-\alpha\delta]z & 1+\delta\beta' y+\delta\beta z-(\beta\beta'+\alpha\alpha'\gamma)yz \end{pmatrix}$$

(2.4.34)

with

$$\Delta(y,z) = 1 + y\delta\beta' + z\delta\beta - 2yz(\beta\beta'+\alpha\alpha'\gamma) + y^2 z\delta\beta + yz^2\delta\beta' + y^2 z^2 \qquad (2.4.35)$$

where γ , δ , α , α' , β and β' are defined in (2.3.12). Note that if we put $y = e^{i\theta}$ and $z = e^{i\phi}$, (2.4.35) becomes

$$\Delta(y,z) = \frac{-2yz}{\sinh 2K_1} (\cosh 2K_1 \cosh 2K_2 \cosh 2K_3 + \sinh 2K_1 \sinh 2K_2 \sinh 2K_3 - \sinh 2K_2 \cos\theta - \sinh 2K_1 \cos(\theta+\phi) - \sinh 2K_3 \cos\phi)$$

(2.4.36)

The logarithm of the expression in brackets is just the integrand of the double integral for the free energy of the triangular lattice [Temperley, 1950: Eqt. 10].

As for the generating function $\mathcal{A}'(y,z)$, from (2.4.33)

$$\mathcal{A}'(y,z) = \frac{1}{\Delta(y,z)} \begin{pmatrix} \alpha\alpha'+\beta\beta'\gamma-\gamma yz & i\,(\alpha\beta'+\alpha'\beta\gamma-\delta\alpha y) \\ -i(\alpha'\beta+\alpha\beta'\gamma-\delta\alpha' z) & \beta\beta'+\alpha\alpha'\gamma-\delta\beta y-\delta\beta' z \\ & -yz \end{pmatrix} \tag{2.4.37}$$

Using (2.2.11) and (2.3.14), we have

$$a_{\ell,j} = \ell_\alpha\, a'_{\ell,j} \quad , \quad \ell,\ j = 1,\ 2,\ \ldots \tag{2.4.38}$$

where

$$\ell_\alpha = \begin{pmatrix} \alpha & -i\beta \\ i\beta & \alpha \end{pmatrix} \tag{2.4.39}$$

or equivalently, we may write

$$\mathcal{A}(y,z) = \ell_\alpha\, \mathcal{A}'(y,z) \quad . \tag{2.4.40}$$

We have therefore in fact obtained the generating function $\mathcal{A}(y,z)$:

$$\mathcal{A}(y,z) = \frac{1}{\Delta(y,z)} \begin{pmatrix} \alpha'(1+z\delta\beta)-yz\alpha\gamma & i\{\beta'(1+z\delta\beta)+yz\beta-y\delta\} \\ -i(\beta'\gamma+yz\beta\gamma-z\alpha\alpha'\delta) & \alpha'\gamma-z\alpha(\delta\beta'+y) \end{pmatrix} \tag{2.4.41}$$

Similarly, $\mathcal{B}(z,x)$ and $\mathcal{C}(x,y)$ can be evaluated explicitly. The elements of $\hat{A}$ (and similarly $\hat{B}$ and $\hat{C}$) can now in principle be obtained by Taylor expanding

$\mathcal{A}(y,z)$ (respectively $\mathcal{B}(z,x)$ and $\mathcal{C}(x,y)$) in powers of y and z .

§ 4.3 ELLIPTIC FUNCTION PARAMETRIZATION

To solve the coupled integral equations (2.4.15a-c), we apply the elliptic function parametrization which occurs naturally for the triangular lattice as follows :

$$\cosh 2K_j = \mathrm{cn}(2v_j)$$

$$\sinh 2K_j = -\,i\,\mathrm{sn}(2v_j) \quad , \quad j = 1, 2, 3 \quad . \tag{2.4.42}$$

where sn , cn and dn are Jacobian elliptic functions with modulus k given by (Stephenson, 1964) :

$$k^2 = \frac{\left[(1-t_1^2)(1-t_2^2)(1-t_3^2)\right]^2}{16(1+t_1t_2t_3)(t_1+t_2t_3)(t_2+t_3t_1)(t_3+t_1t_2)} \tag{2.4.43}$$

where $t_j = \tanh K_j$, $j = 1, 2, 3$.

Now if we restrict ourselves to the regime where all the K_j are real and positive (i.e. we consider only the pure ferromagnetic case), the v_j will be all purely imaginary and are subjected to the following conditions :

$$0 < \mathrm{Im}(v_j) < K'/2 \quad \text{and} \quad v_1 + v_2 + v_3 = iK'/2$$

where K , K' are the complete elliptic integrals of the first kind of moduli k , $k' = (1-k^2)^{\frac{1}{2}}$, respectively.

(These are not to be confused with the energy coefficients K_1 , K_2 and K_3 used above.) If we apply the following transformations to the variables of the integral equations (2.4.15a-c),

$$\begin{aligned} x &= k \ \mathrm{sn}(u_1+v_1) \ \mathrm{sn}(u_1-v_1) \\ y &= k \ \mathrm{sn}(u_2+v_2) \ \mathrm{sn}(u_2-v_2) \\ z &= k \ \mathrm{sn}(u_3+v_3) \ \mathrm{sn}(u_3-v_3) \end{aligned} \qquad (2.4.44)$$

we can solve the equations in terms of the new variables u_1, u_2, u_3 . It is more convenient to work on the new kernel defined by

$$W_1(u_2,u_3)\ du_3 = \mathcal{A}\ (y,z^{-1})\ dz/z \qquad (2.4.45a)$$

$$W_2(u_3,u_1)\ du_1 = \mathcal{B}\ (z,x^{-1})\ dx/x \qquad (2.4.45b)$$

$$W_3(u_1,u_2)\ du_2 = \mathcal{C}\ (x,y^{-1})\ dy/y \qquad (2.4.45c)$$

We now restrict the analysis to $\mathcal{A}\ (y,z)$.
We are able to factorize $\Delta(y,z^{-1})$ in terms of the variables u_2 and u_3 . Using the transformation given in (2.4.44) and considering the sum and product of the roots of the expression in (2.4.35) as a function of y , we obtain

$$\begin{aligned} z^2\Delta(y,z^{-1}) = k^2 \ &(1 - k^2\mathrm{sn}(u_3+v_3)\mathrm{sn}(u_3-v_3)\mathrm{sn}(2v_2+2v_3)\mathrm{sn}(2v_2)) \\ &\times (\mathrm{sn}(u_2+v_2)\mathrm{sn}(u_2-v_2) - \mathrm{sn}(u_3+v_3)\mathrm{sn}(u_3+v_3+2v_2)) \\ &\times (\mathrm{sn}(u_2+v_2)\mathrm{sn}(u_2-v_2) - \mathrm{sn}(u_3-v_3)\mathrm{sn}(u_3-v_3-2v_2)) \end{aligned} \qquad (2.4.46)$$

[Appendix IIB] .

Similarly, we may obtain $W_1(u_2,u_3)$ as a function of u_2 and u_3 . Consider the following matrix

$$D^{-1}(u_2,v_2)\ M_1(u_2,u_3)\ D(u_3,v_3)$$

where $D(u,v)$ and $M_i(u_j,u_\ell)$ are 2×2 matrices given by

$$D(u,v) = \begin{pmatrix} -cn(u-v) & dn(u+v)\,sn(u-v) \\ cn(u+v) & sn(u+v)\,dn(u-v) \end{pmatrix} \qquad (2.4.47)$$

$$M_i(u_j,u_\ell) = \begin{pmatrix} \phi(u_\ell-u_j+v_j+v_\ell) & -\phi(u_j+u_\ell-v_j-v_\ell) \\ -\phi(u_j+u_\ell+v_j+v_\ell) & \phi(u_\ell-u_j-v_j-v_\ell) \end{pmatrix} \qquad (2.4.48)$$

with

$$\phi(u) = dn(u)/sn(u) \qquad (2.4.49)$$

and $i\ \ j\ \ \ell$ cyclic permutation of $1\ 2\ 3$.

It can be shown that this matrix has the same poles and residues as $W_1(u_2,u_3)$ and hence by Liouville's theorem and their periodicity, they are in fact the same matrix [Appendix IIA, B] . We may then write the kernels as

$$W_i(u_j,u_\ell) = D^{-1}(u_j,v_j)\ M_i(u_j,u_\ell)\ D(u_\ell,v_\ell) \qquad (2.4.50)$$

where $i\ j\ \ell$ are cyclic permutations of $1\ 2\ 3$.

The coupled integral equations (2.4.15a-c) become

$$(2\pi i)^{-1} \int_{c'_\ell} W_i(u_j,u_\ell)\ p_m^{(\ell)}(u_\ell)\ du_\ell = p_m^{(j)}(u_j)\ \lambda_m^{(i)}$$
$$m = 1,\ 2,\ \ldots \qquad (2.4.51)$$

with $i\ j\ \ell$ being cyclic permutations of $1\ 2\ 3$.

§ 4.4 THE CONTOUR OF INTEGRATION

Before we proceed any further, we would like to comment on the contour of integration for the coupled integral equations in (2.4.15a-c) and hence for (2.4.51). We would like to focus our attention on the z plane for the integration of (2.4.15a) . Similar arguments can be applied to the integrations of (2.4.15b) and (2.4.15c) in the x and y plane respectively with necessary change of variables.

Suppose that the radius of convergence for $p_m^{(3)}(z)$, ($m = 1, 2, \ldots$) as defined in (2.4.12) is R . By the orthogonality requirements for $\hat{P}_3$, we have

$$\sum_{m=1}^{\infty} p_{m,\ell}^{(3)^T} p_{m,j}^{(3)} = \delta_{\ell,j} \quad , \quad \ell, j = 1, 2, \ldots \qquad (2.4.52)$$

This implies that we must have $p_{\ell,j}^{(3)} \to 0$ as $\ell \to \infty$ and so, the radius of convergence R cannot less than unity. The contour of integration c_3 must then be a circle of radius less than R and yet, it must be sufficiently large that $\mathcal{A}(y, z^{-1})$ is an analytic function of z for z outside and on c_3 .

For $y = 0$, $\mathcal{A}(y, z^{-1})$ has poles at $z = 0$ and $z = -\delta\beta$ only. Hence, we may choose the radius of the contour to be greater than $|-\delta\beta|$ surrounding the origin. By continuity, for a small circular domain D surrounding the origin in the y plane, the integral equation (2.4.15a)

is valid by choosing c_3 such that

(i) c_3 is a simple closed curve surrounding the origin;

(ii) $p_m^{(3)}(z)$ is analytic for z inside and on c_3 ;

(iii) for $y \in D$, both poles of $\mathcal{A}(y,z^{-1})$ in the z plane lie inside c_3 .

Under the transformation from z to u_3 , we find that provided

$$v_3 < \eta' < iK' - v_3 \qquad (2.4.53)$$

we have

(i) a straight line with $\mathrm{Im}(u) = \eta'$ maps to a simple closed curve c in the z plane surrounding the origin;

(ii) the domain $v_3 < |\mathrm{Im}(u)| < \eta'$ maps to the interior of c ;

(iii) as u moves from left to right a distance $2K$ along the line $\mathrm{Im}(u) = \eta'$, z moves monotonically once around c in an clockwise-direction.

So, the contour of integration in the complex u_3 plane for (2.4.51) becomes a line segment $(i\eta_3+K, i\eta_3-K)$, where η_3 is such that the corresponding contour c_3 in the original z plane surrounds the poles of the kernel $\mathcal{A}(y,z^{-1})$. An appropriate choice of η_3 for (2.4.51) is

$$|\mathrm{Im}(u_2)| + |\mathrm{Im}(v_2+v_3)| < \eta_3 < \min(2iK'-|\mathrm{Im}(u_2)|-\mathrm{Im}(v_2+v_3), iK'-v_3) \qquad (2.4.54)$$

Using this, we may solve the coupled integral equations (2.4.51) in the complex u_ℓ plane using Fourier transforms.

5 SOLUTION OF THE INTEGRAL EQUATIONS

The coupled integral equations of (2.4.51) can be solved in the complex u_1, u_2 and u_3 planes for $\lambda_m^{(\ell)}$ and $p_m^{(\ell)}(u_\ell)$ ($\ell = 1, 2, 3$) with the assumption that the corresponding $p_m^{(1)}(x)$, $p_m^{(2)}(y)$ and $p_m^{(3)}(z)$ are analytic within and on the contour of integrations c_ℓ ($\ell = 1, 2, 3$) in the x, y and z planes respectively. We will check the analyticity of our result on $p_m^{(\ell)}(x)$, $\ell = 1, 2, 3$ in Section II.5.3.

§ 5.1 SOLUTION BY FOURIER TRANSFORMS

Define

$$f_m^{(\ell)}(u_\ell) = D(u_\ell, v_\ell)\, p_m^{(\ell)}(u_\ell) \qquad \ell = 1, 2, 3 . \quad m = 1, 2, \ldots . \tag{2.5.1}$$

Substituting this to (2.4.51), we have

$$-(2\pi i)^{-1} \int_{i\eta_\ell - K}^{i\eta_\ell + K} M_i(u_j, u_\ell)\, f_m^{(\ell)}(u_\ell)\, du_\ell = f_m^{(j)}(u_j)\, \lambda_m^{(i)} \qquad m = 1, 2, \ldots \tag{2.5.2}$$

where $M_i(u_j, u_\ell)$ is defined in (2.4.48) and i j ℓ are

cyclic permutations of $1\ 2\ 3$. Note that the elements of $M_i(u_j,u_\ell)$ depend only on either (u_j-u_ℓ) or (u_j+u_ℓ) , but not both, so the transformation from x , y , $z \to u_1$, u_2 , u_3 can be regarded as reducing the integral equations (2.4.15a-c) to a difference kernel form (Onsager, 1970).

Consider the case $i\ j\ \ell = 1\ 2\ 3$ for (2.5.2). Since $p_j^{(3)}(z)$ is analytic within and on c_3 , $f_j^{(3)}(u_3)$ must be analytic in the region $v_3 \leq |\mathrm{Im}(u_3)| \leq \eta_3$. Further, $p_m^{(3)}(z)$ is a single-valued function of z . Incrementing u_3 by $2K$ negates $D(u_3,v_3)$ while leaves z unchanged. This implies that $f_m^{(3)}(u_3)$ is a periodic function with period $4K$ and therefore must have a Fourier series. Similar arguments can be applied to $f_m^{(1)}(u_1)$ and $f_m^{(2)}(u_2)$. Hence, we may write

$$f_m^{(\ell)}(u_\ell) = \sum_{n=-\infty}^{\infty} F_{n,m}^{(\ell)} \exp(in\pi u_\ell/2K) \qquad \begin{matrix} \ell = 1,\ 2,\ 3\ . \\ m = 1,\ 2,\ \ldots \end{matrix} \tag{2.5.3}$$

for some 2×2 matrices $F_{n,m}^{(\ell)}$. This should be convergent for $v_\ell \leq \mathrm{Im}(u_\ell) \leq \eta_\ell$. From the definition of $\phi(u)$, we have

$$\begin{aligned} \phi(u) &= \mathrm{dn}(u) \ / \ \mathrm{sn}(u) \\ &= -i\pi/K \sum_{n=-\infty}^{\infty} \exp\{i\pi(2n-1)u/2K\} \ / \ (1+q^{2n-1}) \end{aligned} \tag{2.5.4}$$

provided that $0 < \mathrm{Im}(u) < 2K'$. q is the "nome" of the

elliptic functions given by

$$q = \exp(- \pi K'/K) \quad . \tag{2.5.5}$$

Provided that u_j is in D and u_ℓ is on c_ℓ, the imaginary parts of the arguments of all the functions ϕ in $M_i(u_j, u_\ell)$ lie in the region $(0 , 2K')$. Thus we may substitute (2.5.3) and (2.5.4) to (2.5.2) to give

$$\frac{1}{2K} \int_{i\eta_\ell - K}^{i\eta_\ell + K} \sum_{n=-\infty}^{\infty} \sum_{r=-\infty}^{\infty} \frac{du_\ell}{(1+q^{2n-1})} \begin{pmatrix} \exp\{i(2n-1)\pi(u_\ell - u_j + v_j + v_\ell)/2K\} \\ -\exp\{i(2n-1)\pi(u_j + u_\ell + v_j + v_\ell)/2K\} \\ \vdots \\ -\exp\{i(2n-1)\pi(u_j + u_\ell - v_j - v_\ell)/2K\} \\ \exp\{i(2n-1)\pi(u_\ell - u_j - v_j - v_\ell)/2K\} \end{pmatrix} F^{(\ell)}_{r,m} \exp(i\pi r u_\ell/2K)$$

$$= \sum_{n=-\infty}^{\infty} F^{(j)}_{n,m} \exp(i\pi n u_j/2K) \lambda^{(i)}_m \quad . \qquad m = 1, 2, \ldots \tag{2.5.6}$$

After performing the integration, we have

$$\sum_{n=-\infty}^{\infty} \frac{1}{(1+q^{2n-1})} \begin{pmatrix} \exp\{i(2n-1)\pi(-u_j + v_j + v_\ell)/2K\} \\ -\exp\{i(2n-1)\pi(u_j + v_j + v_\ell)/2K\} \\ \vdots \\ -\exp\{i(2n-1)\pi(u_j - v_j - v_\ell)/2K\} \\ \exp\{i(2n-1)\pi(-u_j - v_j - v_\ell)/2K\} \end{pmatrix} F^{(\ell)}_{-2n+1,m}$$

$$= \sum_{n=-\infty}^{\infty} F^{(j)}_{n,m} \exp(i\pi n u_j/2K) \lambda^{(i)}_m \quad . \qquad m = 1, 2, \ldots \tag{2.5.7}$$

Define ω_ℓ by

$$\omega_\ell = q^{\frac{1}{2}} \exp(-i\pi v_\ell/K) , \ \ell = 1, 2, 3. \tag{2.5.8}$$

Noting that

$$\omega_1 \omega_2 \omega_3 = q \quad , \tag{2.5.9}$$

and equating terms in (2.5.7) we have

$$F^{(j)}_{2n,m} = 0 \tag{2.5.10}$$

and

$$\frac{1}{(1+q^{-2n+1})} \begin{pmatrix} \omega_i^{-n+\frac{1}{2}} & 0 \\ 0 & \omega_i^{n-\frac{1}{2}} \end{pmatrix} F^{(\ell)}_{2n-1,m} - \frac{1}{(1+q^{2n-1})} \begin{pmatrix} 0 & \omega_i^{-n+\frac{1}{2}} \\ \omega_i^{n-\frac{1}{2}} & 0 \end{pmatrix} F^{(\ell)}_{-2n+1,m}$$

$$= F^{(j)}_{2n-1,m} \lambda^{(i)}_m \qquad \begin{matrix} n = 1, 2, \ldots \\ m = 1, 2, \ldots \end{matrix} \tag{2.5.11}$$

The left-hand side of the equation is unchanged if we change $(2n-1)$ to $(-2n+1)$ and at the same time premultiply it by $-\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Thus, requiring that all the $\lambda^{(i)}_m$ to be non-singular,

$$F^{(j)}_{2n-1,m} = -\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} F^{(j)}_{-2n+1,m} \quad . \tag{2.5.12}$$

Substituting back to (2.5.11) gives

$$\begin{pmatrix} \omega_i^{-n+\frac{1}{2}} & 0 \\ 0 & \omega_i^{n-\frac{1}{2}} \end{pmatrix} F^{(\ell)}_{2n-1,m} = F^{(j)}_{2n-1,m} \lambda^{(i)}_m \quad . \tag{2.5.13}$$

Using all three cyclic permutations of $1\ 2\ 3$ for $i\ j\ \ell$, we obtained three coupled equations :

$$\begin{pmatrix} \omega_1^{-n+\frac{1}{2}} & 0 \\ 0 & \omega_1^{n-\frac{1}{2}} \end{pmatrix} F^{(3)}_{2n-1,m} = F^{(2)}_{2n-1,m}\ \lambda^{(1)}_m$$

$$\begin{pmatrix} \omega_2^{-n+\frac{1}{2}} & 0 \\ 0 & \omega_2^{n-\frac{1}{2}} \end{pmatrix} F^{(1)}_{2n-1,m} = F^{(3)}_{2n-1,m}\ \lambda^{(2)}_m$$

$$\begin{pmatrix} \omega_3^{-n+\frac{1}{2}} & 0 \\ 0 & \omega_3^{n-\frac{1}{2}} \end{pmatrix} F^{(2)}_{2n-1,m} = F^{(1)}_{2n-1,m}\ \lambda^{(3)}_m$$

$$n,\ m = 1,\ 2,\ \ldots \quad . \qquad (2.5.14)$$

Combining the three equations and noting that from (2.4.6)

$$\lambda_m = \lambda^{(1)}_m\ \lambda^{(2)}_m\ \lambda^{(3)}_m \qquad (2.5.15)$$

and all the $\lambda^{(\ell)}_m$s commute with each other, we obtain

$$\begin{pmatrix} q^{-n+\frac{1}{2}} & 0 \\ 0 & q^{n-\frac{1}{2}} \end{pmatrix} F^{(\ell)}_{2n-1,m} = F^{(\ell)}_{2n-1,m}\ \lambda_m$$

$$\ell = 1,\ 2,\ 3\ ;\quad n,\ m = 1,\ 2,\ \ldots \qquad (2.5.16)$$

Hence, each λ_m has eigenvalues which are odd integer powers of $q^{\frac{1}{2}}$. Arrange the λ_m s in such a way that the eigenvalues for λ_m ($m = 1,\ 2,\ \ldots$) are $q^{-m+\frac{1}{2}}$ and $q^{m-\frac{1}{2}}$, then, for a given m, we must have

$$F_{n,m} = 0 \quad \text{unless} \quad n = \pm\,(2m-1) \quad . \qquad (2.5.17)$$

In view of the structure of λ_m defined in (2.4.3) we may write

$$\lambda_m = \tfrac{1}{2} \begin{pmatrix} q^{-m+\frac{1}{2}}+q^{m-\frac{1}{2}} & i(q^{-m+\frac{1}{2}}-q^{m-\frac{1}{2}}) \\ -i(q^{-m+\frac{1}{2}}-q^{m-\frac{1}{2}}) & q^{-m+\frac{1}{2}}+q^{m-\frac{1}{2}} \end{pmatrix}$$

$$(2.5.18)$$

From (2.5.16), $F^{(\ell)}_{2m-1,m}$ must then take up the form

$$F^{(\ell)}_{2m-1,m} = \begin{pmatrix} -i\rho^{(\ell)}_m & \rho^{(\ell)}_m \\ i\nu^{(\ell)}_m & \nu^{(\ell)}_m \end{pmatrix} \qquad (2.5.19a)$$

and hence

$$F^{(\ell)}_{-2m+1,m} = \begin{pmatrix} -i\nu^{(\ell)}_m & -\nu^{(\ell)}_m \\ i\rho^{(\ell)}_m & -\rho^{(\ell)}_m \end{pmatrix} \qquad (2.5.19b)$$

$$\ell = 1, 2, 3 ; \quad m = 1, 2, \ldots$$

for some $\rho^{(\ell)}_m$ and $\nu^{(\ell)}_m$, ($\ell = 1, 2, 3$). Also, we have

$$f^{(\ell)}_m(u) = \left[\exp(i\pi(2m-1)u/2K) - \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\exp(-i\pi(2m-1)u/2K)\right] F^{(\ell)}_{2m-1,m}$$

$$\ell = 1, 2, 3 \ .$$
$$m = 1, 2, \ldots \ . \qquad (2.5.20)$$

§ 5.2 ORTHOGONALITY PROPERTIES OF P_ℓ

$\rho^{(\ell)}_m$ and $\nu^{(\ell)}_m$ may be determined explicitly by the orthogonality properties of P_ℓ and $\hat{P}_\ell$. Since all the $\hat{P}_\ell$ s are orthogonal matrices, using (2.4.52) and (2.4.13), we may write

$$(2\pi i)^{-1} \int_{C_\ell} p^{(\ell)T}_m(x)\, p^{(\ell)}_n(x^{-1})\, x^{-1}\, dx = \delta_{m,n} \qquad (2.5.21)$$

$$\ell = 1, 2, 3 \ .$$
$$m, n = 1, 2, \ldots \ .$$

Using (2.5.1) and applying the transformation of variable from x to u_ℓ through

$$x = k \ \mathrm{sn}(u_\ell+v_\ell) \ \mathrm{sn}(u_\ell-v_\ell) \quad , \qquad (2.5.22)$$

(2.5.2) becomes

$$-(2\pi i)^{-1} \int_{i\eta_\ell-K}^{i\eta_\ell+K} f_m^{(\ell)T}(u_\ell) \ \{D^{-1}(u_\ell,v_\ell)\}^T \ D^{-1}(iK'-u_\ell,v_\ell) \ f_n^{(\ell)}(iK'-u_\ell) \ \frac{dx}{x \ du_\ell} \ du_\ell = \delta_{m,n} \qquad (2.5.23)$$

By the definition of $D(u_\ell,v_\ell)$ in (2.4.47), we have

$$\{D^{-1}(u_\ell,v_\ell)\}^T \ D^{-1}(iK'-u_\ell,v_\ell) = \frac{i\,k \ \mathrm{sn}(u_\ell-v_\ell) \ \mathrm{sn}(u_\ell+v_\ell)}{\mathrm{sn}(2u_\ell)\{1-k^2\mathrm{sn}^2(u_\ell+v_\ell)\mathrm{sn}^2(u_\ell-v_\ell)\}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad (2.5.24)$$

and so the left-hand side of the integral equation becomes

$$-(k/2\pi) \int_{i\eta_\ell-K}^{i\eta_\ell+K} f_m^{(\ell)T}(u_\ell) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} f_n^{(\ell)}(iK'-u_\ell) \ du_\ell$$

$$= -(2kK/\pi) \ (q^{-m+\frac{1}{2}} + q^{m-\frac{1}{2}}) \ \rho_m^{(\ell)} \ \nu_m^{(\ell)} \ \delta_{m,n} \quad . \qquad (2.5.25)$$

Thus,

$$\rho_m^{(\ell)} \ \nu_m^{(\ell)} = -\pi \ / \ \{2kK \ (q^{-m+\frac{1}{2}}+q^{m-\frac{1}{2}}) \ \} \ . \qquad (2.5.26)$$

Further, it can be seen readily that the matrix $L_A^{-\frac{1}{2}} \mathcal{D} L_A^{\frac{1}{2}}$ is symmetric, so, it is natural to require that $L_A^{-\frac{1}{2}} P_2$ be orthogonal. From properties (iv) of the representatives,

the representative of an orthogonal matrix X is made up of two by two diagonal subblocks. This implies that $\ell_a^{-\frac{1}{2}} p_m^{(2)}(u_2)$ is diagonal. We may impose similar condition on P_1 and P_3 also.

Noting that

$$\ell_a^{-\frac{1}{2}} = \begin{pmatrix} \cosh K_2 & i \sinh K_2 \\ -i \sinh K_2 & \cosh K_2 \end{pmatrix}$$

$$= \frac{1}{(1-k^2 \mathrm{sn}^4(v_2))^{\frac{1}{2}}} \begin{pmatrix} \mathrm{cn}(v_2) & \mathrm{sn}(v_2)\mathrm{dn}(v_2) \\ -\mathrm{sn}(v_2)\mathrm{dn}(v_2) & \mathrm{cn}(v_2) \end{pmatrix} \tag{2.5.27}$$

we have

$$\ell_a^{-\frac{1}{2}} p_m^{(2)}(u_2) = \ell_a^{-\frac{1}{2}} D^{-1}(u_2, v_2) f_m^{(2)}(u_2)$$

$$= -(1-k^2 \mathrm{sn}^4(v_2))^{-\frac{1}{2}} \{\mathrm{sn}(2u_2)(1-k^2 \mathrm{sn}^2(u_2+v_2)\mathrm{sn}^2(u_2-v_2))\}^{-1}$$

$$\times \left(\begin{array}{l|l} \{\mathrm{cn}(v_2)\mathrm{sn}(u_2+v_2)\mathrm{dn}(u_2-v_2) - \mathrm{cn}(u_2+v_2)\mathrm{sn}(v_2)\mathrm{dn}(v_2)\} & -\{\mathrm{cn}(v_2)\mathrm{dn}(u_2+v_2)\mathrm{sn}(u_2-v_2) + \mathrm{cn}(u_2-v_2)\mathrm{sn}(v_2)\mathrm{dn}(v_2)\} \\ -\{\mathrm{sn}(v_2)\mathrm{dn}(v_2)\mathrm{sn}(u_2+v_2)\mathrm{dn}(u_2-v_2) + \mathrm{cn}(u_2+v_2)\mathrm{cn}(v_2)\} & \{\mathrm{dn}(u_2+v_2)\mathrm{sn}(u_2-v_2)\mathrm{sn}(v_2)\mathrm{dn}(v_2) - \mathrm{cn}(v_2)\mathrm{cn}(u_2-v_2)\} \end{array} \right)$$

$$\times f_m^{(2)}(u_2) \tag{2.5.28}$$

Using the identity given in (II.A.6) of Appendix IIA, we may simplify (2.5.28) to

$$\ell_a^{-\frac{1}{2}} p_m^{(2)}(u_2) = \frac{\{1-k^2\mathrm{sn}^2(u_2+v_2)\mathrm{sn}^2(u_2-v_2)\}}{2\ (1-k^2\mathrm{sn}^4(v_2))^{\frac{1}{2}}} \begin{pmatrix} i(\rho_m^{(2)}+\nu_m^{(2)})(e^{-r}+e^{r})/\mathrm{cn}(u_2) \\ i(\rho_m^{(2)}-\nu_m^{(2)})(e^{-r}-e^{r})/\mathrm{sn}(u_2)\mathrm{dn}(u_2) \\ \vdots \\ (\rho_m^{(2)}-\nu_m^{(2)})(e^{-r}+e^{r})/\mathrm{cn}(u_2) \\ (\rho_m^{(2)}+\nu_m^{(2)})(e^{-r}-e^{r})/\mathrm{sn}(u_2)\mathrm{dn}(u_2) \end{pmatrix}$$

$$m = 1, 2, \ldots \qquad (2.5.29)$$

where $r = i\pi(2m-1)u_2/2K$. Hence, requiring that $\ell_a^{-\frac{1}{2}} p_m^{(2)}(u_2)$ to be diagonal implies that $\rho_m^{(2)}$ and $\nu_m^{(2)}$ must be equal. Similar results may be obtained for $\rho_m^{(1)}$, $\nu_m^{(1)}$ and $\rho_m^{(3)}$, $\nu_m^{(3)}$. So from (2.5.26)

$$\rho_m^{(\ell)} = \nu_m^{(\ell)} = \pm i\ \{\pi/2kK(q^{-m+\frac{1}{2}}+q^{m-\frac{1}{2}})\}^{\frac{1}{2}} \qquad (2.5.30)$$

$$\ell = 1, 2, 3 ; \quad m = 1, 2, \ldots$$

independent of ℓ . This simplifies $f_m^{(\ell)}(u)$ to

$$f_m^{(\ell)}(u) = \pm\left[\frac{\pi}{2kK(q^{-m+\frac{1}{2}}-q^{m-\frac{1}{2}})}\right]^{\frac{1}{2}} \begin{pmatrix} (e^{r}+e^{-r}) & i(e^{r}-e^{-r}) \\ -(e^{r}+e^{-r}) & i(e^{r}-e^{-r}) \end{pmatrix} \qquad (2.5.31)$$

where $r = i\pi(2m-1)u/2K$. Finally, if we substitute (2.5.30) to (2.5.13) for $n = m$, we obtain

$$\lambda_m^{(\ell)} = \tfrac{1}{2} \begin{pmatrix} \omega_\ell^{-m+\frac{1}{2}}+\omega_\ell^{m-\frac{1}{2}} & i(\omega_\ell^{-m+\frac{1}{2}}-\omega_\ell^{m-\frac{1}{2}}) \\ -i(\omega_\ell^{-m+\frac{1}{2}}-\omega_\ell^{m-\frac{1}{2}}) & \omega_\ell^{-m+\frac{1}{2}}+\omega_\ell^{m-\frac{1}{2}} \end{pmatrix}$$

$$\ell = 1, 2, 3 ; \quad m = 1, 2, \ldots \qquad (2.5.32)$$

§ 5.3 ANALYTICITY OF $p_m^{(\ell)}(x)$

We still need to check the analyticity of $p_m^{(\ell)}(x)$ within and on the contour of integration.

Since the solution for $f_m^{(\ell)}(u_\ell)$ in (2.5.31) is an entire function of u_ℓ, $p_m^{(\ell)}(u_\ell)$ is analytic except at the simple poles of $D^{-1}(u_\ell, v_\ell)$, i.e. at $u_\ell = nK + in'K'$ for any integers n and n'. Consider the residue of $p_m^{(\ell)}(u_\ell)$ at the pole $u_\ell = 2nK$:

$$\lim_{u_\ell \to 2nK} D^{-1}(u_\ell, v_\ell)\, f_m^{(\ell)}(u_\ell) = \frac{-\rho_m^{(\ell)}}{(1-k^2 sn^4(v_\ell))} \begin{pmatrix} sn(v_\ell)dn(v_\ell) & sn(v_\ell)dn(v_\ell) \\ -cn(v_\ell) & -cn(v_\ell) \end{pmatrix}$$

$$\times \begin{pmatrix} -2i & 0 \\ 2i & 0 \end{pmatrix}$$

$$= 0 \quad . \tag{2.5.33a}$$

Also, at $u_\ell = (2n+1)K$,

$$\lim_{u_\ell \to (2n+1)K} D^{-1}(u_\ell, v_\ell)\, f_m^{(\ell)}(u_\ell) = \frac{\rho_m^{(\ell)} k' dn^2(v_\ell)}{(dn^4(v_\ell) - k^2 cn^4(v_\ell))} \times$$

$$\begin{pmatrix} -cn(v_\ell) & cn(v_\ell) \\ -sn(v_\ell)dn(v_\ell) & sn(v_\ell)dn(v_\ell) \end{pmatrix} \times \begin{pmatrix} 0 & 2(-1)^m i \\ 0 & 2(-1)^m i \end{pmatrix}$$

$$= 0 \quad . \tag{2.5.33b}$$

Hence, $p_m^{(\ell)}(u_\ell)$ is in fact analytic at $u_\ell = nK$ for all integers n and so it is analytic in the strip $0 < u_\ell < iK'$. However, the mapping from x to u_ℓ as given in (2.5.22) is not conformal at $u_\ell = nK$ since (dx/du_ℓ) is zero at

this point also. Yet, from (2.5.31) and (2.4.47)

$$f_m^{(\ell)}(-u_\ell) = -\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} f_m^{(\ell)}(u_\ell) \qquad (2.5.34)$$

and

$$D(-u_\ell, v_\ell) = -\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} D(u_\ell, v_\ell) \quad , \qquad (2.5.35)$$

so,

$$p_m^{(\ell)}(u_\ell) = p_m^{(\ell)}(-u_\ell) \quad . \qquad (2.5.36)$$

By periodicity of $p_m^{(\ell)}(u_\ell)$ and $x(u_\ell)$, we then have

$$\begin{aligned} p_m^{(\ell)}(nK+u_\ell-nK) &= p_m^{(\ell)}(-u_\ell+2nK) \\ &= p_m^{(\ell)}(nK-(u_\ell-nK)) \end{aligned} \qquad (2.5.37)$$

So, $p_m^{(\ell)}(u_\ell)$ is an even function of $(u_\ell-nK)$ for any integer n and so $p_m^{(\ell)}(x)$ is analytic at the point

$$x = -k\ \mathrm{sn}^2(v_\ell) \quad . \qquad (2.5.38)$$

Hence, $p_m^{(\ell)}(x)$ is analytic inside and on c_ℓ . In fact, the only singularity of $p_m^{(\ell)}(x)$ are branch points at the points in the x plane corresponding to $u_\ell = nK \pm iK'$, i.e.

$$x = -(k\ \mathrm{sn}^2(v_\ell))^{-1} \quad . \qquad (2.5.39)$$

When $T < T_c$, $0 < k < 1$, this is greater than unity and so is R the radius of convergence. Hence the summation in (2.4.12) is convergent at least inside and on the unit circle.

THE DIAGONAL FORM OF THE CORNER TRANSFER MATRICES AND THE SPONTANEOUS MAGNETIZATION

6

§ 6.1 THE DIAGONAL FORM OF THE CTM

In Section II.5, we have obtained $\lambda_m^{(\ell)}$, $\ell = 1, 2, 3$ and λ_m and hence $\hat{A}_d$, $\hat{B}_d$, $\hat{C}_d$ and $\hat{\mathcal{D}}_d$. Using property (v) of the representatives, we can determine A_d , B_d , C_d and $\mathcal{D}_d$ within a multiplicative constant. For instance, the matrix $\mathcal{D}_d$ can be written as

$$\mathcal{D}_d = \text{const.} \times \prod_{j=1}^{\infty} \tfrac{1}{2}\{(1+q^{j-\frac{1}{2}})+(1-q^{j-\frac{1}{2}})s_j s_{j+1}\} \quad (2.6.1)$$

We now consider the following transformation of the representation (which corresponds to merely re-arranging the rows and columns of the matrices). We replace σ_1 , σ_2 , ... , σ_n and σ_1' , σ_2' , ... , σ_n' by the new spin variables μ_1 , μ_2 , ... , μ_n and μ_1' , μ_2' , ... , μ_n' through

$$\mu_j = \sigma_j \sigma_{j+1} \; ; \quad \mu_j' = \sigma_j' \sigma_{j+1}' \; ; \qquad j = 1, 2, \ldots, n-1 \quad (2.6.2)$$

and $\mu_n = \sigma_n$, $\mu_n' = \sigma_n'$.

Under this transformation, we have

$$s_j s_{j+1} \to s_j \; ; \quad s_1 \to s_1 s_2 \ldots s_n \quad (2.6.3)$$

with the new s_j , c_j , d_j defined under the new spin representation μ_j and μ_j' . Hence, the matrix S in (2.2.9) under the new representation is given by

$$S = s_1 s_2 \ldots s_n$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \ldots \qquad (2.6.4)$$

and also, (2.6.1) becomes

$$\mathscr{D}_d = \text{const.} \times \prod_{j=1}^{n} \tfrac{1}{2}\{(1+q^{j-\frac{1}{2}})+(1-q^{j-\frac{1}{2}})s_j\} \qquad (2.6.5)$$

The diagonal form of the matrix $\mathscr{D}$ can therefore be written in a direct product form

$$\mathscr{D}_d = \text{const.} \times \begin{pmatrix} 1 & 0 \\ 0 & q^{\frac{1}{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & q^{\frac{3}{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & q^{\frac{5}{2}} \end{pmatrix} \otimes \ldots \qquad (2.6.6)$$

Using a similar argument, A_d , B_d and C_d can also be written in this form under the new representation :

$$A_d = \text{const.} \times \begin{pmatrix} 1 & 0 \\ 0 & \omega_1^{\frac{1}{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & \omega_1^{\frac{3}{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & \omega_1^{\frac{5}{2}} \end{pmatrix} \otimes \ldots$$

$$B_d = \text{const.} \times \begin{pmatrix} 1 & 0 \\ 0 & \omega_2^{\frac{1}{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & \omega_2^{\frac{3}{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & \omega_2^{\frac{5}{2}} \end{pmatrix} \otimes \ldots$$

$$C_d = \text{const.} \times \begin{pmatrix} 1 & 0 \\ 0 & \omega_3^{\frac{1}{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & \omega_3^{\frac{3}{2}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & \omega_3^{\frac{5}{2}} \end{pmatrix} \otimes \ldots \qquad (2.6.7)$$

The matrix A_d (similarly B_d or C_d) obtained depends on v_1 (v_2 or v_3 respectively) only through $\omega_1 = \exp\{-i\pi(v_1-\frac{1}{2}iK')/K\}$. Hence it can be written in the form $\exp\{(v_1-\frac{1}{2}iK')\mathcal{H}\}$, where $\mathcal{H}$ is a diagonal matrix independent of v_1 , v_2 and v_3 .

$$\mathcal{H} = -\frac{i\pi}{4K} \sum_{j=1}^{\infty} (2j-1)\ (1-s_j s_{j+1}) \quad . \qquad (2.6.8)$$

Unfortunately, the matrices P_1 , P_2 and P_3 do not appear to have any simple structure, but we do note from (2.5.1) and (2.5.31) that P_1 depends only on k and v_1 (not on v_2 or v_3), and similarly for P_2 and P_3 .

Although each CTM A (B or C) depends on all the three parameters v_1 , v_2 and v_3 , yet as seen from (2.4.7) ,

$$A = P_2\ A_d\ P_3^{-1} \qquad (2.6.9)$$

and from the fact that P_j depends only on v_j ($j = 1$, 2 or 3) , the CTMs can be factorized into a product of three matrices each of which depends on only one of the parameters in the limit of an infinite lattice. For example

$$A = P(v_2)\ A_d(v_1)\ P^{-1}(v_3) \quad . \qquad (2.6.10)$$

§ 6.2 THE SPONTANEOUS MAGNETIZATION

In the original representation, all the matrices A , B and C break into two diagonal blocks corresponding to $\sigma_1 = +1$ or -1 and so are all the P_ℓ s . Also, in this representation

$$S = \begin{pmatrix} I & \\ & -I \end{pmatrix} \quad . \tag{2.6.11}$$

Hence, all the matrices (A , B , C and P_ℓ , $\ell = 1, 2, 3$) commute with S . This is still true when we go to the new spin representation μ_j and μ_j' as suggested in (2.6.2) . Hence from (2.2.8) , we may write the spontaneous magnetization as

$$\begin{aligned} M &= \frac{\text{Trace}\{ S(ABC)^2 \}}{\text{Trace}\{ (ABC)^2 \}} \\ &= \prod_{j=1}^{\infty} \left[\frac{1-q^{2j-1}}{1+q^{2j-1}} \right] \\ &= (k')^{\frac{1}{4}} \\ &= (1-k^2)^{\frac{1}{8}} \end{aligned} \tag{2.6.12}$$

which is just the exact result obtained by other methods (Stephenson, 1964).

CONCLUSION

The most interesting result obtained in this work is the diagonal form of the CTMs A , B , C and their products. The fact that $\mathcal{D}_d$ can be written in a direct product form in essentially the same way as the square lattice suggests that this may be an inherent characteristic of a ferromagnetic Ising model independent of the type of lattice.

No new thermodynamic result has yet been obtained by this approach. For this, we will need to have a better knowledge of the diagonalizing matrices P_ℓ ($\ell = 1, 2, 3$) . However, it is hoped that the simplicity of the final expression for the diagonal form of the corner transfer matrices may provide illuminating insights into the model.

THE JACOBIAN ELLIPTIC FUNCTIONS AND THETA FUNCTIONS

The technique of elliptic functions has played an important role in the evaluation of the CTMs. For the convenience of the reader, we give here some of the properties and relations between the three Jacobian elliptic functions as well as their relations with the Theta functions. This account is by no means complete and only relations relevant to the derivations for the work are quoted here. For a more complete understanding of the functions, the reader is referred to Byrd and Friedman (1954); Gradstein and Ryshik (1965); Neville (1971).

The Jacobian elliptic functions sn , cn and dn (with modulus k) are double-periodic functions with two poles of first order in each period parallelogram. Their periods, zeros, poles and residues are given in Table IIA.1.

The elliptic functions are related to the Theta functions through

$$\mathrm{sn}(u) = \mathrm{H}(u) \,/\, k^{\frac{1}{2}}\, \Theta(u)$$

$$\mathrm{cn}(u) = (k'/k)^{\frac{1}{2}}\, \mathrm{H}_1(u) \,/\, \Theta(u)$$

and

$$\mathrm{dn}(u) = k'^{\frac{1}{2}}\, \Theta_1(u) \,/\, \Theta(u) \qquad \text{(II.A.1)}$$

Table IIA.1. Periods, zeros, poles and residues of $sn(u,k)$, $cn(u,k)$ and $dn(u,k)$. (Gradstein and Ryshik, 1965)

	Periods	Zeros	Poles	Residues
$sn(u)$	$4mK+2niK'$	$2mK+2niK'$	$2mK+(2n+1)iK'$	$(-1)^m/k$
$cn(u)$	$4mK+2n(K+iK')$	$(2m+1)K+2niK'$	$2mK+(2n+1)iK'$	$(-1)^{m-1}i/k$
$dn(u)$	$2mK+4niK'$	$(2m+1)K+(2n+1)iK'$	$2mK+(2n+1)iK'$	$(-1)^{n-1}i$

(K and K' are the complete elliptic integral of the first kind with moduli k and $k' = (1-k^2)^{\frac{1}{2}}$ respectively.)

The following relations between the Jacobian elliptic functions and Theta functions are useful for our analysis :

(i) $$sn^2(u) + cn^2(u) = 1$$
$$k^2 cn^2(u) + dn^2(u) = 1 \qquad \text{(II.A.2)}$$

(ii) $$sn(a)sn(b) - sn(c)sn(d) = \frac{\Theta(0)\Theta(a+b)H(a-d)H(b-d)}{k\,\Theta(a)\Theta(b)\Theta(c)\Theta(d)}$$
$$1 - k^2 sn(a)sn(b)sn(c)sn(d) = \frac{\Theta(0)\Theta(a+b)\Theta(a-d)\Theta(b-d)}{\Theta(a)\Theta(b)\Theta(c)\Theta(d)} \qquad \text{(II.A.3)}$$

where $a+b = c+d$ (Baxter, 1972).

(iii) $$sn(a\pm b) = (sn(a)cn(b)dn(b) \pm sn(b)cn(a)dn(a))/(1-k^2sn^2(a)sn^2(b))$$
$$cn(a\pm b) = (cn(a)cn(b) \mp sn(a)sn(b)dn(a)dn(b))/(1-k^2sn^2(a)sn^2(b))$$
$$dn(a\pm b) = (dn(a)dn(b) \mp k^2 sn(a)sn(b)cn(a)cn(b))/(1-k^2sn^2(a)sn^2(b)) \qquad \text{(II.A.4)}$$

(iv) $$cn(a)cn(b) - dn(a+b)sn(a)sn(b) = cn(a+b)$$
$$dn(a)dn(b) - k^2 cn(a+b)sn(a)sn(b) = dn(a+b) \qquad \text{(II.A.5)}$$

(v) Using (iv) above, we may further establish the identities

$$\mathrm{cn}(b)\,\mathrm{sn}(a+b)\,\mathrm{dn}(a-b) - \mathrm{cn}(a+b)\,\mathrm{sn}(b)\,\mathrm{dn}(b)$$
$$= \mathrm{cn}(b)\,\mathrm{sn}(a-b)\,\mathrm{dn}(a+b) + \mathrm{cn}(a-b)\,\mathrm{sn}(b)\,\mathrm{dn}(b)$$

and

$$\mathrm{cn}(a+b)\,\mathrm{cn}(b) + \mathrm{sn}(a+b)\,\mathrm{dn}(a-b)\,\mathrm{sn}(b)\,\mathrm{dn}(b)$$
$$= \mathrm{cn}(a-b)\,\mathrm{cn}(b) - \mathrm{sn}(a-b)\,\mathrm{dn}(a+b)\,\mathrm{sn}(b)\,\mathrm{dn}(b)\ . \qquad \text{(II.A.6)}$$

We state also the Liouville's theorem for analytic functions which is useful in various parts of the calculations :

Liouville's theorem

If a function of z is analytic at all points in the complex z plane and is bounded everywhere, including everywhere at $|z| = \infty$, then the function is a mere constant, independent of z.

It is a direct consequence of this theorem that a doubly periodic function without singularity is a constant.

THE KERNEL $W_i(u_j, u_\ell)$

We apply the following transformation as given in (2.4.44) to the variables x , y and z .

$$\begin{aligned} x &= k\ \mathrm{sn}(u_1+v_1)\ \mathrm{sn}(u_1-v_1) \\ y &= k\ \mathrm{sn}(u_2+v_2)\ \mathrm{sn}(u_2-v_2) \\ z &= k\ \mathrm{sn}(u_3+v_3)\ \mathrm{sn}(u_3-v_3) \end{aligned} \qquad \text{(II.B.1)}$$

and substitute it into (2.4.41) to obtain the corresponding kernel of the integrals in the u_ℓ plane.

Firstly, consider $\Delta(y, z^{-1})$ as a quadratic function in y .

$$z^2\Delta(y,z^{-1}) = y^2(1+z\delta\beta) + y\{\delta\beta'(1+z^2)-2z(\beta\beta'+\alpha\alpha'\gamma)\} + z^2 + z\delta\beta \qquad \text{(II.B.2)}$$

Let y_1 , y_2 be the roots of the equation. The product of the roots is given by

$$\begin{aligned} y_1\ y_2 &= \frac{z\ (z+\delta\beta)}{(1+z\,\delta\beta)} \\ &= \frac{k^2\mathrm{sn}(u_3+v_3)\mathrm{sn}(u_3-v_3)(\mathrm{sn}(u_3+v_3)\mathrm{sn}(u_3-v_3)-\mathrm{sn}(2v_2+2v_3)\mathrm{sn}(2v_2))}{(\ 1\ -\ k^2\mathrm{sn}(u_3+v_3)\mathrm{sn}(u_3-v_3)\mathrm{sn}(2v_2+2v_3)\mathrm{sn}(2v_2)\ )} \\ &= k^2\mathrm{sn}(u_3+v_3)\mathrm{sn}(u_3-v_3)\mathrm{sn}(u_3+v_3+2v_2)\mathrm{sn}(u_3-v_3-2v_2) \end{aligned} \qquad \text{(II.B.3)}$$

(using identities (II.A.3)).

The sum of the roots is

$$y_1 + y_2 = -\{\delta\beta'(1+z^2)-2z(\beta\beta'+\alpha\alpha'\gamma)\} / (1+z\delta\beta)$$

$$= k\{\mathrm{sn}(2v_2+2v_3)\,\mathrm{sn}(2v_3)(1+k^2\mathrm{sn}^2(u_3+v_3)\,\mathrm{sn}^2(u_3-v_3)) +$$

$$2\mathrm{sn}(u_3+v_3)\,\mathrm{sn}(u_3-v_3)(\mathrm{cn}(2v_2)\,\mathrm{cn}(2v_3)\,\mathrm{dn}(2v_2+2v_3)-\mathrm{sn}(2v_2)\,\mathrm{sn}(2v_3))\}$$

$$/\ (\ 1 - k^2\mathrm{sn}(u_3+v_3)\,\mathrm{sn}(u_3-v_3)\,\mathrm{sn}(2v_2+2v_3)\,\mathrm{sn}(2v_2)\ )$$

$$= f(u_3) \quad . \qquad \text{(II.B.4)}$$

$f(u_3)$ is a doubly-periodic function of u_3 with period $(\ 2mK\ ,\ 2inK'\ )$ with

(i) $u_3 + v_3 = 2mK + (2n+1)iK'$;

(ii) $u_3 - v_3 = 2mK + (2n+1)iK'$;

(iii) $u_3 + v_3 + 2v_2 = 2mK + (2n+1)iK'$;

(iv) $u_3 - v_3 - 2v_2 = 2mK + (2n+1)iK'$;

for all integers m and n , as its poles of singularities. The residues of the function at these poles are given by :

(i) at $u_3 + v_3 = iK'$,

$$\lim_{u_3 \to iK'-v_3} (u_3+v_3-iK')\, f(u_3) = 1/k\,\mathrm{sn}(2v_2) \qquad \text{(II.B.5a)}$$

(ii) at $u_3 - v_3 = iK'$,

$$\lim_{u_3 \to iK'+v_3} (u_3-v_3-iK')\, f(u_3) = -1/k\,\mathrm{sn}(2v_2) \qquad \text{(II.B.5b)}$$

(iii) at $u_3 + v_3 + 2v_2 = iK'$,

$$\lim_{u_3 \to iK'-v_3-2v_2} (u_3+v_3+2v_2-iK')\, f(u_3) = -1/k\,\mathrm{sn}(2v_2) \qquad \text{(II.B.5c)}$$

and

(iv) at $u_3 - v_3 - 2v_2 = iK'$,

$$\lim_{u_3 \to iK' + v_3 + 2v_2} (u_3 - v_3 - 2v_2 - iK')\, f(u_3) = 1/k\,\mathrm{sn}(2v_2) \quad . \tag{II.B.5d}$$

So, $f(u_3)$ has the same poles and residues as the following function

$$g(u_3) = k\,(\mathrm{sn}(u_3+v_3)\,\mathrm{sn}(u_3+v_3+2v_2) + \mathrm{sn}(u_3-v_3)\,\mathrm{sn}(u_3-v_3-2v_2)) \tag{II.B.6}$$

and hence by Liouville's theorem, $f(u_3)$ must be differ from $g(u_3)$ by a constant only (independent of u_3). Consider the point at $u_3 + v_3 = 0$, we have

$$\begin{aligned} f(-v_3) &= k\ \mathrm{sn}(2v_3)\ \mathrm{sn}(2v_2+2v_3) \\ &= g(-v_3) \quad . \end{aligned} \tag{II.B.7}$$

So, we must have $f(u_3)$ the same as $g(u_3)$ or

$$f(u_3) = k\mathrm{sn}(u_3+v_3)\,\mathrm{sn}(u_3+v_3+2v_2) + k\mathrm{sn}(u_3-v_3)\,\mathrm{sn}(u_3-v_3-2v_2) \tag{II.B.8}$$

Together with (II.B.3), we conclude that

$$y_1 = k\ \mathrm{sn}(u_3+v_3)\ \mathrm{sn}(u_3+v_3+2v_2)$$

and

$$y_2 = k\ \mathrm{sn}(u_3-v_3)\ \mathrm{sn}(u_3-v_3-2v_2) \tag{II.B.9}$$

and $\Delta(y, z^{-1})$ is given by

$$\begin{aligned} z^2\Delta(y,z^{-1}) &= k^2(1-k^2\mathrm{sn}(u_3+v_3)\,\mathrm{sn}(u_3-v_3)\,\mathrm{sn}(2v_2+2v_3)\,\mathrm{sn}(2v_2)) \\ &\quad \times (\mathrm{sn}(u_2+v_2)\,\mathrm{sn}(u_2-v_2) - \mathrm{sn}(u_3+v_3)\,\mathrm{sn}(u_3+v_3+2v_2)) \\ &\quad \times (\mathrm{sn}(u_2+v_2)\,\mathrm{sn}(u_2-v_2) - \mathrm{sn}(u_3-v_3)\,\mathrm{sn}(u_3-v_3-2v_2)) \end{aligned} \tag{II.B.10}$$

[cf. (2.4.46)] .

Now, the kernel $W_1(u_2,u_3)$ is given by

$$W_1(u_2,u_3) = \frac{dz}{z\,du_3}\,\Phi(y,z^{-1}) \qquad \text{(II.B.11)}$$

Substitute (2.4.41) and (II.B.1) to it,

$$W_1(u_2,u_3) = \eta k \left\{ \begin{array}{l} \{cn(2v_3)(sn(u_3+v_3)sn(u_3-v_3)-sn(2v_2)sn(2v_2+2v_3)) \\ \quad - cn(2v_2)dn(2v_2+2v_3)sn(u_2+v_2)sn(u_2-v_2)\} \\ \\ \{cn(2v_2)cn(2v_3)sn(2v_2+2v_3)-sn(2v_3)dn(2v_2+2v_3)sn(u_3+v_3) \\ \quad sn(u_3-v_3) - sn(2v_2)dn(2v_2+2v_3)sn(u_2+v_2)sn(u_2-v_2)\} \end{array} \right.$$

$$\left. \begin{array}{l} \{sn(2v_3)(sn(u_3+v_3)sn(u_3-v_3)-sn(2v_2)sn(2v_2+2v_3)) + \\ sn(u_2+v_2)sn(u_2-v_2)(sn(2v_2)-k^2sn(2v_2+2v_3)sn(u_3+v_3)sn(u_3-v_3))\} \\ \\ \{cn(2v_3)dn(2v_2+2v_3)sn(u_3+v_3)sn(u_3-v_3) - \\ \quad cn(2v_2)(sn(u_2+v_2)sn(u_2-v_2)-sn(2v_3)sn(2v_2+2v_3))\} \end{array} \right.$$

$$= k\,\eta\,R(u_2,u_3) \qquad \text{(II.B.12)}$$

where

$$\eta = \frac{dz}{du_3}\,\left(\, z^2\,\Delta(y,z^{-1})\,\right)^{-1}$$

$$= \frac{sn(2u_3)\,\left(\,1 - k^2 sn^2(u_3+v_3)sn^2(u_3-v_3)\,\right)}{k\,z^2\,\Delta(y,z^{-1})} \qquad \text{(II.B.13)}$$

If we temporarily regard $W_1(u_2,u_3)$ ($\equiv W(u_3)$) as a function of u_3 only, with u_2 , v_2 and v_3 being fixed, then $W(u_3)$ is a doubly-periodic function of period $(2K\ ,\ 2iK')$ and also

$$W(u_3) = -\,W(-u_3) \quad . \qquad \text{(II.B.14)}$$

The only poles of $W(u_3)$ are simple poles of η at

$$\begin{aligned}
&\text{(i)} \quad u_3 = u_2 - v_2 - v_3 + 2mK + 2niK' \ , \\
&\text{(ii)} \quad u_3 = u_2 + v_2 + v_3 + 2mK + 2niK' \ , \\
&\text{(iii)} \quad u_3 = -u_2 + v_2 + v_3 + 2mK + 2niK' \ , \\
&\text{(iv)} \quad u_3 = -u_2 - v_2 - v_3 + 2mK + 2niK' \ .
\end{aligned} \tag{II.B.15}$$

Note that the matrix R in (II.B.12) has zero determinants at these poles. For the residues at these poles, by periodicity of $W(u_3)$, we may just consider the case in which $m = n = 0$.

(i) At $u_3 = u_2 - v_2 - v_3$, with repeated usage of (II.A.3) to (II.A.5), we find that

$$\begin{aligned}
&\lim_{u_3-u_2+v_2+v_3\to 0} (u_3-u_2+v_2+v_3)\, k\, \eta \\
&= -1 \,/\, \{\mathrm{sn}(2u_2)\,\mathrm{sn}(2v_2+2v_3)(1-k^2\mathrm{sn}^2(u_2+v_2)\,\mathrm{sn}^2(u_2-v_2))\}
\end{aligned} \tag{II.B.16}$$

and the matrix R at $u_3 = u_2 - v_2 - v_3$ becomes

$$R = \mathrm{sn}(2v_2+2v_3) \begin{pmatrix} -\mathrm{sn}(u_2+v_2)\,\mathrm{dn}(u_2-v_2)\,\mathrm{cn}(u_2-v_2-2v_3) & \vdots & \mathrm{sn}(u_2+v_2)\,\mathrm{dn}^2(u_2-v_2)\,\mathrm{sn}(u_2-v_2-2v_3) \\ \mathrm{cn}(u_2+v_2)\,\mathrm{cn}(u_2-v_2-2v_3) & \vdots & -\mathrm{cn}(u_2+v_2)\,\mathrm{dn}(u_2-v_2)\,\mathrm{sn}(u_2-v_2-2v_3) \end{pmatrix} \tag{II.B.17}$$

Noting that in this case $u_3 + v_3 = u_2 - v_2$ and $u_3 - v_3 = u_2 - v_2 - 2v_3$, the residue of $W(u_3)$ at $u_3 = u_2 - v_2 - v_3$ is

$$-\{\mathrm{sn}(2u_2)(1-k^2\mathrm{sn}^2(u_2+v_2)\mathrm{sn}^2(u_2-v_2))\}^{-1}\begin{pmatrix}\mathrm{sn}(u_2+v_2)\mathrm{dn}(u_2-v_2)\\ -\mathrm{cn}(u_2+v_2)\end{pmatrix}$$

$$\times\quad(\ -\mathrm{cn}(u_3-v_3)\quad \mathrm{sn}(u_3-v_3)\mathrm{dn}(u_3+v_3)\ )$$

(ii) Similarly at $u_3 = u_2 + v_2 + v_3$, the residue of $W(u_3)$ is

$$\{\mathrm{sn}(2u_2)(1-k^2\mathrm{sn}^2(u_2+v_2)\mathrm{sn}^2(u_2-v_2))\}^{-1}\ \times$$

$$\begin{pmatrix}\mathrm{sn}(u_2-v_2)\mathrm{dn}(u_2+v_2)\mathrm{cn}(u_2+v_2+2v_3) & \mathrm{sn}(u_2+v_2+2v_3)\mathrm{sn}(u_2-v_2)\mathrm{dn}^2(u_2+v_2)\\ \mathrm{cn}(u_2+v_2+2v_3)\mathrm{cn}(u_2-v_2) & \mathrm{cn}(u_2-v_2)\mathrm{dn}(u_2+v_2)\mathrm{sn}(u_2+v_2+2v_3)\end{pmatrix}$$

$$= -\{\mathrm{sn}(2u_2)(1-k^2\mathrm{sn}^2(u_2+v_2)\mathrm{sn}^2(u_2-v_2))\}^{-1}$$

$$\times\begin{pmatrix}-\mathrm{sn}(u_2-v_2)\mathrm{dn}(u_2+v_2)\\ -\mathrm{cn}(u_2-v_2)\end{pmatrix}\ (\ \mathrm{cn}(u_3+v_3)\quad \mathrm{sn}(u_3+v_3)\mathrm{dn}(u_3-v_3)\ )$$

(II.B.18)

(using the fact that $u_3 + v_3 = u_2 + v_2 + 2v_3$ and $u_3 - v_3 = u_2 + v_2$.)

(iii) At $u_3 = -u_2 + v_2 + v_3$, since $W(u_3) = -W(-u_3)$, therefore ,

$$\lim_{u_3\to t}(u_3-t)\ W(u_3) = -\lim_{u_3\to -t}(u_3+t)\ W(-u_3)$$

$$= \lim_{u_3\to -t}(u_3-(-t))\ W(u_3)$$

(II.B.19)

Hence the residue in this case is the same as (i) given in (II.B.16) and (II.B.17) except that in this case, we have $u_3 + v_3 = -u_2 + v_2 + 2v_3$ and

$u_3 - v_3 = - u_2 + v_2$. So, the residue becomes

$$\{\mathrm{sn}(2u_2)(1-k^2\mathrm{sn}^2(u_2+v_2)\mathrm{sn}^2(u_2-v_2))\}^{-1} \times$$

$$\begin{pmatrix} \mathrm{sn}(u_2+v_2)\mathrm{dn}(u_2-v_2) \\ -\mathrm{cn}(u_2+v_2) \end{pmatrix} \begin{pmatrix} \mathrm{cn}(u_3+v_3) & \mathrm{sn}(u_3+v_3)\mathrm{dn}(u_3-v_3) \end{pmatrix} \qquad \text{(II.B.20)}$$

(iv) Similarly at $u_3 = - u_2 - v_2 - v_3$, the residue of $W(u_3)$ is

$$\{\mathrm{sn}(2u_2)(1-k^2\mathrm{sn}^2(u_2+v_2)\mathrm{sn}^2(u_2-v_2))\}^{-1} \times$$

$$\begin{pmatrix} -\mathrm{sn}(u_2-v_2)\mathrm{dn}(u_2+v_2) \\ -\mathrm{cn}(u_2-v_2) \end{pmatrix} \begin{pmatrix} -\mathrm{cn}(u_3-v_3) & \mathrm{sn}(u_3-v_3)\mathrm{dn}(u_3+v_3) \end{pmatrix} \qquad \text{(II.B.21)}$$

Hence, it is clear that $W(u_3)$ has the same poles and residues as the following matrix product :

$$-\{\mathrm{sn}(2u_2)(1-k^2\mathrm{sn}^2(u_2+v_2)\mathrm{sn}^2(u_2-v_2))\}^{-1} \begin{pmatrix} \mathrm{sn}(u_2+v_2)\mathrm{dn}(u_2-v_2) \\ -\mathrm{cn}(u_2+v_2) \end{pmatrix}$$

$$\vdots \begin{pmatrix} -\mathrm{sn}(u_2-v_2)\mathrm{dn}(u_2+v_2) \\ -\mathrm{cn}(u_2-v_2) \end{pmatrix} \times \begin{pmatrix} \phi(u_3-u_2+v_2+v_3) & -\phi(u_3+u_2-v_2-v_3) \\ -\phi(u_3+u_2+v_2+v_3) & \phi(u_3-u_2-v_2-v_3) \end{pmatrix}$$

$$\times \begin{pmatrix} -\mathrm{cn}(u_3-v_3) & \mathrm{sn}(u_3-v_3)\mathrm{dn}(u_3+v_3) \\ \mathrm{cn}(u_3+v_3) & \mathrm{sn}(u_3+v_3)\mathrm{dn}(u_3-v_3) \end{pmatrix}$$

$$= D^{-1}(u_2, v_2)\, M_1(u_2, u_3)\, D(u_3, v_3) \qquad \text{(II.B.22)}$$

where $D(u_\ell, v_\ell)$ and $M_i(u_j, u_\ell)$ are as defined in (2.4.47) and (2.4.48) . We require that $\phi(u)$ has simple poles of residue unity at $u = 2mK + 2inK'$ as its only singularities

for any integers m and n . The periodicity of $W_1(u_2,u_3)$ requires that

$$\phi(u+2iK') = \phi(u+2K) = -\phi(u) \quad . \qquad \text{(II.B.23)}$$

These conditions define $\phi(u)$ uniquely as

$$\phi(u) = \mathrm{dn}(u) \,/\, \mathrm{sn}(u) \quad . \qquad \text{(II.B.24)}$$

[cf. (2.4.49)] .

By Liouville's theorem, the difference of $W_1(u_2,u_3)$ from the matrix product in (II.B.22) is a constant independent of u_3 . The constant may depend on u_2 , v_2 and v_3 , however, changing u_3 to $-u_3$ negated both $W(u_3)$ and (II.B.22) . Hence, their difference must be zero or we may write

$$W_1(u_2,u_3) = D^{-1}(u_2,v_2)\; M_1(u_2,u_3)\; D(u_3,v_3) \qquad \text{(II.B.25)}$$

[cf. (2.4.50)] .

SECTION III

square lattice variational approximations applied to the Ising model

1 INTRODUCTION

In Section II, we have shown that the partition function of a lattice may be written as the trace of a product of corner transfer matrices. In fact, the partition function can also be written as the trace of a product of row (or column) transfer matrices as shown by Kramers and Wannier (1941a) and Montroll (1941). The transfer matrix method, besides giving suggestive ideas for solving several lattice models of statistical mechanics exactly, also enables the use of variational approximations to tackle the problem. From the fact that the trace of a matrix is simply given by the algebraic sum of the eigenvalues of the matrix involved, in the thermodynamic limit, the partition function per site of the lattice is proportional to the maximum eigenvalue of the row (or column) transfer matrix of the lattice. This obviously suggests the use of the variational principle for solving the eigenvalue problem.

This idea was first applied to the Ising problem by Kramers and Wannier (1941b). Using the variational method, they were able to obtain approximations for the critical temperature and the partition function per site of the system. The idea was again taken up by Baxter (1968) for solving the monomer-dimer system on a rectangular lattice numerically in 1968. A set of matrix equations was derived from the

variational method which gives the statistical mechanical properties of the system in the thermodynamic limit. Very good estimates of the free energy of the system was obtained. In 1976, Kelland used a similar approach for the square lattice Potts model and hence was able to obtain estimates for the critical exponent β of the model (Kelland, 1976).

Recently, Baxter (1978) extended the method to a fairly general Ising model on the square lattice. A similar set of matrix equations was obtained and a rapidly convergent sequence of approximations to the free energy was developed. This approach is interesting as it provides a way of locating the critical point of the system and gives very good numerical estimates of some thermodynamic properties of the system.

It is the purpose of the following work to test the convergence of this approach. We apply the method to the zero field square lattice Ising model. With this system, it is possible for us to compare the result of the various approximations with the exact solution of the model. The variational method developed by Kramers and Wannier (1941b) is a special case of this method (Baxter, 1978).

The sequence of approximations generated by the method is solved numerically for the spontaneous magnetization below the critical point and for the critical temperature of the system. The convergence of the results to the exact values and the critical behaviour of the spontaneous magnetization are studied. The variational

method is found to give good estimates to the thermodynamic properties of the system.

We formulate the method and hence derive the set of variational equations for the square lattice Ising model in Section III.2. Some thermodynamic functions of the system may be obtained from the equations. They are given in Section III.3. In Section III.4, we calculate the lowest order of the sequence of variational approximations in a leading order expansion. The result is proved to be the same as Kramers and Wannier approximation. An iterative procedure for the solution of the equations is also given. From Section III.5 onwards, we focus on the case of zero magnetic field. The technique of spinor representations is used to simplify the matrix equations, thereby reducing the problem to one of solving a relatively small system of non-linear equations. The analytic solution of these equations for the infinite system is given in Section III.6. For the finite system, the equations are solved numerically for the spontaneous magnetization and the critical temperature. The method is given in Section III.7 and the results in Section III.8. They support a scaling hypothesis for the spontaneous magnetization.

2 THE VARIATIONAL APPROXIMATION

We outline below the variational approach for the square lattice models developed by Baxter (1978). We restrict the derivation to the Ising model with nearest-neighbour interactions only. However, it can be readily seen that the result can be easily generalised to a more general Ising model as considered by Baxter (1978).

§ 2.1 THE TRANSFER MATRIX

Consider a square Ising lattice of n_r rows and n_c columns with interaction energies J_1 and J_2 along the horizontal and vertical direction respectively (Fig. 3.1). Associated with each lattice site is a spin variable σ_i with value $+1$ or -1 . The energy of the system in the configuration specified by $\{\sigma\}$ is

$$E\{\sigma\} = - \sum_{\text{n.n.}} J_{i,j}\, \sigma_i\, \sigma_j - H \sum_{<i>} \sigma_i \qquad (3.2.1)$$

where the summation is over all nearest neighbours with $J_{i,j} = J_1$ or J_2 if the bond connecting spins σ_i and σ_j is in the horizontal or vertical direction respectively. The second summation is over all spins σ_i

of the lattice. The partition function of the system is then given by

$$Z_{n_r,n_c} = \sum \exp(- E/k_B T) \qquad (3.2.2)$$

where k_B is the Boltzmann's constant and T the temperature. The summation here is over all possible spin configurations of the lattice.

Impose toroidal boundary conditions on the lattice, i.e. require that the spin configuration of the (n_r+1) th row and (n_c+1) th column of the lattice is identical with that of the first row and column of the lattice, respectively. Denote the spin configuration of the j th row by

$$\underline{\alpha}^{(j)} = \{ \alpha_1^{(j)}, \alpha_2^{(j)}, \ldots, \alpha_{n_c}^{(j)} \}, \quad j=1,2,\ldots,n_r. \qquad (3.2.3)$$

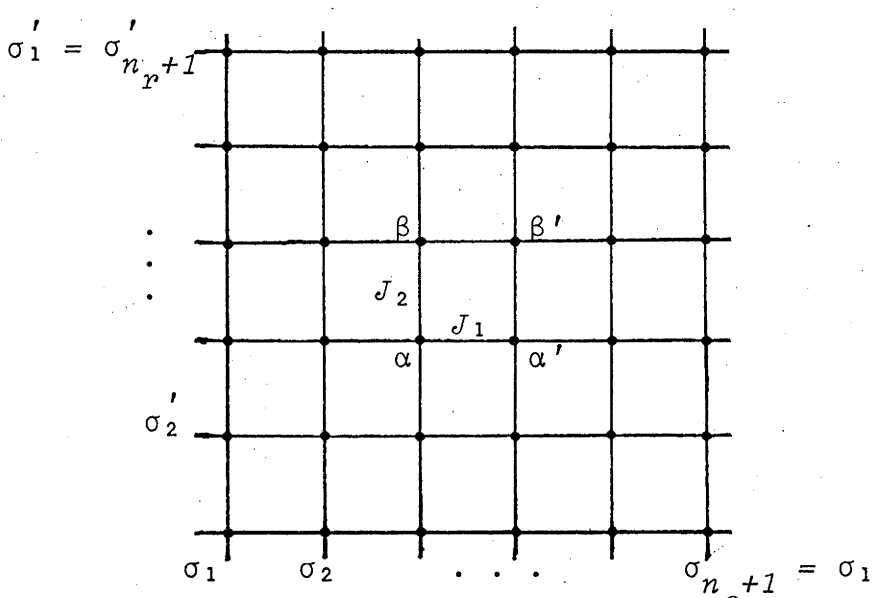


Fig. 3.1 The square Ising lattice with toroidal boundary conditions.

where $\alpha_\ell^{(j)}$ ($= +$ or -1) is the spin value of the ℓ th site of the j th row of the lattice. If we define

$$V(\underline{\alpha} \mid \underline{\alpha}') = \prod_{\ell=1}^{n_c} w(\alpha_\ell, \alpha_{\ell+1}, \alpha'_\ell, \alpha'_{\ell+1}) \qquad (3.2.4)$$

where

$$w(\alpha,\alpha',\beta,\beta') = \exp\{[2J_1(\alpha\alpha'+\beta\beta')+2J_2(\alpha\beta+\alpha'\beta')+H(\alpha+\alpha'+\beta+\beta')]/4k_BT\} \qquad (3.2.5)$$

is the weight function of a square face of the lattice, then (3.2.2) becomes

$$\begin{aligned} Z_{n_r,n_c} &= \sum_{\underline{\alpha}^{(1)}} \sum_{\underline{\alpha}^{(2)}} \cdots \sum_{\underline{\alpha}^{(n_r)}} \exp(- E\{\underline{\alpha}\}/k_BT) \\ &= \sum_{\underline{\alpha}^{(1)}} \sum_{\underline{\alpha}^{(2)}} \cdots \sum_{\underline{\alpha}^{(n_r)}} \prod_{j=1}^{n_r} \prod_{\ell=1}^{n_c} w(\alpha_\ell^{(j)}, \alpha_{\ell+1}^{(j)}, \alpha_\ell^{(j+1)}, \alpha_{\ell+1}^{(j+1)}) \\ &= \sum_{\underline{\alpha}^{(1)}} \sum_{\underline{\alpha}^{(2)}} \cdots \sum_{\underline{\alpha}^{(n_r)}} V(\underline{\alpha}^{(1)} \mid \underline{\alpha}^{(2)})\, V(\underline{\alpha}^{(2)} \mid \underline{\alpha}^{(3)}) \\ &\qquad \cdots V(\underline{\alpha}^{(n_r)} \mid \underline{\alpha}^{(1)}) \\ &= \text{Trace}\ (V^{n_r}) \end{aligned} \qquad (3.2.6)$$

Hence, the partition function of the system is written as the trace of the n_r th power of the $2^{n_c} \times 2^{n_c}$ matrix V. V is called the row transfer matrix of the lattice.

§ 2.2 THE VARIATIONAL APPROACH

The object of statistical mechanics is to calculate the partition function per site of the system in the thermodynamic limit (i.e. as n_r and n_c approach infinity).

It is a fundamental fact in matrix theory that the trace of a matrix is merely the sum of its eigenvalues and the eigenvalues of V^m are the eigenvalues of V raised to the m th power. So, from (3.2.6)

$$Z_{n_r,n_c} = \sum_{j=1}^{n_c} \lambda_j^{n_r} \tag{3.2.7}$$

where λ_j ($j = 1, 2, \ldots, n_c$) are the eigenvalues of the matrix V . In the thermodynamic limit, we may write

$$Z_{n_r,n_c} \sim \lambda_{\max}^{n_r} \tag{3.2.8}$$

where $\lambda_{\max}$ is the maximum eigenvalue of V . Hence the partition function per site of the system becomes

$$\kappa = Z_{n_r,n_c}^{1/n_r n_c} \sim \lambda_{\max}^{1/n_c} \tag{3.2.9}$$

Since V is symmetric, we may apply the variational principle to obtain its maximum eigenvalue $\lambda_{\max}$.

Given an arbitrary non-zero column vector Ψ , we define a function L by

$$L = \frac{\Psi^T V \Psi}{\Psi^T \Psi} \tag{3.2.10}$$

The derivative of L with respect to Ψ is

$$\frac{dL}{d\Psi} = \frac{2}{\Psi^T\Psi} (V\Psi - L\Psi) \quad . \qquad (3.2.11)$$

L is stationary if and only if

$$V\Psi = L\Psi \qquad (3.2.12)$$

i.e. if L is an eigenvalue of V and Ψ the corresponding eigenvector. So, the greatest eigenvalue of the matrix V is simply the maximum of all the stationary values of the expression (3.2.10) with respect to Ψ , i.e.

$$\lambda_{max} = \max \{ \text{stat.} \frac{\Psi^T V\Psi}{\Psi^T\Psi} \} \qquad (3.2.13)$$

Let Ψ_{max} be the eigenvector of V corresponding to its greatest eigenvalue. We have in the limit of m large

$$\Psi_{max} \propto V^m \phi \qquad (3.2.14)$$

for any arbitrary vector ϕ which is not orthogonal to Ψ_{max}. Hence, choosing any arbitrary ϕ not orthogonal to Ψ_{max} , $V^m\phi$ gives a reasonable approximation to the unnormalised eigenvector Ψ_{max} and is exact if m becomes infinitely large.

If ϕ is chosen so that each of its elements is unity, then using the definition (3.2.4) of V , we have

$$V^m\phi(\sigma_1,\sigma_2,\ldots,\sigma_{n_c}) = \sum_{\underline{\alpha}^{(1)},\underline{\alpha}^{(2)},\ldots,\underline{\alpha}^{(m)}} V(\sigma_1,\sigma_2,\ldots,\sigma_{n_c}|\underline{\alpha}^{(1)}) V(\underline{\alpha}^{(1)}|\underline{\alpha}^{(2)})\ldots V(\underline{\alpha}^{(m-1)}|\underline{\alpha}^{(m)})$$

$$= \sum_{\substack{\alpha_1^{(1)},\alpha_1^{(2)},\ldots,\alpha_1^{(m)} \\ \alpha_2^{(1)},\alpha_2^{(2)},\ldots,\alpha_2^{(m)} \\ \vdots \quad \vdots \quad \vdots \\ \alpha_{n_c}^{(1)},\alpha_{n_c}^{(2)},\ldots,\alpha_{n_c}^{(m)}}} \prod_{\ell=1}^{n_c} \{w(\sigma_\ell,\sigma_{\ell+1},\alpha_\ell^{(1)},\alpha_{\ell+1}^{(1)}) \times w(\alpha_\ell^{(1)},\alpha_{\ell+1}^{(1)},\alpha_\ell^{(2)},\alpha_{\ell+1}^{(2)}) \ldots \times w(\alpha_\ell^{(m-1)},\alpha_{\ell+1}^{(m-1)},\alpha_\ell^{(m)},\alpha_{\ell+1}^{(m)})\}$$

(3.2.15)

where $\sigma_{n_c+1} = \sigma_1$ and $\alpha_{n_c+1}^{(j)} = \alpha_1^{(j)}$ ($j = 1, 2, \ldots, m$)

Define a new set of indices $\underline{\mu}_j$ by

$$\underline{\mu}_j = (\alpha_j^{(1)},\alpha_j^{(2)},\ldots,\alpha_j^{(m)}) , \quad j = 1, 2, \ldots, n_c.$$

(3.2.16)

Then, (3.2.15) can be written as

$$V^m \phi(\sigma_1,\sigma_2,\ldots,\sigma_{n_c}) = \sum_{\underline{\mu}_1,\underline{\mu}_2,\ldots,\underline{\mu}_{n_c}} F_{\underline{\mu}_1,\underline{\mu}_2}^{\sigma_1,\sigma_2} F_{\underline{\mu}_2,\underline{\mu}_3}^{\sigma_2,\sigma_3} \ldots F_{\underline{\mu}_{n_c},\underline{\mu}_1}^{\sigma_{n_c},\sigma_1}$$

(3.2.17)

where

$$F_{\underline{\mu},\underline{\mu}'}^{\sigma,\sigma'} = w(\sigma,\sigma',\alpha^{(1)},\beta^{(1)})\, w(\alpha^{(1)},\beta^{(1)},\alpha^{(2)},\beta^{(2)}) \ldots w(\alpha^{(m-1)},\beta^{(m-1)},\alpha^{(m)},\beta^{(m)}) \qquad (3.2.18)$$

with $\underline{\mu} = (\alpha^{(1)},\alpha^{(2)},\ldots,\alpha^{(m)})$ and $\underline{\mu}' = (\beta^{(1)},\beta^{(2)},\ldots,\beta^{(m)})$. The summation in (3.2.17) is over all possible configurations of $\underline{\mu}_\ell$ s . We may write (3.2.17) as

$$V^m \phi(\sigma_1,\sigma_2,\ldots,\sigma_{n_c}) = \text{Trace}\,\{F(\sigma_1,\sigma_2)F(\sigma_2,\sigma_3)\ldots F(\sigma_{n_c},\sigma_1)\}$$

(3.2.19)

where each of $F(+,+)$, $F(+,-)$, $F(-,+)$, $F(-,-)$ is a $2^m \times 2^m$ matrix with the $(\underline{\mu},\underline{\mu}')$ th element given by

$$F_{\underline{\mu},\underline{\mu}'}(\sigma,\sigma') = F^{\sigma,\sigma'}_{\underline{\mu},\underline{\mu}'} \; ; \quad \sigma, \sigma' = + \text{ or } - \; . \tag{3.2.20}$$

As m tends towards infinity, the eigenvector Ψ_{max} is proportional to $V^m\phi$ and hence it must be of the form

$$\Psi_{max}(\sigma_1,\sigma_2,\ldots,\sigma_{n_c}) \propto \text{Trace}\{F(\sigma_1,\sigma_2)F(\sigma_2,\sigma_3)\ldots F(\sigma_{n_c},\sigma_1)\} \tag{3.2.21}$$

where, here, the matrices $F(\sigma,\sigma')$ are infinite dimensional matrices. It follows that even for small dimensionality, by taking the matrices $F(\sigma,\sigma')$ to be arbitrary, (3.2.21) provides a reasonable form for the trial function Ψ_{max} of the variational principle.

Further, we note from (3.2.18) that $F^{\sigma,\sigma'}_{\underline{\mu},\underline{\mu}'}$ is symmetric with respect to interchanging σ and $\underline{\mu}$ with σ' and $\underline{\mu}'$ provided that

$$w(\alpha,\alpha',\beta,\beta') = w(\alpha',\alpha,\beta',\beta) \tag{3.2.22}$$

which is obviously true in this case. It is natural to keep this property even in the case $F(\sigma,\sigma')$ being arbitrary, that is, we require that

$$F(\sigma,\sigma') = F^T(\sigma',\sigma) \quad . \tag{3.2.23}$$

The problem now reduces to finding the maximum of all the stationary values of the expression (3.2.10) with respect to Ψ while keeping Ψ to be of the form (3.2.21) with $F(\sigma,\sigma')$ being $2^m \times 2^m$ matrices satisfying (3.2.23)

but otherwise arbitrary. Using (3.2.21), we have

$$\Psi^T\Psi = \sum_{\substack{\underline{\mu}_j\ \underline{\nu}_j\ \alpha_j \\ j=1,2,\ldots,n_c}} \sum \sum \sum F^{\alpha_1,\alpha_2}_{\underline{\mu}_1,\underline{\mu}_2} F^{\alpha_2,\alpha_3}_{\underline{\mu}_2,\underline{\mu}_3} \cdots F^{\alpha_{n_c},\alpha_1}_{\underline{\mu}_{n_c},\underline{\mu}_1} F^{\alpha_1,\alpha_2}_{\underline{\nu}_1,\underline{\nu}_2} F^{\alpha_2,\alpha_3}_{\underline{\nu}_2,\underline{\nu}_3} \cdots F^{\alpha_{n_c},\alpha_1}_{\underline{\nu}_{n_c},\underline{\nu}_1}$$

$$= \sum_{\substack{\underline{\mu}_j\ \underline{\nu}_j\ \alpha_j \\ j=1,2,\ldots,n_c}} \sum \sum \sum R(\alpha_1,\underline{\mu}_1,\underline{\nu}_1|\alpha_2,\underline{\mu}_2,\underline{\nu}_2)\, R(\alpha_2,\underline{\mu}_2,\underline{\nu}_2|\alpha_3,\underline{\mu}_3,\underline{\nu}_3) \cdots R(\alpha_{n_c},\underline{\mu}_{n_c},\underline{\nu}_{n_c}|\alpha_1,\underline{\mu}_1,\underline{\nu}_1)$$

$$= \text{Trace } (R^{n_c}) \qquad (3.2.24)$$

where R is a $2^{2m+1} \times 2^{2m+1}$ matrix with elements

$$R(\alpha,\underline{\mu},\underline{\nu}|\alpha',\underline{\mu}',\underline{\nu}') = F^{\alpha,\alpha'}_{\underline{\mu},\underline{\mu}'} F^{\alpha,\alpha'}_{\underline{\nu},\underline{\nu}'} \quad ; \quad \alpha,\ \alpha' = + \text{ or } - \qquad (3.2.25)$$

Similarly,

$$\Psi^T V \Psi = \sum_{\substack{\underline{\mu}_j\ \underline{\nu}_j\ \alpha_j\ \beta_j \\ j=1,2,\ldots,n_c}} \sum \sum \sum \sum \prod_{j=1}^{n_c} F^{\alpha_j,\alpha_{j+1}}_{\underline{\mu}_j,\underline{\mu}_{j+1}}\, w(\alpha_j,\alpha_{j+1},\beta_j,\beta_{j+1})\, F^{\beta_j,\beta_{j+1}}_{\underline{\nu}_j,\underline{\nu}_{j+1}}$$

$$= \text{Trace } (S^{n_c}) \qquad (3.2.26)$$

where S is a $2^{2m+2} \times 2^{2m+2}$ matrix with elements

$$S(\alpha,\beta,\underline{\mu},\underline{\nu}|\alpha',\beta',\underline{\mu}',\underline{\nu}') = F^{\alpha,\alpha'}_{\underline{\mu},\underline{\mu}'}\, w(\alpha,\alpha',\beta,\beta')\, F^{\beta,\beta'}_{\underline{\nu},\underline{\nu}'}$$

$$\alpha,\ \beta,\ \alpha',\ \beta' = + \text{ or } - . \qquad (3.2.27)$$

So, (3.2.13) reduces to

$$\lambda_{max} = \max \{ \text{stat.} \frac{\text{Trace } (S^{n_c})}{\text{Trace } (R^{n_c})} \} \qquad (3.2.28)$$

In the limit of large n_c ,

$$\lambda_{max} \sim (\eta / \xi)^{n_c} \qquad (3.2.29)$$

where ξ and η are the maximum eigenvalues of R and S respectively. In this case, the partition function per site as given in (3.2.9) becomes

$$\kappa = \lambda_{max}^{1/n_c} = \eta/\xi \quad . \qquad (3.2.30)$$

As for the maximum eigenvalues of R and S , let the column vectors defined by $\overline{X} \equiv (X^{\alpha}_{\underline{\mu},\underline{\nu}})$ and $\overline{P} \equiv (P^{\alpha,\beta}_{\underline{\mu},\underline{\nu}})$ be the associated eigenvectors of R and S respectively, and define $2^m \times 2^m$ matrices $X(\alpha)$ and $P(\alpha,\beta)$ (α,β = + or -) with $X^{\alpha}_{\underline{\mu},\underline{\nu}}$ and $P^{\alpha,\beta}_{\underline{\mu},\underline{\nu}}$ as their ($\underline{\mu},\underline{\nu}$) th element. Obviously, we may write

$$\sum_{\underline{\mu}'} \sum_{\underline{\nu}'} \sum_{\alpha'} R(\alpha,\underline{\mu},\underline{\nu}|\alpha',\underline{\mu}',\underline{\nu}') \, X^{\alpha'}_{\underline{\mu}',\underline{\nu}'} = \xi \, X^{\alpha}_{\underline{\mu},\underline{\nu}} \qquad (3.2.31a)$$

and

$$\sum_{\underline{\mu}'} \sum_{\underline{\nu}'} \sum_{\alpha'} \sum_{\beta'} S(\alpha,\beta,\underline{\mu},\underline{\nu}|\alpha',\beta',\underline{\mu}',\underline{\nu}') \, P^{\alpha',\beta'}_{\underline{\mu}',\underline{\nu}'} = \eta \, P^{\alpha,\beta}_{\underline{\mu},\underline{\nu}} \qquad (3.2.31b)$$

or equivalently (from (3.2.25) and (3.2.27)) we have

$$\sum_{\underline{\mu}'} \sum_{\underline{\nu}'} \sum_{\alpha'} F^{\alpha,\alpha'}_{\underline{\mu},\underline{\mu}'} \, X^{\alpha'}_{\underline{\mu}',\underline{\nu}'} \, F^{\alpha,\alpha'}_{\underline{\nu},\underline{\nu}'} = \xi \, X^{\alpha}_{\underline{\mu},\underline{\nu}} \qquad (3.2.32a)$$

and

$$\sum_{\underline{\mu}'} \sum_{\underline{\nu}'} \sum_{\alpha'} \sum_{\beta'} w(\alpha,\alpha',\beta,\beta') \, F^{\alpha,\alpha'}_{\underline{\mu},\underline{\mu}'} \, P^{\alpha',\beta'}_{\underline{\mu}',\underline{\nu}'} \, F^{\beta,\beta'}_{\underline{\nu},\underline{\nu}'} = \eta \, P^{\alpha,\beta}_{\underline{\mu},\underline{\nu}} \qquad (3.2.32b)$$

Using the symmetric properties of $F(\alpha,\beta)$ in (3.2.23) , (3.2.32a,b) reduces to

$$\sum_{\alpha'} F(\alpha,\alpha')\, X(\alpha')\, F(\alpha',\alpha) = \xi\, X(\alpha) \qquad (3.2.33a)$$

and

$$\sum_{\alpha'}\sum_{\beta'} w(\alpha,\alpha',\beta,\beta')\, F(\alpha,\alpha')\, P(\alpha',\beta')\, F(\beta',\beta) = \eta\, P(\alpha,\beta) \qquad (3.2.33b)$$

The equations (3.2.33a,b) are consistent with the conditions

$$X(\alpha) = X^T(\alpha)$$

and (3.2.34)

$$P(\alpha,\beta) = P^T(\beta,\alpha) \quad ,$$

provided that

$$w(\alpha,\alpha',\beta,\beta') = w(\beta,\beta',\alpha,\alpha') \qquad (3.2.35)$$

which is obviously true in our case also. So, for simplicity, we will choose the solution for $X(\alpha)$ and $P(\alpha,\beta)$ with this symmetry.

§ 2.3 MAXIMIZATION OF κ

As illustrated in the last section, to obtain λ_{max}, we need to determine the maximum eigenvalues of R and S. Since R and S are themselves symmetric matrices, we may again apply the variational principle.

Similarly to (3.2.13), the maximum eigenvalue of R

is given by

$$\xi = \max \{ \text{stat.} \ \frac{\overline{X}^T R \overline{X}}{\overline{X}^T \overline{X}} \} \qquad (3.2.36)$$

With $\overline{X}$ being defined to be the eigenvector corresponding to ξ and using (3.2.25), we may write

$$\xi = \max \{ \text{stat.} \ \frac{\text{Trace} \left(\sum_{\alpha,\alpha'} X(\alpha) F(\alpha,\alpha') X(\alpha') F(\alpha',\alpha) \right)}{\text{Trace} \left(\sum_{\alpha} X^2(\alpha) \right)} \} \qquad (3.2.37)$$

From the definition of $\overline{X}$ in (3.2.32a), the expression in the right-hand side of (3.2.37) is in fact stationary with respect to the variation of any arbitrary element of $\overline{X}$.

Similarly for the matrix S, its maximum eigenvalue is given by

$$\eta = \max \{ \text{stat.} \ \frac{\overline{P}^T S \overline{P}}{\overline{P}^T \overline{P}} \}$$

$$= \max \{ \text{stat.} \ \frac{\text{Trace} \left(\sum_{\alpha,\beta,\alpha',\beta'} w(\alpha,\alpha',\beta,\beta') P(\beta,\alpha) F(\alpha,\alpha') P(\alpha',\beta') F(\beta',\beta) \right)}{\text{Trace} \left(\sum_{\alpha,\beta} P(\beta,\alpha) P(\alpha,\beta) \right)} \} \qquad (3.2.38)$$

Again, the right-hand side of (3.2.38) is stationary with respect to variation of any of the elements of $\overline{P}$ by its definition. Hence, from (3.2.30),

$$\kappa = \max \{ \text{stat.} \frac{\text{Trace} \left(\sum_{\alpha} X^2(\alpha) \right)}{\text{Trace} \left(\sum_{\alpha,\alpha'} X(\alpha)\, F(\alpha,\alpha')\, X(\alpha')\, F(\alpha',\alpha) \right)}$$

$$\times \frac{\text{Trace} \left(\sum_{\alpha,\beta,\alpha',\beta'} w(\alpha,\alpha',\beta,\beta') P(\beta,\alpha) F(\alpha,\alpha') P(\alpha',\beta') F(\beta',\beta) \right)}{\text{Trace} \left(\sum_{\alpha,\beta} P(\beta,\alpha)\, P(\alpha,\beta) \right)} \} \tag{3.2.39}$$

Since this expression is stationary with respect to the variation of $X(\alpha)$ and $P(\alpha,\beta)$, so, the remaining requirement for κ is that it has to be stationary with respect to the variation of any of the $F(\alpha,\beta)$ (α,β = + or -) also. Let $G(F)$ =

$$\frac{\text{Trace}(\sum_{\alpha} X^2(\alpha)) \times \text{Trace}(\sum_{\alpha,\beta,\alpha',\beta'} w(\alpha,\alpha',\beta,\beta') P(\beta,\alpha) F(\alpha,\alpha') P(\alpha',\beta') F(\beta',\beta))}{\text{Trace}(\sum_{\alpha,\alpha'} X(\alpha) F(\alpha,\alpha') X(\alpha') F(\alpha',\alpha)) \times \text{Trace}(\sum_{\alpha,\beta} P(\beta,\alpha) P(\alpha,\beta))} \tag{3.2.40}$$

and

$$\zeta = \kappa \frac{\text{Trace} \left(\sum_{\alpha,\beta} P(\beta,\alpha)\, P(\alpha,\beta) \right)}{\text{Trace} \left(\sum_{\alpha} X^2(\alpha) \right)} \tag{3.2.41}$$

If we vary a particular element $F^{\sigma,\sigma'}_{\underline{\tau}_1,\underline{\tau}_2}$ of $F(\alpha,\beta)$ such that

$$(F^{\alpha,\beta}_{\underline{\mu},\underline{\nu}})^* = \begin{cases} F^{\alpha,\beta}_{\underline{\mu},\underline{\nu}} + \varepsilon, & \text{if } \alpha=\sigma,\ \beta=\sigma',\ \underline{\mu}=\underline{\tau}_1 \text{ and } \underline{\nu}=\underline{\tau}_2. \\ F^{\alpha,\beta}_{\underline{\mu},\underline{\nu}}, & \text{otherwise .} \end{cases} \tag{3.2.42}$$

then

$$\frac{\partial G(F)}{\partial \varepsilon}\Big|_{\varepsilon=0} \propto \sum_{\underline{\mu},\underline{\mu}',\beta,\beta'} w(\sigma,\sigma',\beta,\beta')\, P^{\sigma,\beta}_{\underline{\tau}_1,\underline{\mu}}\, P^{\sigma',\beta'}_{\underline{\tau}_2,\underline{\mu}'}\, F^{\beta,\beta'}_{\underline{\mu},\underline{\mu}'}$$

$$- \zeta \sum_{\underline{\mu},\underline{\mu}'} X^{\sigma}_{\underline{\tau}_1,\underline{\mu}}\, X^{\sigma'}_{\underline{\tau}_2,\underline{\mu}'}\, F^{\sigma,\sigma'}_{\underline{\mu},\underline{\mu}'} \tag{3.2.43}$$

For $G(F)$ to be stationary, we require that (3.2.43) equal to zero or equivalently

$$\sum_{\beta}\sum_{\beta'} w(\alpha,\alpha',\beta,\beta')P(\alpha,\beta)F(\beta,\beta')P(\beta',\alpha') = \zeta\, X(\alpha)F(\alpha,\alpha')X(\alpha') \tag{3.2.44}$$

Hence, κ will be stationary with respect to all its parameters if (3.2.33a,b) and (3.2.44) are satisfied. Solving this set of equations for η , ξ , ζ and the matrices $X(\alpha)$, $F(\alpha,\beta)$ and $P(\alpha,\beta)$ (α, β = + or -) we should be able to obtain estimates for κ using (3.2.30) . All the matrices in these equations are of $2^m \times 2^m$ dimensions. They should give us the exact result for κ if all the matrices are infinite in size. Hence, a sequence of variational approximations may be obtained for κ by taking $m = 0, 1, 2, \ldots$.

The arguments so far do not depend on the exact form of $w(\alpha,\alpha',\beta,\beta')$ as long as it satisfies conditions (3.2.22) and (3.2.35). So, they may equally be applied to a more generalised square Ising lattice such as that considered by Baxter (1978).

3 THERMODYNAMIC PROPERTIES OF THE SYSTEM

In this section, we shall examine some of the thermodynamic properties of the system that can readily be obtained from the matrices $X(\alpha)$, $F(\alpha,\beta)$ and $P(\alpha,\beta)$.

§ 3.1 ROW-COLUMN SYMMETRY

It is interesting that the symmetry of rows and columns in the lattice is reflected in the expression of κ obtained.

If we introduce matrices $A(+)$, $A(-)$, $F^*(+,+)$, $F^*(+,-)$, $F^*(-,+)$ and $F^*(-,-)$ such that

$$X(\alpha) = A^T(\alpha)\, A(\alpha) \tag{3.3.1a}$$

and

$$P(\alpha,\beta) = A^T(\alpha)\, F^*(\alpha,\beta)\, A(\beta) \tag{3.3.1b}$$

with

$$F^*(\alpha,\beta) = F^{*T}(\beta,\alpha) \tag{3.3.2}$$

$$\alpha,\ \beta = + \text{ or } -$$

then, κ in (3.2.39) becomes

$$\kappa = \max\{\ \text{stat.}\ \frac{\text{Trace}\left(\sum_{\alpha}\left(A^{T}(\alpha)A(\alpha)\right)^{2}\right)}{\text{Trace}\left(\sum_{\alpha,\alpha'} A^{T}(\alpha)A(\alpha)F(\alpha,\alpha')A^{T}(\alpha')A(\alpha')F(\alpha',\alpha)\right)} \times$$

$$\frac{\text{Trace}\left(\sum_{\alpha,\beta,\alpha',\beta'} w(\alpha,\alpha',\beta,\beta')A^{T}(\beta)F^{*}(\beta,\alpha)A(\alpha)F(\alpha,\alpha')A^{T}(\alpha')F^{*}(\alpha',\beta')A(\beta')F(\beta',\beta)\right)}{\text{Trace}\left(\sum_{\alpha,\beta} A^{T}(\beta)F^{*}(\beta,\alpha)A(\alpha)A^{T}(\alpha)F^{*}(\alpha,\beta)A(\beta)\right)}\}$$

(3.3.3)

Equation (3.3.3) is essentially unaltered by the interchange of $F(\alpha,\beta)$ with $F^{*}(\alpha,\beta)$ and $A(\alpha)$ with $A^{T}(\alpha)$ while simultaneously replacing $w(\alpha,\alpha',\beta,\beta')$ by $w(\alpha,\beta,\alpha',\beta')$. From the definition of the function w in (3.2.5), this is equivalent to interchanging the columns with the rows in the lattice. κ is therefore symmetric with respect to row and column interactions.

§ 3.2 THERMODYNAMIC FUNCTIONS

Some of the thermodynamic functions can be easily written in terms of the matrices $A(\alpha)$, $F(\alpha,\beta)$ and $F^{*}(\alpha,\beta)$.

Firstly, it is readily seen from (3.2.9) that the free energy per site of the system is given by

$$f = -\frac{k_B T}{n_r n_c} \ln Z_{n_r,n_c}$$

$$= -k_B T \ln \kappa \quad . \tag{3.3.4}$$

Many of the thermodynamic functions can be written in terms of derivatives of the free energy per site f of the system.

Since κ is stationary with respect to the matrices $A(\alpha)$, $F(\alpha,\beta)$ and $F^*(\alpha,\beta)$ (α,β = + or -), the differentiations of κ with respect to H, J_1, J_2 or T can be carried out as if these matrices were constants.

Before we perform any such differentiation, it is more convenient to write the expression of κ in (3.3.3) in terms of the following new matrix variables :

$$\begin{aligned} A_1(\alpha) &= \exp(-H\alpha/4k_BT)\ A(\alpha) \\ F_1(\alpha,\beta) &= \exp(H(\alpha+\beta)/4k_BT)\ \exp(J_1\alpha\beta/2k_BT)\ F(\alpha,\beta) \\ F_1^*(\alpha,\beta) &= \exp(H(\alpha+\beta)/4k_BT)\ \exp(J_2\alpha\beta/2k_BT)\ F^*(\alpha,\beta) \end{aligned} \tag{3.3.5}$$

Using the above variables, κ can then be written as

$$\kappa = \max\{\text{stat.}\frac{\text{Trace}(\sum_{\alpha}\exp(H\alpha/k_BT)\ (A_1^T(\alpha)A_1(\alpha))^2)}{\text{Trace}(\sum_{\alpha,\alpha'}\exp(\frac{-J_1\alpha\alpha'}{k_BT})A_1^T(\alpha)A_1(\alpha)F_1(\alpha,\alpha')A_1^T(\alpha')A_1(\alpha')F_1(\alpha',\alpha))}$$

$$\times\frac{\text{Trace}(\sum_{\alpha,\beta,\alpha',\beta'}A_1^T(\beta)F_1^*(\beta,\alpha)A_1(\alpha)F_1(\alpha,\alpha')A_1^T(\alpha')F_1^*(\alpha',\beta')A_1(\beta')F_1(\beta',\beta))}{\text{Trace}(\sum_{\alpha,\beta}\exp(\frac{-J_2\alpha\beta}{k_BT})A_1^T(\beta)F_1^*(\beta,\alpha)A_1(\alpha)A_1^T(\alpha)F_1^*(\alpha,\beta)A_1(\beta))}\} \tag{3.3.6}$$

From the fact that κ is stationary with respect to variations in $A(\alpha)$, $F(\alpha,\beta)$ and $F^*(\alpha,\beta)$, it can be shown that it is stationary with respect to the newly defined matrices $A_1(\alpha)$, $F_1(\alpha,\beta)$ and $F_1^*(\alpha,\beta)$ also. Hence, the differentiations with respect to H, J_1, J_2 or T can be performed as if they were constants also.

Using (3.3.6), some of the thermodynamic functions can be calculated readily.

Magnetization

The magnetization per site of the lattice is given by

$$
\begin{aligned}
M &= \langle \sigma_1 \rangle \\
&= k_B T \, \frac{\partial \ln(\kappa)}{\partial H} \\
&= \frac{\mathrm{Trace}\left(\sum_{\alpha} \alpha \exp(H\alpha/k_B T) \, (A_1^T(\alpha) A_1(\alpha))^2 \right)}{\mathrm{Trace}\left(\sum_{\alpha} \exp(H\alpha/k_B T) \, (A_1^T(\alpha) A_1(\alpha))^2 \right)}
\end{aligned}
\tag{3.3.7}
$$

which using (3.3.5) gives

$$
M = \frac{\mathrm{Trace}\left(\sum_{\alpha} \alpha \, (A^T(\alpha) A(\alpha))^2 \right)}{\mathrm{Trace}\left(\sum_{\alpha} (A^T(\alpha) A(\alpha))^2 \right)} \tag{3.3.8}
$$

Nearest-neighbour correlation

The horizontal nearest-neighbour correlation is

$$
\begin{aligned}
\langle \sigma_i \sigma_j \rangle_{\text{hori.}} &= k_B T \; \partial(\ln \kappa)/\partial J_1 \\
&= \frac{\mathrm{Trace}\left(\sum_{\alpha,\alpha'} \alpha\alpha' \exp(-J_1\alpha\alpha'/k_B T) A_1^T(\alpha) A_1(\alpha) F_1(\alpha,\alpha') A_1^T(\alpha') A_1(\alpha') F_1(\alpha',\alpha) \right)}{\mathrm{Trace}\left(\sum_{\alpha,\alpha'} \exp(-J_1\alpha\alpha'/k_B T) A^T{}_1(\alpha) A_1(\alpha) F_1(\alpha,\alpha') A_1^T(\alpha') A_1(\alpha') F_1(\alpha',\alpha) \right)} \\
&= \frac{\mathrm{Trace}\left(\sum_{\alpha,\alpha'} \alpha\alpha' \, A^T(\alpha) A(\alpha) F(\alpha,\alpha') A^T(\alpha') A(\alpha') F(\alpha',\alpha) \right)}{\mathrm{Trace}\left(\sum_{\alpha,\alpha'} A^T(\alpha) A(\alpha) F(\alpha,\alpha') A^T(\alpha') A(\alpha') F(\alpha',\alpha) \right)}
\end{aligned}
\tag{3.3.9}
$$

The vertical nearest-neighbour correlation can be obtained similarly by replacing $F(\alpha,\alpha')$ with $F^{*}(\alpha,\alpha')$ and $A(\alpha)$ with $A^{T}(\alpha)$.

Internal energy

Finally, the internal energy per site of the system is

$$U = k_B T^2 \, \partial(\ln \kappa)/\partial T$$

$$= \frac{\mathrm{Trace}\left(\sum_{\alpha} H\alpha \exp(H\alpha/k_B T) \, (A_1^T(\alpha) A_1(\alpha))^2 \right)}{\mathrm{Trace}\left(\sum_{\alpha} \exp(H\alpha/k_B T) \, (A_1^T(\alpha) A_1(\alpha))^2 \right)}$$

$$+ \frac{\mathrm{Trace}\left(\sum_{\alpha,\alpha'} J_1\alpha\alpha' \exp(-J_1\alpha\alpha'/k_B T) A_1^T(\alpha) A_1(\alpha) F_1(\alpha,\alpha') A_1^T(\alpha') A_1(\alpha') F_1(\alpha',\alpha) \right)}{\mathrm{Trace}\left(\sum_{\alpha,\alpha'} \exp(-J_1\alpha\alpha'/k_B T) \, A_1^T(\alpha) A_1(\alpha) F_1(\alpha,\alpha') A_1^T(\alpha') A_1(\alpha') F_1(\alpha',\alpha) \right)}$$

$$+ \frac{\mathrm{Trace}\left(\sum_{\alpha,\beta} J_2\alpha\beta \exp(-J_2\alpha\beta/k_B T) \, A_1^T(\alpha) F_1^{*}(\alpha,\beta) A_1(\beta) A_1^T(\beta) F_1^{*}(\beta,\alpha) A_1(\alpha) \right)}{\mathrm{Trace}\left(\sum_{\alpha,\beta} \exp(-J_2\alpha\beta/k_B T) \, A_1^T(\alpha) F_1^{*}(\alpha,\beta) A_1(\beta) A_1^T(\beta) F_1^{*}(\beta,\alpha) A_1(\alpha) \right)}$$

$$= HM + J_1 \langle \sigma_i \sigma_j \rangle_{\mathrm{hori.}} + J_2 \langle \sigma_i \sigma_j \rangle_{\mathrm{vert.}} \qquad (3.3.10)$$

The result reflects the fact that the only contributions to the internal energy of the system are those from the magnetic field and the nearest-neighbour interactions of the system (Onsager, 1944).

§ 3.3 GRAPHICAL INTERPRETATION OF THE MATRICES

When m approaches infinity, the form (3.2.21) of Ψ_{max} is exact with the elements of $F(\alpha,\beta)$ as given in (3.2.18). So, if we consider the case when all the matrices are of infinite dimensions (i.e. $m = \infty$), $F(\alpha,\beta)$ may be interpreted as the half-column transfer matrices whose elements being the Boltzmann weight of half of a lattice column with (α,β) as their bottom spins (Fig. 3.2a). From (3.2.25), R is then the column-to-column transfer matrix with its element $R(\alpha,\underline{\mu},\underline{\nu}|\beta,\underline{\mu}',\underline{\nu}')$ being the weight of the full column as given in Fig. 3.2b. Similar interpretation can be given for $S(\alpha,\beta,\underline{\mu},\underline{\nu}|\alpha',\beta',\underline{\mu}',\underline{\nu}')$ (Fig. 3.2c).

Since, in the limit of m' large,

$$\overline{X} \propto R^{m'}\phi \qquad (3.3.11)$$

for some vector ϕ not orthogonal to $\overline{X}$, the elements $X^{\alpha}_{\underline{\mu},\underline{\nu}}$ of the maximal eigenvector $\overline{X}$ of R can be interpreted as the weight for half of the lattice, as shown in Fig. 3.3a, summing over spins of solid circles. That is, it is the probability that the left-hand edge of a lattice with $(2m+1)$ rows and $(m'+1)$ columns has the spin configuration $(\underline{\mu},\alpha,\underline{\nu})$. In view of (3.3.1a), the element $A^{\alpha}_{\underline{\mu},\underline{\mu}'}$ is then the weight of the spins of the corner shown in Fig. 3.3b (summing over dotted spins). Hence apart from the outer boundary which is irrelevant in the limit when m approaches infinity,

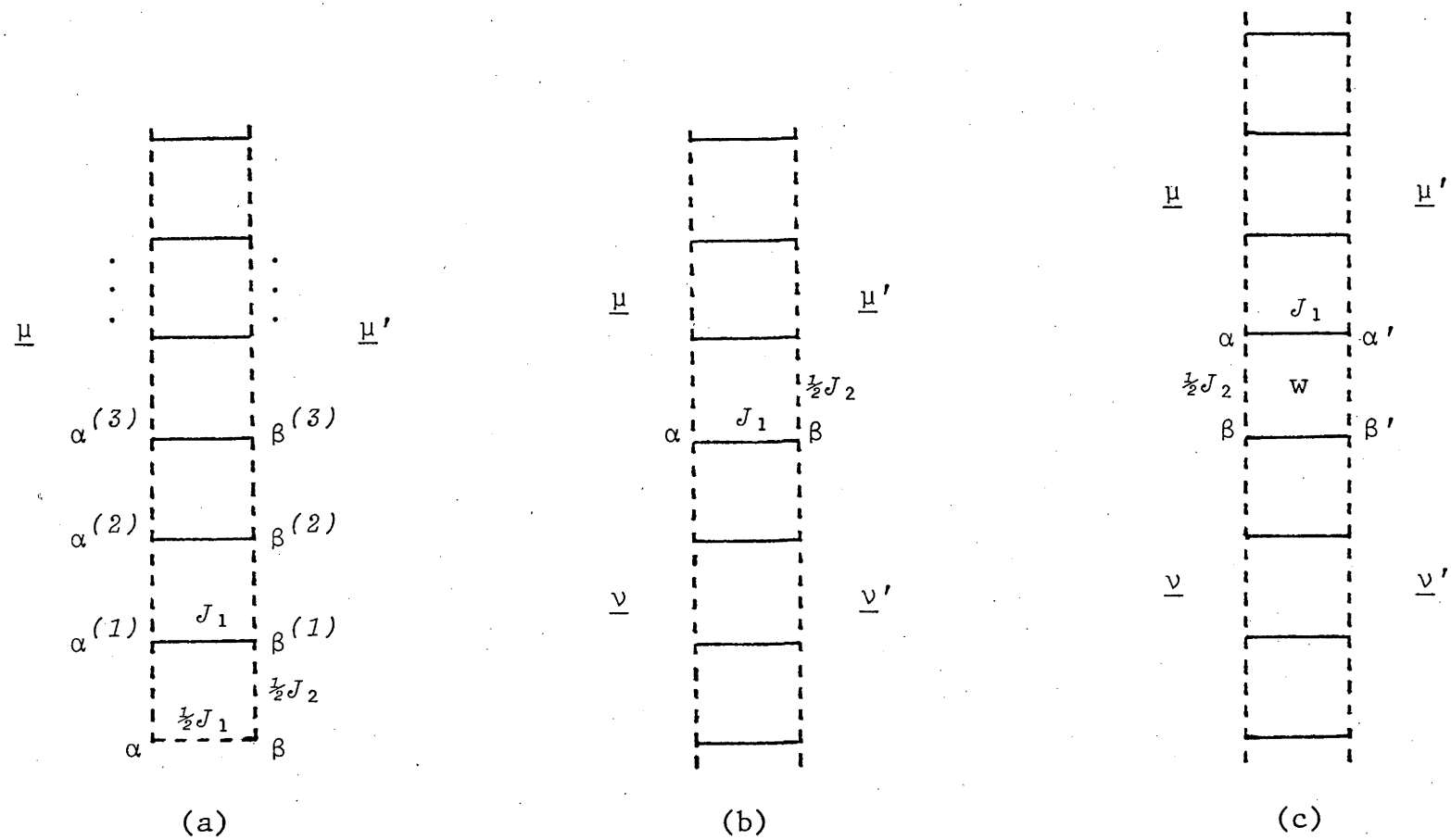
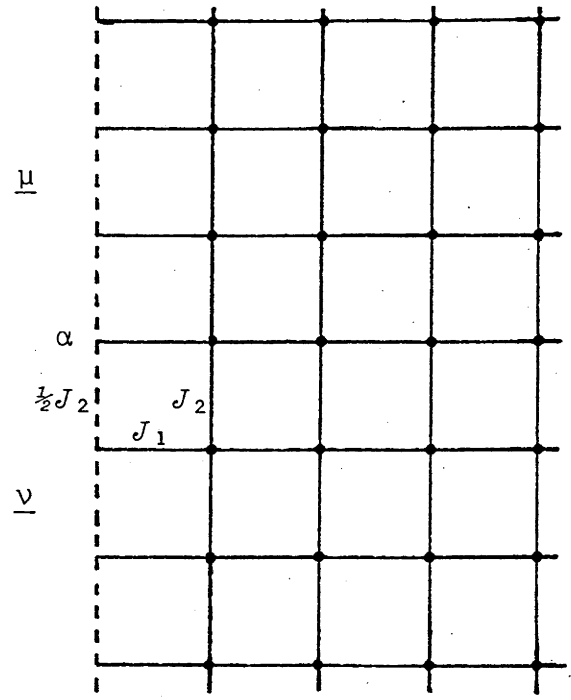


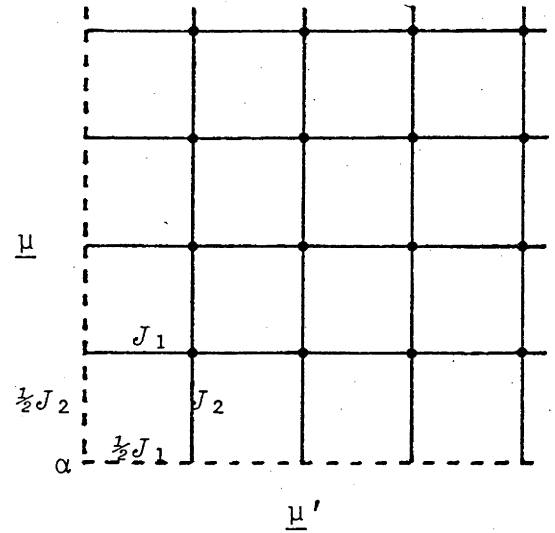
Fig. 3.2 The lattice weight corresponds to the elements : (a) $F^{\alpha,\beta}_{\underline{\mu},\underline{\mu}'}$;

(b) $R(\alpha,\underline{\mu},\underline{\nu}|\beta,\underline{\mu}',\underline{\nu}')$; (c) $S(\alpha,\beta,\underline{\mu},\underline{\nu}|\alpha',\beta',\underline{\mu}',\underline{\nu}')$.

(N.B. Bonds connected by full lines are given the full interaction energies ($J_{ij}\sigma_i\sigma_j$) between the spins connected by the bonds whereas only half of the interaction energies ($\frac{1}{2}J_{ij}\sigma_i\sigma_j$) are considered for bonds connected by broken lines.)



(a)



(b)

Fig. 3.3 The lattice segments correspond to the weight of the spins represented by $X^{\alpha}_{\underline{\mu},\underline{\nu}}$ and $A^{\alpha}_{\underline{\mu},\underline{\mu}'}$, summing over the dotted spins.

the $2^{m+1} \times 2^{m+1}$ matrix

$$\mathcal{A}' = \begin{pmatrix} A(+) & 0 \\ 0 & A(-) \end{pmatrix} \qquad (3.3.12)$$

and its transpose is the corner transfer matrix for the square lattice (Baxter, 1977). Also, by (3.3.1b), $F^*(\alpha,\beta)$ may then be interpreted as the "half-row" transfer matrix of the lattice.

With the above graphical interpretation for the matrices, each term in the expression (3.3.3) of κ can be interpreted as a partition function for the lattice of a certain size with a different partition (see Fig. 3.4). If we still adopt this definition of $A(\alpha)$, $F(\alpha,\beta)$ and $F^*(\alpha,\beta)$ for a given finite m, then (3.3.3) implies

$$\kappa = \frac{Z_{2m+1,2m+1}\, Z_{2m+2,2m+2}}{Z_{2m+1,2m+2}\, Z_{2m+2,2m+1}} \qquad (3.3.13)$$

where Z_{n_r,n_c} is the partition function of a lattice of n_r rows and n_c columns as defined in (3.2.2). This provides an approximate formula for κ and is exact if m is infinite (Woodbury, 1969; Enting and Baxter, 1977).

As proposed in Section III.2, for finite m, by taking the matrices $A(\alpha)$, $F(\alpha,\beta)$ and $F^*(\alpha,\beta)$ to be arbitrary, a sequence of variational approximations for κ of the infinite system may be obtained. When m is finite, one may imagine a similar graphical interpretation for the matrices in the finite lattice, except that now the interactions between sites of the lattice are more

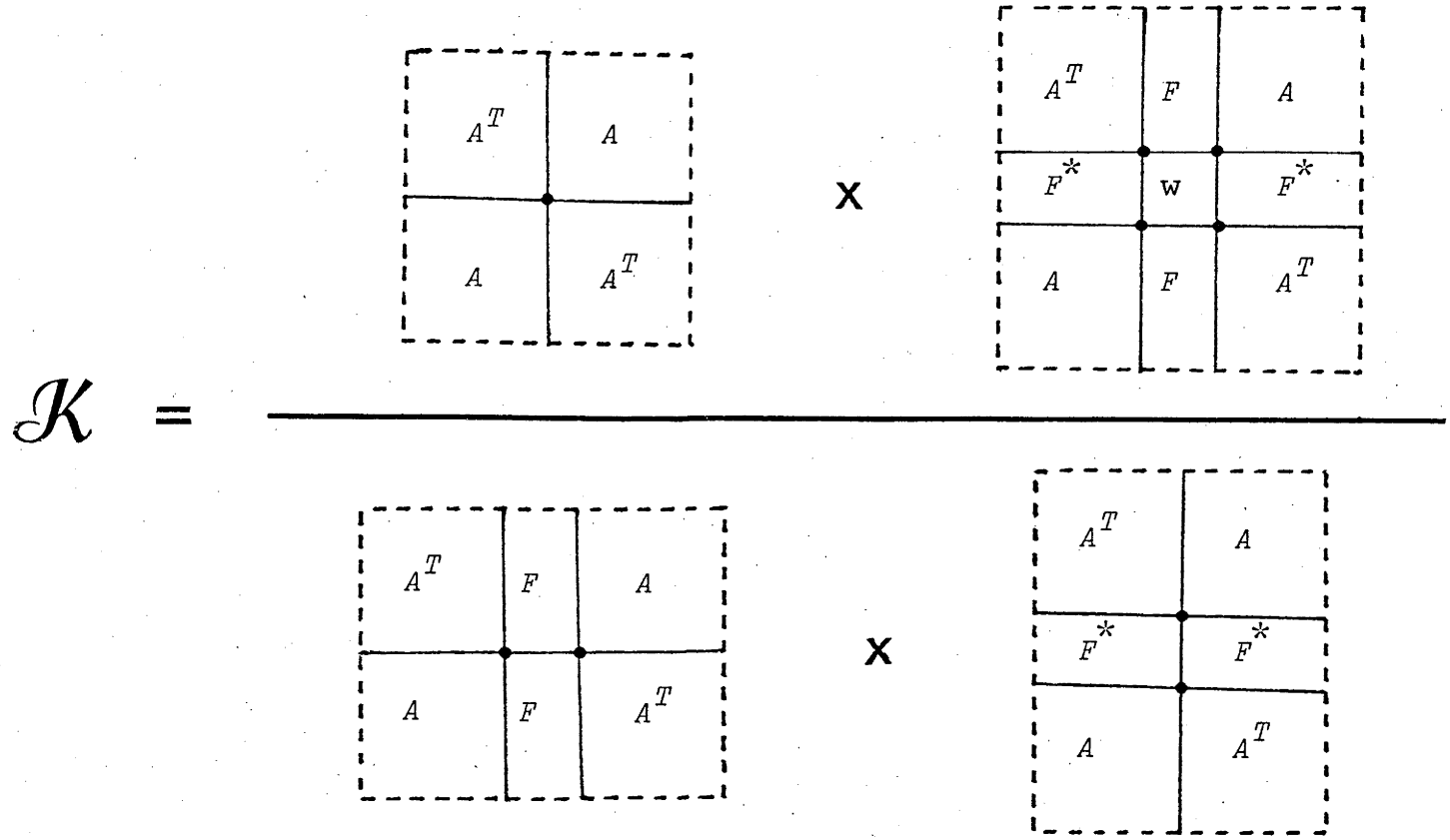


Fig. 3.4 Graphical representation of the variational expression (3.3.3) for κ .

complicated and are such as to maximize the free energy of the system at a given temperature. Moreover, the interpretation of the matrices as corner (row or column) transfer matrices of the system may provide a good initial guess to the solution of the sequence of variational approximations.

4 THE SEQUENCE OF VARIATIONAL APPROXIMATIONS FOR THE ISOTROPIC SQUARE ISING MODEL

§ 4.1 REPRESENTATIONS IN WHICH $A(\pm)$ DIAGONAL

The variational method reduces the calculation of the partition function of the system to the evaluation of equations (3.2.33a,b) and (3.2.44) . In terms of matrices $A(\alpha)$, $F(\alpha,\beta)$ and $F^*(\alpha,\beta)$ ($\alpha,\beta = +$ or $-$) , they can be written as

$$\sum_{\alpha'} F(\alpha,\alpha')\, A^T(\alpha')\, A(\alpha')\, F(\alpha',\alpha) = \xi\, A^T(\alpha)\, A(\alpha) \qquad (3.4.1a)$$

$$\sum_{\alpha'}\sum_{\beta'} w(\alpha,\alpha',\beta,\beta')F(\alpha,\alpha')A^T(\alpha')F^*(\alpha',\beta')A(\beta')F(\beta',\beta) = \eta\, A^T(\alpha)F^*(\alpha,\beta)A(\beta) \qquad (3.4.1b)$$

and

$$\sum_{\alpha'}\sum_{\beta'} w(\alpha,\beta,\alpha',\beta')F^*(\alpha,\alpha')A(\alpha')F(\alpha',\beta')A^T(\beta')F^*(\beta',\beta) = \zeta\, A(\alpha)F(\alpha,\beta)A^T(\beta) \qquad (3.4.1c)$$

The set of equations (3.4.1a-c) , (3.2.23) and (3.3.2) are unchanged by the following transformations:

$$\begin{aligned} A(\alpha) &\to c\, Q(\alpha)\, A(\alpha)\, P^T(\alpha) \quad ; \\ F(\alpha,\beta) &\to P(\alpha)\, F(\alpha,\beta)\, P^T(\beta) \quad ; \\ F^*(\alpha,\beta) &\to Q(\alpha)\, F^*(\alpha,\beta)\, Q^T(\beta) \quad ; \end{aligned} \qquad (3.4.2)$$

where $P(+)$, $P(-)$, $Q(+)$ and $Q(-)$ are $2^m \times 2^m$ orthogonal ($\alpha,\beta = +$ or $-$)

matrices and c is some scalar. Hence, without loss of generality, the matrices $A(+)$ and $A(-)$ can be chosen to be diagonal with the maximum diagonal element of $A(+)$ being unity. In this case, we have

$$A(\alpha) = A^T(\alpha) \quad , \quad \alpha = + \text{ or } - \quad . \tag{3.4.3}$$

Since multiplying the matrices $F(\alpha,\beta)$ and $F^*(\alpha,\beta)$ ($\alpha,\beta = +$ or $-$) by some scalar constants c_1 and c_2 respectively only changes the value of ξ , η and ζ accordingly without any change in the structure of the equation, we may normalise the equations such that

$$\xi = 1$$

and (3.4.4)

$$\zeta = \eta \quad .$$

It follows that, in this case, we have

$$\kappa = \eta = \zeta \quad . \tag{3.4.5}$$

We have shown the symmetry of the row and column interactions in the expression of κ in (3.3.3) . So, for simplicity, we will just consider the isotropic case in which the horizontal and vertical nearest-neighbour interactions of the lattice are the same, bearing in mind that all the derivations may be generalised to the anisotropic case.

For the isotropic case, we have

$$J = J_1 = J_2 \quad \text{and} \quad F^*(\alpha,\beta) = F(\alpha,\beta) \quad , \quad \alpha,\beta = + \text{ or } - \quad . \tag{3.4.6}$$

Equations (3.4.1b) and (3.4.1c) become identical and we may write (3.4.1a-c) as

$$\sum_{\alpha'} F(\alpha,\alpha')\, A^2(\alpha')\, F(\alpha',\alpha) = A^2(\alpha) \qquad (3.4.7a)$$

and

$$\sum_{\alpha'} \sum_{\beta'} w(\alpha,\alpha',\beta,\beta') F(\alpha,\alpha') A(\alpha') F(\alpha',\beta') A(\beta') F(\beta',\beta) = \kappa\, A(\alpha) F(\alpha,\beta) A(\beta) \qquad (3.4.7b)$$

From this set of equations, we may then evaluate $A(+)$, $A(-)$, $F(+,+)$, $F(+,-)$ ($= F^T(-,+)$) , $F(-,-)$ and hence κ with $A(+)$ and $A(-)$ being in the diagonal representation.

§ 4.2 ZEROTH ORDER APPROXIMATION

Equations (3.4.7a,b) provide a sequence of variational approximations for κ by taking the size of the matrices to be 2^m with $m = 0, 1, 2, \ldots$. The case for $m = 0$ in zero magnetic field is found to be the same as the Kramers-Wannier approximation.

For $m = 0$, all the matrices that occur in (3.4.7a,b) are just simple scalars. To simplify the notation, let

$$\begin{aligned} A(+) &= a_+ \quad ; \quad A(-) = a_- \quad ; \\ F(+,+) &= f_+ \quad ; \quad F(-,-) = f_- \quad ; \\ F(+,-) &= F(-,+) = f_o \end{aligned} \qquad (3.4.8)$$

where a_+ , a_- , f_+ , f_- and f_o are all scalars. It is obvious that in the representation defined above, we must

have

$$a_+ = 1 \quad . \tag{3.4.9}$$

Define

$$\begin{aligned} z &= \exp(-2J/k_B T) \\ u &= \exp(-2H/k_B T) \end{aligned} \tag{3.4.10}$$

then (3.4.7a) gives

$$f_+^2 + f_0^2 a_-^2 = 1 \tag{3.4.11a}$$

$$f_0^2 + f_-^2 a_-^2 = a_-^2 \tag{3.4.11b}$$

and (3.4.7b) gives

$$z^{-1}u^{-\frac{1}{2}}f_+^3 + 2u^{-\frac{1}{4}}f_+f_0^2a_- + f_0^2a_-^2f_- = \kappa f_+ \tag{3.4.12a}$$

$$u^{-\frac{1}{4}}f_+^2 + f_+a_-f_- + za_-f_0^2 + u^{\frac{1}{4}}a_-^2f_-^2 = \kappa a_- \tag{3.4.12b}$$

$$f_0^2f_+ + 2u^{\frac{1}{4}}f_0^2f_-a_- + z^{-1}u^{\frac{1}{2}}f_-^3a_-^2 = \kappa a_-^2f_- \tag{3.4.12c}$$

For z small (i.e. in the low temperature region) and H positive, a series expansion in z of the solution may be obtained for κ .

Firstly, to leading order, equations (3.4.11a,b) and (3.4.12a-c) imply [footnote 3]

$$\kappa \sim z^{-1} u^{-\frac{1}{2}} \quad ; \quad f_+ \sim 1 \quad ;$$

$$f_0 \sim a_- \sim z\, u^{\frac{1}{4}} \quad ;$$

and

$$f_- \sim z\, u^{\frac{1}{2}} \quad . \tag{3.4.13}$$

Assuming that

$$\begin{aligned} \kappa &= z^{-1} u^{-\frac{1}{2}} (1 + \delta\kappa) \\ f_+ &= 1 + \delta f_+ \\ f_0 &= z u^{\frac{1}{4}} (1 + \delta f_0) \\ f_- &= z u^{\frac{1}{2}} (1 + \delta f_-) \\ a_- &= z u^{\frac{1}{4}} (1 + \delta a_-) \end{aligned} \qquad (3.4.14)$$

and equating subsequent higher order terms in the equations, we find that at low temperatures,

$$\begin{aligned} \kappa = z^{-1} u^{-\frac{1}{2}} \{ & 1 + z^4 u + 2z^6 u^2 \\ & + z^8 (- 2u^2 + 6u^3 + u^4) \\ & + z^{10} (- 14u^3 + 18u^4 + 8u^5 + 2u^6) \\ & + z^{12} (8u^3 - 77u^4 + 44u^5 + 40u^6 + 22u^7 + 6u^8) \\ & + \ldots \quad \} \end{aligned} \qquad (3.4.15a)$$

or equivalently

$$\begin{aligned} \ln \kappa = & (2J+H)/k_B T + z^4 u + 2z^6 u^2 \\ & + z^8 (- 2\tfrac{1}{2} u^2 + 6u^3 + u^4) \\ & + z^{10} (- 16u^3 + 18u^4 + 8u^5 + 2u^6) \\ & + z^{12} (10\tfrac{1}{3} u^3 - 85u^4 + 43u^5 + 40u^6 + 22u^7 + 6u^8) \\ & + \ldots \end{aligned} \qquad (3.4.15b)$$

Compared with the exact series expansions for the square Ising lattice (Sykes, Essam and Gaunt, 1965),

$$\ln \kappa = (2J+H)/k_B T + z^4 u + 2z^6 u^2$$
$$+ z^8 \left(- 2\tfrac{1}{2} u^2 + 6u^3 + u^4 \right)$$
$$+ z^{10} \left(- 16u^3 + 18u^4 + 8u^5 + 2u^6 \right)$$
$$+ z^{12} \left(10\tfrac{1}{3} u^3 - 85u^4 + 43u^5 + 40u^6 + 22u^7 + 6u^8 + u^9 \right)$$
$$+ \ldots \quad , \qquad (3.4.16)$$

the result for $m = 0$ already agrees with the exact result up to terms of order z^{10} in the expansion.

It can be shown that our equations are in fact identical with those given by Kramers and Wannier (1941b) if we make the following transformations of variables

$$e^{4H} \rightarrow f_+ f_- / f_0^2$$
and $$(3.4.17)$$
$$e^{A} \rightarrow f_+ / f_-$$

for the variational function in equation (75) of Kramers and Wannier (1941b).

§ 4.3 ITERATIVE METHOD OF SOLUTION

With a reasonable initial guess to the solution of the equations (3.4.7a,b) for a given m, an iterative procedure for the solution similar to Baxter (1978) may be obtained.

Define matrices

$$H(\alpha, \beta' | \beta) = \sum_{\alpha'} w(\alpha, \alpha', \beta, \beta') F(\alpha, \alpha') A(\alpha') F(\alpha', \beta') \qquad (3.4.18)$$

$$F_o(\beta) = \begin{pmatrix} A(+)F(+,\beta)A^{-1}(\beta) \\ A(-)F(-,\beta)A^{-1}(\beta) \end{pmatrix} \qquad (3.4.19)$$

and

$$U(\beta) = \begin{pmatrix} H(+,+|\beta) & H(+,-|\beta) \\ H(-,+|\beta) & H(-,-|\beta) \end{pmatrix} \qquad (3.4.20)$$

$$\alpha,\ \beta = + \text{ or } - \ .$$

Equation (3.4.7b) can be written as

$$U(\beta)\ F_o(\beta) = \kappa\ F_o(\beta)\ A(\beta) \quad ,\quad \beta = + \text{ or } - \ . \qquad (3.4.21)$$

It follows that the elements of $\kappa A(\alpha)$ are contained in the set of eigenvalues of $U(\alpha)$ and all the column vectors of $F_o(\alpha)$ are eigenvectors of $U(\alpha)$. So, with a knowledge of the leading order behaviour of the elements of $A(\alpha)$, we are able to select from the set of eigenvalues of $U(\alpha)$, the appropriate elements for the matrices $\kappa A(\alpha)$ and hence obtain the solution for $F(\alpha,\alpha')$ also from the corresponding eigenvectors of $U(\alpha)$.

This suggests the following iterative procedure for solving the equations for a given value of m. Given a reasonable initial guess at the solution for $A(\alpha)$ and $F(\alpha,\beta)$:

(i) Calculate $U(+)$ and $U(-)$ and obtain their normalised eigenvectors and eigenvalues.

(ii) Since the maximum eigenvalue for $A(+)$ is unity, κ is equal to the largest eigenvalue of $U(+)$.

(iii) From the 2^{m+1} eigenvalues of $U(\alpha)$ ($\alpha = +$ or $-$)

select the 2^m of these which are closest to the previous values of the elements of $\kappa\, A(\alpha)$ and hence redefine $A(\alpha)$ accordingly.

(iv) Using this selection and ordering of the eigenvalues, obtain the matrices $F_0(\alpha)$ from the corresponding set of eigenvectors.

(v) The matrices $F(\alpha,\beta)$ may be obtained from the elements of

$$\begin{pmatrix} A^{-1}(+) & \\ & A^{-1}(-) \end{pmatrix} F_0(\alpha)A(\alpha) \equiv \begin{pmatrix} F(+,\alpha) \\ F(-,\alpha) \end{pmatrix} \quad (3.4.22)$$

by (3.4.19).

§ 4.4 LEADING ORDER CONSIDERATIONS

It is more convenient to define matrices

$$\mathscr{A} = \begin{pmatrix} A(+) & \\ & u^{-\frac{1}{4}}A(-) \end{pmatrix} \quad (3.4.23)$$

and

$$\mathscr{F} = \begin{pmatrix} F(+,+) & z^{\frac{1}{2}}u^{\frac{1}{4}}F(+,-) \\ z^{\frac{1}{2}}u^{\frac{1}{4}}F(-,+) & u^{\frac{1}{2}}F(-,-) \end{pmatrix} \quad (3.4.24)$$

where z and u are defined in (3.4.10). It can be shown readily that

$$\begin{aligned} U(+) &= z^{-1}u^{-\frac{1}{2}} \begin{pmatrix} I & \\ & z^{\frac{1}{2}}I \end{pmatrix} \mathcal{U} \begin{pmatrix} I & \\ & z^{\frac{1}{2}}I \end{pmatrix} \\ U(-) &= z^{-1}u^{-\frac{1}{4}} \begin{pmatrix} z^{\frac{1}{2}}I & \\ & I \end{pmatrix} \mathcal{U} \begin{pmatrix} z^{\frac{1}{2}}I & \\ & I \end{pmatrix} \end{aligned} \quad (3.4.25)$$

where

$$\mathcal{U} = \mathcal{Z}^T \mathcal{A} \mathcal{Z} \tag{3.4.26}$$

and I is the identity matrix.

Define a $2^{m+2} \times 2^{m+2}$ matrix V by

$$V = zu^{\frac{1}{2}} \begin{pmatrix} U(+) & \\ & u^{-\frac{1}{4}} U(-) \end{pmatrix} \tag{3.4.27}$$

then (3.4.21) can equivalently be written as

$$V \begin{pmatrix} F_0(+) & 0 \\ 0 & F_0(-) \end{pmatrix} = zu^{\frac{1}{2}} \kappa \begin{pmatrix} F_0(+) & 0 \\ 0 & F_0(-) \end{pmatrix} \mathcal{A} \tag{3.4.28}$$

Also define matrix P to be the orthogonal matrix which diagonalizes V and let the corresponding diagonal matrix containing the eigenvalues of V to be

$$C \equiv (d_j) \quad ; \quad j = 1, 2, \ldots, 2^{m+2} \quad . \tag{3.4.29}$$

With this set of matrix variables, we have obtained the leading order solution of $\mathcal{A}$, $\mathcal{Z}$ and κ for $m = 0$ and $m = 1$ using the iterative procedure defined previously, in Appendix III.A .

If we order the column vectors of P in such a way that at low temperatures, P is almost diagonal (i.e. $p_{\ell,\ell} \simeq 1$ and $p_{\ell,j} << p_{\ell,\ell}$ for $\ell \neq j$) , then from the leading order behaviour of the matrices involved (see Appendix III.A), for small values of m , we find that

$$\kappa = d_1 \; / \; zu^{\frac{1}{2}} \tag{3.4.30}$$

and with

$$\mathcal{A} \equiv (a'_j) \quad , \quad j = 1, 2, \ldots, 2^{m+1} \quad , \qquad (3.4.31a)$$

we have

$$a'_j = d_{2j-1} / d_1 \quad , \quad j = 1, 2, \ldots, 2^{m+1} \; . \qquad (3.4.31b)$$

We may form $F_0(+)$ and $F_0(-)$ from the corresponding odd column vectors of P . Let

$$\mathcal{H} = \mathcal{A}^{-1} \left(F_0(+) \, , \, F_0(-) \right) \mathcal{A}$$

$$= \begin{pmatrix} F(+,+) & u^{-\frac{1}{4}} F(+,-) \\ u^{\frac{1}{4}} F(-,+) & F(-,-) \end{pmatrix} \qquad (3.4.32)$$

$\mathcal{L}$ can then be obtained from its definition (3.4.24) .

5 THE VARIATIONAL EQUATIONS IN THEIR REPRESENTATIVES

The argument up to now is still applicable even in the presence of a magnetic field. However, since we are interested in the convergence of the sequence of approximations to the exact solution as m increases, we will focus our attention on the case in which the magnetic field is zero. In this case, we are able to apply Kaufman's technique of spinor representations, as defined in Section II.3.1.

§ 5.1 THE REPRESENTATIVES OF THE MATRICES

In order to formulate the problem in the spinor representations, we define a set of $(2p+1)$ spin operators,

$$\Gamma_1 = s_1 \quad ; \quad \Gamma_2 = (c_1 s_2 + i d_1)/\sqrt{2} \quad ; \quad \Gamma_3 = (c_1 s_2 - i d_1)/\sqrt{2} \quad ;$$

$$\Gamma_{2j} = c_1 c_2 \ldots c_{j-1} \, (c_j s_{j+1} + i d_j)/\sqrt{2} \quad ;$$

$$\Gamma_{2j+1} = c_1 c_2 \ldots c_{j-1} \, (c_j s_{j+1} - i d_j)/\sqrt{2} \quad ;$$

$$j = 2, 3, \ldots, p \, . \qquad (3.5.1)$$

where s_j , c_j and d_j are the Pauli spin operators acting on the j th spin as defined in (2.2.18) and $s_{p+1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$,

the identity matrix ($i = \sqrt{-1}$). The set of operators is not totally anticommuting with each other, yet the representatives under this set of operators can be obtained by a similarity transformation from the following set of $(2p+1)$ anticommuting operators :

$$\Gamma'_1 = s_1 \quad ; \quad \Gamma'_2 = d_1 \quad ; \quad \Gamma'_3 = c_1 s_2 \quad ;$$

$$\Gamma'_{2j} = c_1 c_2 \ldots c_{j-1} d_j \quad ; \quad \Gamma'_{2j+1} = c_1 c_2 \ldots c_j s_{j+1} \quad ;$$

$$j = 2, 3, \ldots, p \quad . \qquad (3.5.2)$$

The representatives $\hat{X}$ under Γ_j s are related to those ($\hat{X}'$) under Γ'_j s by

$$\hat{X} = R^{-1} \hat{X}' R \qquad (3.5.3)$$

where

$$R = \begin{pmatrix} 1 & & & & & & \\ & i/\sqrt{2} & -i/\sqrt{2} & & & & \\ & 1/\sqrt{2} & 1/\sqrt{2} & & & & \\ & & & i/\sqrt{2} & -i/\sqrt{2} & & \\ & & & 1/\sqrt{2} & 1/\sqrt{2} & & \\ & & & & & \ddots & \\ & & & & & & \ddots \end{pmatrix} \qquad (3.5.4)$$

Clearly, the representatives under (3.5.1) also form a group $\mathcal{G}$. Similar to the case in Section II.3.1, we can establish the following corresponding properties of the representatives :

(i) The inverse of any $\hat{X}$ in $\mathcal{G}$ is given by

$$\hat{X}^{-1} = L\,\hat{X}^{T}\,L \tag{3.5.5}$$

where

$$L = \begin{pmatrix} 1 & & & & & & \\ & 0 & 1 & & & & \\ & 1 & 0 & & & & \\ & & & 0 & 1 & & \\ & & & 1 & 0 & & \\ & & & & & \ddots & \\ & & & & & & \ddots \end{pmatrix} \tag{3.5.6}$$

(ii) Each representative determines its parent matrix to within a multiplicative constant. Furthermore, if X_1 , X_2 , ... , X_j , Y are members of the group such that $X_1X_2\ldots X_j = Y$, then the corresponding representatives $\hat{X}_1$, $\hat{X}_2$, ... , $\hat{X}_j$, $\hat{Y}$ satisfy the same relationship, i.e. $\hat{X}_1\hat{X}_2\ldots\hat{X}_j = \hat{Y}$.

(iii) If X is real and symmetric, then $\hat{X}$ is real and symmetric.

(iv) If X is orthogonal, $\hat{X}$ is orthogonal and has the following structure

$$\hat{X} = \begin{pmatrix} a & q & q & r & r & \cdots \\ s & u & v & f & g & \\ s & v & u & g & f & \\ t & y & z & \ell & h & \\ t & z & y & h & \ell & \\ \vdots & & & & & \ddots \end{pmatrix} \tag{3.5.7}$$

(v) If X is diagonal, it must be of the form

$$X = \rho \times \prod_{j=1}^{p} \tfrac{1}{2}\{(1+y_j) + (1-y_j)s_j s_{j+1}\} \qquad (3.5.8)$$

where ρ is some scalar factor, and $\hat{X}$ is diagonal, with diagonal elements $x_1 , x_2 , \ldots , x_{2p+1}$ satisfying

$$x_1 = 1 \quad ; \quad x_{2j+1} = 1/x_{2j} = y_j \quad ; \quad j=1,2,\ldots,p . \qquad (3.5.9)$$

It can be verified that the representatives of $\mathscr{A}$ and $\mathscr{Y}$ exist under (3.5.1) with $p = m+1$. For matrices V , P and C , we apply an enlarged set of operators Γ_j^{en} defined similarly in (3.5.1) with $p = m+2$. From the definitions of the matrices V , P and C , and the representatives, one can obtain $\hat{V}$ from $\hat{\mathscr{Y}}$ and also $\hat{\mathscr{Y}}$ from $\hat{P}$ [Appendix III.B] . So, in a similar way to above, an analogous iterative procedure for the equations in their representatives may be developed.

§ 5.2 ITERATIVE METHOD OF SOLUTION

Given a reasonable initial guess of $\hat{\mathscr{A}}$ and $\hat{\mathscr{Y}}$ at a particular value of z and setting $n = m+2$:

(i) Define $\hat{U}$ by

$$\hat{U} = \hat{\mathscr{Y}}^T \hat{\mathscr{A}} \hat{\mathscr{Y}} \equiv (u_{\ell,j}) \quad , \quad \ell,j=1,2,\ldots,2n-1 . \qquad (3.5.10)$$

Then $\hat{V}$ is given by

$$\hat{V} = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & (u_{1,1}+1)/2z & (u_{1,1}-1)/2 & (2z)^{-\frac{1}{2}}u_{1,j-2} & \cdots \\ \vdots & & z(u_{1,1}+1)/2 & (z/2)^{\frac{1}{2}}u_{1,j-2} & \cdots \\ & & & u_{\ell-2,j-2} & \\ & & & & \ddots \end{pmatrix}$$

$$\ell, j = 4, 5, \ldots, 2n+1 \ . \qquad (3.5.11)$$

Note that $\hat{V}$ is symmetric.

(ii) Solve the eigenvalue equation

$$\hat{V}\,\hat{P} = \hat{P}\,\hat{C} \qquad (3.5.12)$$

for $\hat{C}$ and $\hat{P}$ such that $\hat{C}$ is diagonal and $\hat{P}$ is orthogonal and almost diagonal.

(iii) With $\hat{C} \equiv (a_j)$, $j = 1, 2, \ldots, 2n+1$, $\hat{\mathcal{A}}$ is obtained by truncating the last two rows and columns of $\hat{C}$, i.e. $\hat{\mathcal{A}} = (a_j)$, $j = 1, 2, \ldots, 2n-1$. (3.5.13)

(iv) Given

$$\hat{P} \equiv (p_{\ell,j}) \quad , \quad \ell, j = 1, 2, \ldots, 2n+1 \qquad (3.5.14)$$

and let

$$\hat{\mathcal{H}} \equiv (h_{\ell,j}) \quad , \quad \ell, j = 1, 2, \ldots, 2n-1 \qquad (3.5.15)$$

then, we have

$$h_{1,1} = (p_{2,2n}+p_{3,2n}) \ / \ (p_{2,2n}-p_{3,2n}) \quad ,$$

$$h_{1,j} = \frac{a_j}{\sqrt{2}} \{ (p_{2,j}+p_{3,j}) - \frac{(p_{2,j}-p_{3,j})(p_{2,2n}+p_{3,2n})}{(p_{2,2n}-p_{3,2n})} \} \quad ,$$

$$h_{j,1} = a_j^{-1}\sqrt{2} \{ p_{j+2,2n} / (p_{2,2n}-p_{3,2n}) \} \qquad (3.5.16)$$

and

$$h_{\ell,j} = a_\ell^{-1} \{ p_{\ell+2,j} - p_{\ell+2,2n} \frac{(p_{2,j}-p_{3,j})}{(p_{2,2n}-p_{3,2n})} \} a_j$$
$$\ell,j=2,3,\ldots,2n-1 \quad . \qquad (3.5.17)$$

From (3.4.24) and (3.4.32) ,

$$\hat{\mathcal{J}} = \left(\begin{array}{c|c} \frac{h_{1,1}+v}{1+vh_{1,1}} & \frac{h_{1,j}}{\mathrm{ch}(J/k_BT)\ (1+vh_{1,1})} \\ \hline & h_{\ell,j} - \frac{vh_{1,j}h_{\ell,1}}{1+vh_{1,1}} \\ & \ell,j=2,3,\ldots,2n-1 \ . \end{array} \right) \qquad (3.5.18)$$

where $v = \tanh(J/k_BT)$. [Appendix III.B]

The whole procedure may be repeated until we arrive at a solution of $\mathcal{A}$ and $\hat{\mathcal{J}}$ with satisfactory accuracy.

§ 5.3 SYMMETRY PROPERTIES OF $\hat{\mathcal{H}}$

The problem can be further simplified by using the symmetry properties of $\hat{\mathcal{H}}$. By definition, $\mathcal{H}$ is symmetric and hence using property (iii) of the representatives, $\hat{\mathcal{H}}$ is symmetric. That is, we have,

$$h_{\ell,j} = h_{j,\ell} \quad , \quad \text{for} \quad \ell,j=1,2,\ldots,2n-1. \tag{3.5.19}$$

Firstly, since V breaks into two diagonal blocks, we must have

$$p_{1,1} = 1 \quad \text{and} \quad p_{1,j} = p_{j,1} = 0 \quad , \quad j = 2, 3, \ldots, 2n+1 \ . \tag{3.5.20}$$

In view of (3.5.16) and (3.5.17), (3.5.19) implies that

$$p_{j+2,2n} = a_j^2 \left(p_{2,2n}p_{3,j} - p_{2,j}p_{3,2n} \right) \quad j = 2, 3, \ldots, 2n-1 \ , \tag{3.5.21}$$

and

$$a_\ell^2 p_{j+2,\ell} - a_j^2 p_{\ell+2,j} = a_j^2 a_\ell^2 \left(p_{2,\ell}p_{3,j} - p_{2,j}p_{3,\ell}\right) \quad \ell, j = 2, 3, \ldots, 2n-1 \ . \tag{3.5.22}$$

Noting the special structure of $\hat{P}$ from property (iv) of the representatives, we define

$$\begin{aligned} \mu_{j,\ell} &= p_{2j,2\ell} = p_{2j+1,2\ell+1} \\ \nu_{j,\ell} &= p_{2j,2\ell+1} = p_{2j+1,2\ell} \end{aligned} \qquad \ell,j=1,2,\ldots,n \ . \tag{3.5.23}$$

and also

$$c_j = a_{2j+1} = 1/a_{2j} \quad . \tag{3.5.24}$$

If we put $\ell \to 2\ell$ and $j \to 2j$ in (3.5.22), we have

$$\mu_{j+1,\ell}c_\ell^{-2} - \mu_{\ell+1,j}c_j^{-2} = (\mu_{1,\ell}\nu_{1,j} - \mu_{1,j}\nu_{1,\ell})\, c_\ell^{-2}c_j^{-2} \quad \ell,j=1,2,\ldots,n-1 \ . \tag{3.5.25a}$$

Also, if we put $\ell \to 2\ell+1$ and $j \to 2j+1$, then (3.5.22)

gives

$$\mu_{j+1,\ell}c_\ell^2 - \mu_{\ell+1,j}c_j^2 = (\mu_{1,j}\nu_{1,\ell} - \mu_{1,\ell}\nu_{1,j})\, c_\ell^2 c_j^2$$
$$\ell,j=1,2,\ldots,n-1 \ . \qquad (3.5.25b)$$

Hence, combining both equations, we have

$$\mu_{\ell+1,j} = c_\ell^2(1+c_j^4)\,(\mu_{1,j}\nu_{1,\ell} - \mu_{1,\ell}\nu_{1,j}) \,/\, (c_\ell^4 - c_j^4)$$
$$\ell \neq j \ ; \quad \ell,j=1,2,\ldots,n-1 \ . \qquad (3.5.26)$$

Similarly, by putting $\ell \to 2\ell$, $j \to 2j+1$ and $\ell \to 2\ell+1$, $j \to 2j$ respectively in (3.5.22), we obtain

$$\nu_{j+1,\ell}c_\ell^{-2} - \nu_{\ell+1,j}c_j^2 = (\mu_{1,\ell}\mu_{1,j} - \nu_{1,\ell}\nu_{1,j})\, c_\ell^{-2} c_j^2$$

and

$$\nu_{j+1,\ell}c_\ell^2 - \nu_{\ell+1,j}c_j^{-2} = (\nu_{1,\ell}\nu_{1,j} - \mu_{1,\ell}\mu_{1,j})\, c_\ell^2 c_j^{-2} \qquad (3.5.27)$$

Thus, combining, we have

$$\nu_{\ell+1,j} = c_\ell^2(1+c_j^4)\,(\mu_{1,\ell}\mu_{1,j} - \nu_{1,\ell}\nu_{1,j}) \,/\, (1-c_\ell^4 c_j^4)$$
$$\ell,j=1,2,\ldots,n-1 \ . \qquad (3.5.28)$$

(3.5.26) and (3.5.28) can be combined into one equation given by

$$p_{\ell+2,j} = a_\ell^2(1+a_j^4)\,(p_{2,j}p_{3,\ell} - p_{2,\ell}p_{3,j}) \,/\, (a_j^4 - a_\ell^4)$$
$$\ell \neq j \ ; \quad \ell,j=2,3,\ldots,2n-1 \ . \qquad (3.5.29)$$

In view of (3.5.21) , we may extend the equation to include the case when $j = 2n$ and $2n+1$ also. If we define

$$\beta_j = (1 + a_j^4) \ , \quad j=2,3,\ldots,2n-1 \qquad (3.5.30)$$

and $\beta_{2n} = \infty$, $\beta_{2n+1} = 1$, then, we may write

$$p_{\ell+2,j} = \alpha_\ell^2 \beta_j \, (p_{2,j}p_{3,\ell} - p_{2,\ell}p_{3,j}) \, / \, (\beta_j - \beta_\ell) \quad ,$$

$$\ell \neq j \quad ; \quad \ell = 2,3,\ldots,2n-1 \; , \quad j = 2,3,\ldots,2n+1 \; , \tag{3.5.31a}$$

where

$$\text{and} \quad \begin{matrix} p_{3,2j} = p_{2,2j+1} \\ p_{3,2j+1} = p_{2,2j} \end{matrix} \quad , \text{ for } \; j = 1,2,\ldots,n \; . \tag{3.5.31b}$$

Hence, the only independent elements of $\hat{P}$ are $p_{2,j}$ for $j = 2, 3, \ldots, 2n+1$ and $p_{j+2,j}$ for $j = 2, 3, \ldots, 2n-1$.

One can substitute (3.5.31a,b) into (3.5.18) to obtain $\hat{\mathscr{Z}}$. If we write

$$\hat{\mathscr{Z}} \equiv (f_{\ell,j}) \quad , \quad \ell,j = 1,2,\ldots,2n-1 \quad , \tag{3.5.32}$$

then

$$f_{1,1} = (p_{2,2n} + zp_{2,2n+1}) \, / \, g_{2n} \quad ,$$

$$f_{1,j} = f_{j,1} = (2z)^{\frac{1}{2}} \, \alpha_j r_j \, / \, (\beta_j g_{2n}) \quad ,$$

$$f_{j,j} = p_{j+2,j} - \alpha_j^2 g_j r_j \, / \, (\beta_j g_{2n}) \quad ,$$

$$f_{\ell,j} = f_{j,\ell} = \alpha_j \alpha_\ell \, (g_j r_\ell - g_\ell r_j) \, / \, (\beta_j - \beta_\ell) g_{2n}$$

$$\ell \neq j \quad ; \quad \ell,j = 2,3,\ldots,2n-1 \; , \tag{3.5.33}$$

where

$$\begin{aligned} g_j &= p_{2,j} - zp_{3,j} \\ r_j &= \beta_j \, (p_{2,2n}p_{3,j} - p_{2,j}p_{3,2n}) \end{aligned} \tag{3.5.34}$$

§ 5.4 REDUCTION OF THE MATRIX EQUATIONS

The main problem in the iterative procedure is to solve for $\hat{C}$ and $\hat{P}$ in equation (3.5.12) . However, the elements of $\hat{V}$ is related to the elements of $\hat{U}$ through (3.5.11) . Also, the elements of $\hat{U}$, from (3.5.10) and (3.5.33) , can again be written in terms of elements of $\hat{C}$ and $\hat{P}$. Hence, equation (3.5.12) provides a set of equations relating elements of $\hat{C}$ and $\hat{P}$ only.

(3.5.12) implies that with

$$\hat{V} \equiv (v_{\ell,j}) \quad , \qquad \ell,j=1,2,\ldots,2n+1 \ , \tag{3.5.35}$$

we have

$$v_{\ell,j} = \sum_{i=1}^{2n+1} p_{\ell,i}\, a_i\, p_{j,i} \quad ; \quad \ell,j=1,2,\ldots,2n+1. \tag{3.5.36}$$

However, the special structure of $\hat{V}$ from (3.5.11) requires that

$$\begin{aligned} v_{3,3} &= z^2\, v_{2,2} \\ v_{2,3} &= z v_{2,2} - 1 \end{aligned} \tag{3.5.37}$$

and

$$v_{3,j} = z\, v_{2,j} \ , \qquad j=4,5,\ldots,2n+1 \ . \tag{3.5.38}$$

Combining the various cases for (ℓ,j) being equal to $(2,2)$, $(3,3)$ and $(2,3)$ in (3.5.36) , we obtain

$$\begin{aligned} \sum_{i=2}^{2n+1} a_i\, p_{3,i}^2 &= z^2\, \sigma \\ \text{and} \\ \sum_{i=2}^{2n+1} a_i\, p_{2,i}\, p_{3,i} &= z\sigma - 1 \end{aligned} \tag{3.5.39}$$

where

$$\sigma = \sum_{i=1}^{2n+1} a_i \, p_{2,i}^2 \quad . \tag{3.5.40}$$

Also, if we take the square of (3.5.12), bearing in mind that $\hat{P}$ is orthogonal, we have

$$\hat{V}^2 = \hat{P} \, \hat{C}^2 \, \hat{P}^T \tag{3.5.41}$$

Hence, using (3.5.37) and (3.5.38), we obtain

$$\sum_{i=1}^{2n+1} a_i^2 \, p_{3,i}^2 = z^2\rho - 2z(1-z^2)\sigma + 1 - z^2$$

and (3.5.42)

$$\sum_{i=1}^{2n+1} a_i^2 \, p_{2,i} \, p_{3,i} = z\rho - (1-z^2)\sigma - z$$

where

$$\rho = \sum_{j=1}^{2n+1} a_j^2 \, p_{2,j}^2 \quad . \tag{3.5.43}$$

Let

$$x_j = p_{2,j} - z p_{3,j}$$

and (3.5.44)

$$y_j = a_j \, (z p_{2,j} - p_{3,j})$$

then, from (3.5.39) to (3.5.43), one can easily arrive at

$$\sum_{j=1}^{2n+1} x_j^2 = \sum_{j=1}^{2n+1} y_j^2 = \sum_{j=1}^{2n+1} x_j y_j = 1 + z^2 \quad . \tag{3.5.45}$$

Hence, we may write

$$\sum_{j=1}^{2n+1} (x_j - y_j)^2 = 0 \quad . \tag{3.5.46}$$

However, since C and P are real matrices and hence $\hat{C}$

and $\hat{P}$ are real, we have x_j and y_j real also. So, (3.5.46) implies

$$x_j = y_j \quad , \quad j=1,2,\ldots,2n+1 \quad . \tag{3.5.47}$$

That is, we have

$$p_{3,j} = p_{2,j}\,(1-za_j)/(z-a_j) \quad , \quad j=1,2,\ldots,2n+1 \quad . \tag{3.5.48}$$

Equation (3.5.48) enables us to simplify the matrix equations a lot. The main conditions for the matrices can be summarized in the following equations :

$$\hat{V} = \hat{P}\,\hat{C}\,\hat{P}^T = f(\hat{\mathcal{Y}}^T \hat{\mathcal{A}}\,\hat{\mathcal{Y}}) \tag{3.5.49}$$

and also the orthogonality condition for $\hat{P}$, i.e.

$$\hat{P}\,\hat{P}^T = \mathrm{I} \quad . \tag{3.5.50}$$

Using (3.5.48) , equation (3.5.39) reduces to

$$(1-z^2)^2 \sum_{j=2}^{2n+1} \frac{a_j p_{2,j}^2}{(z-a_j)^2} + 2z(1-z^2) \sum_{j=2}^{2n+1} \frac{a_j p_{2,j}^2}{(z-a_j)} = 0 \tag{3.5.51a}$$

and

$$(1-z^2) \sum_{j=2}^{2n+1} \frac{a_j p_{2,j}^2}{(z-a_j)} = -1 \quad . \tag{3.5.51b}$$

Combining, we obtain

$$\sum_{j=2}^{2n+1} \frac{a_j p_{2,j}^2}{(z-a_j)^2} = 2z/(1-z^2)^2 \quad . \tag{3.5.52}$$

Similarly, (3.5.42) implies

$$\sum_{j=2}^{2n+1} \frac{a_j^2 p_{2,j}^2}{(z-a_j)^2} = (1+z^2)/(1-z^2)^2 \qquad (3.5.53)$$

The orthogonality condition of $\hat{P}$ provides us the normalization equation for the elements $p_{2,j}$.

$$\sum_{j=2}^{2n+1} p_{2,j}^2 = 1 \qquad . \qquad (3.5.54)$$

The conditions that

$$\sum_{j=2}^{2n+1} p_{3,j}^2 = 1$$

and (3.5.55)

$$\sum_{j=2}^{2n+1} p_{2,j}\, p_{3,j} = 0$$

are automatically satisfied provided that (3.5.52) and (3.5.53) are satisfied. The orthogonality of other row vectors of $\hat{P}$ with the vector formed by $p_{2,j}$ provides us additional conditions on elements of $p_{2,j}$. The fact that

$$\sum_{\ell=2}^{2n+1} p_{i,\ell}\, p_{j,\ell} = \delta_{i,j} \qquad (3.5.56)$$

implies that for $i = 2$,

$$\sum_{\ell=2\neq j}^{2n+1} \frac{\beta_\ell p_{2,\ell}^2 a_j^2 (a_\ell - a_j)}{(\beta_\ell - \beta_j)\ (z-a_\ell)} = p_{j+2,j}\ (z-a_j)/(1-z^2) \qquad (3.5.57)$$

and for $i = 3$,

$$\sum_{\ell=2\neq j}^{2n+1} \frac{\beta_\ell p_{2,\ell}^2 a_j^2 (a_\ell - a_j)(1-z a_\ell)}{(\beta_\ell - \beta_j)\ (z-a_\ell)^2} = p_{j+2,j}\ (1-z a_j)/(1-z^2) \qquad (3.5.58)$$

Multiplying (3.5.57) by z and subtracting it from

(3.5.58) gives

$$\sum_{\ell=2\neq j}^{2n+1} \frac{\beta_\ell p_{2,\ell}^2 a_j^2 (a_\ell - a_j)}{(\beta_\ell - \beta_j)(z-a_\ell)^2} = p_{j+2,j} / (1-z^2)$$

$$j = 2, 3, \ldots, 2n+1 \quad . \qquad (3.5.59a)$$

Similarly multiplying (3.5.58) by z and subtracting it from (3.5.57) gives

$$\sum_{\ell=2\neq j}^{2n+1} \frac{\beta_\ell p_{2,\ell}^2 a_\ell a_j (a_\ell - a_j)}{(\beta_\ell - \beta_j)(z-a_\ell)^2} = p_{j+2,j} / (1-z^2)$$

$$j = 2, 3, \ldots, 2n+1 \quad . \qquad (3.5.59b)$$

Noting the condition

$$a_{2j+1} = 1/a_{2j} \qquad (3.5.60)$$

from the properties of a diagonal matrix in its representatives and also the relation (3.5.48), we find that (3.5.59b) is just an equivalent form of (3.5.59a).

Equation (3.5.59a) provides us a relation between the elements a_j ($j = 2, 3, \ldots, 2n+1$), $p_{2,j}$ ($j = 2, 3, \ldots, 2n+1$) and $p_{j+2,j}$ ($j = 2, 3, \ldots, 2n-1$). However, another set of equations relating them is given by (3.5.49). Consider equations for $v_{2,j+2}$ (and hence $u_{1,j}$) $j = 2, 3, \ldots, 2n-1$. From (3.5.11) we have

$$(2z)^{-\frac{1}{2}} u_{1,j} = a_j p_{2,j} \{ p_{j+2,j} - \frac{a_j(1-z^2)}{(z-a_j)} \sum_{\ell=2\neq j}^{2n+1} \frac{\beta_\ell p_{2,\ell}^2 a_\ell (a_\ell - a_j)}{(\beta_\ell - \beta_j)(z-a_\ell)} \} \qquad (3.5.61)$$

whereas, from (3.5.10) and (3.5.33), we have

$$(2z)^{-\frac{1}{2}}u_{1,j} = 2z^{\frac{1}{2}}a_j g_{2n}^{-2}\{[p_{j+2,j}r_j + (p_{2,2n}+zp_{2,2n+1})\beta_j r_j - a_j^2 g_j r_j^2]/\beta_j^2 + \sum_{\ell=2\neq j}^{2n-1} \frac{r_\ell a_\ell^2 (g_j r_\ell - g_\ell r_j)}{\beta_\ell(\beta_j-\beta_\ell)}\} \quad (3.5.62)$$

which on simplification using (3.5.34), (3.5.52), (3.5.53), (3.5.59a) etc., reduces to

$$(2z)^{-\frac{1}{2}}u_{1,j} = a_j p_{2,j}\{p_{j+2,j}\left[1+\frac{4a_j}{z-a_j}\right] - \frac{(1+z^2)^2 a_j}{z(1-z^2)(z-a_j)} + \frac{\beta_j(1-z^2)}{(z-a_j)}\left[\frac{p_{2,j}^2}{(z-a_j)^2} + \frac{p_{2,2n}^2\beta_j}{(z-a_{2n})^2 a_{2n}a_j^3}\right] - \frac{a_j(1-z^2)}{(z-a_j)}\sum_{\ell=2\neq j}^{2n+1}\frac{\beta_\ell p_{2,\ell}^2 a_\ell(a_\ell-a_j)}{(\beta_\ell-\beta_j)(z-a_\ell)}\} \quad (3.5.63)$$

Comparing with (3.5.61), we obtain

$$p_{j+2,j} = \frac{(1+z^2)^2}{4z(1-z^2)} - \frac{\beta_j(1-z^2)}{4a_j}\left[\frac{p_{2,j}^2}{(z-a_j)^2} + \frac{p_{2,2n}^2\beta_j}{(z-a_{2n})^2 a_{2n}a_j^3}\right] \quad j=2,3,\ldots,2n-1 \quad . \quad (3.5.64)$$

Hence, the matrix equations involve only $2n$ independent variables, namely, a_{2j+1} and $p_{2,2j+1}$ for $j = 1, 2, \ldots, n$.

We still have the equations for the elements $v_{\ell+2,j+2}$ ($\ell, j \geq 2$) from equation (3.5.49). However, after some tedious, yet straightforward simplifications on the summations involved, they can be proved to be identities provided that (3.5.52), (3.5.53), (3.5.59a) and (3.5.64) are all satisfied. Hence, we are left with $2n$ independent equations involving the $2n$ variables a_{2j+1} and $p_{2,2j+1}$ for $j = 1, 2, \ldots, n$. To simplify the notation, we

define

$$c_j = a_{2j+1}$$

and

$$c_{1-j} = 1/c_j = a_{2j} \quad , \quad j=1,2,\ldots,n \quad , \tag{3.5.65}$$

$$w_j = w_{1-j} = \beta_{2j+1} p^2_{2,2j+1} \; / \; a_{2j+1}(z-a_{2j+1})^2$$

$$j=1,2,\ldots,n-1 \quad . \tag{3.5.66a}$$

and

$$w_n = p^2_{2,2n+1} / \; a_{2n+1}(z-a_{2n+1})^2 \quad . \tag{3.5.66b}$$

For convenience, we choose only $(n-1)$ equations from (3.5.59a) and take another set of $(n-1)$ independent equations from (3.5.59b) . The equations then become

$$\frac{w_j}{4} + \sum_{\ell=2-n\neq j}^{n-1} \frac{w_\ell c_\ell c_j^2 (c_\ell - c_j)}{(c_\ell^4 - c_j^4)} + w_n \left[\frac{c_n}{c_j} - \frac{c_n^2}{c_j^2} + c_n^2 c_j^2 - c_n^3 c_j^3 \right] = \tfrac{1}{4} \phi(c_j)$$

$$j=1,2,\ldots,n-1 \; , \tag{3.5.67a}$$

$$\frac{w_j}{4} + \sum_{\ell=2-n\neq j}^{n-1} \frac{w_\ell c_\ell^2 c_j (c_\ell - c_j)}{(c_\ell^4 - c_j^4)} + w_n \left[c_n c_j - c_n^2 c_j^2 + \frac{c_n^2}{c_j^2} - \frac{c_n^3}{c_j^3} \right] = \tfrac{1}{4} \phi(c_j)$$

$$j=1,2,\ldots,n-1 \; , \tag{3.5.67b}$$

$$\sum_{\ell=2-n}^{n-1} w_\ell c_\ell^3/(1+c_\ell^4) + w_n c_n (1+c_n^2) = (1+z^2)/(1-z^2)^2 \quad , \tag{3.5.67c}$$

and

$$\sum_{\ell=2-n}^{n-1} w_\ell c_\ell^2/(1+c_\ell^4) + 2w_n c_n^2 = 2z/(1-z^2)^2 \tag{3.5.67d}$$

where

$$\phi(u) = \frac{(1+z^2)^2}{z(1-z^2)^2} - w_n c_n^4 \, (u^4 + 2 + u^{-4}) \quad . \tag{3.5.68}$$

The iterative procedure for the solution is replaced by solving the system of equations (3.5.67a-d) for the c_j s and w_j s .

6 THE INFINITE SOLUTION AND THE THERMODYNAMIC FUNCTIONS

§ 6.1 THE INFINITE SOLUTION

It is possible to solve the problem for the infinite system by noting the fact that the matrices $\mathscr{A}$ and $\mathscr{Z}$ should tend towards the corresponding corner transfer matrix and row (or column) transfer matrix of the infinite lattice as their limit, when n approaches infinity.

Since $\hat{\mathscr{A}}$ is diagonal, from property (v) of the spin representations, with an appropriate normalization and arrangement of rows and columns, $\mathscr{A}$ can be written as

$$\mathscr{A} = \begin{pmatrix} 1 & 0 \\ 0 & c_1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & c_2 \end{pmatrix} \otimes \ldots \otimes \begin{pmatrix} 1 & 0 \\ 0 & c_{n-1} \end{pmatrix} \tag{3.6.1}$$

for $n = 1, 2, \ldots$.

The corner transfer matrices for the square lattice Ising model were obtained by Baxter (1977). For the case $n = \infty$, the corresponding corner transfer matrix for $\mathscr{A}$ is similar to that considered by Baxter (1977) except that instead of having diagonal interaction energy coefficients J and J' , we have interaction energy coefficient J in both the horizontal and vertical directions (Fig. 3.3b).

Instead of going through the whole derivation again,

we note that if we put $J_3 = 0$ and let $J = J_1 = J_2$ in the case of the triangular Ising lattice considered in Section II, the system reduces to that of a square lattice. Let $\mathcal{A}_{sq}$ be the corner transfer matrix representing the corner shown in Fig. 3.3b. We have

$$\begin{aligned} \mathcal{A}_{sq}^2 &= L_A^{-\frac{1}{2}} A_\Delta B_\Delta C_\Delta L_A^{\frac{1}{2}} \\ &= L_A^{-\frac{1}{2}} \mathcal{D} L_A^{\frac{1}{2}} \end{aligned} \tag{3.6.2}$$

where A_Δ , B_Δ , C_Δ are the matrices A , B , C defined in (2.2.3) and (2.2.4) , and, L_A and $\mathcal{D}$ are as defined in (2.2.12) and (2.4.1) . Since, by (2.4.2), P_2 is the matrix which diagonizes $\mathcal{D}$, it is obvious that the matrix $L_A^{-\frac{1}{2}} P_2$ brings $\mathcal{A}_{sq}^2$ to a diagonal form. Hence we have

$$(\mathcal{A}_{sq})_d^2 = \mathcal{D}_d \tag{3.6.3}$$

where $(\mathcal{A}_{sq})_d$ is the corresponding diagonal form of $\mathcal{A}_{sq}$. By (2.6.6) , we may write, within a normalisation constant,

$$\mathcal{A}_{sq} = \text{const.} \times \begin{pmatrix} 1 & 0 \\ 0 & q^{\frac{1}{4}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & q^{\frac{3}{4}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & q^{\frac{5}{4}} \end{pmatrix} \otimes \ldots \tag{3.6.4}$$

where q is the nome of the elliptic function. Here the elliptic modulus k defined in (2.4.43) reduces to

$$k = \{ \sinh(2J/k_B T) \}^{-2} \tag{3.6.5}$$

In the diagonal representation of $\mathcal{A}$, for $n = \infty$, $\mathcal{A}$ is in fact equal to $\mathcal{A}_{sq}$ apart from a constant factor.

So, in view of (3.6.1), we have

$$c_j = q^{\frac{1}{4}(2j-1)} \quad , \quad j=1,2,3,\ldots \quad . \tag{3.6.6}$$

We may solve for w_j from the set of equations (3.5.67a-d) when $n = \infty$. Adding (3.5.67a) with (3.5.67b), we have

$$\sum_{\ell=2-n}^{n-1} \frac{w_\ell c_\ell c_j}{(c_\ell^2+c_j^2)} + w_n\{c_n(c_j+c_j^{-1}) - c_n^3(c_j^3+c_j^{-3})\} = \tfrac{1}{2}\phi(c_j)$$
$$j=2-n,3-n,\ldots,n-1 \quad . \tag{3.6.7}$$

Using the fact that the determinant of a $N \times N$ matrix X with elements $X_{\ell,j} = (\mu_\ell+\nu_j)^{-1}$ is given by

$$\det X = \prod_{0\le\ell<j\le N} (\mu_\ell-\mu_j)(\nu_\ell-\nu_j) \times \prod_{\ell=0}^{N}\prod_{j=0}^{N} (\mu_\ell+\nu_j)^{-1} \tag{3.6.8}$$

we may solve the equation (3.6.7) by Cramer's rule of linear equations to obtain

$$w_j c_j = (\det M^{(j)}) / (\det M^{(0)})$$
$$j=2-n,3-n,\ldots,n-1 \tag{3.6.9}$$

where $M^{(0)}$ is the $(2n-2) \times (2n-2)$ matrix with $(c_\ell^2+c_j^2)^{-1}$ as its elements and $M^{(j)}$ is the corresponding matrix with the $(n-1+j)$ th column of the matrix $M^{(0)}$ being replaced by the column vector formed by

$$f(c_j) = \tfrac{1}{2}c_j^{-1}\phi(c_j) - w_n c_j^{-1}\{c_n(c_j+c_j^{-1}) - c_n^3(c_j^3+c_j^{-3})\}$$
$$j=2-n,3-n,\ldots,n-1 \quad . \tag{3.6.10}$$

Hence by (3.6.8), we may write

$$w_j c_j = \prod_{m_1=2-n}^{n-1} \prod_{m_2=2-n}^{n-1} (c_{m_1}^2 + c_{m_2}^2) \prod_{2-n \le m_1 < m_2 \le n-1} (c_{m_1}^2 - c_{m_2}^2)^{-2}$$

$$\times \sum_{\ell=2-n}^{n-1} (-1)^{j+\ell} f(c_\ell) \frac{\prod_{\substack{2-n \le m_1 < m_2 \le n-1 \\ m_1, m_2 \neq \ell}} (c_{m_1}^2 - c_{m_2}^2) \prod_{\substack{2-n \le m_1 < m_2 \le n-1 \\ m_1, m_2 \neq j}} (c_{m_1}^2 - c_{m_2}^2)}{\prod_{\substack{m_1=2-n \\ \neq \ell}}^{n-1} \prod_{\substack{m_2=2-n \\ \neq j}}^{n-1} (c_{m_1}^2 + c_{m_2}^2)} \tag{3.6.11}$$

For the case $n = \infty$, we have c_n being zero and the summation and product being from negative infinity to positive infinity. So, (3.6.10) becomes

$$f(c_j) = \frac{(1+z^2)^2}{2z c_j (1-z^2)^2} \tag{3.6.12}$$

Substituting (3.6.6) to the equations and using the properties of elliptic functions, we have

$$\frac{\prod_{\ell=2-n}^{n-1} (c_\ell^2 + c_j^2)}{\prod_{\substack{\ell=2-n \\ \neq j}}^{n-1} (c_j^2 - c_\ell^2)} = \frac{\prod_{\ell=2-n}^{n-1} (q^{\ell-\frac{1}{2}} + q^{j-\frac{1}{2}})}{\prod_{\substack{\ell=2-n \\ \neq j}}^{n-1} (q^{j-\frac{1}{2}} - q^{\ell-\frac{1}{2}})}$$

$$= 2(-1)^{n-2+j} q^{j-\frac{1}{2}} \prod_{\ell=1}^{n-1-j} \left[\frac{1+q^\ell}{1-q^\ell}\right]^2 \prod_{\ell=n-1-j}^{n-2+j} \left[\frac{1+q^\ell}{1-q^\ell}\right]$$

$$j = 2-n, 3-n, \ldots, n-1 \quad . \tag{3.6.13}$$

Letting $n = \infty$ in (3.6.11), we have

$$w_j c_j = \frac{(-1)^j q^{j-\frac{1}{2}} (1+z^2)^2}{z\,(1-z^2)^2} \prod_{\ell=1}^{\infty} \left[\frac{1+q^\ell}{1-q^\ell}\right]^4 \sum_{\ell=-\infty}^{\infty} \frac{2(-1)^\ell q^{\frac{1}{2}(\ell-\frac{1}{2})}}{(q^{\ell-\frac{1}{2}} + q^{j-\frac{1}{2}})} \tag{3.6.14}$$

$$j = 1, 2, \ldots \quad .$$

Since

$$\prod_{\ell=1}^{\infty} \left[\frac{1+q^{\ell}}{1-q^{\ell}}\right]^2 = \pi/(2Kk') \qquad (3.6.15)$$

and

$$\sum_{\ell=-\infty}^{\infty} \frac{(-1)^{\ell} q^{\frac{1}{2}(\ell-\frac{1}{2})}}{(q^{\ell-\frac{1}{2}}+q^{j-\frac{1}{2}})} = \tfrac{1}{2} + q^{-\frac{1}{2}(j-\frac{1}{2})} \sum_{\ell=1}^{\infty} \frac{(-1)^{\ell+j} q^{\frac{1}{2}\ell}}{(1+q^{\ell})}$$

$$= (-1)^{j} \; q^{-\frac{1}{2}(j-\frac{1}{2})} \; (1-k)K/\pi \qquad (3.6.16)$$

where K is the complete elliptic integral of the first kind of modulus k and k' ($= \sqrt{1-k^2}$) is the associated elliptic modulus of the elliptic functions, we obtain from (3.6.14),

$$w_j \; c_j = q^{\frac{1}{2}(j-\frac{1}{2})} \pi/2zK$$

or

$$w_j = \pi/2zK \quad , \quad \forall \; j \qquad (3.6.17)$$

Hence, apart from a sign of multiplication, we can determine $p_{2,j}$ through (3.5.66a). From (3.5.48), it is obvious that

$$p_{2,2j} \; / \; (z-a_{2j}) = - \; p_{2,2j+1} \; / \; (z-a_{2j+1}) \qquad (3.6.18)$$

Also, as pointed out in step (ii) of the iterative procedure (p. 119), $\hat{P}$ is almost diagonal and it is natural to take $p_{j,j}$ to be positive. By (3.5.31a), we have

$$p_{j,j} = \beta_j a_{j-2}^2 \; (p_{2,j}p_{3,j-2} - p_{2,j-2}p_{3,j})/(\beta_j-\beta_{j-2})$$

$$= - \frac{\beta_j a_{j-2}^2 p_{2,j} p_{2,j-2} (a_j-a_{j-2})(1-z^2)}{(z-a_j)\;(z-a_{j-2})\;(\beta_j-\beta_{j-2})} \qquad (3.6.19)$$

$$j=4,5,\ldots,2n+1.$$

Taking $p_{j,j}$ to be positive implies that we require

$$\frac{p_{2,j}}{(z-a_j)} \times \frac{p_{2,j-2}}{(z-a_{j-2})} \leq 0 \quad , \qquad j=4,5,\ldots,2n+1. \tag{3.6.20}$$

Also requiring $p_{2,2}$ and $p_{3,3}$ to be positive, (3.6.18) and (3.6.20) will both be satisfied if we take

$$\frac{p_{2,2j+1}}{(z-a_{2j+1})} = -\frac{p_{2,2j}}{(z-a_{2j})} = (-1)^{j+1} \frac{\pi\, q^{\frac{1}{2}(j-\frac{1}{2})}}{2zK(1+q^{2j-1})} \qquad j=1,2,3,\ldots \tag{3.6.21}$$

We may then obtain $\hat{\mathcal{F}}$ from (3.5.33) with

$$f_{1,1} = (1+z^2)/(1-z^2) \quad ,$$

$$f_{1,j} = f_{j,1} = (2z)^{\frac{1}{2}}\, y_j \quad ,$$

$$f_{j,j} = \tfrac{1}{4}(1+z^2)^2/z(1-z^2) + \tfrac{1}{4}y_j^2 a_j^{-3}(1-z^2)(3a_j^4-1) \quad ,$$

and

$$f_{\ell,j} = f_{j,\ell} = y_\ell y_j (1-z^2)(\beta_j a_\ell - \beta_\ell a_j)/(\beta_j - \beta_\ell) \quad , \qquad \ell \neq j \;\; ; \;\; \ell, j \geq 2 \tag{3.6.22}$$

where a_j is related to c_j through (3.5.65) and is given by

$$a_{2j+1} = 1/a_{2j} = q^{\frac{1}{2}(j-\frac{1}{2})} \quad , \qquad j=1,2,3,\ldots \tag{3.6.23a}$$

$$\beta_j = 1 + a_j^4 \quad , \tag{3.6.23b}$$

and

$$y_j = \mathrm{sgn}(j)\, \{\pi a_j^3/(2zK\beta_j)\}^{\frac{1}{2}} \tag{3.6.24}$$

with

$$\mathrm{sgn}(j) = \begin{cases} +1 & \text{if } j = 1 \text{ or } 2 \text{ (modulo 4)} \\ -1 & \text{if } j = 0 \text{ or } 3 \text{ (modulo 4)} \end{cases} \tag{3.6.25}$$

For finite n , we are able to solve the equations numerically only. However, the $n = \infty$ solution for a given matrix element is approximately correct for finite n at low temperature, at least to leading order. Hence, they serve as a good initial guess to the solution for numerical calculations.

§ 6.2 THE THERMODYNAMIC FUNCTIONS IN THEIR REPRESENTATIVES

In Section III.3.2, it was shown that most of the thermodynamic functions can be written in terms of the traces of products of matrices. Using the set of operators defined in (3.5.1) , the trace of a matrix in the original representation can be conveniently expressed in terms of the determinants of the matrix itself and of its representative.

Consider the $2^p \times 2^p$ diagonal matrix X defined in (3.5.8) . The trace of the matrix is

$$\text{Trace } X = \rho \prod_{j=1}^{p} (1+y_j) \tag{3.6.26}$$

and the determinant of the matrix is given by

$$\det X = \rho^{2^p} \prod_{j=1}^{p} y_j^{2^{p-1}} \tag{3.6.27}$$

and by (3.5.9)

$$\det (I + \hat{X}) = 2 \prod_{j=1}^{p} (1+y_j)(1+y_j^{-1}) = 2 \prod_{j=1}^{p} (1+y_j)^2/y_j \tag{3.6.28}$$

So combining the equations (3.6.26) with (3.6.28), we have

$$\frac{\text{Trace } X}{(\det X)^{2-p}} = \prod_{j=1}^{p} (1+y_j)/y_j^{\frac{1}{2}}$$

$$= \{ \tfrac{1}{2} \det (I + \hat{X}) \}^{\frac{1}{2}} \qquad (3.6.29)$$

Since both the trace and determinant of a matrix are invariant under similar transformations, equation (3.6.29) is true for any matrix X in group $\mathcal{G}$. So, we may write the thermodynamic functions of the system in terms of determinants.

Spontaneous magnetization

When the magnetic field is zero, (3.3.8) can be written as

$$M = \frac{\text{Trace } (s_1 \mathcal{A}^4)}{\text{Trace } (\mathcal{A}^4)} \qquad (3.6.30)$$

Since $\mathcal{A}$ is already diagonal, in the representation considered in (3.6.1), the spontaneous magnetization is given by

$$M = \prod_{j=1}^{n-1} \frac{(1-c_j^4)}{(1+c_j^4)} \quad . \qquad (3.6.31)$$

The partition function and free energy

For the isotropic case, in the absence of any magnetic field, using (3.3.3), the partition function per

site of the system can be written as

$$\kappa = \frac{\mathrm{Trace}(\sum_{\alpha} A^4(\alpha)) \times \mathrm{Trace}\Big(\sum_{\alpha,\beta,\alpha',\beta'} w(\alpha,\alpha',\beta,\beta') A(\beta) F(\beta,\alpha) A(\alpha) F(\alpha,\alpha') A(\alpha') F(\alpha',\beta') A(\beta') F(\beta',\beta) \Big)}{\Big\{ \mathrm{Trace}\Big(\sum_{\alpha,\alpha'} A^2(\alpha) F(\alpha,\alpha') A^2(\alpha') F(\alpha',\alpha) \Big) \Big\}^2} \tag{3.6.32}$$

which in terms of the matrices $\mathcal{A}$, $\mathcal{Z}$ and $\mathcal{H}$ can be written as

$$\kappa = \frac{\exp(2J/k_B T)\ \mathrm{Trace}(\mathcal{A}^4) \times \mathrm{Trace}(\mathcal{A}\mathcal{Z})^4}{\{\ \mathrm{Trace}\ (\mathcal{A}^2\mathcal{H})^2\ \}^2} \tag{3.6.33}$$

Thus, using (3.6.29) , we have

$$\kappa = \frac{z^{-1}\ \{\det(I + \hat{\mathcal{A}}^4) \times \det\ [I + (\hat{\mathcal{A}}\hat{\mathcal{Z}})^4]\}^{\frac{1}{2}}}{\det\{\ I + (\hat{\mathcal{A}}^2\hat{\mathcal{H}})^2\}} \times \left[\frac{\det(\mathcal{Z})}{\det(\mathcal{H})}\right]^{2^{-p+2}} \tag{3.6.34}$$

However, from (3.4.24) and (3.4.32) , we note that

$$\mathrm{Trace}\ \mathcal{Z} = \mathrm{Trace}\ \mathcal{H} \quad . \tag{3.6.35}$$

So, we may write

$$\kappa = \frac{z^{-1}\ \{\det(I + \hat{\mathcal{A}}^4) \times \det[I + (\hat{\mathcal{A}}\hat{\mathcal{Z}})^4]\}^{\frac{1}{2}}}{\det\{\ I + (\hat{\mathcal{A}}^2\hat{\mathcal{H}})^2\}} \times \left[\frac{\det(I + \hat{\mathcal{H}})}{\det(I + \hat{\mathcal{Z}})}\right]^2 \tag{3.6.36}$$

The free energy per site of the system can be written similarly in terms of determinants by (3.3.4).

Nearest-neighbour correlation

In a similar way for κ, we may write the nearest-neighbour correlation in (3.3.9) as

$$\langle \sigma_i \sigma_j \rangle_{\text{hori.}} = \frac{\text{Trace } (s_1 \mathcal{A}^2 \mathcal{H})^2}{\text{Trace } (\mathcal{A}^2 \mathcal{H})^2}$$

$$= \left[\frac{\det\{I + (\hat{s}_1 \hat{\mathcal{A}}^2 \hat{\mathcal{H}})^2\}}{\det\{I + (\hat{\mathcal{A}}^2 \hat{\mathcal{H}})^2\}} \right]^{\frac{1}{2}} . \qquad (3.6.37)$$

Internal energy

Similarly, from (3.3.10), the internal energy per site of the system is given by

$$U = 2J \left[\frac{\det\{I + (\hat{s}_1 \hat{\mathcal{A}}^2 \hat{\mathcal{H}})^2\}}{\det\{I + (\hat{\mathcal{A}}^2 \hat{\mathcal{H}})^2\}} \right]^{\frac{1}{2}} . \qquad (3.6.38)$$

7 THE NUMERICAL METHOD OF SOLUTION

§ 7.1 POLYNOMIAL FORM OF EQUATIONS

It is possible to further reduce the number of variables in (3.5.67a-d) to n by expressing the equations in polynomials.

Define, for all complex numbers u ,

$$G(u) = w_n\{c_n(u-u^{-1}) + c_n^2(u^2-u^{-2}) + c_n^3(u^3-u^{-3})\} + \tfrac{1}{2}\sum_{j=2-n}^{n-1} w_j(c_j+u)/(c_j-u) \quad . \tag{3.7.1}$$

From (3.5.65) , $G(u)$ satisfies the relation

$$G(u) + G(u^{-1}) = 0 \quad . \tag{3.7.2}$$

In terms of this function, the equations (3.5.67a) and (3.5.67b) can be written as

$$2G(-u) - (1+i)G(iu) - (1-i)G(-iu) = \phi(u) \quad , \tag{3.7.3a}$$

$$-2G(-u) + (1-i)G(iu) + (1+i)G(-iu) = \phi(u) \quad , \tag{3.7.3b}$$

for $u = c_{2-n}$, c_{3-n} ,... , c_{n-1} , where $\phi(u)$ is defined by (3.5.68) and $i = \sqrt{-1}$. An equivalent and simpler form of this pair of equations is

$$2i\ \{\ G(-u)\ -\ G(iu)\ \}\ =\ \phi(u)\quad , \tag{3.7.4a}$$

$$-\ 2i\ \{\ G(-u)\ -\ G(-iu)\ \}\ =\ \phi(u)\quad , \tag{3.7.4b}$$

for $u = c_{2-n}\ ,\ c_{3-n}\ ,\ \ldots\ ,\ c_{n-1}$. We now define $f(u)$ by

$$f(u)\ =\ \prod_{j=2-n}^{n-1}\ (u-c_j)\quad , \tag{3.7.5}$$

and the function $R(u)$ by

$$R(u)\ =\ 2i\{G(-u)\ -\ G(iu)\}\ -\ \phi(u)\quad . \tag{3.7.6}$$

$R(u)$ is a ratio of two polynomials of degree $4n$ in u and satisfies

$$R^{*}(u)\ =\ R(iu)\ =\ R(u^{-1})\quad . \tag{3.7.7}$$

By examining $G(u)$ in (3.7.1) , the zeros of $f(-u)$ and $f(iu)$ are $(4n-4)$ simple poles of $R(u)$ and by (3.7.4a,b), the zeros of $f(u)$ and $f(-iu)$ are also zeros of $R(u)$. So, $R(u)$ can be factorized into the form

$$R(u)\ =\ -\frac{f(u)\ f(-iu)}{f(-u)\ f(iu)}\ \alpha(u) \tag{3.7.8}$$

where $u^{4}\alpha(u)$ is a polynomial in u of degree eight. Hence we obtain the following identity, true for all complex numbers u :

$$2i\{G(-u)\ -\ G(iu)\}\ \equiv\ \phi(u)\ -\ \frac{f(u)\ f(-iu)}{f(-u)\ f(iu)}\ \alpha(u)\quad . \tag{3.7.9}$$

Further, since $f(u)$ satisfies condition similar to (3.7.7), $\alpha(u)$ must also satisfy

$$\alpha^*(u) = \alpha(iu) = \alpha(u^{-1}) \quad . \tag{3.7.10}$$

Hence, $\alpha(-\omega u)$ is a polynomial in $(u+u^{-1})$ and

$$\alpha(\omega)\ \alpha(-\omega) = \alpha(\omega^{-1})\ \alpha(-\omega^{-1}) \tag{3.7.11}$$

where

$$\omega^4 = -1 \quad ; \quad \omega = (1+i)/\sqrt{2} \quad . \tag{3.7.12}$$

It is therefore clear that $u^8\alpha(u)\alpha(-u)$ is a polynomial in u^4 and $u^4\alpha(-\omega u)$ must factorize into the form

$$u^4\alpha(-\omega u) = \text{const.} \times (u+\omega a)(u+1/\omega a)(u+a/\omega)(u+\omega/a)(u+\omega b)(u+1/\omega b) \times (u+b/\omega)(u+\omega/b) \tag{3.7.13}$$

for some scalars a and b. Thus, we have

$$\alpha(u) = \text{const.} \times \rho(u)\ \rho(-iu) \tag{3.7.14}$$

with $\rho(u)$ given by

$$\rho(u) = (a+a^{-1}-u-u^{-1})\ (b+b^{-1}-u-u^{-1}) \quad . \tag{3.7.15}$$

We can identity the constant in (3.7.14) to be $w_n c_n^4$ by equating terms in (3.7.9).

Three additional equations can be obtained from (3.7.9) by replacing u by iu, $-u$ and $-iu$ respectively. The function $G(u)$ can be eliminated between these four forms of (3.7.9) giving

$$4\phi(u) = \frac{f(u)\{f^2(-iu)\alpha(u)+f^2(iu)\alpha(iu)\}}{f(-u)\ f(iu)\ f(-iu)} + \frac{f(-u)\{f^2(iu)\alpha(-u)+f^2(-iu)\alpha(-iu)\}}{f(u)\ f(iu)\ f(-iu)} \quad . \tag{3.7.16}$$

If we consider poles of $f(-u)$ in the equation, it can be easily seen that $f(-u)$ must be a factor of $\{f^2(-iu)\alpha(u) + f^2(iu)\alpha(iu)\}$ and since $\rho(u)$ is a factor of both $\alpha(u)$ and $\alpha(iu)$ from (3.7.14), we obtain

$$f^2(-iu)\rho(-iu) + f^2(iu)\rho(iu) = f(-u)R(u) \qquad (3.7.17)$$

for some polynomial $R(u)$. The left-hand side of (3.7.17) is unaltered by negating u, so $f(u)$ must be a factor of $R(u)$, i.e.

$$R(u) = f(u)\ \sigma(u) \qquad (3.7.18)$$

where $\sigma(u)$ is an even function of u. Substituting (3.7.17) and (3.7.18) to (3.7.16), we find that

$$4w_n c_n^4\ \phi(u) = \sigma(iu)\ \sigma(u) \quad . \qquad (3.7.19)$$

It follows that

$$\sigma(u) = -2w_n c_n^4\ (u^2 - m_o + u^{-2}) \qquad (3.7.20)$$

where

$$m_o = \left[\frac{(1+z^2)^2}{z(1-z^2)^2 w_n c_n^4}\right]^{\frac{1}{2}} \quad . \qquad (3.7.21)$$

The negative sign of (3.7.20) is chosen so as to fit the limit of the left-hand side of (3.7.17) as u approaches zero.

We can solve for $\rho(u)$ from equations (3.5.67c) and (3.5.67d). From (3.5.67c), we have

$$\{\omega^{-1}G(\omega) - \omega^{-1}G(-\omega) + \omega G(\omega^{-1}) - \omega G(-\omega^{-1})\} = 4(1+z^2)/(1-z^2)^2 \qquad (3.7.22a)$$

and from (3.5.67d), we have

$$\omega^2\{ - G(\omega) - G(-\omega) + G(\omega^{-1}) + G(-\omega^{-1})\} = 8z/(1-z^2)^2 \tag{3.7.22b}$$

Since by (3.7.2),

$$G(\omega^{-1}) = - G(\omega)$$

and (3.7.23)

$$G(-\omega^{-1}) = - G(-\omega) \quad ,$$

(3.7.22a,b) can be written as

$$(\omega^{-1}-\omega)\{G(\omega) - G(-\omega)\} = 4(1+z^2)/(1-z^2)^2 \tag{3.7.24a}$$

and

$$- \omega^2\{G(\omega) + G(-\omega)\} = 4z/(1-z^2)^2 \quad . \tag{3.7.24b}$$

On solving, we obtain

$$G(\omega) = -G(\omega^{-1}) = \sqrt{2}i(1+\sqrt{2}z+z^2)/(1-z^2)^2 \tag{3.7.25a}$$

and

$$G(-\omega) = -G(-\omega^{-1}) = -\sqrt{2}i(1-\sqrt{2}z+z^2)/(1-z^2)^2 \tag{3.7.25b}$$

If we put u to be ω^{-1} and $-\omega^{-1}$ respectively in (3.7.9), we obtain

$$\alpha(\omega^{-1}) = \alpha(-\omega^{-1}) = (1-6z^2+z^4)/z(1-z^2)^2 \tag{3.7.26}$$

Let

$$h_1 = a + a^{-1}$$

and (3.7.27)

$$h_2 = b + b^{-1}$$

in (3.7.15), then (3.7.26) implies that

$$(h_1^2-2)(h_2^2-2) = m_0^2\,(1-6z^2+z^4)/(1+z^2)^2 \quad . \tag{3.7.28}$$

Equating coefficients of powers of u in (3.7.9), we have for terms of the order

(i) u^{-3} :

$$(h_1 + h_2) = 2\,(c_n^{-1} - \sum_{j=2-n}^{n-1} c_j) \qquad (3.7.29a)$$

(ii) u^{-1} :

$$(h_1+h_2)(h_1h_2+1) = \frac{2}{3}\{4(c_n^{-1} - \sum_{j=2-n}^{n-1} c_j)^3 + \sum_{j=2-n}^{n-1} c_j^3 - c_n^{-3}\} \qquad (3.7.29b)$$

(iii) u^{o} :

$$h_1^2h_2^2+4h_1h_2+2 = m_o^2 - 2 + \frac{8}{3}(c_n^{-1} - \sum_{j=2-n}^{n-1} c_j) \times \{(c_n^{-1} - \sum_{j=2-n}^{n-1} c_j)^3 + \sum_{j=2-n}^{n-1} c_j^3 - c_n^{-3}\} \qquad (3.7.29c)$$

Hence eliminating all the summations of c_j in the equations, we have

$$(h_1^2-2)^2 + (h_2^2-2)^2 = 2m_o^2 \quad . \qquad (3.7.30)$$

Together with (3.7.28), we can solve the equations to give

$$h_1^2 = 2 + m_o\,(1+2z-z^2)/(1+z^2) \qquad (3.7.31a)$$

and

$$h_2^2 = 2 + m_o\,(1-2z-z^2)/(1+z^2) \quad . \qquad (3.7.31b)$$

In summary, the matrix equations are reduced to the following polynomial equation involving c_j , $j=1,2,\ldots,n-1$ and m_o only :

$$\rho(iu)f^2(iu) + \rho(-iu)f^2(-iu) = -2(u^2-m_o+u^{-2})f(u)f(-u) \qquad (3.7.32)$$

where $f(u)$, $\rho(u)$ and m_0 are given by (3.7.5) , (3.7.15) and (3.7.21) respectively.

§ 7.2 THE CRITICAL POINT OF THE SYSTEM

Before proceeding any further, it is convenient to define the critical point of the system at this stage.

In the thermodynamic limit, the critical point can be defined to be the point at which the spontaneous magnetization of the system vanishes as the temperature increases. A similar definition may be used for the case when n is finite. From (3.6.31) , the spontaneous magnetization will vanish if any of the c_j s is unity. Since, both from the infinite solution (i.e. when $n = \infty$) and the low temperature expansions from the equations, all the c_j s are less than unity and decrease as j increases for all temperatures below the critical temperature, for any finite n , we expect

$$1 \geq c_1 > c_2 > \ldots > c_n \quad . \tag{3.7.33}$$

Also, c_j increases as z increases for any given j . Hence, one can equivalently define the critical point for a system with finite n to be the point at which $c_1 = 1$. As seen from (3.6.1) , it is also the point at which the maximum eigenvalue of the matrix $\mathcal{A}$ degenerates.

It is interesting to note that at the critical

temperature of the system, $f(1) = 0$ from (3.7.5) . Since $f(u) \propto f(u^{-1})$ and $\rho(i) = \rho(-i)$, if we set $u = 1$ in (3.7.32) , we have

$$\rho(i)\, f^2(i) = 0 \tag{3.7.34}$$

which implies that

$$\rho(i) = 0 \quad \text{or} \quad h_1 h_2 = 0 \tag{3.7.35}$$

at the critical temperature. Now $h_1 > h_2$, so h_2 must vanish at the critical point of the system for all finite values of n .

§ 7.3 THE $n = 2$ SOLUTION

We can solve the polynomial equation (3.7.32) for c_j s when $n = 2$.

Let $\rho(u)$ be given by

$$\rho(u) = \rho_0 - b_0(u+u^{-1}) + u^2 + u^{-2} \quad . \tag{3.7.36}$$

We can identify ρ_0 and b_0 as

$$\begin{aligned} \rho_0 &= h_1 h_2 + 2 \\ b_0 &= h_1 + h_2 \end{aligned} \tag{3.7.37}$$

For $n = 2$, we may write (3.7.5) as

$$f(u) = u \{ (u+u^{-1}) - c \} \tag{3.7.38}$$

where

$$c = (c_1 + c_1^{-1}) \quad . \tag{3.7.39}$$

Equating coefficients in (3.7.32) gives

$$m_0 - \rho_0 = 4 + 2b_0 c \tag{3.7.40a}$$

and

$$m_0 + \rho_0 = 2c^2 + b_0 c^3 - 2b_0 c \quad . \tag{3.7.40b}$$

Also (3.7.30) implies

$$m_0^2 = \rho_0^2 - 2b_0^2(\rho_0 - 1) + \tfrac{1}{2}b_0^4 \quad . \tag{3.7.40c}$$

Hence, if we make the following transformations of variables:

$$y = b_0/c$$

and $$r = b_0 c/4 \quad , \tag{3.7.41}$$

we obtain from (3.7.40a-c)

$$4(1+2r)(1+2r-y) = ry^3 + 8ry^2 + 3y^2 - 4ry - 8r^2 y \tag{3.7.42}$$

which implies that

$$(y+2)\{ry^2 + (6r+3)y - 2(4r^2+4r+1)\} = 0 \quad . \tag{3.7.43}$$

The zeros of the expression inside the brackets { } occur at

$$r = \{y^2+6y-8 \pm y(y^2+12y+20)^{\frac{1}{2}}\}/16 \quad . \tag{3.7.44}$$

So, if we make the parametrization

$$s + s^{-1} = \tfrac{1}{2}(y+6) \quad ; \quad |s| \leq 1 \tag{3.7.45}$$

then from (3.7.44)

$$r = s(s-3)/2 \tag{3.7.46a}$$

or

$$r = (1-3s)/2s^2 \quad . \tag{3.7.46b}$$

If we put $u = i$ in (3.7.32), we note that

$$h_1 h_2 \geq 0 \tag{3.7.47}$$

provided that $m_0 \geq 2$ (which we would justify later in Section III.7.4). Also, from the low temperature expansion on c_j s , the left-hand side of (3.7.29a) is positive, or we have

$$h_1 + h_2 \geq 0 \quad . \tag{3.7.48}$$

Hence, with h_1 being greater than h_2 for all temperatures from (3.7.31a,b) and h_2 being zero at the critical point, we expect that, by continuity, (3.7.48) holds for all temperatures below the critical temperature. So, from (3.7.37) and (3.7.41) ,

$$r \geq 0 \quad . \tag{3.7.49}$$

Hence, from (3.7.46a,b) with $s \leq 1$, the only acceptable solution is

$$r = (1-3s)/2s^2 \quad . \tag{3.7.50}$$

Also, this implies that we must have

$$s \leq 1/3 \quad . \tag{3.7.51}$$

The parameter s is related to z by the side condition

(3.7.28) which on simplification gives

$$z^2 = s(1-3s)/(1-3s+s^2) \quad . \tag{3.7.52}$$

Also, we obtain the solution for c and m_0 as

$$c^2 = (1-3s)/s(1-3s+s^2) \tag{3.7.53a}$$

and

$$m_0 = (1-3s+2s^3)/s^3 \tag{3.7.53b}$$

At the critical temperature, $c_1 = 1$. So, by (3.7.39)

$$c = 2 \tag{3.7.54}$$

which by (3.7.53a) implies that

$$s = (5\pm\sqrt{17})/4 \quad . \tag{3.7.55}$$

With the condition in (3.7.51) , we must have

$$s = (5-\sqrt{17})/4 \tag{3.7.56}$$

and so the critical temperature of the $n = 2$ system is given by

$$\begin{aligned} z_c &= (5-\sqrt{17})/2 \\ &= 0.4384471872 \end{aligned} \tag{3.7.57}$$

As expected, this is the same as predicted by the Kramers and Wannier (1941) approximation.

§ 7.4 THE NUMERICAL APPROACH

We may note from (3.5.67c) that each term of the left-hand side of (3.5.67c) is greater than $w_n c_n^3$. So we must have

$$2nw_n c_n^3 \leq (1+z^2)/(1-z^2)^2 < (1+z^2)^2/z(1-z^2)^2 \qquad (3.7.58)$$

for $z \leq 1$. Since the minimum value for n is 2 and c_n is less than 1 , we must have

$$w_n c_n^4 < (1+z^2)^2/4z(1-z^2)^2 \quad . \qquad (3.7.59)$$

In view of the definition of m_o in (3.7.21) , this implies that

$$m_o > 2 \qquad (3.7.60)$$

for all finite n . So, we can define a real parameter c_n by

$$m_o = c_n^2 + c_n^{-2} \quad ; \quad 0 < c_n < 1 \quad . \qquad (3.7.61)$$

(The c_n defined here is different from that used previously.) The zeros of the right-hand side of equation (3.7.32) occur at c_1 , c_2 ,..., c_n , so

$$\frac{\rho(ic_j)\ f^2(ic_j)}{\rho(-ic_j)\ f^2(-ic_j)} = -1 \quad ; \quad j = 1, 2, \ldots, n. \qquad (3.7.62)$$

We consider now the low temperature expansions for the polynomials in (3.7.62) . We may write

$$\frac{f(ic_j)}{f(-ic_j)} = i(-1)^{n-j} \prod_{\ell=1}^{n-1} \frac{(1-ic_jc_\ell)}{(1+ic_jc_\ell)} \prod_{\ell=1}^{j-1} \frac{(1-ic_j/c_\ell)}{(1+ic_j/c_\ell)} \prod_{\ell=j+1}^{n-1} \frac{(1+ic_\ell/c_j)}{(1-ic_\ell/c_j)}$$

$$j=1,2,\ldots,n-1 \qquad (3.7.63a)$$

and

$$\frac{f(ic_n)}{f(-ic_n)} = \prod_{\ell=1}^{n-1} \frac{(1-ic_nc_\ell)(1-ic_n/c_\ell)}{(1+ic_nc_\ell)(1+ic_n/c_\ell)} \qquad (3.7.63b)$$

Also,

$$\frac{\rho(ic_j)}{\rho(-ic_j)} = \frac{(h_1-ic_j+i/c_j)(h_2-ic_j+i/c_j)}{(h_1+ic_j-i/c_j)(h_2+ic_j-i/c_j)} \quad . \qquad (3.7.64)$$

Taking logarithms of both sides of (3.7.62), we consider the branch for the principal value of the logarithmic function in the complex plane and equate the imaginary part of the expression. Then, we obtain the equation

$$\tan^{-1}\left[\frac{c_j^{-1}-c_j}{h_1}\right] + \tan^{-1}\left[\frac{c_j^{-1}-c_j}{h_2}\right] - 2\sum_{\ell=1}^{n-1}\tan^{-1}(c_jc_\ell) - 2\sum_{\ell=1}^{j-1}\tan^{-1}(c_j/c_\ell)$$

$$+ 2\sum_{\ell=j+1}^{n-1}\tan^{-1}(c_\ell/c_j) = \begin{cases} 0 & , \quad j=1,2,\ldots,n-1 \\ \pi/2 & , \quad j=n \end{cases} . \qquad (3.7.65)$$

Using the fact that

$$\tan^{-1}x = \pi/2 - \tan^{-1}(x^{-1}) \qquad (3.7.66)$$

and

$$\tan^{-1}x_1 + \tan^{-1}x_2 = \tan^{-1}\left[\frac{x_1+x_2}{1-x_1x_2}\right] \quad ,$$

we may write (3.7.65) equivalently as

$$2\sum_{\ell=1}^{n-1}\tan^{-1}\left[\frac{c_\ell^{-1}+c_\ell}{c_j^{-1}-c_j}\right] + \tan^{-1}\left[\frac{h_1}{c_j^{-1}-c_j}\right] + \tan^{-1}\left[\frac{h_2}{c_j^{-1}-c_j}\right] = (n-j+\tfrac{1}{2})\,\pi$$

$$j=1,2,\ldots,n \quad . \qquad (3.7.67)$$

where h_1 and h_2 are given by (3.7.31a,b).

Equation (3.7.67) provides a system of n non-linear equations in n unknowns. We are able to solve the equations numerically only. Since the Jacobian matrix of the functions with respect to a_j s can be calculated readily, it is natural to apply the Newton-Raphson method of numerical analysis.

Given a system of equations

$$f_j(\underline{x}) = 0 \quad , \quad j=1,2,\ldots,n \tag{3.7.68}$$

with $\underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$.

Let the approximation to the solution of the equations at the n th iteration be $\underline{x}_n$. Then, Newton-Raphson iterative procedure gives the $(n+1)$ th approximation of the solution as

$$\underline{x}_{n+1} = \underline{x}_n - (\mathcal{J}^{-1}F)_{\text{at } \underline{x}=\underline{x}_n} \tag{3.7.69}$$

where F is the column vector formed by $(f_j(\underline{x}))$ and $\mathcal{J}$ is the Jacobian matrix formed by the partial derivatives of F with respect to the parameters x_j .

$$\mathcal{J}_{i,j} = (\partial f_i / \partial x_j) \tag{3.7.70}$$

The convergence of the method usually depends on having a good starting approximation. For our case, the infinite solution of the equations provides a good initial

guess to the solution for finite n at least for temperatures far enough from the critical region. Hence, at low temperature, for a given n , we may use the following as a starting approximation for the method :

$$c_1 \sim q^{\frac{1}{4}} \sim z$$

and (3.7.71)

$$c_j \sim c_1^{2j-1} \quad , \quad j=2,3,\ldots,n \ .$$

However, for temperatures nearer to the critical point, we need a better initial approximation for convergence. This is achieved by using quadratic extrapolation on the variables, as a function of z . Since at the critical point $c_1 = 1$ for any n , it is more convenient to treat c_1 as the fixed parameter and z as the variable in the equation . Also, z only occurs in the equation through h_1 and h_2 . So, we may equally treat h_2 as the variable of the equation and write h_1 as a function of h_2 and c_n , given by

$$h_1^2 = h_2^2 + 4z(c_n^2+c_n^{-2})/(1+z^2) \qquad (3.7.72)$$

Using this set of variables, we are able to solve the equation (3.7.67) , using the UNIVAC 1100/42 computer, for z and c_j , $j = 2, 3, \ldots, n$, up to the critical point of the system.

8 THE NUMERICAL SOLUTION

Equation (3.7.67) has been solved numerically for a range of values of z below the critical point using the Newton-Raphson method. The computation was done on a UNIVAC 1100/42 computer using double-precision floating point arithmetic with 18 significant digits. A solution was assumed to have converged only when the relative change of each variable, through one iteration, was less than 10^{-14}. As a measure of the degree to which an equation was satisfied, we calculated also the difference between the right- and left-hand sides divided by the absolute sum of all the additive terms in the equation. This was never greater than 10^{-16}.

Solutions were obtained for $n = 2$ up to 20. Since the $n = 2$ case can be solved analytically, it serves as a guide to the degree of accuracy of the solution. Another plausible guide to the accuracy is provided by the fact that some quantities tend very rapidly to their known $n = \infty$ values, differing from them only in the last few digits (see, for example, column 2 in Table III.1). Combining both, we are able to conclude that the numerical results we obtained are accurate at least to 11 significant figures.

§ 8.1 SPONTANEOUS MAGNETIZATION

The spontaneous magnetization of the system is given by (3.6.31). We tabulate in Table III.1 the difference of the spontaneous magnetization calculated at a given n from the exact value, at some particular values of z .

The exact value of the spontaneous magnetization of the system is given by (Yang, 1952)

$$M = (1 - k^2)^{\frac{1}{8}} \tag{3.8.1}$$

where k is as defined in (3.6.5). The convergence of the approximations for the spontaneous magnetization per site to the exact value is extremely rapid away from the critical temperature of the infinite system (denoted by $T_{c,\infty}$) and even for temperatures very close to $T_{c,\infty}$ (e.g. column 5 of Table III.1), the convergence is still at least geometric.

§ 8.2 THE CRITICAL TEMPERATURE

Another quantity of interest is the estimation of the critical temperature of the system and the way it converges towards the exact result.

A more convenient temperature parameter to be used is

$$t = \operatorname{cosech}^4(2J/k_B T) - 1 \tag{3.8.2}$$

Table III.1. Approximations to the spontaneous magnetization for various values of z with $n = 2$ to 20 .†

	$M_n - M_\infty$			
n	$z = 0.4$	$z = 0.414$	$z = 0.4142$	$z = 0.414213$
2	0.02392802714	0.27069383063	0.40964931899	0.52166267553
3	0.00114718221	0.13961159480	0.27329853612	0.38495721146
4	0.00003110890	0.06200532571	0.18216108501	0.29280635216
5	0.00000064786	0.02135243598	0.11642461140	0.22459790868
6	0.00000001171	0.00548872105	0.06856599103	0.17146657416
7	0.00000000193	0.00110682362	0.03561995801	0.12882150103
8	0.0	0.00018921799	0.01572474294	0.09408287799
9	.	0.00002906023	0.00583086002	0.06581275992
10	.	0.00000415274	0.00185340100	0.04330353924
11	.	0.00000056384	0.00052339043	0.02626341718
12		0.00000007370	0.00013571881	0.01441855726
13		0.00000000935	0.00003310139	0.00709879411
14		0.00000000116	0.00000771716	0.00314589825
15		0.00000000014	0.00000173848	0.00127286235
16		0.00000000002	0.00000038124	0.00047878871
17		0.0	0.00000008182	0.00017022932
18		.	0.00000001725	0.00005796032
19		.	0.00000000358	0.00001908212
20	0.0	0.0	0.00000000073	0.00000611736
M_∞	0.80554134201	0.48198594815	0.34155136722	0.22944135750

† The rate of convergence to the exact value is at least geometric.

$$z_{c,\infty} = 0.414213562373$$

Table III.2. The values of $t_{c,n}$ and c_n at the critical point for $n = 2$ up to 20 .

n	$t_{c,n}$	c_n
2	0.38883618289	0.17034166992
3	0.055708351974	0.069221620115
4	0.013533606104	0.034470127987
5	0.0041397721372	0.019108958190
6	0.0014589742584	0.011351755016
7	0.00056804454817	0.0070847910329
8	0.00023846971442	0.0045907985350
9	0.00010626511883	0.0030646532019
10	0.000049720759649	0.0020963364563
11	0.000024234867745	0.0014635757443
12	0.000012232230534	0.0010397980729
13	0.0000063637896075	0.00074998870553
14	0.0000033998957695	0.00054818852449
15	0.0000018597394040	0.00040543697430
16	0.0000010389642033	0.00030303841587
17	0.00000059157832392	0.00022866703980
18	0.00000034270961999	0.00017404462601
19	0.00000020169352724	0.00013351912150
20	0.00000012043354466	0.00010317422824

(for T near $T_{c,\infty}$, this is proportional to $T - T_{c,\infty}$) .

From (3.7.31b) , we have

$$t = \frac{(1+2z-z^2)(1+z^2)^3(2-h_2^2)}{(1-z^2)^4\ (c_n^2+c_n^{-2})} \quad . \qquad (3.8.3)$$

Also, at the critical point of the infinite system ($n = \infty$),

$$t = t_{c,\infty} = 0 \quad . \qquad (3.8.4)$$

Let $t_{c,n}$ be the critical value of t for finite n . At $t = t_{c,n}$, h_2 vanishes for all finite values of n . So, from (3.8.3)

$$t_{c,n} = \frac{2(1+2z-z^2)(1+z^2)^3}{(1-z^2)^4(c_n^2+c_n^{-2})} \quad . \qquad (3.8.5)$$

For n large, z is then close to the limiting critical value $(\sqrt{2}-1)$, so from (3.8.5)

$$t_{c,n} \simeq 8\sqrt{2}\, c_n^2 \quad . \qquad (3.8.6)$$

In Table III.2, the critical value of t calculated at the n th level ($t_{c,n}$) is given. We give also the value of c_n at the critical point of the system. We find numerically that we are able to fit the c_n s extremely accurately to the formula

$$c_n = 1.6817928304 \exp(-\sqrt{4.9348022005\, n - 4.6263770635}) \quad . \qquad (3.8.7)$$

For $n \geq 5$, this fits to our numerical accuracy of 11 significant figures. (Even for $n = 2$ it is accurate to 7 figures.) It is almost certainly the large n asymptotic form of c_n . The corresponding asymptotic form for $t_{c,n}$ follows immediately from (3.8.6) .

§ 8.3 CROSS-OVER PHENOMENON

It is interesting to study the critical behaviour of the spontaneous magnetization per site below the critical point of the system. In terms of the t defined in (3.8.2), the exact $n = \infty$ result is

$$M = (-t)^{\beta} \qquad (3.8.8)$$

where β is the critical exponent and is equal to $1/8$. However, for finite n, and t very close to $t_{c,n}$, M vanishes according to the classical law

$$M \propto (t_{c,n} - t)^{\frac{1}{2}} \quad . \qquad (3.8.9)$$

For large, but fixed, n, the cross-over from (3.8.8) to (3.8.9) is easily seen in Fig. 3.5, when $\log M$ is plotted against $\log \tau$ for various values of n, where

$$\tau = (t_{c,n} - t)/t_{c,n} \quad . \qquad (3.8.10)$$

For t sufficiently less than $t_{c,n}$, this plot is almost a straight line, with slope $1/8$, while for t very close to $t_{c,n}$ it changes to one with slope $1/2$. The cross-over occurs when $(t_{c,n} - t) \sim t_{c,n}$.

We give in Table III.3 rough estimates of the slope of the curve at various values of τ for $n = 3$ and 6. It is readily seen for quite small values of n, the cross-over is already predominant, and it is possible to get very good estimates of β provided that we work in the low temperature region away from the critical point. This is not surprising, since we have chosen the temperature

Fig. 3.5 Log-log plot of spontaneous magnetization M *v.s.* the temperature parameter τ for $n = 3, 6, 10, 20$. The cross-over can be seen easily even for quite small values of n .

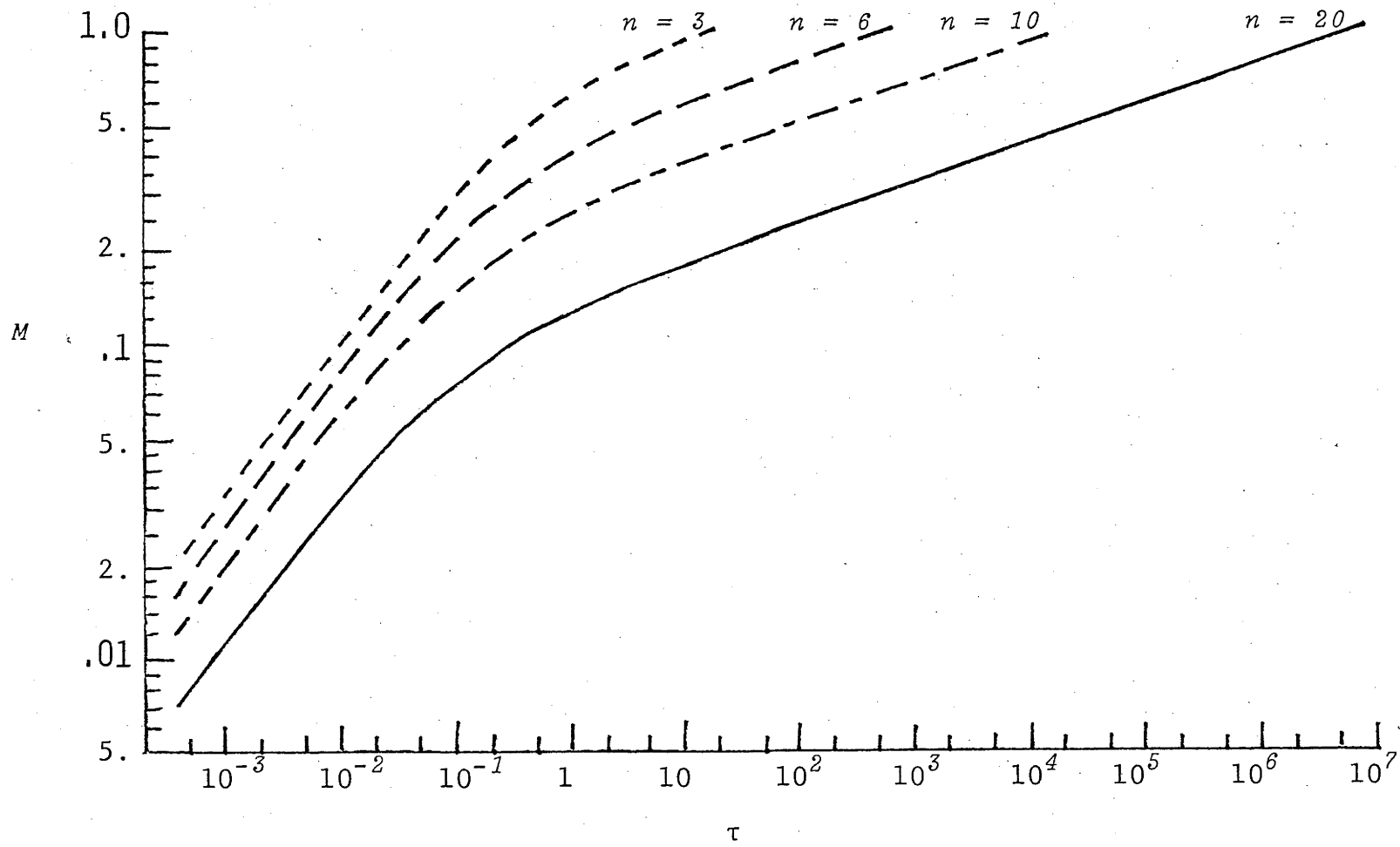


Table III.3. Estimates of β from slope of log-log plot of log M *v.s.* log τ for $n = 3$ and 6 .

$n = 3$		$n = 6$	
τ	β	τ	β
18.936	*0.13197*	*685.87*	*0.12518*
15.943	*0.13338*	*406.01*	*0.12531*
11.607	*0.13687*	*120.07*	*0.12612*
6.3175	*0.14795*	*59.493*	*0.12740*
2.4218	*0.18212*	*23.767*	*0.13151*
0.70898	*0.26037*	*7.3456*	*0.14618*
0.17427	*0.37496*	*1.8116*	*0.18763*
0.075442	*0.43114*	*0.43840*	*0.26202*
0.025400	*0.47476*	*0.12021*	*0.35373*
0.0075640	*0.49062*	*0.031410*	*0.44075*
0.0023273	*0.49715*	*0.0048358*	*0.48612*
0.00088441	*0.49901*	*0.00092492*	*0.49752*

parameter t such that M is exactly equal to $(t_{c,n} - t)^{\frac{1}{8}}$ at all temperatures below the critical point for $n = \infty$.

To describe the cross-over phenomenon, we propose a scaling hypothesis similar to that used by Hankey and Stanley for describing the cross-over of a system from two dimensions to three (Hankey and Stanley, 1972; Liu and Stanley, 1972). We assume that the spontaneous magnetization per site as a function of n and the temperature parameter t ($= t - t_{c,\infty}$) satisfies the scaling hypothesis, i.e. for temperature near to the critical point and for n large, the spontaneous magnetization per site is asymptotically a generalized

homogeneous function,

$$M(t,n) = |t|^{\beta} g(1,\lambda_n t) \quad , \tag{3.8.11}$$

where $\beta = 1/8$ and λ_n is a monotonic increasing function of n. At $t_{c,n}$, the left-hand side of (3.8.11) vanishes for all values of n. Since t is non-zero at $t = t_{c,n}$, the scaling function $g(1,x)$ must have a zero for some fixed value of x called x_o and at x_o,

$$\lambda_n = x_o / t_{c,n} \quad . \tag{3.8.12}$$

Equation (3.8.11) now becomes

$$\begin{aligned} M(t,n) &= |t|^{\beta} g(1,x_o t/t_{c,n}) \\ &= |t|^{\beta} g(1,x_o(1-\tau)) \end{aligned} \tag{3.8.13}$$

where τ is defined by (3.8.10). Hence, we have

$$M(t,n)/|t|^{\beta} = \text{a function of } \tau \text{ only.} \tag{3.8.14}$$

If the left-hand side of (3.8.14) is plotted against τ, scaling predicts that all the data points near the critical point should collapse asymptotically into a single curve. In Fig. 3.6, $\log(1 + t/M^8)$ is plotted against τ for $n = 4, 6, 10$ and 20. The data supports the scaling hypothesis very well.

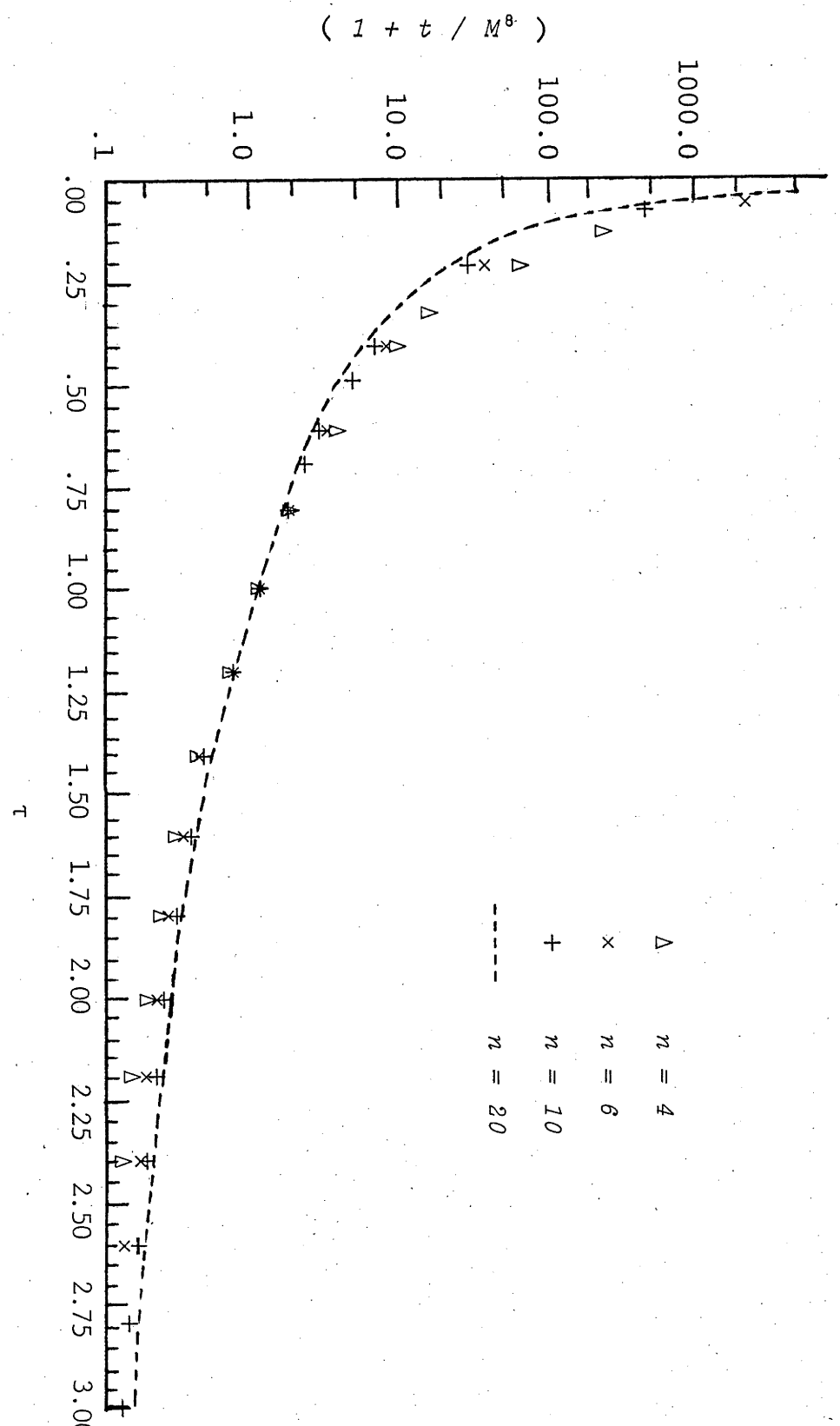


Fig. 3.6 Plot of $\log(1 + t/M^8)$ *v.s.* τ for $n = 4, 6, 10$ and 20 .

§ 8.4 ESTIMATION OF THE CRITICAL EXPONENT β

The scaling hypothesis suggests a way for estimating the critical exponent β of the spontaneous magnetization.

From (3.8.13), we have

$$\ln M(t,n) = \beta \ln |t| + g_1(\tau) \qquad (3.8.15)$$

where g_1 is a function of τ only. Consider the spontaneous magnetization in (3.8.15) for a particular value of τ and denote t by $t_\tau(n)$ (as a function of τ and n). If we compare the value of the spontaneous magnetization at successive values of n, we obtain

$$\begin{aligned} &\ln M(t_\tau(n+1),n+1) - \ln M(t_\tau(n),n) \\ &\quad = \beta \left(\ln |t_\tau(n+1)| - \ln |t_\tau(n)| \right) \\ &\quad = \beta \left(\ln |t_{c,n+1}| - \ln |t_{c,n}| \right) \end{aligned} \qquad (3.8.16)$$

(using (3.8.10) and the fact that τ is fixed).

Since (3.8.13) is asymptotically correct, we should be able to obtain reasonable good estimates for β from (3.8.16) for large n. In Table III.4, the estimation of β from (3.8.16) at $t = t_{c,\infty}$ for $n = 2$ to 19 is given. The data suggests the following asymptotic form for the approximations :

$$\beta_n \sim \beta_\infty \exp(- a/n) \qquad (3.8.17)$$

where β_∞ should correspond to the exact value for the

Table III.4. Estimates of β from (3.8.16) for $n = 2$ to 19 at $t = t_{c,\infty}$.

n	β from (3.8.16)	β_∞ from (3.8.17)
2	0.10340900	
3	0.11490989	0.14189122
4	0.11837555	0.12941239
5	0.11997858	0.12661076
6	0.12091610	0.12571473
7	0.12154229	0.12536813
8	0.12199537	0.12521458
9	0.12234067	0.12513849
10	0.12261354	0.12509692
11	0.12283505	0.12507228
12	0.12301865	0.12505642
13	0.12317340	0.12504563
14	0.12330565	0.12503788
15	0.12342000	0.12503209
16	0.12351987	0.12502761
17	0.12360785	0.12502406
18	0.12368594	0.12502117
19	0.12375574	0.12501880

geometric extrapolation = 0.1250076

critical exponent β . We give in column 3, the estimation of β_∞ and hence extrapolate to obtain a better estimate for β by geometric extrapolation. The result is reasonably accurate as compare with the exact value of 0.125 .

CONCLUSION

For the zero field Ising model, the variational method converges rapidly to the exact results and gives quite good estimates with only a moderate amount of computational effort. The approximations for M at a given n appear to agree with exact series expansions up to and including terms of the order z^{8n-6} [footnote 2]. It has been shown that the system with finite n exhibits a cross-over phenomenon, and good estimates for the exponent β can be obtained. Since the free energy and internal energy per site of the system can be written in terms of determinants involving $\hat{\mathcal{A}}$ and $\hat{\mathcal{Z}}$, their behaviour can also be studied using this method.

Most recently, Baxter and Enting (1979) studied the variational equation of the square Ising lattice in the original representation for the case of non-zero magnetic field and are able to obtain a series expansion of the free energy of the system up to terms of the order z^{46}.

This method proves to be a very efficient method for estimating the thermodynamic properties of the square lattice Ising model. The method has the advantages over many other closed form approximation methods in its rapid convergence towards the exact result of the model even for temperatures quite near to the critical region of the system and also in

the possibility of obtaining as much accuracy as one wishes by increasing m , the order of approximation. Hence, it may be useful to generalize the method to apply to other models also.

The technique can be applied to many other square lattice models e.g. the monomer-dimer system, the Potts model. Essentially, the variational approximation method can be applied on any system whose partition function can be written as the trace of some transfer matrix. However, the possible simplification of the equations and hence the form of the trial function involved depend on the possibility of writing the transfer matrix as a product of weight functions of a square face of the lattice. This makes the generalization of the technique to other lattices without this property quite difficult. Futhermore, the variational equations (3.4.1a-c) require the symmetry conditions (3.2.22) and (3.2.35) of the weight function $w(\alpha,\alpha',\beta,\beta')$. Without these conditions, the equations may be a bit more complicated as the symmetry conditions for $F(\alpha,\beta)$, $P(\alpha,\beta)$ etc. will not hold also.

The formulation of the equations does not depend on the number of values taken up by the spin variable. Hence, the method can easily be generalized to systems in which the spin variable takes up more than two values, for instance, ℓ values. In this case, it would be necessary to require the matrices $X(\alpha)$, $F(\alpha,\beta)$, $P(\alpha,\beta)$ etc. to be $\ell^m \times \ell^m$ matrices.

Nevertheless, this method is interesting as it not only provides a sequence of variational approximations which converges rapidly and gives good estimates of many thermodynamic properties such as the spontaneous magnetization and the critical temperature, but also exhibits cross -over of the predictions from the behaviour of the infinite lattice to those from classical theories as the system approaches the critical temperature of the system for finite m .

LOW TEMPERATURE LEADING ORDER BEHAVIOUR OF THE VARIATIONAL EQUATIONS

We may deduce some relations between the matrices $\mathcal{A}$ and C from the leading order behaviour of the equations in the iterative procedure.

We start from the lowest order of approximation with $m = 0$. For the low temperature case, we try the initial guess

$$\mathcal{A} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

and (III.A.1)

$$\mathcal{Y} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

Following the iterative procedure in Section III.4.3, using the matrices defined in Section III.4.4, we have

$$\mathcal{U} = \mathcal{Y}^T \mathcal{A} \mathcal{Y} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad \text{(III.A.2)}$$

and

$$V = \begin{pmatrix} 1 & 0 & & \\ 0 & 0 & & \\ & & z & 0 \\ & & 0 & 0 \end{pmatrix} \qquad \text{(III.A.3)}$$

and so, on solving for C and P, we have

$$C = \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & z & \\ & & & 0 \end{pmatrix}$$

and (III.A.4)

$$P = I_4$$

As there are only two non-zero eigenvalues of C, it is natural to choose the two non-zero eigenvalues of C to be the elements of $\kappa\mathcal{A}$. In fact, we know from previous low temperature expansions (Section III.4.2) that to leading order in z,

$$\kappa \sim z^{-1} u^{-\frac{1}{2}}$$

and (III.A.5)

$$\mathcal{A} \sim \begin{pmatrix} 1 & 0 \\ 0 & z \end{pmatrix} .$$

Hence, our choice is correct at least to leading order and we obtain

$$\mathcal{H} \sim \begin{pmatrix} 1 & z \\ 0 & 0 \end{pmatrix}$$

and (III.A.6)

$$\mathcal{I} \sim \begin{pmatrix} 1 & z^{\frac{3}{2}} u^{\frac{1}{2}} \\ 0 & 0 \end{pmatrix} .$$

If we repeat the procedure once again, we have

$$\mathcal{U} \sim \begin{pmatrix} 1 & z^{\frac{3}{2}} u^{\frac{1}{2}} \\ z^{\frac{3}{2}} u^{\frac{1}{2}} & z^3 u \end{pmatrix} \qquad \text{(III.A.7a)}$$

$$V \sim \begin{pmatrix} 1 & z^2u^{\frac{1}{2}} & & \\ z^2u^{\frac{1}{2}} & z^4u & & \\ & & z & z^2u^{\frac{1}{2}} \\ & & z^2u^{\frac{1}{2}} & z^3u \end{pmatrix} \qquad \text{(III.A.7b)}$$

and hence

$$P \sim \begin{pmatrix} 1 & -z^2u^{\frac{1}{2}} & & \\ z^2u^{\frac{1}{2}} & 1 & & \\ & & 1 & -zu^{\frac{1}{2}} \\ & & zu^{\frac{1}{2}} & 1 \end{pmatrix} . \qquad \text{(III.A.8a)}$$

Also

$$C \sim \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & z & \\ & & & 0 \end{pmatrix} . \qquad \text{(III.A.8b)}$$

Choosing the eigenvalues in the same way as the last iteration, we obtain

$$\mathcal{A} \sim \begin{pmatrix} 1 & 0 \\ 0 & z \end{pmatrix}$$

$$\mathcal{H} \sim \begin{pmatrix} 1 & z \\ zu^{\frac{1}{2}} & zu^{\frac{1}{2}} \end{pmatrix} \qquad \text{(III.A.9)}$$

and

$$\mathcal{Y} \sim \begin{pmatrix} 1 & z^{\frac{3}{2}}u^{\frac{1}{2}} \\ z^{\frac{3}{2}}u^{\frac{1}{2}} & zu \end{pmatrix}$$

which is correct already to leading order.

We may estimate the leading order behaviour similarly for the higher order approximations. For example, for the

$m = 1$ case, we may use the initial guess as

$$\mathcal{A} = \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & z & \\ & & & 0 \end{pmatrix}$$

and (III.A.10)

$$\mathcal{I} = \begin{pmatrix} 1 & 0 & z^{\frac{3}{2}}u^{\frac{1}{2}} & 0 \\ 0 & 0 & 0 & 0 \\ z^{\frac{3}{2}}u^{\frac{1}{2}} & 0 & zu & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and repeat the whole procedure again. For the first iteration, we have

$$\mathcal{U} \sim \begin{pmatrix} 1 & 0 & z^{\frac{3}{2}}u^{\frac{1}{2}} & 0 \\ 0 & 0 & 0 & 0 \\ z^{\frac{3}{2}}u^{\frac{1}{2}} & 0 & 2z^3u^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and (III.A.11)

$$V \sim \begin{pmatrix} 1 & 0 & z^2u^{\frac{1}{2}} & 0 & & & & \\ 0 & 0 & 0 & 0 & & & & \\ z^2u^{\frac{1}{2}} & 0 & 2z^4u & 0 & & & & \\ 0 & 0 & 0 & 0 & & & & \\ & & & & z & 0 & z^2u^{\frac{1}{2}} & 0 \\ & & & & 0 & 0 & 0 & 0 \\ & & & & z^2u^{\frac{1}{2}} & 0 & 2z^3u & 0 \\ & & & & 0 & 0 & 0 & 0 \end{pmatrix}$$

So,

$$C \sim \begin{pmatrix} 1 & & & & & & \\ & 0 & & & & & \\ & & z^4u^2 & & & & \\ & & & 0 & & & \\ & & & & z & & \\ & & & & & 0 & \\ & & & & & & z^3u^2 \end{pmatrix}$$ (III.A.12a)

and

$$P \sim \begin{pmatrix} 1 & 0 & -z^2u^{\frac{1}{2}} & 0 & & & & \\ 0 & 1 & 0 & 0 & & & & \\ z^2u^{\frac{1}{2}} & 0 & 1 & 0 & & & & \\ 0 & 0 & 0 & 1 & & & & \\ & & & & 1 & 0 & -zu^{\frac{1}{2}} & 0 \\ & & & & 0 & 1 & 0 & 0 \\ & & & & zu^{\frac{1}{2}} & 0 & 1 & 0 \\ & & & & 0 & 0 & 0 & 1 \end{pmatrix} . \qquad \text{(III.A.12b)}$$

Hence with a similar choice of eigenvalues from C, we have to leading order

$$\kappa \sim z^{-1}\, u^{-\frac{1}{2}}$$

$$\mathcal{A} \sim \begin{pmatrix} 1 & & & \\ & z^4u^2 & & \\ & & z & \\ & & & z^3u^2 \end{pmatrix}$$

and

$$\mathcal{L} \sim \begin{pmatrix} 1 & -z^6u^{\frac{5}{2}} & z^{\frac{3}{2}}u^{\frac{1}{2}} & -z^{\frac{9}{2}}u^3 \\ 0 & 0 & 0 & 0 \\ z^{\frac{3}{2}}u^{\frac{1}{2}} & z^{\frac{7}{2}}u^2 & zu & z^2u^{\frac{5}{2}} \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \text{(III.A.13)}$$

If we repeat the process again, we obtain to leading order

$$\mathcal{A} \sim \begin{pmatrix} 1 & & & \\ & z^4u^2 & & \\ & & z & \\ & & & z^3u^2 \end{pmatrix}$$

and (III.A.14)

$$\mathcal{L} \sim \begin{pmatrix} 1 & -z^6u^{\frac{5}{2}} & z^{\frac{3}{2}}u^{\frac{1}{2}} & -z^{\frac{9}{2}}u^3 \\ -z^6u^{\frac{5}{2}} & z^2u & z^{\frac{7}{2}}u^2 & z^{\frac{5}{2}}u^{\frac{3}{2}} \\ z^{\frac{3}{2}}u^{\frac{1}{2}} & z^{\frac{7}{2}}u^2 & zu & z^2u^{\frac{5}{2}} \\ -z^{\frac{9}{2}}u^3 & z^{\frac{5}{2}}u^{\frac{3}{2}} & z^2u^{\frac{5}{2}} & zu^2 \end{pmatrix}$$

This again agrees with the variational equations at least to leading order in z . So, from the structure of C and P , we then conjecture that with P being almost diagonal ($p_{\ell,\ell} \simeq 1$ and $p_{\ell,j} << p_{\ell,\ell}$ for $\ell \neq j$) and C given by

$$C \equiv (d_j) \quad , \quad j=1,2,3,\ldots,2^{m+2} \quad , \qquad \text{(III.A.15)}$$

κ and $\mathcal{A}$ are given by

$$\kappa = d_1 \, z^{-1} \, u^{-\frac{1}{2}} \qquad \text{(III.A.16)}$$

and

$$\mathcal{A} \equiv (a'_j) \quad , \quad j=1,2,3,\ldots,2^{m+1}$$

where

$$a'_j = d_{2j-1} / d_1 \quad , \quad j=1,2,3,\ldots,2^{m+1} \quad . \qquad \text{(III.A.17)}$$

RELATIONS BETWEEN MATRICES IN THEIR REPRESENTATIVES

In order to formulate the iterative procedure of Section III.4.3 in terms of the matrices in the representatives, we must establish the relations between the matrices $\hat{\mathcal{U}}$ and $\hat{V}$, $\hat{\mathcal{Z}}$ and $\hat{P}$ under the set of operators Γ_j and Γ_j^{en} respectively.

It may be seen readily that Γ_j^{en} ($j = 1, 2, \ldots, 2n+1$) can be related to Γ_j ($j = 1, 2, \ldots, 2n-1$) through

$$\Gamma_1^{en} = \begin{pmatrix} I_{2^{n-1}} & 0 \\ 0 & -I_{2^{n-1}} \end{pmatrix}$$

$$\Gamma_2^{en} + \Gamma_3^{en} = \sqrt{2} \begin{pmatrix} 0 & \Gamma_1 \\ \Gamma_1 & 0 \end{pmatrix}$$

$$\Gamma_2^{en} - \Gamma_3^{en} = \sqrt{2} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

and

$$\Gamma_j^{en} = \begin{pmatrix} 0 & \Gamma_{j-2} \\ \Gamma_{j-2} & 0 \end{pmatrix}, \quad j=4,5,\ldots,2n+1 . \tag{III.B.1}$$

Define

$$\chi = \begin{pmatrix} I_\mu & & & \\ & z^{\frac{1}{2}} I_\mu & & \\ & & z^{\frac{1}{2}} I_\mu & \\ & & & I_\mu \end{pmatrix} \tag{III.B.2a}$$

where $\mu = 2^{n-2}$, and

$$\mathcal{U}^{en} = \begin{pmatrix} \mathcal{U} & \\ & \mathcal{U} \end{pmatrix} \qquad \text{(III.B.2b)}$$

then by (3.4.27)

$$V = \chi \mathcal{U}^{en} \chi \qquad \text{(III.B.3)}$$

Using the set Γ_j^{en} defined above in (3.5.1) , we have

$$\hat{\chi} = \begin{pmatrix} 1 & & & & & & & \\ & z^{-\frac{1}{2}} & & & & & & \\ & & z^{\frac{1}{2}} & & & & & \\ & & & 1 & & & & \\ & & & & 1 & & & \\ & & & & & \ddots & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{pmatrix} . \qquad \text{(III.B.4)}$$

Let the representative of $\mathcal{U}$ under Γ_j s be

$$\hat{\mathcal{U}} \equiv (u_{\ell,j}) \quad , \quad \ell,j=1,2,\ldots,2n-1 \qquad \text{(III.B.5)}$$

and let the representative of $\mathcal{U}^{en}$ under Γ_j^{en} s be

$$\hat{\mathcal{U}}^{en} \equiv (\psi_{\ell,j}) \quad , \quad \ell,j=1,2,\ldots,2n+1 . \qquad \text{(III.B.6)}$$

By the definition of representatives,

$$\mathcal{U}^{en} \Gamma_j^{en} (\mathcal{U}^{en})^{-1} = \sum_{\ell=1}^{2n+1} \psi_{\ell,j} \Gamma_\ell^{en} \quad , \quad j=1,2,\ldots,2n+1 . \qquad \text{(III.B.7)}$$

Using (III.B.1) , the right-hand side of the equation is given by

$$\sum_{\ell=1}^{2n+1} \psi_{\ell,j}\Gamma_\ell^{en} = \psi_{1,j}\Gamma_1^{en} + \psi_{2,j}\Gamma_2^{en} + \psi_{3,j}\Gamma_3^{en} + \sum_{\ell=4}^{2n+1} \begin{pmatrix} 0 & \psi_{\ell,j}\Gamma_{\ell-2} \\ \psi_{\ell,j}\Gamma_{\ell-2} & 0 \end{pmatrix}$$

$$j=1,2,\ldots,2n+1 . \qquad \text{(III.B.8)}$$

For $j = 1$, the left-hand side gives

$$\mathcal{U}^{en}\,\Gamma_1^{en}(\mathcal{U}^{en})^{-1} = \begin{pmatrix} I_{2n-1} & \\ & -I_{2n-1} \end{pmatrix} = \Gamma_1^{en} \quad . \tag{III.B.9}$$

This implies that

$$\psi_{j,1} = \delta_{j,1} \quad , \quad j=1,2,\ldots,2n+1 \quad . \tag{III.B.10}$$

For $j \geq 4$, the left-hand side of the equation gives

$$\mathcal{U}^{en}\,\Gamma_j^{en}(\mathcal{U}^{en})^{-1} = \begin{pmatrix} 0 & \mathcal{U}\Gamma_{j-2}\mathcal{U}^{-1} \\ \mathcal{U}\Gamma_{j-2}\mathcal{U}^{-1} & 0 \end{pmatrix}$$

$$= \sum_{\ell=1}^{2n-1} u_{\ell,j-2} \begin{pmatrix} 0 & \Gamma_\ell \\ \Gamma_\ell & 0 \end{pmatrix} \tag{III.B.11}$$

Equating it with (III.B.8) , we obtain

$$(\psi_{2,j} + \psi_{3,j})/\sqrt{2} = u_{1,j-2} \quad ,$$

$$\psi_{2,j} = \psi_{3,j}$$

and

$$\psi_{\ell,j} = u_{\ell-2,j-2} \quad , \quad \ell,j=4,5,\ldots,2n+1 \quad . \tag{III.B.12}$$

For the cases $j = 2$ and $j = 3$, we consider

$$\mathcal{U}^{en}\,(\Gamma_2^{en} + \Gamma_3^{en})(\mathcal{U}^{en})^{-1} = \sqrt{2}\begin{pmatrix} 0 & \mathcal{U}\Gamma_1\mathcal{U}^{-1} \\ \mathcal{U}\Gamma_1\mathcal{U}^{-1} & 0 \end{pmatrix}$$

$$= \sqrt{2}\sum_{\ell=1}^{2n-1} u_{\ell,1} \begin{pmatrix} 0 & \Gamma_\ell \\ \Gamma_\ell & 0 \end{pmatrix} \tag{III.B.13}$$

Hence,

$$\psi_{2,2} = \psi_{3,3}$$

and

$$\psi_{2,2} + \psi_{3,3} + 2\psi_{2,3} = 2u_{1,1} \quad . \qquad \text{(III.B.14)}$$

Also from

$$\mathcal{U}^{en} \left(\Gamma_2^{en} - \Gamma_3^{en} \right) \left(\mathcal{U}^{en} \right)^{-1} = \sqrt{2} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \qquad \text{(III.B.15)}$$

we have

$$\psi_{2,2} + \psi_{3,3} - 2\psi_{2,3} = 2 \quad . \qquad \text{(III.B.16)}$$

On solving, we obtain

$$\begin{aligned} \psi_{2,2} &= \psi_{3,3} = (1+u_{1,1})/2 \\ \text{and} \qquad & \qquad \text{(III.B.17)} \\ \psi_{3,2} &= \psi_{2,3} = (u_{1,1}-1)/2 \quad . \end{aligned}$$

Hence, from (III.B.3) ,

$$\hat{V} = \left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \quad \cdots \\ 0 & (u_{1,1}+1)/2z & (u_{1,1}-1)/2 & (2z)^{-\frac{1}{2}} u_{1,j-2} \quad \cdots \\ 0 & (u_{1,1}-1)/2 & z(u_{1,1}+1)/2 & (z/2)^{\frac{1}{2}} u_{1,j-2} \\ \hline & & & u_{\ell-2,j-2} \\ & & & \ell,j=4,5,\ldots,2n+1. \end{array}\right] \qquad \text{(III.B.18)}$$

(Compare with (3.5.11)).

After diagonalization of $\hat{V}$, the next step in the iterative procedure is to obtain $\hat{\mathcal{A}}$ from $\hat{C}$ and $\hat{\mathcal{F}}$ from $\hat{P}$.

To obtain $\hat{\mathcal{A}}$ from $\hat{C}$, we note that Γ_j^{en} can be recognized from Γ_j in another way :

$$\Gamma_j^{en} = \Gamma_j \otimes I_2 \quad , \quad j=1,2,\ldots,2n-1 \quad . \qquad \text{(III.B.19)}$$

Since $\mathcal{A}$ is diagonal, we have

$$\mathcal{A}\,\Gamma_j\,\mathcal{A}^{-1} = a_j^{o}\,\Gamma_j \qquad \text{(III.B.20)}$$

where

$$\hat{\mathcal{A}} \equiv (a_j^{o}) \quad , \quad j=1,2,\ldots,2n-1 \quad .$$

It is obvious that

$$a_1^{o} = 1 \quad . \qquad \text{(III.B.21)}$$

With a given j ($j \geq 2$) , we must have for any non-zero element (ℓ , ℓ') of Γ_j ,

$$a_j^{o} = a'_{\ell}\, a'^{-1}_{\ell'} = d_{2\ell-1}\, d^{-1}_{2\ell'-1} \qquad \text{(III.B.22)}$$

where a'_j s are elements of $\mathcal{A}$ as given in (3.4.31a,b) . However, by (III.B.19) , if the (ℓ , ℓ') th element of Γ_j is non-zero, then the ($2\ell-1$, $2\ell'-1$) th and (2ℓ , $2\ell'$) th element of Γ_j^{en} are non-zero. Since, with

$$\hat{C} \equiv (a_j) \quad , \quad j=1,2,\ldots,2n+1 \quad , \qquad \text{(III.B.23)}$$

we have

$$\hat{C}\,\Gamma_j^{en}\,\hat{C}^{-1} = a_j\,\Gamma_j^{en} \quad , \qquad \text{(III.B.24)}$$

so, the ($2\ell-1$, $2\ell'-1$) th element of the matrix equation is given by

$$d_{2\ell-1}\, d^{-1}_{2\ell'-1} = a_j \quad . \qquad \text{(III.B.25)}$$

By (III.B.22) , we then obtain

$$a_j^{o} = a_j \quad , \quad j=2,3,\ldots,2n-1 \quad . \qquad \text{(III.B.26)}$$

Hence, $\hat{\mathcal{A}}$ is obtained from $\hat{C}$ by truncating the last two

rows and columns of $\hat{C}$.

As for $\hat{\mathcal{F}}$, we form the matrix

$$Q = (F_o(+) , F_o(-)) \qquad \text{(III.B.27)}$$

from the odd eigenvectors of P and let

$$\hat{Q} \equiv (q_{\ell,j}) \quad , \quad \ell,j=1,2,\ldots,2n-1 \ . \qquad \text{(III.B.28)}$$

Write P as

$$P = \begin{pmatrix} \phi_1,\phi_2,\ldots,\phi_{2^{n-1}} & \\ & \theta_1,\theta_2,\ldots,\theta_{2^{n-1}} \end{pmatrix} \qquad \text{(III.B.29)}$$

where ϕ_j and θ_j are column vectors, and let

$$\Phi = (\phi_1,\phi_3,\ldots,\phi_{2^{n-1}-1})$$
and $$\qquad \text{(III.B.30)}$$
$$\Theta = (\theta_1,\theta_3,\ldots,\theta_{2^{n-1}-1}) \ .$$

Then Q is given by

$$Q = (\Phi , \Theta) \qquad \text{(III.B.31)}$$

Next, we consider the representative of P .

$$\begin{aligned} P\Gamma_j^{en} &= \sum_{\ell=1}^{2n+1} p_{\ell,j}\, \Gamma_\ell^{en}\, P \\ &= \{ p_{1,j} \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} + (p_{2,j}-p_{3,j})/\sqrt{2} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \\ &\quad + (p_{2,j}+p_{3,j})/\sqrt{2} \begin{pmatrix} 0 & \Gamma_1 \\ \Gamma_1 & 0 \end{pmatrix} + \sum_{\ell=4}^{2n+1} p_{\ell,j} \begin{pmatrix} 0 & \Gamma_{\ell-2} \\ \Gamma_{\ell-2} & 0 \end{pmatrix} \} P \end{aligned}$$

$$j=1,2,\ldots,2n+1 \ . \qquad \text{(III.B.32)}$$

Let Γ_j^t ($j = 1, 2, \ldots, 2n-3$) be a set of $2^{n-2} \times 2^{n-2}$ spin operators as defined in (3.5.1) . So,

$$\Gamma_j = \Gamma_j^t \otimes I_2 \quad , \quad j=1,2,\ldots,2n-3 \ . \qquad \text{(III.B.33)}$$

Hence, for $j \geq 4$, the odd columns of (III.B.32) imply

$$\Phi\, \Gamma_{j-2}^t = \{(p_{2,j}-p_{3,j})/\sqrt{2} + \Gamma_1(p_{2,j}+p_{3,j})/\sqrt{2} + \sum_{\ell=4}^{2n+1} p_{\ell,j}\Gamma_{\ell-2} \}\, \Theta \qquad \text{(III.B.34)}$$

and

$$\Theta\, \Gamma_{j-2}^t = \{-(p_{2,j}-p_{3,j})/\sqrt{2} + \Gamma_1(p_{2,j}+p_{3,j})/\sqrt{2} + \sum_{\ell=4}^{2n+1} p_{\ell,j}\Gamma_{\ell-2} \}\, \Phi$$

$$j=4,5,\ldots,2n-1 \ . \qquad \text{(III.B.35)}$$

However, if we consider the representative of Q , we have

$$\begin{aligned} Q\Gamma_j &= \sum_{\ell=1}^{2n-1} q_{\ell,j}\, \Gamma_\ell \ (\ \Phi\ ,\ \Theta\ ) \\ &= (\ \Phi\ ,\ \Theta\ ) \begin{pmatrix} 0 & \Gamma_{j-2}^t \\ \Gamma_{j-2}^t & 0 \end{pmatrix} \\ &= (-\Phi,\Theta)(p_{2,j}-p_{3,j})/\sqrt{2} + \Gamma_1(\Phi,\Theta)(p_{2,j}+p_{3,j})/\sqrt{2} \\ &\quad + \sum_{\ell=4}^{2n+1} p_{\ell,j}\Gamma_{\ell-2}(\Phi,\Theta) \quad , \quad j=4,5,\ldots,2n-1 \ . \end{aligned} \qquad \text{(III.B.36)}$$

For $j = 2$ and $j = 3$, using the fact that

$$\Gamma_2^{en} + \Gamma_3^{en} = \sqrt{2} \begin{pmatrix} 0 & \Gamma_1 \\ \Gamma_1 & 0 \end{pmatrix} = \sqrt{2} \begin{pmatrix} 0 & \Gamma_1^t \\ \Gamma_1^t & 0 \end{pmatrix} \otimes I_2 \qquad \text{(III.B.37)}$$

and

$$\Gamma_2^{en} - \Gamma_3^{en} = \sqrt{2} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \quad ,$$

we have

$$\Gamma_2^{en} = \tfrac{1}{2}\sqrt{2}\begin{pmatrix} 0 & \Gamma_1+I \\ \Gamma_1-I & 0 \end{pmatrix} = \tfrac{1}{2}\sqrt{2}\begin{pmatrix} 0 & \Gamma_1^t+I \\ \Gamma_1^t-I & 0 \end{pmatrix} \otimes I_2$$

and (III.B.38)

$$\Gamma_3^{en} = \tfrac{1}{2}\sqrt{2}\begin{pmatrix} 0 & \Gamma_1-I \\ \Gamma_1+I & 0 \end{pmatrix} = \tfrac{1}{2}\sqrt{2}\begin{pmatrix} 0 & \Gamma_1^t-I \\ \Gamma_1^t+I & 0 \end{pmatrix} \otimes I_2$$

Result similar to (III.B.36) can be obtained for $j = 2$ and $j = 3$ by substituting (III.B.38) to (III.B.32). Hence, (III.B.36) in fact holds for $j = 2$ and 3 also, or we have

$$\sum_{\ell=1}^{2n-1} q_{\ell,j}\Gamma_\ell(\Phi,\Theta) = -(\Phi,\Theta)\Gamma_1(p_{2,j}-p_{3,j})/\sqrt{2} + \Gamma_1(\Phi,\Theta)(p_{2,j}+p_{3,j})/\sqrt{2} + \sum_{\ell=2}^{2n-1} p_{\ell+2,j}\,\Gamma_\ell(\Phi,\Theta) \quad , \quad j=2,3,\ldots,2n-1 \ . \tag{III.B.39}$$

As for the $j = 2n$ case, we note that

$$\Gamma_{2n}^{en} = \sqrt{2}\begin{pmatrix} & & & & & & & 1 \\ & & & & & & 0 & \\ & & & & & 1 & & \\ & & & & 0 & & & \\ & & & 1 & & & & \\ & & 0 & & & & & \\ & \iddots & & & & & & \\ 1 & & & & & & & \\ 0 & & & & & & & \end{pmatrix} \ . \tag{III.B.40}$$

So, in combining the odd columns of (III.B.32) only, we obtain

$$(\Phi,\Theta)\Gamma_1(p_{2,2n}-p_{3,2n})/\sqrt{2} = \Gamma_1(\Phi,\Theta)(p_{2,2n}+p_{3,2n})/\sqrt{2} + \sum_{\ell=2}^{2n-1} p_{\ell+2,2n}\Gamma_\ell(\Phi,\Theta). \tag{III.B.41}$$

Thus, provided that

$$p_{2,2n} \neq p_{3,2n} \quad , \tag{III.B.42}$$

(III.B.39) becomes

$$\sum_{\ell=1}^{2n-1} q_{\ell,j}\Gamma_\ell(\Phi,\Theta) = \left\{ \left[(p_{2,j}+p_{3,j})/\sqrt{2} - \frac{(p_{2,j}-p_{3,j})(p_{2,2n}+p_{3,2n})}{\sqrt{2}\,(p_{2,2n}-p_{3,2n})} \right] \Gamma_1 \right.$$

$$\left. + \sum_{\ell=2}^{2n-1} \left(p_{\ell+2,j} - \frac{(p_{2,j}-p_{3,j})}{(p_{2,2n}-p_{3,2n})} p_{\ell+2,2n} \right) \Gamma_\ell \right\} (\Phi,\Theta)$$

$$j=2,3,\ldots,2n-1 \ . \tag{III.B.43}$$

From (III.B.41) and (III.B.43) , we obtain

$$q_{1,1} = (p_{2,2n}+p_{3,2n}) / (p_{2,2n}-p_{3,2n})$$

$$q_{\ell,1} = \sqrt{2}\, p_{\ell+2,2n} / (p_{2,2n}-p_{3,2n})$$

$$q_{1,j} = \frac{1}{\sqrt{2}} \left\{ (p_{2,j}+p_{3,j}) - \frac{(p_{2,j}-p_{3,j})(p_{2,2n}+p_{3,2n})}{(p_{2,2n}-p_{3,2n})} \right\}$$

and

$$q_{\ell,j} = p_{\ell+2,j} - p_{\ell+2,2n}(p_{2,j}-p_{3,j})/(p_{2,2n}-p_{3,2n}) \ .$$

$$\ell,j=2,3,\ldots,2n-1 \ . \tag{III.B.44}$$

Hence, one can easily obtain $\hat{\mathcal{H}}$ as given by (3.5.16) from the fact that

$$\hat{\mathcal{H}} = \hat{\mathcal{A}}^{-1}\, \hat{Q}\, \hat{\mathcal{A}} \quad . \tag{III.B.45}$$

In the original representation, in the absence of magnetic field (i.e. $u = 1$) ,

$$\mathcal{H} = \begin{pmatrix} F(+,+) & F(+,-) \\ F(-,+) & F(-,-) \end{pmatrix} \tag{III.B.46}$$

and

$$\mathcal{F} = \begin{pmatrix} F(+,+) & z^{\frac{1}{2}}F(+,-) \\ z^{\frac{1}{2}}F(-,+) & F(-,-) \end{pmatrix} . \qquad \text{(III.B.47)}$$

Hence,

$$\mathcal{H} = (1+v_o)^{-1}(\mathcal{F} + v_o\Gamma_1\mathcal{F}\Gamma_1) \qquad \text{(III.B.48a)}$$

or equivalently

$$\mathcal{F} = (1-v_o)^{-1}(\mathcal{H} - v_o\Gamma_1\mathcal{H}\Gamma_1) \qquad \text{(III.B.48b)}$$

where

$$v_o = \tanh(J/2k_BT) . \qquad \text{(III.B.49)}$$

So, obviously, we have

$$\mathcal{F}\Gamma_1 = (1+v_o)\mathcal{H}\Gamma_1 - v_o\Gamma_1\mathcal{F} \qquad \text{(III.B.50)}$$

and also

$$\mathcal{F}\Gamma_j = \sum_{\ell=1}^{2n-1} h_{\ell,j}\Gamma_\ell\mathcal{F} + \frac{2v_o h_{1,j}}{(1-v_o)}\mathcal{H}\Gamma_1$$

$$j=2,3,\ldots,2n-1 . \qquad \text{(III.B.51)}$$

Combining the equations, we have

$$\mathcal{F}\Gamma_j + \frac{2v_o h_{1,j}}{(1-v_o^2)}\mathcal{F}\Gamma_1 = \sum_{\ell=1}^{2n-1} h_{\ell,j}\Gamma_\ell\mathcal{F} + \frac{2v_o^2 h_{1,j}}{(1-v_o^2)}\Gamma_1\mathcal{F} .$$

(III.B.52)

Hence with $\hat{\mathcal{F}}$ given by $\hat{\mathcal{F}} \equiv (f_{\ell,j})$, $\ell,j=1,2,\ldots,2n-1$,

$$f_{1,j} = h_{1,j}\,(1+v_o^2-2v_o f_{1,1})/(1-v_o^2) \qquad \text{(III.B.53)}$$

and

$$f_{\ell,j} = h_{\ell,j} - 2v_o h_{\ell,1}h_{1,j}\,\frac{(1+v_o^2-2v_o f_{1,1})}{(1-v_o^2)^2}$$

$$\ell,j=2,3,\ldots,2n-1 . \qquad \text{(III.B.54)}$$

by noting that both $\hat{\mathcal{F}}$ and $\hat{\mathcal{H}}$ are symmetric.

Since from (III.B.48a)', $\mathcal{H}$ can be obtained from $\mathcal{F}$ in a similar way by negating v_o, we may obtain equation for $h_{1,j}$ similar to (III.B.53) :

$$h_{1,j} = f_{1,j}\,(1+v_o^2+2v_o h_{1,1})/(1-v_o^2) \quad . \qquad \text{(III.B.55)}$$

Hence,

$$f_{1,j} = h_{1,j} \,/\, \{\cosh(J/k_BT)(1+vh_{1,1})\} \quad . \qquad \text{(III.B.56a)}$$

where $v = \tanh(J/k_BT)$. Comparing with (III.B.53) , we have

$$f_{1,1} = (h_{1,1}+v)/(1+vh_{1,1}) \qquad \text{(III.B.56b)}$$

and from (III.B.54b)

$$f_{\ell,j} = h_{\ell,j} - vh_{1,\ell}h_{j,1}/(1+vh_{1,1}) \qquad \text{(III.B.56c)}$$

$$\ell,j=2,3,\ldots,2n-1 \quad .$$

which is as given in (3.5.18) .

FOOTNOTES :

1. RENORMALIZATION GROUP.

Consider a lattice A of spins σ_i with Hamiltonian $\mathcal{H}\{\sigma\}$. The partition function is defined as a sum over the $\{\sigma\}$ space

$$Z(N, \mathcal{H}) = \sum_{\{\sigma\}} \exp(-\beta \mathcal{H}\{\sigma\}) \quad . \tag{1a}$$

If we group the spins in cells and associate each cell of spins a new spin variable μ_i for cell i, we have for the new lattice B formed

$$Z(N', \mathcal{H}') = \sum_{\{\mu\}} \exp(-\beta \mathcal{H}'\{\mu\}) \quad . \tag{1b}$$

The renormalization group can be considered to be a set of transformations from the old variables σ to the new variables μ and from the old Hamiltonian $\mathcal{H}\{\sigma\}$ to the new Hamiltonian $\mathcal{H}'\{\mu\}$ of the system while leaving the free energy invariant. We may write

$$\mathcal{H}'\{\mu\} = R(\mathcal{H}\{\sigma\}) \quad . \tag{1c}$$

In effect, the transformation is a change of length scale of the system. The absolute correlation length is the same for both systems but the relative correlation length has decreased.

If the system is not originally critical, then successive transformations of this form reduce the relative correlation length to the inter-cell spacing, and the properties can then readily be determined. By choosing a good approximation on the transformation, good estimates on the thermodynamic functions and properties may be obtained. Further, for near-critical systems, this procedure is dominated by the fixed points of the transformations, and from these one can in principle obtain the critical behaviour.

2. ACCURACY OF SERIES EXPANSION .

The number of terms reliable in the series expansion can be obtained empirically.

Since the eigenvalues are obtained through the trace of a product of matrices, from a leading order calculation of each element of the matrices, the order (say z^n) to which each term of the expression contributes to the eigenvalues (e.g. η) can be determined. The required accuracy of each element of the matrix to attain a certain accuracy of η can also be determined. This in term can also be used to determine to which order the series expansion is reliable.

Also, by comparing the series in successive approximation, the terms that remain unchanged in successive higher order of approximations can be assumed to be accurate to that order of approximation.

3. DERIVATION OF (3.4.13) .

The set of equation (3.4.11-3.4.12) naturally consists of at least two solutions, one corresponds to the state of the system with most of its spins pointing to the positive direction (i.e. most $\sigma_i = +1$) and the other corresponds to the state with most spins in the negative direction (i.e. most $\sigma_i = -1$) .

Consider the solution for the state with most spins positive and normalise a_+ to be $+1$, we may assume that f_+ is higher order in magnitude (at least for small z) than f_o , f_- and a_- . From (3.4.11a) , this immediately implies that $f_+ \sim 1$ to leading order. Using this, the leading order term for $\mathcal{K}$ (from (3.4.12a)), a_- (from (3.4.12b)), f_o (from (3.4.11b)) and f_- (from (3.4.12c)) can then be obtained to give (3.4.13).

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