A NEW APPROACH TO PROBLEMS IN LATTICE STATISTICS

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CONTENTS

SUMMARY

This thesis deals extensively with the field theoretical approach to the soluble two dimensional Ising lattice, which has recently been developed by Hurst and the author. The aim of this work has been to extend this approach to all statistical lattice problems, and in particular to look at the unsolved lattice problems. The problems considered in detail are the two dimensional square lattice Ising model, the two-dimensional next-nearest neighbour Ising model, the Dimer problem, Slater's model of the ferro-electric K.D.P. and the Rys antiferro-electric model.

In establishing a unified treatment for all lattice problems the formalism of Hurst is presented in a comparatively new and simple fashion. It is shown that the partition function for the models can be written in the general form

$$Z = \langle o | \; T \exp(\Sigma_j H(j)) \; | o \rangle$$

where $H(j)$ is a quadratic function of fermion operators for soluble models and is a quartic function of fermion operators for unsolved models. General field theoretical techniques such as Green's functions and diagonalization of the Hamiltonian, $H(j)$, are discussed in relation to the above expression. The exact results for the partition function,

spontaneous magnetization of the square Ising lattice and the partition function of the Dimer problem are derived using Green's functions.

The next-nearest neighbour Ising lattice and the ferro-electric and antiferro-electric models are not completely solved in terms of this formalism. However, approximate results can be obtained by making a perturbation expansion for the partition function. There is reason to believe that the analytic behaviour of the partition function is closely related to the analytic behaviour of the first few terms of the perturbation expansion. This is particularly so for the cases considered, where the results agree exactly with the expected results.

The first term of the perturbation series for the next-nearest Ising lattice is considered, and the values of the critical indices α, α', β are found to be the same as the two-dimensional soluble lattices. These results agree with the "scaling law" approach of Kadanoff. For the ferro-electric problem, the first-order term contains the exact critical temperature and analytic behaviour of the specific heat as given by Lieb. Higher order terms are calculated and are found to contain no new singularities. The exact solution is obtained for temperatures below the critical temperature and an exact relation between the critical temperature and electric field is obtained using Green's functions.

STATEMENT

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

(R. W. GIBBERD)

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CHAPTER I

INTRODUCTION

1.1 Review of Present Status

One of the most active fields of theoretical physics at the present time is the study of co-operative phenomena in systems of large numbers of interacting particles. Powerful mathematical methods, borrowed in part from quantum field theory, have been developed to treat these phenomena, such as the phase transitions in superconductivity and superfluidity and the order-disorder transition in the Heisenberg model of ferro-magnetism. However, when analysis by approximate mathematical methods indicates a phase change it must then be ascertained whether these results are a consequence of the system considered or of the approximation used in the mathematics. For this reason, some exactly soluble models exhibiting a phase transition have been devised; in particular the Ising model as a model of ferro-magnetism, and the Slater and Rys models as examples of ferro-electricity and antiferro-electricity. It is a coincidence that these simple, classical models can also be treated by methods based on the techniques of quantum field theory. This work is concerned with one of these methods.

The Ising model is well known as a model of magnetism. It is interesting not only as one of the few non-trivial many-body problems that is exactly soluble and shows a phase

transition, but also it has recently been shown experimentally[1] that many systems behave as Ising systems, particularly near the critical temperature. Although the exact solution in the absence of an external magnetic field was given originally over twenty years ago by Onsager[2] using the language of Lie algebras, the flow of papers on exact solutions is still strong today. The reason is, no doubt, the difficulty of the original Onsager method and the subsequent calculation by Yang[3] of the spontaneous magnetization. Kaufman[4], Newell and Montroll[5], Green and Hurst[6], have helped to clarify the Onsager method, but it was Shultz, Mattis and Lieb[7] (herinafter referred to as S.M.L.) who finally made the solution comparatively simple using field-theoretical many fermion techniques. The original Lie algebra is cast into fermion second quantization operators, which for the soluble Ising lattices reduces to a quadratic form resembling a system of non-interacting fermions, but for the unsolved lattices reduces to a form resembling interacting fermions. Kadanoff[8] has introduced the concept of a Green's function into the S.M.L. formalism, which apart from giving an alternative evaluation of the partition function and magnetization, may prove to be a powerful tool in developing approximate procedures for unsolved problems. Although the approaches of S.M.L. and Kadanoff will not be discussed in detail, it is intriguing to notice the many

similarities between their techniques and those given in this work.

The alternative approach to the algebraic solution is to transform the Ising model to a problem of counting polygons on a lattice. Kac and Ward[9] were the first to indicate that the polygons could be summed to give the Onsager solution, although this method was only made rigorous years later by Sherman[10] and Burgoyne[11]. Hurst and Green[12] (see also Kasteleyn[13] and Fisher[14]) simplified considerably the combinatorial approach by showing that the polygons could be counted exactly by a mathematical entity called a pfaffian. The pfaffian technique has gained considerable popularity, being used by Montroll, Potts and Ward[15] to calculate the magnetization and by Stephenson[16] to solve the triangular Ising lattice problem. Hurst[17] has derived pfaffians for generalized Ising lattices. Also Kasteleyn[18], Fisher[19] and Stephenson[20] have solved the dimer problem, and Wu[21], a model of a ferro-electric, with pfaffians.

The technique to be given in this work is obviously related to the pfaffian method, but there will be a greater emphasis on its connection with quantum field theory methods, with the aim of using the powerful mathematical tools of quantum field theory. This approach has recently been published by Hurst[22] and Gibberd and Hurst[23] for the square lattice Ising model, where the partition function and magnetization were obtained by Green's function techniques. This

is analogous to the work of Kadanoff, though the approaches are different.

A disappointing feature of the existing methods of solving the Ising model is that they cannot solve any more complicated problems than those solved by the original Onsager method. As examples of this, the three dimensional and next-nearest neighbour Ising lattices cannot be formulated in the Onsager-Lie algebra approach; the pfaffian method gives the wrong answer, counting some of the graphs with the wrong sign; and the S.M.L. and the present approach cast the models into a a form analogous to the unsolved interacting fermion problem. However, one hopes that the approximation techniques associated with the fermion problem will give useful results. In any case, as was stated by Wannier[24]:

> "It is unwise to suppress successful techniques when discussing a subject in mathematical physics, for in the last analysis a subject grows with the techniques available to handle it."

Two other exactly soluble models of co-operative phenomena, exhibiting a phase transition, are Slater's model of ferro-electric crystals, in particular $KH_2\ PO_4$ (K.D.P.) and the Rys model or F-model of antiferro-electric materials such as $NH_4\ H_2\ PO_4$. The ferro-electric model was originally proposed by Slater[25] in 1941, and the antiferro-electric model by Rys[26] in 1963, and until very recently neither of these models could be solved exactly. Much approximate numerical

work has been done on these models, the most recent being that of Nagle[27], who developed high and low temperature series approximations for both models. For the ferroelectric case, Nagle was able to derive exact results for the critical temperature and the thermodynamic quantities for temperatures below the critical temperature, but was unable to determine the transition temperature for the Rys model. In fact, in this case, the series expansion and Pade approximate methods predicted the wrong transition temperature[28], given by

$$\exp\left(-\epsilon/kTc\right) = .486$$

$$\text{instead of} = \tfrac{1}{2}$$

The lack of an exact solution was particularly disturbing since the models, though resembling the Ising model in many details, failed to yield to the existing Ising techniques. Recently Lieb[29] and Sutherland[30] have solved both models exactly. The initial setting up of Lieb's solution resembles closely the algebraic approach or transfer matrix formalism used by S.M.L. to solve the Ising model. However, the operator belonging to the transfer matrix is no longer typical of the operator of a system of non-interacting fermions, as in the Ising model case, but instead resembles a system of interacting fermions. Thus, the operator cannot be diagonalized, but the situation is saved because the eigenstates of this operator are the

same as the eigenstates of the anisotropic one dimensional Heisenberg model. The solution then is more involved than the Ising model solution, since the so-called Hamiltonian contains an interaction term, and this is why these models have not yielded to the standard Ising model treatments. That a solution is possible relies on the fortuitous fact that the maximum eigenstate corresponds to the known ground state of the Heisenberg chain.

In this work the abovementioned models of co-operative phenomena are to be treated in a unified way which is intimately connected with the methods of quantum field theory. The progress and advancement of quantum field theory occurred in the early fifties when many of the problems that had previously been put aside due to the computational difficulties were approached anew with a more powerful perturbation technique. This so-called Feynman diagrammatic perturbation theory was able to produce experimentally verifiable numerical results in the field of Quantum Electrodynamics. As a result of this success, a vast number of mathematical methods, manipulations, expansions and partial summations have been developed. These techniques have been applied not only to all aspects of quantum field theory but also to problems of statistical mechanics. Matsubara[31] pointed the way by showing that the partition function of a system of particles, written as the trace of a density operator, can be expanded as a series

whose terms can be represented by Feynman diagrams. This method has been developed in many ways, as seen in the works of Martin and Schwinger[32], Kadanoff and Baym[33], and Bloch[34]. Also, Goldstone[35] obtained a graphical representation of the perturbation theory of Brueckner[36], for the ground state energy of a many-particle system. In the last twelve years the quantum field theory approach has been used for almost all many-body problems, the only requirement being that the Hamiltonian of the system is known and can be written in terms of second quantization operators. In most cases the results are good and often they appear to have further application beyond their apparent validity. For example, straightforward perturbation treatments fail in the theory of superconductivity, but more elaborate techniques involving selective summation of certain classes of Feynman diagrams yield the correct results[37], [38].

In regard to the Ising model, field theoretical perturbation methods fall into two classes. The first can be regarded as the application of the above general diagrammatic techniques to the Ising model. So far none of these methods have been able to reproduce the exact solutions of Onsager, but rather give the molecular field solution as the first order approximation. The second-order approximations have been shown by Horwitz and Callen[39] to agree with the high and low temperature series expansions. (Brout[40], Englert[41], Bloch and Langer[42], Bell[43], Oguchi and Ono[44], and Abe[45] have all used

diagrammatic techniques).

The second class of field theory approaches to the Ising model is considered in this thesis. These are the exact methods, already discussed, of S.M.L. Kadanoff and Hurst and Gibberd. Although the rigorous solutions obtained by these methods contain the most successful description of phase transitions so far, these approaches have not been extended beyond the limitations of the simple models they solve. In particular, it is very difficult to draw any conclusions about real systems from these solutions.

On the other hand, it is felt that the field theory techniques are the best approach to phase transitions, which are characterized by the non-analytic behaviour of their thermodynamic quantities, such as specific heat and susceptibility. This is because other practical methods of approximation, such as a rapidly convergent expansion technique, cannot hope to work for functions which are non-analytic in the most interesting temperature range, the critical point. The quantity which could handle this non-analytical behaviour is the Green's function. The Green's function first arose as a powerful tool in quantum field theory, where its own analytic properties govern many of the properties of the system. As examples, in the field of elementary particle physics, a simple pole in the Green's functions correspond to elementary particles, complex poles correspond to unstable elementary particles depending on which Riemann sheet they lie, while branch points generally

start at energies corresponding to the lowest energies of multi-particle states. In the study of the ground state of a many-body problem, the singularity occurs at the energy of the first excited state. In this thesis it is shown how the position of the singularity of the Green's function determines the value of the transition temperature. It would appear that an expansion in terms of Green's functions, which already contain the non-analytic behaviour of the system, is likely to be the most fruitful approach.

1.2 A Brief Outline of the Contents

The aim of this work has been to extend the approach of Gibberd and Hurst[23] to all statistical lattice problems, and in particular to look at the unsolved lattice problems. The problems considered in detail are the two dimensional square lattice Ising model, the two dimensional next-nearest neighbour Ising model, the Dimer problem, Slater's model of a ferro-electric, and the Rys model of an antiferro-electric.

In establishing a unified treatment for all lattice problems the original formalism of Hurst[22] is presented in a comparatively new and simple fashion. In chapter two the counting of graphs on a given Ising lattice is shown to be equivalent to summing a larger class of graphs, which we have called Feynman graphs. The sum of these Feynman graphs is written as the vacuum expectation value of a time-ordered

product of exponentials, and the partition functions for the lattice problems can be written in the general form

$$Z = \langle o|\ T \exp\ (\Sigma_j\ H(j))\ |o\rangle$$

where H(j) is a quadratic function of fermion creation and annihilation operators for the soluble models, and is a quartic function of fermion operators for the unsolved models.

In chapter three, use is made of the strong similarity of the above expression to the S-matrix expressions obtained in field theory. Free and pertubed Green's functions are defined, and some of their general properties discussed. The free Green's functions are evaluated explicitly, and Dyson's integral equation is derived for the pertubed Green's function. The free Green's functions are used in the next chapter to evaluate the partition function and magnetization of the square lattice Ising model. The well-known results of Onsager are obtained, although the derivation is considerably simpler.

Chapter five considers the unsolved problem of the next-nearest neighbour Ising model. Perturbation expansions for the partition function and magnetization are developed. The first term of these expansions reproduces the critical behaviour expected of this model; which is the same as the soluble two-dimensional lattices : a logarithmic singularity in the specific heat, and the magnetization behaving as $(Tc - T)^{\frac{1}{8}}$ near the critical temperature. The critical temperature is calculated

and compared to the results of Potts[51].

In chapter six, an extra field theoretical technique is developed. The S-matrix is simplified by taking the Fourier transform of the fermi operators, and the resulting expression is very similar to those of non-interacting and interacting fermion systems. From this expression a "reduced Hamiltonian" approximation is used on the unsolved problems.

The ferro-electric problem is considered in Chapter seven. This problem has not been completely solved using the combinatorial approach. However, using the Green's function techniques developed in the preceding chapters, it is shown that the low temperature case can be solved exactly, and that the high temperature critical behaviour is given exactly by the first order approximation. Higher order terms of the perturbation series are shown not to contain any new singularities. It is shown that the boundary conditions of this model are important, and that for a model containing helical boundary conditions an exact relation between the critical temperature and the electric field can be derived. The recent exact solution of Lieb is discussed, and comparison between the two methods is made. For the antiferro-electric problem, the first order approximation is shown to predict the exact critical temperature.

The Dimer problem is solved using this new approach, in chapter eight.

In attempting to develop some of the potential that this new formalism would appear to have, we have found the important

result that the first order approximation contains the correct critical point behaviour for some of the unsolved problems, e.g., next-nearest neighbour Ising lattice, ferro-electric and antiferro-electric models. (For soluble Ising models the first order approximation is equivalent to the exact solution and hence must give the correct behaviour). We have also been able to obtain, for the first time, a relation between the critical temperature and electric field for the ferro-electric problem. However, although this technique is more powerful than other methods, there remain many problems, a few of which are discussed in the last chapter.

This thesis contains nine chapters numbered one to nine. The pages are numbered consecutively and the equations (n, m), n being the chapter number and m the number of the equation in that chapter. The references to other literature are collected at the end of the thesis.

CHAPTER 2. REFORMULATION OF THE ISING MODEL

2.1 The Square Lattice

The reformulation of the Ising model to be given in this chapter is based on the combinatorial solution of Kac and Ward[9], who obtained an exact solution for the partition function by summing all the graphs that could be drawn on the lattice. Hurst and Green[12] have since shown that the process of summing all the graphs can be carried out with the use of pfaffians, and a second quantization formalism. This approach had some advantage over other methods, but the more interesting work was to follow when Hurst[21] modified the second quantization formalism to produce an analogy between the expression for the partition function of the Ising model and expressions commonly obtained in the field theory approach to many-body problems. This chapter is concerned with giving an alternative derivation of the partition function as a vacuum to vacuum expectation value of time-ordered exponentials. It is felt that, in comparison to the method already published, the following approach is more concise and elegant, and displays the principles involved in a more transparent form, particularly the analogy with the quantum field theory of many particles.

Essentially, the method shows that the process of summing all Ising graphs is equivalent to summing a larger class of graphs, which are called Feynman graphs. These Feynman graphs can then be summed by a vacuum to vacuum expectation value of

an expression resembling the S-matrix in field theory. For ease of presentation, we shall work in the reverse order, writing down the S-matrix and then showing that this is equal to the sum of all Feynman graphs, which in turn is equivalent to the sum of all the Ising graphs.

Starting with the combinatorial approach of Kac and Ward, the partition function, Z, can be written as

$$Z = \sum_{r,s} g(r,s)\, x^r y^s \qquad (2.1)$$

where $x = \tanh \beta K_1 \quad y = \tanh \beta K_2$

and K_1, K_2 are the horizontal and vertical bond energies and $g(r,s)$ is the number of graphs (closed polygons) that can be constructed from r horizontal bonds and s vertical bonds on a square lattice. These graphs are called Ising graphs to distinguish them from the Feynman diagrams which will be introduced later.

An important feature of these graphs is that they must contain no repeated bonds. In many-body theory, no two identical fermions are allowed to occupy the same state, and the particles are said to obey fermi-statistics. Hence, the Ising graphs can be regarded as obeying fermi-statistics since no bond can be repeated in a given graph. The fact that the partition function can be reduced to counting fermion type graphs is a useful coincidence, for it is this analogy which enables

the Ising graphs to be counted by a many-fermion type expression. A typical many-fermion expression which can be evaluated by the Feynman diagram technique is

$$\langle o|\ T \exp\left(\int_{t_1}^{t_2} H(t)\ dt \right) |o\rangle \qquad (2.2)$$

where $|o\rangle$ represents the vacuum state and H(t) is the Hamiltonian of the system, written in terms of second quantization operators.

Our present aim is to show that we can consider an expression, similar to eq. (2.2), which when expanded in terms of Feynman diagrams will exactly count the Ising graphs associated with the Ising problem. This expression is

$$\langle o|\ T \exp\left(\sum_{j=1}^{N} H(j) \right) |o\rangle \qquad (2.3)$$

where $H(j) = xy\, a_j^{2*}\, a_j^{1*} + y a_j^{2*}\, a_{j-m}^{2} + y a_j^{2*}\, a_{j-1}^{1}$

$$+ x a_j^{1*}\, a_{j-m}^{2} + x a_j^{1*}\, a_{j-1}^{1} + a_{j-m}^{2}\, a_{j-1}^{1}$$

In this expression the variable j is to be regarded as representing the j^{th} lattice point on the Ising lattice, and the operators appearing in H(j) above are associated with this lattice point. Thus, the lattice coordinate, j, takes the place of the time variable, t, in eq. (2.2). The operators a_j^{1*}, a_j^{2*} are fermi-creation operators and a_j^1, a_j^2 are annihilation

operators, which obey the following commutation rules

$$\left[a_j^{p*},\ a_k^{q} \right]_+ = \delta_{p,q}\ \delta_{j,k}$$

$$\left[a_j^{p*},\ a_k^{q*} \right]_+ = \left[a_j^{p},\ a_k^{q} \right]_+ = 0 \qquad (2.4)$$

The symbol, T, is similar to the chronological ordering symbol of Dyson[46] and requires that the operators associated with the various lattice points be arranged in order of increasing j from the right, and an over-all sign factor affixed, according to the parity of the permutation from the standard order given. The symbols $|o\rangle$, $\langle o|$ represent vacuum states such that

$$a_j|o\rangle = 0 \quad ; \quad \langle o|a_j^{*} = 0$$

$$\langle o|o\rangle = 1 \qquad (2.5)$$

The exponential in eq. (2.3) is expanded as a series to give

$$Z = \langle o|T \sum_{n=o}^{\infty} \frac{1}{n!} \left(\sum_{j=1}^{N} H(j) \right)^n |o\rangle \qquad (2.6)$$

A term such as

$$\langle o|T \frac{1}{n!} \left(\sum_{j=1}^{N} H(j) \right)^n |o\rangle \qquad (2.7)$$

which occurs in eq. (2.6) consists of products of creation and

annihilation operators. As can be seen from the relations in eq. (2.5), the vacuum to vacuum expectation value of a product is zero unless every creation operator has, situated to its left, its conjugate operator, the annihilation operator. The time-ordering operator, T, makes certain that, for a product consisting of pairs of creation and annihilation operators, the creation operator stands to the right of the annihilation operator. If the product consists only of pairs of operators, these pairs can be removed by means of the commutation relations in eq. (2.4), leaving a factor $(-1)^l x^r y^s \frac{1}{n!}$, where r is the number of pairs of $a_j^1\ a_j^{1*}$ operators, s is the number of $a_j^2\ a_j^{2*}$ operators. The $\frac{1}{n!}$ term comes from eq. (2.7), and the factor $(-1)^l$ is due to the anticommutation relations. For example

$$\langle o|T\ x\ a_j^{1*}\ a_j^1\ |o\rangle = -\langle o|T\ x\ a_j^1\ a_j^{1*}\ |o\rangle$$

$$= \langle o|\ (a_j^{1*}\ a_j^1 - 1)\ x\ |o\rangle = -x$$

The non-zero contributions which occur in eq. (2.7) can be best represented by the Feynman diagram technique. To see this, we represent each of the terms in H(j) by a vertex, as shown in Fig. 1.

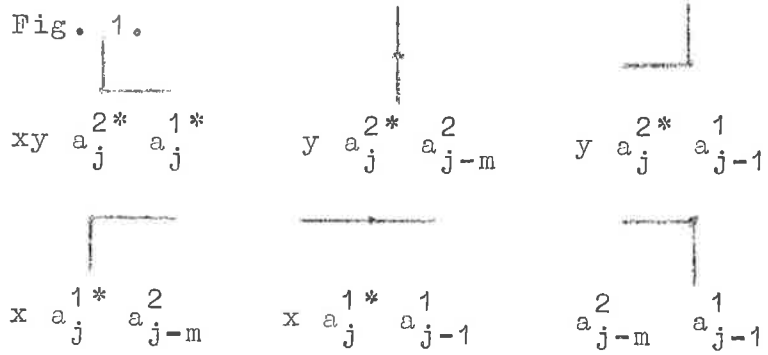


Fig. 1.

Then any product contributing to eq. (2.6) can be represented by a closed diagram drawn on the lattice. As an example the graph drawn in Fig. 2 corresponds to the product

$$\langle o| \frac{1}{4!} x^2 y^2 \; a^2_{j+1} \; a^1_{j+m} \; a^{1*}_{j+m} \; a^2_j \; a^{2*}_{j+1} \; a^1_j \; a^{2*}_j \; a^{1*}_j \; |o\rangle$$

when written in the time-ordered form.

Fig. 2

Hence, to evaluate eq. (2.6), we have to sum all the Feynman diagrams that can be drawn on the lattice. The contribution arising from each graph is $\frac{1}{n!} (-1)^l x^r y^s$, where r, s are the number of horizontal, vertical bonds. The $\frac{1}{n!}$ comes from the exponential series expansion and the factor $(-1)^l$ arises when the pairs of operators are brought together in the time-ordered product, where l is the number of permutations involved.

The factor $\frac{1}{n!}$ can be eliminated by seeing that a given graph will occur n! times. If the graph consists of n different vertices, then there are n! different ways of obtaining these vertices from the product in eq. (2.7). Hence, there will be n! identical graphs. If the graph contains groups of similar vertices; ν_1 of type 1, ν_2 of type 2 etc., then

this given product can occur $n!(\nu_1!\ \nu_2!\ \ldots)^{-1}$ times. Also, there will be $\nu_1!\ \nu_2!\ \ldots$ identical graphs due to the identical vertex points, and so, by multiplying these two factors, there will be n! identical graphs. Thus, by only counting topologically different graphs, a weighting factor of only $(-1)^l\ x^r y^s$ need be associated with each graph.

We shall now prove that l is the number of crossed bonds in the graph. Consider a graph where j is the lowest point and k the highest vertex on the lattice, and the lines joining j, k do not cross as shown in Fig. 3.

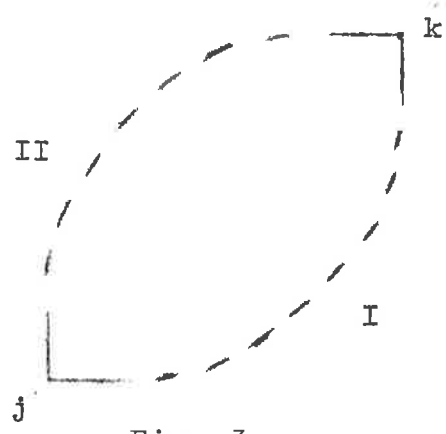


Fig. 3

Then obviously the first pair of operators in the time-ordered product is that associated with the vertex k, $(a^2_{k-m}\ a^1_{k-1})$, and the last pair will be those associated with the vertex j, $(a^{2\,*}_j\ a^{1\,*}_j)$. Thus, the time-ordered product will be

$$a^2_{k-m}\ a^1_{k-1}\ (\ .\ .)\ (\ .\ .)\ \ldots\ldots\ (\ .\ .)\ a^{2\,*}_j\ a^{1\,*}_j$$

where the brackets contain the intermediate pairs of operators. Commuting the operators so that pairs representing vertices of line I are together and those associated with line II are together, we obtain

$$a^2_{k-m}\ (\cdot\ \cdot)\ \ldots\ (\cdot\ \cdot)\ a^{1\,*}_j\ a^1_{k-1}\ (\cdot\ \cdot)\ \ldots\ (\cdot\ \cdot)\ a^{2\,*}_j$$

operators of line I — operators of line II

The sign arising from commuting these operators to this position is positive, since the pairs of fermion operators commute and the single operators anticommute.

Now consider a graph where the lines cross once, as in Fig. 4.

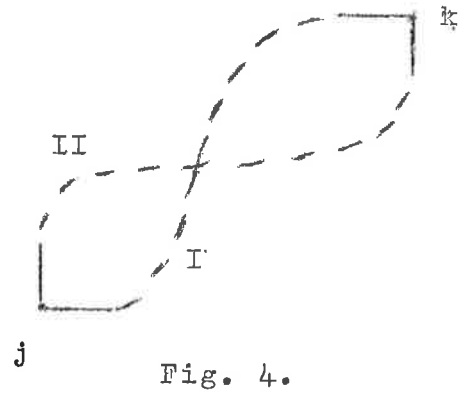


Fig. 4.

These lines may cross at a vertex point, as in the square lattice, or the bonds may cross where there is no lattice point, as in the next-nearest neighbour lattice. In either case, this diagram represents a product of operators similar to that given above, and by commuting the operators associated

with line I to the front of those associated with line II we obtain

$$- a^1_{k-1} (. .) .... (. .) a^{1*}_j \; a^2_{k-m} (. .) ... (. .) a^{2*}_j$$

The minus sign is due to the odd number of permutations. By lengthy but similar considerations it is possible to show that the number of permutations involved in pairing the operators in line I, or II is even. Hence a closed loop with no crossed bonds has a positive sign, while a loop with a single crossed bond has a factor -1. By induction we can see that any graph must have associated with it a factor $(-1)^l$ where l is the number of crossed bonds.

The many-fermion expression in eq. (2.3) can therefore be evaluated by summing all the topologically different Feynman graphs with a weighting factor of $(-1)^l x^r y^s$. In later chapters these graphs are summed using many-fermion techniques, but the remainder of this chapter will be concerned with showing that the sum of all the Feynman graphs associated with eq. (2.3) is equivalent to the sum of all the Ising graphs. There is a similarity between the two classes of graphs, but there is a difference which is now discussed.

The two essential differences are that in the Feynman graphs a given bond may be repeated as frequently as we wish, and that the vertex configuration in Fig. 5 can occur in three alternate ways. For the Ising model, the configuration 5(a)

does not exist, and only one possibility can occur for 5(b)

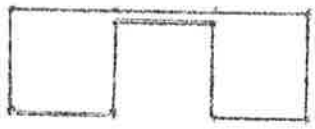


Fig. 5(a)

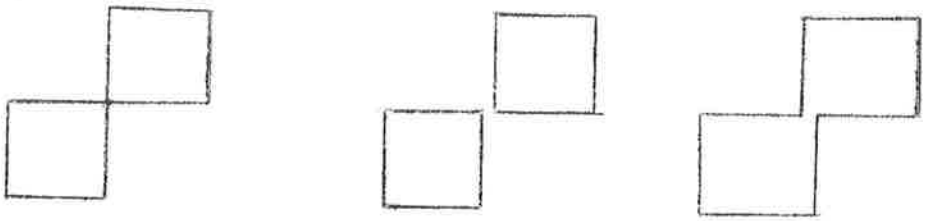


Fig. 5(b)

The first difference, that Feynman graphs do not obey Fermi statistics, was first noticed in the field theory approach to many fermion problems, and the difficulty was easily resolved when it was found that the graphs disobeying Fermi-statistics summed to give a zero contribution, as could be expected from the equation $(a_j^*)^2 = 0$. This same result holds for the above graphs, as can be seen by considering a general example. A graph with a repeated bond can occur in two different ways as shown in Fig. 6.

(a) (b)

Fig. 6

However, the weight factor associated with (a) will be minus that due to (b) since (a) has one less crossed bond. Hence, the total contribution from these two graphs is zero. This reasoning can be extended to any number of repeated bonds, and shows that these graphs do not contribute to the overall sum.

The second difference, concerning the crossed bond configurations can be removed in a similar manner. As the first graph in Fig. 5(b) will have minus the weight of the other two, this leaves a contribution from only one configuration as required by the Ising graphs. The two differences between the sum of the Ising graphs and Feynman graphs have been eliminated, and except for the factor $(-1)^l$ the contributions are the same. For soluble lattices like the square lattice, crossed bonds can only occur at a vertex point, and here they cancel the contribution from an unwanted graph. Hence, it is apparent that for all graphs with non-zero contributions, $l = 0$ and thus,

$$Z = \Sigma g(r,s)\, x^r y^s = \langle o |\, T \exp \left(\sum_{j=1}^{N} H(j) \right) | o \rangle$$

This result was first obtained by Hurst[22] in a direct way, starting from the result of Green and Hurst[47]

$$Z = \langle o | \prod_{j=1}^{N} (1 + xy a_j^{2*} a_j^{1*} + y a_j^{2*} a_{j-m}^{2} + y a_j^{2*} a_{j-1}^{1}$$

$$+ x a_j^{1*} a_{j-1}^{1} + x a_j^{1*} a_{j-m}^{2} + a_{j-m}^{2} a_{j-1}^{1} + xy a_j^{2*} a_j^{1*} a_{j-m}^{2} a_{j-1}^{1}) | o \rangle$$

However, the rigorous justification of this latter expression is quite long and involved.

As is expected, the partition function of all the other soluble Ising lattices can be expressed in terms of a similar quadratic operator H(j).

2.2 Next Nearest Neighbour Lattice

In this section the simplest insoluble Ising lattice is cast into a field theoretic formalism. This problem is the next-nearest neighbour lattice, where the j^{th} spin interacts with its nearest eight neighbours as shown in Fig. 7.

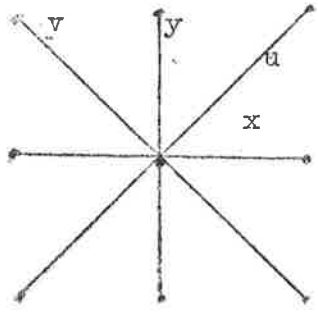


Fig. 7

The partition function can be written as

$$Z = \sum_{p,q,r,s} g(p,q,r,s)\, u^p\, v^q\, x^r\, y^s \qquad (2.8)$$

where $x = \tanh\beta k_1$; $y = \tanh\beta k_2$; $u = \tanh\beta k_3$;

$v = \tanh\beta k_4$; and $g(p,q,r,s)$ is the number of Ising graphs that can be drawn on the lattice with p diagonal

bonds in the u direction, q diagonal bonds in the v direction, r horizontal bonds and s vertical bonds.

Hopefully, we would expect that an expression such as eq. (2.9) would count these graphs.

$$\langle o|\ T \exp\left(\sum_{j=1}^{N} H(j)\right) |o\rangle \qquad (2.9)$$

where $H(j) = va_j^{4*}(ya_j^{2*} + ua_j^{3*} + xa_j^{1*} + a_{j-m+1}^4 + a_{j-m}^2 + a_{j-m-1}^3 + a_{j-1}^1) + ya_j^{2*}(ua_j^{3*} + xa_j^{1*} + a_{j-m+1}^4 + a_{j-m}^2 + a_{j-m-1}^3 + a_{j-1}^1) + ua_j^{3*}(xa_j^{1*} + a_{j-m+1}^4 + a_{j-m}^2 + a_{j-m-1}^3 + a_{j-1}^1) + xa_j^{1*}(a_{j-m+1}^4 + a_{j-m}^2 + a_{j-m-1}^3 + a_{j-1}^1) + a_{j-m+1}^4 (a_{j-m}^2 + a_{j-m-1}^3 + a_{j-1}^1) + a_{j-m}^2 (a_{j-m-1}^3 + a_{j-1}^1) + a_{j-m-1}^3 a_{j-1}^1$

In Fig 8 the bonds to which the operators correspond is shown.

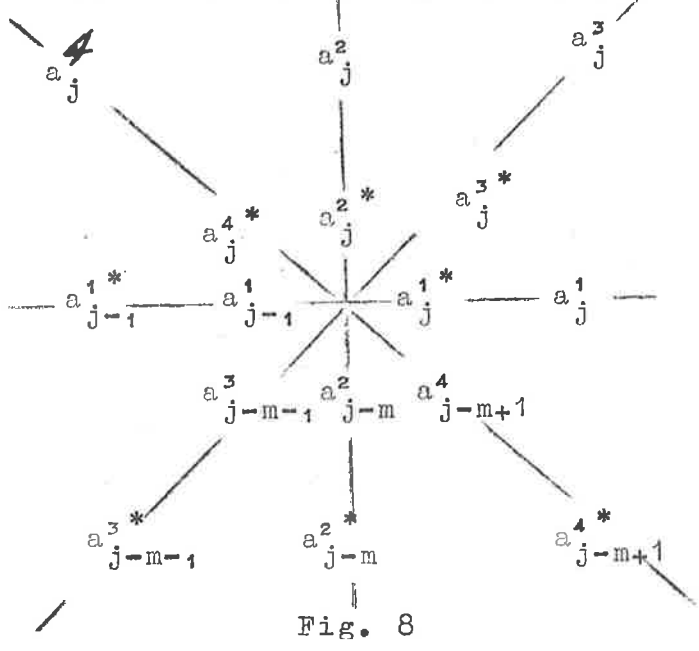


Fig. 8

In analogy with the previous section, we can expand eq. (2.9) in terms of Feynman diagrams and show that they are equivalent to the Ising graphs. However, in this lattice there are graphs contributing to the total sum, which have an odd number of crossed bonds. Fig. 9 contains the simplest example.

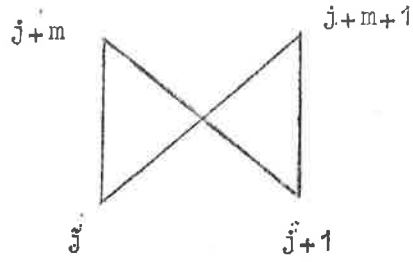


Fig. 9

Thus, expressions (2.8) and (2.9) are the same, except that graphs with an odd number of crossed bonds will be counted with a negative weight by eq. (2.9). Fortunately, we can include in the expression for H(j) extra terms which will count the graphs with an odd number of crossed bonds correctly. However, the form of H(j) is now more complicated as it consists of quartic terms. We write the partition function as

$$Z = \langle o |\ T \exp \left(\sum_{j=1}^{N} H_0(j) + H_1(j) \right) | o \rangle \qquad (2.10)$$

where $H_1(j)$ is the quartic term of operators, and introduce extra lattice points where the bonds cross as shown in Fig. 10.

Fig. 10

Then consider

$$H_0(j) = va_j^{4*}(ya_j^{2*} + ua_j^{3*} + xa_j^{1*} + a_j^6 + a_{j-m}^2 + a_{j-1}^5 + a_{j-1}^1)$$

$$+ ya_j^{2*}(ua_j^{3*} + xa_j^{1*} + a_j^6 + a_{j-m}^2 + a_{j-1}^5 + a_{j-1}^1)$$

$$+ ua_j^{3*}(xa_j^{1*} + a_j^6 + a_{j-m}^2 + a_{j-1}^5 + a_{j-1}^1) + xa_j^{1*}(a_j^6 + a_{j-m}^2 +$$

$$a_{j-1}^5 + a_{j-1}^1) + a_j^6(a_{j-m}^2 + a_{j-1}^5 + a_{j-1}^1) + a_{j-m}^2(a_{j-1}^5 + a_{j-1}^1)$$

$$+ a_{j-1}^5 \; a_{j-1}^1 + a_j^{5*} \; a_{j-m}^3 + a_j^{6*} \; a_{j-m+1}^4$$

$$\text{and } H_1(j) = 2a_j^{6*} \; a_j^{5*} \; a_{j-m+1}^4 \; a_{j-m}^3 \qquad (2.11)$$

where the operators correspond to the bonds as shown in Fig. 11.

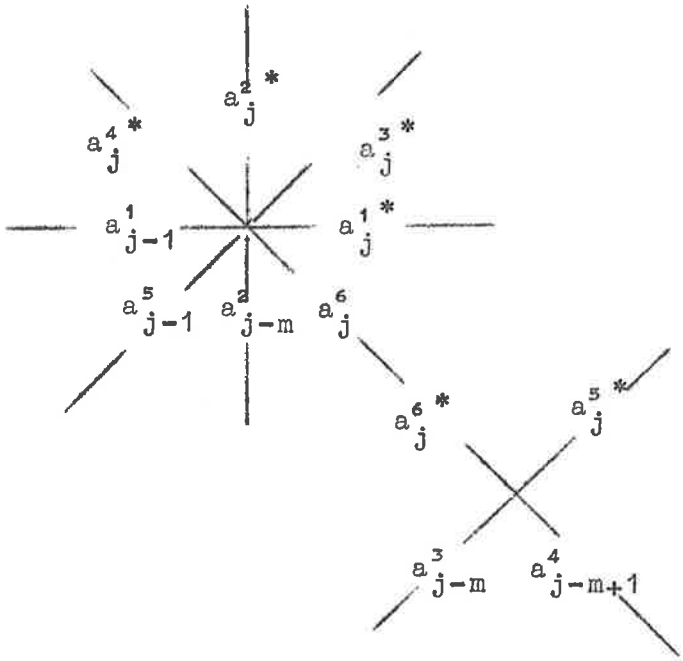
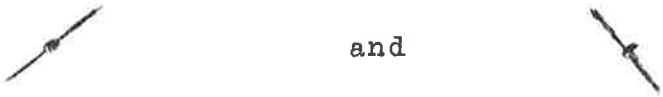


Fig. 11

There are only two pairs of operators in $H_0(j)$ associated with the new lattice point, corresponding to the vertices



This is because any bent vertices going through this point will produce graphs which were not on the original lattice. The quartic term, $H_1(j)$, corresponds to the crossed bond vertex.

To show that expression (2.10) and (2.11) give the correct value for the partition function, we again expand the exponential as a series and look at the sums of products of operators in terms of the Feynman diagrams. Thus eq. (2.10)

can be written

$$Z = \langle o| \; T \sum_{n=o}^{\infty} \frac{1}{n!} \left(\sum_{j=1}^{N} H_1(j) \right)^n \exp \left(\Sigma_j \, H_o(j) \right) |o\rangle \qquad (2.12)$$

The first term in the above series is

$$Z_o = \langle o| \; T \exp \left(\Sigma_j \, H_o(j) \right) |o\rangle \qquad (2.13)$$

It is easily verified that this expression is the same as eq. (2.9) and hence counts some diagrams with the wrong weight. We now introduce some simplifying notation. Call the crossed bonds that do not cross at a vertex point, such as those in Fig. 9, Ising-crossed bonds, to distinguish them from the crossed bonds in Fig. 5(b) which cross at a vertex point. Also let the sum of all Ising graphs with no Ising-crossed bonds be L_o, and the contribution from all Ising graphs with p Ising-crossed bonds be L_p. Hence, from the previous discussion and using the above notation, eq. (2.13) can be written

$$Z_o = L_o - L_1 + L_2 - \ldots\ldots$$

$$= \sum_{i=o}^{\infty} (-1)^i \, L_i$$

The second term in the expansion of eq. (2.12) is

$$Z_1 = \langle o| \; T \left(\Sigma_j \, H_1(j) \right) \exp \left(\Sigma_j \, H_o(j) \right) |o\rangle \qquad (2.14)$$

The Feynman graphs arising from this expression will have an Ising-crossed bond, due to the $H_1(j)$ term, counted with a positive sign and a factor of 2, plus other crossed bonds coming from the exp $(\Sigma_j H_0(j))$ term, with a factor of $(-1)^1$. The expression, Z_1, counts all Ising graphs with a single crossed-bond with a weight factor of +2; graphs with two crossed-bonds with a factor of -4. This last fact can be seen by letting the two crossed-bonds occur at the lattice sites p and q. Then Z_1 will count this graph, firstly, with the crossed bond at the p^{th} site coming from the factor $H_1(p)$ and the q^{th} site from $H_0(q)$ with a factor of -2; and secondly with the cross-bonds coming from $H_1(q)$ and $H_0(p)$ respectively. Thus, the total factor for this graph is -4. Similarly for graphs containing n crossed bonds, Z_1 will count them with a factor $2n(-1)^{n-1}$; the 2 arising from $H_1(j)$, the $(-1)^{n-1}$ coming from $\exp(\Sigma_j H_0(j))$, and the n is due to the summation over j in $H_1(j)$. Hence,

$$Z_1 = 2L_1 - 4L_2 + 6L_3 - \ldots.$$

The k^{th} term in the perturbation series of eq. (2.12) is

$$Z_k = \langle o | \; T \frac{2^k}{k!} \; (\Sigma_j H_1(j))^k \exp(\Sigma_j H_0(j)) \; | o \rangle$$

and can similarly be proved equal to

$$Z_k = 2^k L_k - 2^k L_{k+1} (k+1) + 2^k L_{k+2} (k+2)(k+1) \frac{1}{2!}$$

$$= 2^k \sum_{n=k}^{\infty} (-1)^{n-k} L_n C_k^n$$

To obtain the partition function

$$Z = \sum_{k=o}^{\infty} Z_k$$

in terms of L_j, we sum the coefficients of L_j appearing in $\sum_k Z_k$, which are

$$\sum_{n=1}^{j} 2^n (-1)^{j-n} C_n^j + (-1)^j$$

The last term comes from Z_o. This can be written as

$$(-1)^j \left(1 + \sum_{n=1}^{j} (-2)^n C_n^j\right)$$

which is the binomial expansion of

$$(-1)^j (1 - 2)^j = 1$$

Hence,

$$\sum_{n=o}^{\infty} Z_n = L_o + L_1 + L_2 + \ldots.$$

which is the correct form for the partition function. The partition function for the next-nearest neighbour lattice is therefore given by eqs. (2.10) and (2.11). These expressions are analogous to the many fermion system with interactions, and at the present time can only be evaluated by approximate methods.

2.3 General Ising Lattices

We now consider whether all Ising problems can be represented as a vacuum to vacuum expectation value of a product of exponentials. In section 2.1 it was shown that the partition function for all planar lattices, in which the Ising graphs do not contain crossed bonds, can be written as

$$Z = \langle o |\ T \exp\ (\Sigma_j\ H(j))\ | o \rangle$$

where $H(j)$ will be a quadratic function of fermi operators. For a more general planar lattice containing crossed bonds, the partition function can be written as above, except that $H(j)$ contains quartic terms. Extra vertices have to be included wherever two bonds may cross, and a quartic term is associated with this new vertex. In the case of three-dimensional lattices, these can be considered as an infinite number of planar lattices, where a bond in the z-direction corresponds to a line joining two points on the neighbouring planes. Such a bond will give rise to a large number of crossed bonds, and each vertex will need m extra vertices introduced, to eliminate these crossed bonds, where m is the number of vertices in a row on the lattice. Thus, the partition function can be written in an analogous form to eq. (2.10), but it would appear to be too cumbersome to manipulate successfully. Essentially, the quartic terms, which are regarded as correction terms are too numerous to be neglected in any

approximate calculation (see Chapter 5).

Another unsolved problem is the Ising model in a magnetic field. This problem reduces to counting not only closed graphs but also line graphs, and we have not found a quantity which will count these latter graphs correctly. The one-particle Green's function, defined in the next chapter, counts single line-graphs, however, the sign which it attributes to the weight of each graph is positive or negative, depending on the shape of the graph. This could only be corrected with the inclusion of a quartic term, and so complicates the expression. The many-particle Green's functions would also be required and these have not been evaluated yet. Hence the formalism we have developed here for regarding the Ising problem as a many fermion problem is specific to planar lattices, and does not readily generalize to more difficult Ising problems. However, as shown in later chapters, the approach is perfectly general when dealing with other planar lattice statistical problems, such as the Dimer problem, the two-dimensional ferro-electric and antiferro-electric problems.

Finally, we should briefly mention the work of Vdovichenko[48], as he obtained the partition function of the square lattice Ising model, by showing that one has to sum a larger class of diagrams (corresponding to our Feynman graphs). He did this by means of a determinant. Basically the class of diagrams to be summed are the same, but Vdovichenko avoided as far as

possible the use of concepts not contained in the original combinatorial formulation of the problem. This meant that he could solve the square lattice case, but could not attempt a formulation for lattices with crossed bonds.

CHAPTER 3. GREEN'S FUNCTIONS

3.1 Green's Functions and Thermodynamic Quantities

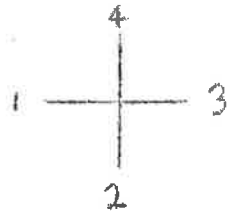
In studying the problems of quantum-field theory, the method of Green's functions has proved to be a very powerful and useful tool. In this chapter it is shown that the Green's function technique is also useful in evaluating the thermodynamic quantities of the Ising model. Our definition of the Green's function for the Ising model is based on the definition of time-dependent Green's functions in field theory. The free or unperturbed Green's function is defined in terms of the Hamiltonian $H_0(j)$, where $H_0(j)$ is only quadratic in the creation and annihilation operators, and is evaluated in Section 3.3 The pertubed Green's function is defined in terms of the full Hamiltonian $H_0(j) + H_1(j)$ and is expressed as a function of the proper-self energy part, Λ, in section 3.4 In this section we shall define the Green's function, and show its relation to the partition function and average energy.

To simplify the expressions, it is necessary to introduce a change in the notation. The following notation was originally used by Hurst[22] and is denoted by

$$A^4(j) = y a_j^{2*} \qquad A^3(j) = x a_j^{1*}$$

$$A^2(j) = a_{j-m}^2 \qquad A^1(j) = a_{j-1}^1$$

The operators belonging to a given lattice point, j, are all labelled by the variable j now, and the superscripts represent the directions of the bonds as shown.



Defining a matrix k by

$$k = \begin{pmatrix} 0 & -1 & -1 & -1 \\ 1 & 0 & -1 & -1 \\ 1 & 1 & 0 & -1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \qquad (3.1a)$$

the eq. (2.3) can be written

$$H_0(j) = \sum_{p,q,=1}^{4} \tfrac{1}{2} k_{pq} A^p(j) A^q(j) \qquad (3.1b)$$

where $H_0(j)$ is the so-called hamiltonian for the square lattice.

For the next-nearest neighbour problem there is a similar change of notation.

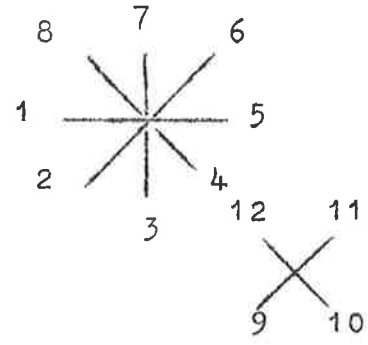
$$A^1(j) = a^1_{j-1} \qquad A^2(j) = a^5_{j-1} \qquad A^3(j) = a^2_{j-m}$$

$$A^4(j) = a^6_j \qquad A^5(j) = a^{1*}_j \qquad A^6(j) = a^{3*}_j$$

$$A^7(j) = a^{2*}_j \qquad A^8(j) = a^{4*}_j \qquad A^9(j) = a^3_{j-m}$$

$$A^{10}(j) = a^4_{j-m+1} \qquad A^{11}(j) = a^{5*}_j \qquad A^{12}(j) = a^{6*}_j$$

where the superscripts represent the bonds shown.



We define k, for this lattice, as the matrix

$$
\begin{array}{cccccccccccc}
0 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\
1 & 0 & -1 & -1 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & -1 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 0 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 0 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 0 & -1 & -1 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 & 0 & -1 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0
\end{array}
\qquad (3.2a)
$$

and then eq. (2.11) can be written

$$H_0(j) = \sum_{p,q} \tfrac{1}{2} k_{pq} A^p(j) A^q(j) \qquad (3.2b)$$

The unpertubed or free Green's function $G_0^{s,t}(l,k)$ is defined for all lattice problems as

$$G_0^{s,t}(l,k) = \langle o| T A^s(l) A^t(k) \exp\left(\Sigma_j H_0(j)\right) |o\rangle \cdot Z_0^{-1}$$

$$\text{where } Z_0 = \langle o| T \exp\left(\Sigma_j H_0(j)\right) |o\rangle \qquad (3.3)$$

This is in direct analogy to

$$G_0(t,t') = \langle o|T\ a^*(t)a(t')\exp\left(\int H_0(t)dt\right)|o\rangle \Big/ \langle o|T\ \exp\left(\int H_0(t)dt\right)|o\rangle$$

which is used in field theory.

The pertubed or exact Green's function is defined in a similar manner as

$$G^{s,t}(l,k) = \langle o|T\ A^s(l)A^t(k)\ \exp\ (\Sigma_j H_0(j) + H_1(j))\ |o\rangle . Z^{-1} \qquad (3.4)$$

Obviously the perturbed Green's function is the same as the free Green's function for the square lattice since $H_1(j) = 0$, but is different for the next-nearest neighbour lattice.

The Green's functions are very simply related to the thermodynamic quantities of the Ising model. To illustrate the relation between the partition function and the Green's functions, we introduce an arbitrary parameter ϵ into the definition of Z.

$$Z(\epsilon) = \langle o|\ T\ \exp\ (\Sigma_j\ \epsilon H_0(j) + H_1(j))\ |o\rangle \qquad (3.5)$$

Therefore

$$\frac{dZ}{d\epsilon}^{(\epsilon)} = \langle o|\ T\ \sum_j H_0(j)\ \exp\ (\sum_j \epsilon H_0(j) + H_1(j))\ |o\rangle$$

where the time-ordering operator, T, allows the differentiation to be carried out without regard to the anti-commutation properties of the operators. Thus

$$Z^{-1}_{(\epsilon)} \cdot \frac{dZ(\epsilon)}{d\epsilon} = \Sigma_j\ \Sigma_{p,q}\ \tfrac{1}{2}\ k_{p,q}\ G^{p,q}\ (j,j,\epsilon)$$

where the definition of the Green's function has been generalized to

$$G^{s,t}(l,k,\epsilon) = \langle o|T\ A^{s}(l)A^{t}(k)\exp(\Sigma_j \epsilon H_o(j)+H_1(j))|o\rangle . Z^{-1}(\epsilon) \quad (3.6)$$

$$\text{Now} \int_o^1 Z(\epsilon)^{-1} \cdot \frac{dZ(\epsilon)}{d\epsilon} \cdot d\epsilon = \log Z$$

and hence

$$\log Z = \int_o^1 d\epsilon \ \Sigma_j \ \Sigma_{p,q} \ \tfrac{1}{2} \ k_{p,q} \ G^{p,q}(j,j,\epsilon) \quad (3.7)$$

It will be seen in Chapter 4 that the integration in this equation can be performed quite simply for the square lattice.

A simple relation exists between the internal energy per particle of the Ising model and the Green's function. This arises from the definition of the internal energy per particle, $\bar{E}$,

$$\bar{E} = -\frac{1}{NZ} \frac{\partial Z}{\partial \beta}$$

$$= -\frac{1}{NZ} \left(\frac{\partial Z}{\partial x} \cdot \frac{\partial x}{\partial \beta} + \frac{\partial Z}{\partial y} \cdot \frac{\partial y}{\partial \beta} \right)$$

for the square lattice. Using eq. (3.4) we obtain

$$Z^{-1} \frac{\partial Z}{\partial x} = \Sigma_j \sum_{p,q} k'_{p,q} \ G^{p,q}(j,j) \ x^{-1}$$

$$Z^{-1} \frac{\partial Z}{\partial y} = \Sigma_j \sum_{p,q} k''_{p,q} \ G^{p,q}(j,j) \ y^{-1}$$

where

$$k' = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 1 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \qquad k'' = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Hence

$$\bar{E} = N^{-1} \Sigma_j \text{ Trace } (k' G(j,j) K_1 (x^{-1}-x) + k'' G(j,j) K_2 (y^{-1}-y))$$

A similar result can be obtained for the next-nearest neighbour problem.

The correlation functions between neighbouring spins can be expressed as linear functions of Green's functions, and in Chapter 4 a determinant, whose elements are Green's functions, is shown to be equal to the magnetization.

These are not the only Green's functions which have been defined in relation to the Ising problem. Both Montroll, Potts and Ward[15] and Kadanoff[8] have defined Green's functions, and there is a direct connection between them, although they all arise in different formalisms.

3.2 Properties of Green's Functions.

In studying the Green's functions which arise in the quantum-many body problems, many useful properties can be derived without requiring very much information about the hamiltonian of

the system. Dispersion relations and sum rules can often be derived. Unfortunately, it has not been possible to obtain similar relations for the Green's function, defined in the previous section, although the following result is necessary. Since we have given the lattice cyclic boundary conditions, such that the lattice is wrapped onto itself helically, the Green's functions are periodic. This is clear from the relation $a_j^{1*} = a_{j\pm N}^{1*}$ where N is the number of lattice points, and hence

$$G^{p,q}(j,k) = G^{p,q}(j\pm N,\ k\pm N)$$

Also, as the hamiltonian, $H_0(j) + H_1(j)$, is translationally invariant with respect to the time variable, j, $G^{p,q}(j,k)$ is a function of (j-k) only. Thus

$$G^{p,q}(j,k) = G^{p,q}(j-k)$$

These two properties enable us to write $G^{p,q}(j-k)$ as a fourier series.

$$G^{p,q}(j-k) = N^{-1} \sum_{r=1}^{N} G^{p,q}(r) \exp\ (2\pi i r(j-k)/N)$$

and conversely

$$G^{p,q}(r) = \sum_{j} G^{p,q}(j) \exp\ (-2\pi i\ r\ j/N) \qquad (3.9)$$

The fact that the Green's function can be written as a fourier series arises very naturally from the work in Chapter

6, where the hamiltonian is diagonalized by a fourier transformation. The fourier transform of the Green's function, $G^{p,q}(r)$ can then be expressed in terms of the diagonalized hamiltonian.

3.3 Evaluation of the Free Green's Function

In this section, a general expression for the unperturbed Green's function is established. This Green's function, given by eq. (3.3) has already been evaluated by Gibberd and Hurst[23], by summing all the Feynman graphs associated with the expression. Here eq. (3.3) is evaluated by a more general method, which involves setting up and solving an integral equation for $G_o^{p,q}(j-k)$. Both methods are typical of those encountered in many-body theory. Eq. (3.3) can be written as

$$G^{s,t}(1-k) = Z_o^{-1} \langle o|T\ A^s(1)\ A^t(k) \sum_{n=o}^{\infty} \frac{1}{n!} (\Sigma_j\ H_o(j))^n\ |o\rangle$$

The vacuum to vacuum expectation value of a time-ordered product of creation and annihilation operators is evaluated by means of Wick's Theorem, which says that the time-ordered product is equal to the normal-ordered product with all possible pairings. This means summing over time-contractions between all possible pairs of operators which appear in the product. The time-contraction of two operators $A^p(1)$ and $A^q(k)$ is written as $A^{p,q}(1,k)$ and is defined by

$$T(A^p(l)\,A^q(k)) = N(A^p(l)\,A^q(k)) + A^{p,q}(l,k) \qquad (3.10a)$$

where T and N are the time and normal ordering operators respectively. If A(l,k) denotes the matrix of time-ordered contractions, we find that for the square lattice

$$A(l,k) = \begin{pmatrix} 0 & 0 & x\delta_{l-1,k} & 0 \\ 0 & 0 & 0 & y\delta_{l-m,k} \\ -x\delta_{l+1,k} & 0 & 0 & 0 \\ 0 & -y\delta_{l+m,k} & 0 & 0 \end{pmatrix}$$

$$= \frac{1}{N} \sum_{r=1}^{N} \omega^{r(l-k)} \begin{pmatrix} 0 & 0 & x\omega^{-r} & 0 \\ 0 & 0 & 0 & y\omega^{-mr} \\ -x\omega^{r} & 0 & 0 & 0 \\ 0 & -y\omega^{mr} & 0 & 0 \end{pmatrix}$$

$$= \frac{1}{N} \sum_{r=1}^{N} \omega^{r(l-k)}\, A(r) \qquad (3.10)$$

where $\omega = \exp(2\pi i/N)$

The corresponding form of A(r) for the next-nearest neighbour lattice is

$$
\begin{array}{cccccccccccc}
0 & 0 & 0 & 0 & x\omega^{-r} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \omega^{-r} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & y\omega^{-mr} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
x\omega^{r} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -u\omega^{+mr} & 0 & 0 & 0 \\
0 & 0 & -y\omega^{mr} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -v\omega^{(m-1)r} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & u\omega^{-m} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & v\omega^{(-m+1)r} & 0 & 0 & 0 & 0 \\
0 & -\omega^{r} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}
$$

The summing over all time contractions is equivalent to summing over all diagrams, and these fall into two categories; those consisting of a line starting and ending with the operators $A^{s}(l)$ and $A^{t}(k)$, and those which are closed loops. Examples of each are given in Fig. 12.

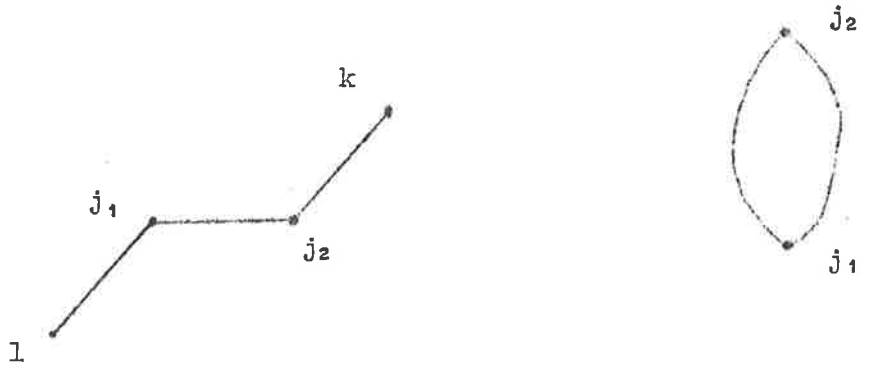


Fig. 12

It is shown in Gibberd and Hurst [23] that, in summing over topologically different diagrams the contribution from a

given diagram depends only on the time contractions represented by the diagram. Hence the contribution from a disconnected diagram is the product of the contributions from its connected components. Thus we can factorize out the summation over all closed loop diagrams.

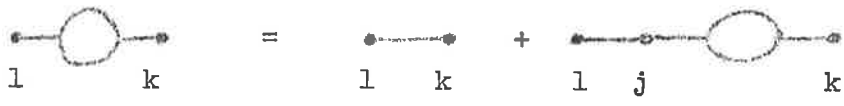
$$\text{Summation over all graphs} = \left[\begin{array}{c}\text{summation over}\\ \text{line graphs}\end{array}\right]\left[\begin{array}{c}\text{summation over}\\ \text{loop graphs}\end{array}\right]$$

But the summation over all loop graphs is equivalent to evaluating the quantity, Z_0, which therefore cancels the Z_0 in the denominator.

Hence to evaluate the Green's function we need to sum only over all line graphs. The contribution from a line graph such as that given by Fig. 12 is

$$A^{s,p_1}(1-j_1)k_{p_1,p_2}\,A^{p_2,q_1}(j_1-j_2)k_{q_1,q_2}\,A^{q_2,t}(j_2-k)$$

The sum over all line graphs can be represented diagrammatically as $G_0{}^{p,q}(1-k) =$  where p,q refer to the directions of the lines at 1,k. Now, we can divide the series of line graphs into the simplest line graph, plus all others minus this graph. Diagrammatically this is represented as



Writing down the contributions of this graphical equation we obtain

$$G_0{}^{p,q}(1-k) = A^{p,q}(1-k) + \sum_{j,s,t} A^{p,s}(1-j)k_{s,t}\,G_0{}^{t,q}(j-k)$$

which is an integral or summation equation for $G_0(l-k)$. This can be written as the following matrix equation

$$G_0(l-k) = A(l-k) + \sum_j A(l-j)\, k\, G_0(j-k)$$

which is solved by taking the Fourier transforms

$$G_0(l-k) = \frac{1}{N} \sum_r \omega^{r(l-k)}\, G_0(r)$$

$$\text{and} \quad A(l-k) = \frac{1}{N} \sum_r \omega^{r(l-k)}\, \Lambda(r)$$

Substituting this into the integral equation, we obtain

$$G_0(r) = \Lambda(r) + \Lambda(r)\, k\, G_0(r)$$

$$\text{and hence } G_0(r) = [1-\Lambda(r)k]^{-1}\, \Lambda(r)$$

$$= [\Lambda^{-1}(r) - k]^{-1} \qquad (3.12)$$

Therefore, the free Green's function has been evaluated as

$$G_0(j-k) = \frac{1}{N} \sum_r \omega^{r(j-k)}\, [\Lambda^{-1}(r)-k]^{-1} \qquad (3.13)$$

The Green's function $G_0(j-k, \epsilon)$, defined by eq. (3.6) can also be evaluated by a similar technique, giving

$$G_0(j-k,\epsilon) = \frac{1}{N} \sum_r \omega^{r(j-k)}\, [\Lambda^{-1}(r)-\epsilon k]^{-1} \qquad (3.14)$$

Equations (3.13) and (3.14) hold for both the Ising lattices that we have been considering, and the elements of the matrix $[\Lambda^{-1}(r) - k]^{-1}$ for the square lattice Ising model are given by

$$\Delta(r)\ (1,1) = x^2 y\ (\omega^{-mr} - \omega^{mr})$$
$$\Delta(r)\ (1,2) = xy\ \omega^{(1-m)r} - x^2 y\ \omega^{-mr} - xy^2 \omega^{r} - x^2 y^2$$
$$\Delta(r)\ (1,3) = x\omega^{r} - xy\ \omega^{r}\ (\omega^{-mr} + \omega^{mr}) - x^2\ (1-y^2) + xy^2\ \omega^{r}$$
$$\Delta(r)\ (1,4) = -xy^2 \omega^{r} - x^2 y^2 + xy\omega^{(m+1)r} - x^2 y\ \omega^{mr}$$
$$\Delta(r)\ (2,1) = -xy\ \omega^{(m-1)r} + xy^2\ \omega^{-r} + x^2 y\ \omega^{mr} + x^2 y^2$$
$$\Delta(r)\ (2,2) = xy^2\ (\omega^{r} - \omega^{-r})$$
$$\Delta(r)\ (2,3) = -x^2 y\ \omega^{mr} - x^2 y^2 + xy\ \omega^{(m+1)r} - xy^2\ \omega^{r}$$
$$\Delta(r)\ (3,1) = -x\omega^{-r} + xy\ \omega^{-r}\ (\omega^{mr} + \omega^{-mr}) + x^2\ (1-y^2) - xy^2 \omega^{-r}$$
$$\Delta(r)\ (3,2) = -xy\ \omega^{-(m+1)r} + x^2 y\ \omega^{-mr} + xy^2 \omega^{-r} + x^2 y^2$$
$$\Delta(r)\ (3,3) = x^2 y\ (\omega^{mr} - \omega^{-mr})$$
$$\Delta(r)\ (3,4) = -xy^2 \omega^{-r} - x^2 y^2 + xy\ \omega^{(m-1)r} - x^2 y\ \omega^{mr}$$
$$\Delta(r)\ (4,1) = -xy\ \omega^{-(m+1)r} + xy^2\ \omega^{-r} + x^2 y\ \omega^{-mr} + x^2 y^2$$
$$\Delta(r)\ (4,2) = -y\ \omega^{-mr} + xy\ \omega^{-mr}\ (\omega^{r} + \omega^{-r}) + y^2\ (1-x^2) - yx^2\ \omega^{-mr}$$
$$\Delta(r)\ (4,3) = -xy\ \omega^{(-m+1)r} + xy^2\ \omega^{r} + y\ x^2 \omega^{-mr} + x^2 y^2$$
$$\Delta(r)\ (4,4) = -xy^2\ (\omega^{r} - \omega^{-r})$$

Where

$$\Delta(r) = (1+x^2)\ (1+y^2) - x(1-y^2)(\omega^{r} + \omega^{-r}) - y(1-x^2)(\omega^{mr} + \omega^{-mr})$$

(3.15)

3.4 The Perturbed Green's Function

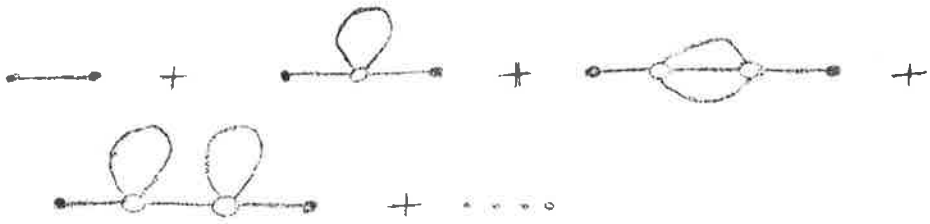
In general the perturbed Green's function cannot be evaluated exactly. Many of the approximation techniques used in many-body theory are based on approximations to the exact Green's function and this section is concerned with developing such a technique for lattice problems. At first sight, it might appear that a systematic approximation procedure for calculating G(j-k) would be to sum the contributions of all diagrams of the first few orders. It has been found in many

fields of physics, however, that the analytic properties (poles, branch points, asymptotic behaviour) are not significantly affected if we include only a finite number of diagrams. Hence, even in the first approximation, it is necessary to include an infinite number of diagrams. We shall consider an infinite partial summation which leads to Dyson's equation, and expresses the Green's function in terms of a proper-self-energy part $\Lambda(j-k)$. As $\Lambda(j-k)$ cannot be evaluated exactly, it is necessary to obtain an approximation for $\Lambda(j-k)$, using physical and mathematical arguments. A simple approximation for $\Lambda(j-k)$ is given in section 7.3 for the ferroelectric problem. However, as has been found in the many-fermion problems, when straightforward perturbation theory fails, the Green's function approach has often had to follow solutions obtained by experiment or other theoretical methods. Often in these problems, Green's function methods are not a reliable guide into unknown fields, but can be used to obtain correct answers to problems whose answers are already known. Consequently, the most appropriate approximation for $\Lambda(j-k)$ has not yet been obtained for lattice problems.

The perturbed Green's function has been defined as

$$G^{p,q}(l-k) = \langle o|T\ A^p(l)A^q(k)\ \exp\ (\sum_j H_o(j)+H_1(j)\ )|o\rangle\ Z^{-1}$$

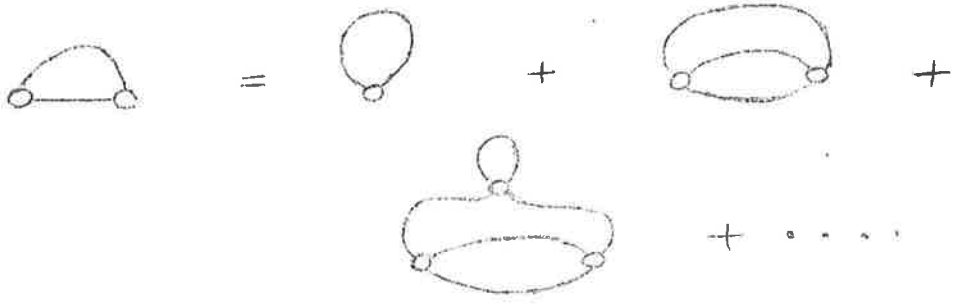
The Feynman graphs associated with the quantity are again line graphs starting and ending with $\Lambda^{p}(1)$ and $\Lambda^{q}(k)$. However, due to the quartic term the graphs are more complex. The lower orders of the graphs are



These are of such a complex nature that they cannot be summed exactly. However, we can still set up diagrammatically an integral equation for the Green's function, which is called Dyson's equation, as follows.

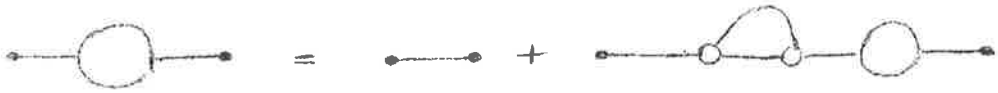
Let us define $\Lambda^{p,q}(j-k)$ as the sum of all diagrams which have the structure

where the semi-circle represents any sub-diagram that is connected to an incoming line in the p^{th} direction at point, j,and to an out-going line in the q^{th} direction at lattice point k, and which cannot be divided into two parts by breaking only one line. Contributions to $\Lambda^{p,q}(j-k)$ are



and such diagrams as

do not belong to the sub-class of diagrams $\Lambda(j-k)$, which is often called in perturbation theory, the proper-self-energy diagrams. The unfilled points in these diagrams represent a quartic term in the product, while the lines represent all contributions from the quadratic terms. Thus the lines in this case represent the free or unperturbed Green's functions. The diagrams which are summed to give $G^{p,q}(j-k)$ can be partially summed and written as



where  represents the exact Green's function and the free Green's function. Written algebraically, the above becomes

$$G^{p,q}(j-k) = G_0{}^{p,q}(j-k) + \sum_{l,m,s,t} G_0{}^{p,s}(j-l)\Lambda^{s,t}(l-m)G^{t,q}(m-k)$$

which can be written as the following matrix equation

$$G(j-k) = G_0(j-k) + \sum_{l,m} G_0(j-l)\ \Lambda\ (l-m)\ G\ (m-k)$$

Using a Fourier transformation to solve the above equation, we obtain

$$G(r) = G_0(r) + G_0(r)\ \Lambda(r)\ G(r)$$

Hence, $$G(r) = [1 - G_0(r)\,\Lambda(r)]^{-1}\, G_0(r)$$

$$= [G_0^{-1}(r) - \Lambda(r)]^{-1}$$

$$= [A^{-1}(r) - k - \Lambda(r)]^{-1} \qquad (3.16)$$

on using eq. (3.13).

When the arbitrary parameter , ϵ, is introduced in the definition of the Green's function, we obtain the result

$$G(r,\epsilon) = [A^{-1}(r) - \epsilon k - \Lambda(r,\epsilon)]^{-1} \qquad (3.17)$$

where $\Lambda(r,\epsilon)$ is also a function of ϵ.

The expressions given here are typical of those used in many-body theory[49], except that generally the Green's functions are not matrices but scalars. Likewise k, and $A^{-1}(r)$ would be scalars, where A(r) is often called the propogator, and k is the vertex part.

The results given in eqs. (3.13) and (3.17) will be used in the rest of this work to obtain the thermodynamic quantities of the models studied.

CHAPTER 4. SOLUTION OF SQUARE LATTICE ISING MODEL

4.1 Partition Function

In this chapter, the thermodynamic quantities of the square lattice Ising model will be evaluated with the use of the Green's functions. The results for the partition function and magnetization are the same a s those obtaincd by Onsager[2] and Yang[3], although the derivation is simpler. Much of this chapter has already been published by the author and Hurst[22].

The partition function is obtained from equations (3.7) and (3.14).

$$\text{Log } Z = \int_0^1 d\epsilon \; \Sigma_j \Sigma_{p,q} \; \tfrac{1}{2} \; k_{p,q} \; G_0{}^{p,q} \; (j-j,\epsilon)$$

$$= - \int_0^1 d\epsilon \; \Sigma_j \text{Trace} \; \tfrac{1}{2} \; k \; G_0 \; (j-j,\epsilon)$$

where the minus sign is because $k_{p,q} = -k_{q,p}$

$$G_0(j-k,\epsilon) = \frac{1}{N} \sum_{r=1}^{N} \omega^{r(j-k)} \; A(r) \; [1-\epsilon k \; A(r)]^{-1}$$

Combining these two results, we obtain

$$\text{Log } Z = -\int_0^1 d\epsilon \; \Sigma_j \; \frac{1}{N} \; \Sigma_{r=1}^{N} \; \text{Trace} \; \tfrac{1}{2} \; kA(r)[1-\epsilon k \; A(r)]^{-1}$$

$$= -\int_0^1 d\epsilon \; \Sigma_{r=1}^{N} \; \text{Trace} \; \tfrac{1}{2} \; kA(r)[1+\epsilon k \; A(r)+\epsilon^2 \; kA(r) \; kA(r) \; +\ldots]$$

The series is convergent for all temperatures and on performing the integration, we obtain

$$\begin{aligned} \text{Log } Z &= -\Sigma_r \text{ Trace } \tfrac{1}{2} [kA(r) + \tfrac{1}{2}(kA(r))^2 + \tfrac{1}{3}(kA(r))^3 + \ldots.] \\ &= \sum_{r=1}^{N} \tfrac{1}{2} \text{ Trace log } (1 - kA(r)) \\ &= \sum_{r=1}^{N} \tfrac{1}{2} \text{ log det. } (1 - kA(r)) \end{aligned} \qquad (4.1)$$

On substituting for k and A(r), (eqs. (3.1), (3,10)), the well-known result follows

$$Z^2 = \prod_{r=1}^{N} \left\{ (1+x^2)(1+y^2) - x(1-y^2)(\omega^r + \omega^{-r}) - y(1-x^2)(\omega^{mr} + \omega^{-mr}) \right\}$$

The critical temperature, mean energy and specific heat can be obtained from this expression. The details of these calculations will be given in the next chapter where an approximation to the next-nearest neighbour lattice will be made.

4.2 Magnetization

The evaluation of the spontaneous magnetization of the Ising model has always been a complicated problem. Onsager was the first to obtain the solution, but he only announced the comparatively simple result. Four years later Yang published the first solution. Since then, alternative derivations have been given by Montroll, Potts and Ward[15], using Toeplitz

determinants; Green[50] using integral equations and Kadanoff[8], who used Green's functions based on the algebraic formalism. In this section, yet another method is given which is based on the field theory approach which has been developed so far. It will be also shown that the methods mentioned above are simply related to each other.

In chapter 2 it was shown how the partition functions of the Ising lattices could be reduced to the vacuum expectation value of a time-ordered operator $\exp(\Sigma_j H(j))$, where $H(j)$ is a quadratic expression of fermion creation and annihilation operators. Here the method is generalized so as to express the correlation functions as the vacuum expectation value of $\exp(\Sigma_j H'(j))$ where $H'(j)$ can be regarded as a perturbed hamiltonian. This can be expanded as a series in analogy with Dyson's perturbation expansion in field theory. The series can be summed, using Green's functions, to give the exact result because $H'(j)$ is quadratic in the fermi-operators.

The correlation function $\langle s_1 s_{k+1} \rangle$ for a pair of spins located at the sites 1 and k+1 is defined as

$$\langle s_1 s_{k+1} \rangle = Z^{-1} (\cosh K_1 \cosh K_2)^N \sum_{\underline{s}=\pm 1} s_1 s_{k+1} \times \prod_{j=1}^{N} (1 + x\, s_j\, s_{j+1})\,(1 + y\, s_j\, s_{j+m}) \qquad (4.2)$$

where Z is the partition function, $s_j = \pm 1$ represents the state of the spins at the lattice site j, $\pm K_1 kT$ and $\pm K_2 kT$ are the interaction energies between horizontal and vertical pairs of spins respectively, and

$$x = \tanh K_1 \qquad y = \tanh K_2 .$$

We shall only consider correlations where the (k+1)-th spin is on the same horizontal row as the first spin. The generalization to other cases is straightforward. Using the identity

$$s_1 s_{k+1} = (s_1 s_2)(s_2 s_3) \cdots\cdots (s_k s_{k+1})$$

equation (4.2) can be written as

$$\langle s_1 s_{k+1} \rangle = Z_1^{-1} x^k \sum_{\underline{s}=\pm 1} \prod_{j=1}^{N} (1+x_j s_j s_{j+1})(1+y s_j s_{j+m}) \qquad (4.3)$$

where $x_j = x^{-1}$ if $j \leq k$

$= x$ if $j > k$

and $Z_1 = Z(\cosh K_1)^{-N} (\cosh K_2)^{-N}$.

Apart from the j dependence of x_j, equation (4.3) is identical with the expression for the partition function. Thus, using the same technique that was used in Chapter II to express the partition function in an S-matrix form, we can

obtain a similar expression for $\langle s, s_{k+1} \rangle$.

$$\langle s, s_{k+1} \rangle = Z_1^{-1} \; x^k \; \langle o | T \exp \left(\sum_{j=1}^{N} H_o(j) + \sum_{j=1}^{k} H'(j) \right) | o \rangle$$

where $H_o(j)$ is the same as for the square lattice partition funotion and is given by equation (3.1) and $H'(j)$ is the perturbation which takes care of the j dependence of x_j, and is given by

$$H'(j) = \sum_{p,q=1}^{4} \tfrac{1}{2} \, k'_{p,q} \; A^p(j) A^q(j) \left(\frac{1}{x^2} - 1 \right)$$

where

$$k' = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 1 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Defining

$$S(N) = \exp \left(\sum_{j=1}^{N} \sum_{p,q=1}^{4} \tfrac{1}{2} \, k_{pq} A^p(j) A^q(j) \right)$$

as the unperturbed S-matrix we have

$$\langle s_1 s_{k+1} \rangle = \langle o | T \exp \left(\sum_{j=1}^{k} \sum_{p,q=1}^{4} \tfrac{1}{2} \, k'_{pq} \; A^p(j) A^q(j) \left(\frac{1}{x^2} - 1 \right) \right) S(N) | o \rangle . Z_1^{-1} x^k$$

If we expand the exponential we obtain the series

$$\langle s_1 s_{k+1} \rangle = \langle o | T [1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(\sum_{j=1}^{k} \sum_{p,q=1}^{4} \tfrac{1}{2} \, k'_{pq} \; A^p(j) A^q(j) \right.$$

$$\left. \left(\frac{1}{x^2} - 1 \right) \right)^n] S(N) | o \rangle . Z_1^{-1} \; x^k \qquad (4.4)$$

To evaluate this we again use Wick's theorem, which means summing all diagrams in the above products. Now, if the factor S(N) were not present in equation (4.4) we would sum over all diagrams, whose contributions would be given by the time contractions $\Lambda^{pq}(j,k)$. These diagrams that arise from the series part of equation (4.4), and not from the factor S(N), we will call skeleton diagrams. It is clear that since the operators appear in pairs the skeleton diagrams are going to be closed loops. Now by a familiar technique used in field theory, when the contributions from S(N) are included, we sum all possible skeleton diagrams, but instead of using the propagator $\Lambda^{pq}(j,k)$ we must now use the Green's function $G^{pq}(j,k)$ to determine the contribution from a diagram. For as we have already seen the Green's function is a summation over all diagrams between two points and so the above technique is equivalent to summing over all skeleton diagrams where now each line in the skeleton diagram represents a partial summation over all possible diagrams between two points. The contribution from the sum over skeleton diagrams will have to be multipled by Z_1, which takes account of all the closed loops arising from the factor S(N).

To sum all the skeleton diagrams which arise from the term $[1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(\sum_{j=1}^{k} \frac{1}{2} k'_{pq} \Lambda^p(j)\Lambda^q(j) \left(\frac{1}{x^2} - 1\right)\right)^n]$ we first notice that the factor $1/2^n n!$ can be removed by summing only

topologically different diagrams. This means that the contribution of a disconnected graph is the product of its connected parts. This fact enables us to use the linked cluster expansion

sum over all diagrams = exp[sum over connected diagrams].

Thus we have to sum over topologically different connected loops. The contribution from a single n-point loop is

$$k'_{p_1 q_1} \cdots k'_{p_n q_n} G^{q_1 p_2}(j_1, j_2)\, G^{q_2 p_3}(j_2, j_3) \cdots G^{q_n p_1}(j_n, j_1) \left(\frac{1}{x^2} - 1\right)^n .$$

Let L_n be the contribution from the sum of topologically different loops with n vertices. Then

$$L_n = \sum_{j_i=1}^{k} \sum_{p_i, q_i=1}^{4} \frac{-1}{2n} k'_{p_1 q_1} \cdots k'_{p_n q_n} G^{q_1 p_2}(j_1, j_2) \cdots G^{q_n p_1}(j_n, j_1) \left(\frac{1}{x^2} - 1\right)^n .$$

where the factor $\frac{1}{2n}$ comes from the fact that in summing over $p_i q_i j_i$ each graph is repeated 2n times since it is a cyclic graph. The minus sign comes from the factor $(-1)^p$ which occurs in the definition of Wick's Theorem. Hence

$$L_n = \sum_{j_i=1}^{k} - \frac{1}{2n} \operatorname{Tr} \left(k' G(j_1, j_2) \cdots k' G(j_n, j_1)\right) \left(\frac{1}{x^2} - 1\right)^n$$

$$= \sum_{j_i=1}^{k} - \frac{1}{n} \sum_{r_i=1}^{N} N^{-n}\, \omega^{r_1(j_1-j_2)+\ldots r_n(j_n-j_1)} [c(r_1)c(r_2)\ldots c(r_n)]$$

$$(\frac{1}{x^2} - 1)^n \qquad (4.5)$$

where $c(r) = [-x^2 - x^2y^2 - x^2y(\omega^{mr}+\omega^{-mr}) + x\omega^{-r}(1-y^2)]/\Delta(r)$.
The last step in equation (4.5) is given in the appendix, at the end of this Chapter.

When the size of the lattice is very large, the summations in equation (4.5) can be converted to integrals. If we write

$$r = s + (t-1)m ,$$

and set

$$\phi = \frac{2\pi ms}{N} \; ; \; \theta = \frac{2\pi(t-1)}{m} + \frac{\phi}{m}$$

we obtain

$$\omega^r = \exp(i\theta); \quad \omega^{mr} = \exp(i\phi).$$

The summation $\sum_{r=1}^{N}$ is equivalent to $\sum_{s=1}^{n} \sum_{t=1}^{m}$, and in the limit of large n,m this can be written as

$$\frac{mn}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} d\theta \; d\phi.$$

Then equation (4.5) becomes

$$L_n = \sum_{j_i=1}^{k} - \frac{1}{n} \cdot \frac{1}{(2\pi)^{2n}} \int_0^{2\pi} d\theta_1 .. d\theta_n \; d\phi_1 ,,, d\phi_n$$

$$e^{i\theta_1(j_1-j_2)+\ldots+i\theta_n(j_n-j_1)}$$

$$\times [c(\theta_1,\phi_1)\ c(\theta_2,\phi_2)\ldots c(\theta_n,\phi_n)]\ (\tfrac{1}{x^2}\ -1)^n\ ,$$

where $c(\theta,\phi) = (-x^2-x^2y^2-2x^2y\cos\phi + xe^{-i\theta(1-y^2)})/\Delta(\theta,\phi)$

with $\Delta(\theta,\phi) = (1+x^2)\ (1+y^2) - 2x(1-y^2)\cos\theta - 2y(1-x^2)\cos\phi.$

The integrals over the ϕ_i can be evaluated immediately since the following relation holds[51]

$$\frac{1}{2\pi}\int_0^{2\pi} d\phi\ c(\theta,\phi)\ (\tfrac{1}{x^2}\ -1) = 1 - f(\theta)/x$$

where $$f(\theta) = u(e^{i\theta})/u(e^{-i\theta}),$$

$$u(e^{i\theta}) = (1-Be^{i\theta})^{\frac{1}{2}}\ (1-Ae^{i\theta})^{-\frac{1}{2}}\ ,$$

$$A = (1-y)/x(1+y),\ \text{and}\ B = x(1-y)/(1+y)\ .$$

Thus,

$$L_n = -\frac{1}{n}\sum_{j_i=1}^{k}\frac{1}{(2\pi)^n}\int_0^{2\pi} d\theta_1..d\theta_n\ e^{i\theta_1(j_1-j_2)+..+i\theta_n(j_n-j_1)}$$

$$\left[1-\frac{f(\theta_1)}{x}\right]\ldots\left[1-\frac{f(\theta_n)}{x}\right]. \qquad (4.6$$

We can simplify this multiple integral by defining the operator P_k by

$$P_k\ h(\phi) = \sum_{j=1}^{k}\frac{1}{2\pi}\int_0^{2\pi} d\theta\ e^{ij(\phi-\theta)}\ h(\theta)\ .$$

P_k is a projection operator which projects out the frequencies 1 to k of the fourier series of $h(\phi)$. We also define $P_k f$ as

an operator which acts on a function $h(\phi)$ as follows:

$$(P_k f)\, h(\phi) = \sum_{j=1}^{k} \frac{1}{2\pi} \int_0^{2\pi} d\theta\; e^{ij(\phi-\theta)} f(\theta)\; h(\theta).$$

If we now introduce an extra integral and delta function $\int_0^{2\pi} d\phi\; \delta(\phi-\theta_n) = \int_0^{2\pi} d\phi \sum_{l=-\infty}^{\infty} e^{il(\phi-\theta_n)}$ into the multiple integral expression in equation (4.6), we obtain

$$L_n = -\frac{1}{n} \sum_{l=-\infty}^{\infty} \sum_{j_i=1}^{k} \frac{1}{(2\pi)^{n+1}} \int_0^{2\pi} d\phi \int_0^{2\pi} d\theta_i e^{il(\phi-\theta_n)} e^{ij_1(\theta_1-\theta_n)} \ldots$$

$$e^{ij_n(\phi-\theta_{n-1})} \left[1 - \frac{f(\theta_1)}{x}\right] \ldots\ldots \left[1 - \frac{f(\theta_n)}{x}\right] .$$

We can then use the above definition of the operator $P_k f$ to write this as

$$L_n = -\frac{1}{n} \sum_{l=-\infty}^{\infty} \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{il\phi} P_k(1-f/x) P_k(1-f/x) \ldots\ldots$$

$$P_k(1-f/x) e^{-il\phi}$$

$$= -\frac{1}{n} \sum_{l=-\infty}^{\infty} \frac{1}{2\pi} \int_0^{2\pi} d\phi\; e^{il\phi} \left[P_k(1-f/x)\right]^n e^{-il\phi}$$

$$= -\frac{1}{n} \mathrm{Tr} \left[P_k\,(1-f/x)\right]^n . \qquad (4.7)$$

Thus we have the result that

$$\sum_{n=1}^{\infty} L_n = \mathrm{Tr} \log(1-P_k(1-f/x))$$

$$= \log\left(\langle s_1 s_{k+1}\rangle x^{-k}\right) \qquad (4.8)$$

This expression is similar to that obtained by Kadanoff[8],

although the derivations are seemingly unrelated. Also, this expression is simply related to the integral equations used by Green[50] and Hartwig[52], and the Toeplitz determinant of Montroll, Potts and Ward[15], to evaluate the correlation functions. The integral equations can be obtained from equation (4.8) by writing

$$\text{Tr log } (1-P_k(1-f(\theta)/x)) = \log \prod_{i=1}^{k} \lambda_i$$

where λ_i are the eigenvalues of the equation

$$(1 - P_k + P_k f(\theta)/x)u_i(\theta) = \lambda_i u_i(\theta) \qquad (4.9)$$

Multiplying by $(1-P_k)$ gives

$$(1-P_k)\, u_i(\theta) = (1-P_k)\, \lambda_i\, u_i(\theta)$$

and hence $u_i(\theta) = P_k u_i(\theta)$ for $\lambda_i \neq 1$.
Multiplying equation (4.9) by P_k, we get

$$P_k x^{-1} f(\theta)\, u_i(\theta) = \lambda_i\, P_k u_i(\theta) = \lambda_i\, u_i(\theta) \quad \lambda_i \neq 1.$$

This is the integral equation which was derived by different methods by Green and Hartwig.

The Toeplitz determinant of Montroll, Potts and Ward can also be written in the form of equation (4.8). We regard $f(e^{i\theta})$ as a Toeplitz matrix with elements f_{i-j} given by the $(i-j)^{th}$ Fourier coefficient of $f(e^{i\theta})$. The projection operators P_k when written in matrix notation have zero elements

everywhere except the diagonal elements (1,1) to (k,k) which are unity. Then equation (4.8) can be written $\log(\langle s_1 s_{k+1}\rangle x^{-k}) = \log \det. (1-P_k + P_k\, x^{-1}\, f)$, which gives the same result as Montroll, Potts and Ward.

The evaluation of equation (4.8) can be carried out in a variety of ways. The generalization of Szegos Theorem enables us to evaluate the Toeplitz Determinant form of equation (4.8). This is the method used by Montroll, Potts and Ward. Green was able to solve the integral equation form exactly because $f(e^{i\theta})$ can be factorized and then its inverse can be found. The method presented here was first given by Kadanoff[8]. It also relies on the fact that we can find the inverse of the operator $P_k\, f(\theta)$ as $k\to\infty$, and hence is related to Green's method. The technique when applied to the matrix representation of $P_k\, f(\theta)$ gives an alternative proof of Szegos Theorem. Thus it appears that all the approaches are closely connected.

To evaluate equation (4.8) we take the perfect differential of the equation with respect to the variables A and B.

$$d \log \langle s_1 s_{k+1}\rangle = \sum_{n=1}^{\infty} d\, L_n + k\, \frac{dx}{x} \qquad (4.10)$$

Using equation (4.7) we obtain

$$d\, L_n = + \mathrm{Tr}\, [P_k\, (1-x^{-1}\, f(\theta))P_k]^{n-1}\, P_k\, d\, (x^{-1} f(\theta)).$$

The extra operator P_k which is inserted simplifies the future work and makes no difference to the expression since $P_k^2 = P_k$.

$$\sum_{n=1}^{\infty} d L_n = Tr \frac{1}{1-P_k + P_k x^{-1} f(\theta) P_k} P_k d (x^{-1} f(\theta)). \quad (4.11)$$

To evaluate the inverse of $(1-P_k + P_k x^{-1} f(\theta) P_k)$ we use some properties of $u(e^{i\theta})$. Now $u(z) = (1-Bz)^{\frac{1}{2}} (1-Az)^{-\frac{1}{2}}$ has a single singularity at the point $z = A^{-1}$, and $u^{-1}(z)$ has a singularity at $z = B^{-1}$. If the low temperature case, $T<T_c$, is considered it can be shown[15] that $B<A<1$. Thus, the singularities of $u(z)$ and $u^{-1}(z)$ lie outside the unit circle. Hence $u^{\pm 1}(z)$ are analytic and can be expanded as a Taylor series inside the unit circle.

$$u(z) = \sum_{n=o}^{\infty} u_n z^n \qquad u^{-1}(z) = \sum_{n=o}^{\infty} u'_n z^n .$$

If we define $P = \lim_{k\to\infty} P_k$ we see that P projects out all positive frequencies of the Fourier Series, and (1-P) the negative frequencies. Since $u^{\pm 1}(e^{i\theta})P$ consists of only positive frequencies the following equations are true.

$$(1-P)u^{\pm 1} (e^{i\theta}) P = 0.$$

$$u^{\pm 1}(e^{i\theta}) P = P u^{\pm 1} (e^{i\theta})P.$$

$$P u^{\pm 1}(e^{-i\theta}) (1-P) = 0.$$

$$P u^{\pm 1} (e^{i\theta}) - u^{\pm 1}(e^{i\theta}) P = P u^{\pm 1} (e^{i\theta}) (1-P) \quad (4.12)$$

Using these equations we can see by multiplication that $(1-P + u^{-1}(e^{i\theta}) P x u(e^{-i\theta}))$ is the right and left inverse of $(1-P + P f(\theta) x^{-1} P)$. Substituting this into equations (4.10), (4.11) we get

$$d \log M = Tr\,(u^{-1}(e^{i\theta}) P x u(e^{-i\theta}) d[f(e^{i\theta})x^{-1}]) + \lim_{k\to\infty} kx^{-1}dx \qquad (4.13)$$

where $M^2 = \lim_{k\to\infty} \langle s_1 s_{k+1}\rangle$ is the magnetization.

$$d[f(e^{i\theta}) x^{-1}] = f(e^{i\theta})\, d(x^{-1}) + u^{-1}(e^{-i\theta})\, x^{-1}\, d\, u(e^{i\theta}) + u(e^{i\theta})\, x^{-1}\, d(u^{-1}(e^{-i\theta})). \qquad (4.14)$$

Substituting equation (4.14) in equation (4.13) means we have to evaluate the trace of three expressions. The first one can be evaluated to give $-\lim_{k\to\infty} k\, x^{-1}\, dx$, which will cancel the last term in equation (4.13). The trace involving the third term in equation (4.14) gives the interesting contribution and shall be evaluated explicitly. Using the last equation in (4.12) we have to evaluate

$$Tr\,(P\, u(e^{-i\theta})\, d(u^{-1}(e^{-i\theta}))$$

$$- Tr(P\, u^{-1}(e^{i\theta})\, (1-P)\, u(e^{i\theta})\, d \log u(e^{-i\theta})) \qquad (4.15)$$

The first term here is similar to the trace obtained from the second term in equation (4.14) and when written out in full is

$$\int_0^{2\pi} \frac{d\phi}{2\pi} \sum_{l=-\infty}^{\infty} e^{il\phi} \int_0^{2\pi} \frac{d\theta}{2\pi} \sum_{j=1}^{\infty} e^{ij(\phi-\theta)} d \log u(e^{-i\theta}) e^{-il\theta}$$

$$= \sum_{j=1}^{\infty} \int \frac{d\theta}{2\pi} \; d \log u(e^{i\theta}) = 0 \text{ since the integral is zero.}$$

The second term of equation (4.15) is

$$- \int_0^{2\pi} \frac{d\phi}{2\pi} \sum_{l=-\infty}^{\infty} e^{il\phi} \int_0^{2\pi} \frac{d\theta_1}{2\pi} \sum_{j_1=1}^{\infty} e^{ij_1(\phi-\theta_1)} \; u^{-1}(e^{i\theta_1})$$

$$\int_0^{2\pi} \frac{d\theta_2}{2\pi} \sum_{j_2=0}^{\infty} e^{-ij_2(\theta_1-\theta_2)} \; u(e^{i\theta_2}) \; d \log u(e^{-i\theta_2}) \; e^{-il\theta_2}$$

$$= - \int_0^{2\pi} \frac{d\theta_1}{2\pi} \sum_{j_1=1}^{\infty} e^{ij_1(\theta_2-\theta_1)} \; u^{-1}(e^{i\theta_1}) \int_0^{2\pi} \frac{d\theta_2}{2\pi} \sum_{j_2=0}^{\infty}$$

$$e^{-ij_2(\theta_1-\theta_2)} u(e^{i\theta_2}) \; d \log u(e^{-i\theta_2})$$

$$= - \sum_{j_1=1}^{\infty} \sum_{j_2=0}^{\infty} \int_0^{2\pi} \frac{d\theta_2}{2\pi} \; e^{i\theta_2(j_1+j_2)} \; u'_{j_1+j_2} \; u(e^{i\theta_2}) \, d\log u(e^{-i\theta_2}).$$

Now the summation over j_1 and j_2 is such that $j_1+j_2 = i$ occurs i times. Hence the above can be written as

$$- \sum_{j=1}^{\infty} \int_0^{2\pi} \frac{d\theta}{2\pi} \; j \; e^{ij\theta} \; u'_j \; u(e^{i\theta}) \; d \log u(e^{-i\theta})$$

$$= i \int \frac{d\theta}{2\pi} \frac{d}{d\theta} \; (u^{-1}(e^{i\theta})) \; u(e^{i\theta}) \; d \log u(e^{-i\theta})$$

$$= i \int \frac{d\theta}{2\pi} \frac{d}{d\theta} \log u(e^{i\theta}) \; d \log u(e^{-i\theta}).$$

Substituting the explicit expressions for $u(e^{i\theta})$ we obtain

$$d \log M = i \int_0^{2\pi} \frac{d\theta}{2\pi} \frac{1}{4} \left[\frac{-iBe^{i\theta}}{1-Be^{i\theta}} + \frac{iAe^{i\theta}}{1-Ae^{i\theta}} \right] \left[\frac{-dBe^{-i\theta}}{1-Be^{-i\theta}} + \frac{d\Lambda e^{-i\theta}}{1-\Lambda e^{-i\theta}} \right]$$

$$= - \oint \frac{dz}{2\pi i z} \cdot \frac{1}{4} \left[\frac{-Bz}{1-Bz} + \frac{\Lambda z}{1-\Lambda z} \right] \left[\frac{-dBz^{-1}}{1-Bz^{-1}} + \frac{d\Lambda z^{-1}}{1-\Lambda z^{-1}} \right]$$

$$= - \frac{1}{4} \left[\frac{dB \cdot B}{1-B^2} - \frac{\Lambda \, dB}{1-\Lambda B} - \frac{d\Lambda \, B}{1-B\Lambda} + \frac{\Lambda \, d\Lambda}{1-\Lambda^2} \right]$$

$$= \frac{1}{8} d \log[(1-B^2)(1-\Lambda^2)/(1-\Lambda B)^2] \cdot$$

Integrating we obtain

$$M^8 = (1-B^2)(1-\Lambda^2)/(1-\Lambda B)^2 \cdot$$

The constant of integration is zero, since M=1 at zero temperature.

This is the exact result for the magnetization of a square lattice for temperatures below the critical temperature. For temperatures above the critical temperature we can show that B<1 but $\Lambda>1$. Hence our expansions for $u^{\pm 1}(z)$ do not hold for the high temperature case. However, we can obtain some similarity between the high and low temperature cases if we consider f(z) as given by

$$f(z) = v(z) \, (z \, v(z^{-1}))^{-1}$$

where $$v(z) = (1-Bz)^{\frac{1}{2}} (1-\Lambda^{-1}z)^{\frac{1}{2}} \cdot$$

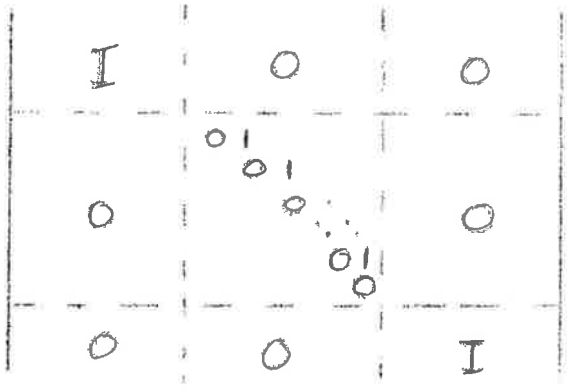
Now $v(z)^{\pm 1}$ are analytic inside the unit circle and hence have expansions which only have positive powers of z.

However, the extra factor z in the definition of f(z) now prevents us from finding an inverse to the operator $(1-P + Pf(e^{i\theta})P)$. In fact the presence of this extra factor z means that this operator has a zero eigenvalue with an eigenfunction $e^{i\theta}v^{-1}(e^{i\theta})$. We have already shown that $M = \prod_{i=1}^{\infty} \lambda_i$ and hence $M = 0$ provided the product of the remaining eigenvalues is finite.

Some justification of the last statement can be provided in the following way. We notice that the operator can be factorized into $(1-P + P\, e^{-i\theta}P) \times (1-P + P\, v(e^{i\theta})\, v^{-1}(e^{-i\theta})P)$. Using the relation Tr ln (AB) = Tr ln A + Tr ln B we get

$$\ln M = \mathrm{Tr}\ \ln(1-P + P\, v\,(e^{i\theta})\, v^{-1}(e^{-i\theta})P) + \mathrm{Tr}\ \ln(1-P + P\, e^{-i\theta}P) \qquad (4.16)$$

If the first term on the right hand side of equation (4.16) is evaluated by the same method as was used in the low temperature case we obtain $\ln\,(1-A^{-2})(1-B^{2})\,(1-A^{-1}B)^{2}$. The second term in equation (4.16) can be evaluated by writing $\mathrm{Tr}\ \ln\,(1-P+P\, e^{-i\theta}P) = \lim_{k\to\infty} \mathrm{Tr}\ \ln\,(1-P_k + P_k\, e^{-i\theta}\, P_k) = \lim_{k\to\infty}$ ln det. $(1-P_k + P_k\, e^{-i\theta}P_k)$. This determinant has ones on the diagonal elements except for the elements (1,1) to (k,k) where there are ones on an off-diagonal. It has the form



This determinant is obviously zero. In the limit as $k \to \infty$ the determinant remains zero. This definition of the value of the infinite determinant is in accordance with the physical representation of an infinite lattice as a limitingcase of a sequence of finite lattices, and so is the most natural one to choose. If instead the infinite determinant were evaluated by just calculating its eigenvalues an ambiguity would arise because the operator $P\, e^{-i\theta} P$ is non-Hermitian and possesses a continuous infinity of eigenvalues in the region of the complex plane $|\lambda|<1$. In a certain sense this approach still leads to the conclusion $M=0$ but it is more difficult to justify. Substituting these results into equation (4.16) we see that the magnetization is zero for all temperatures above the critical point.

Thus, the standard results for the partition function and magnetization have been obtained using Green's functions. Both these methods would be suitable for all Ising models, but as pointed out in Chapter III, the Green's functions for the unsolved models are not known exactly.

4.3 Appendix

We give here an outline of the proof of equation (4. 5). Using equation (3.13) we see that $k'G$ has the structure

$$\begin{pmatrix} a_1 & a_2 & 0 & a_4 \\ a_1 & a_2 & 0 & a_4 \\ 0 & b_2 & b_3 & b_4 \\ -a_1 & -a_2 & 0 & -a_4 \end{pmatrix}$$

where $a_1 = -G^{31}$, $a_2 = -G^{32}$, $a_4 = -G^{34}$ and $b_3 = G^{13} + G^{23} - G^{43}$. The zero entries arise since $\sum_{r=1}^{N} (\omega^r - \omega^{-r}) = 0$. Thus the trace of $k'G$ is $(a_1+a_2-a_4) + b_3$ which on substitution of the values from equation (3.15) gives

$$\mathrm{Tr}\ (k'G) = b_3 + b_3^*$$

where $b_3(j_1, j_2) = \sum_{r=1}^{N} \omega^{(j_1-j_2)r}(-x^2y^2 - x^2 - x^2y(\omega^{nr} + \omega^{-nr}) + x\omega^{-r}(1-y^2))\ \Delta(r)^{-1}$.

Similarly $k'G_1\ k'G_2$ can be written

$$\begin{pmatrix} a_1 & a_2 & 0 & a_4 \\ a_1 & a_2 & 0 & a_4 \\ 0 & b_2 & b_3 & b_4 \\ -a_1 & -a_2 & 0 & -a_4 \end{pmatrix} \qquad \begin{pmatrix} A_1 & A_2 & 0 & A_4 \\ A_1 & A_2 & 0 & A_4 \\ 0 & B_2 & B_3 & B_4 \\ -A_1 & -A_2 & 0 & -A_4 \end{pmatrix}$$

from which we obtain

$$\mathrm{Tr}\ (k'G_1\ k'\ G_2) = b_3^*\ B_3^* + b_3\ B_3.$$

We can repeat this procedure obtaining

$$\mathrm{Tr}\,(k' G_1\, k' G_2 \ldots k' G_n) = b_3(1)\, b_3(2) \ldots b_3(n) + b_3^*(1) b_3^*(1) \ldots b_3^*(n)$$

The summation over r_i means that the contribution from the complex conjugate b^* is the same as that from b. Hence we obtain equation (4.5).

CHAPTER 5. NEXT-NEAREST NEIGHBOUR ISING MODEL

5.1 First Order Approxination to the Critical Temperature

This chapter is concerned with the evaluation of the thermodynamic quantities of the next-nearest neighbour Ising lattice. Although this problem is not solved here, this work derives results for the critical temperature, Tc, and the critical indices α, α', β which are a reasonable first approximation.

The suggested values for the critical temperatures are obtained by examining the singularity of the free or unperturbed Green's function. Although there is no rigorous proof that the singularity of the free Green's function will be the same as that for the perturbed Green's function, evidence in some other areas of physics has shown that this assumption can yield valid answers. For example, in the field of strongly interacting particles, the perturbation method is inapplicable because the coupling constant is very large. Thus the perturbation series cannot necessarily be expected to converge, and no significance is attached to the numerical values of the individual terms. However, Eden, Landshoff, Olive and Polkinghorne[53], Hwa and Teplitz[54] consider that, although the perturbation method may be meaningless outside quantum electrodynamics, the singularity structure of some of the perturbation terms may contain useful

information about the analytical properties of the complete S-matrix. In the case of strong-interaction physics a knowledge of the singularity structure of the first few terms has helped as a useful diagnostic. In many-body problems, Thouless[37] has shown that the transition temperature of a superconducting system can be obtained from the requirement that the "ladder diagrams" of the usual graph theory lead to a divergent sum. Other examples, which have more relevance to the present Ising model approach are the ferro-electric and anti-ferro-electric problems. It has been shown in Chapter 7 that the exact critical temperatures are predicted by the singularities of the free-Green's functions for both these models. In this section, the singularity of the first-order term is suggested as the value of the critical temperature for the next-nearest neighbour lattice.

The critical point, Tc, is determined by the temperature at which the partition function has a singularity, whereas the critical indices α, α', β are determined by the nature of the singularity. Again we assume that the nature of the singularity is the same as the singularity of the first-order approximation. The values we obtain for the critical indices using this assumption are

$$\alpha = \alpha' = 0 \qquad \beta = \tfrac{1}{8}$$

These results are the same as the results for the soluble square lattice model. The idea that the inclusion of the next-nearest neighbour interactions would make no difference to the values of the critical indices has already arisen from the "scaling law" theory of Kadanoff's[55]. One of the consequences of this approach is that the critical indices should not be affected by the details of the interaction, just as the long-range correlations should be insensitive to these details. If a correlation extends over a large number of lattice sites, the correlation should be sensitive only to the grossest features of the interaction and should not be affected by the introduction of some next-nearest neighbour interaction. Our Ising model calculation does in fact help to confirm this hypothesis.

If we use the expression for the perturbed Green's function given by eq. (3.16), the thermodynamic quantities can be given exactly in terms of the unknown quantity, the proper self-energy part, $\Lambda(j-k)$. To obtain the above mentioned results, the approximation, $\Lambda(j-k) = 0$, has been made, which does not appear to be very drastic when discussing the critical phenomena, but is not a good approximation when discussing the absolute values of the thermodynamic quantities. For example, the first order approximation for the partition function agrees with the series expansion only up to terms of order xyuv. The standard perturbation theory

converges for this model since the effective coupling constant is less than one, and by including the second-order terms the partition function will agree with the series expansion up to terms of the order $x^2 y^2 u^2 v^2$. However, there is considerable labour involved in calculating this, and so the next-order calculations have been performed only on the ferro-electric problem where the method is the same, but less tedious. We feel that the next-order term will not change the critical indices, and as these are the most important quantities, there is no immediate necessity to evaluate it.

The partition function can be written as

$$\text{Log } Z = \int_0^1 d\epsilon \sum_{r=1}^{N} \text{Trace } \tfrac{1}{2} k[A^{-1}(r) - \epsilon\, k - \Lambda(r,\epsilon)]^{-1}$$

where we have used equations (3.17) and (3.7).

The term $\Lambda(r,\epsilon)$ prevents the integration over ϵ from being carried out, but if we make the approximation $\Lambda(r,\epsilon)=0$, we obtain in a similar manner to eq. (4.1)

$$\log Z^2 = \sum_{r=1}^{N} \log \det (1-kA(r)) \qquad (5.1)$$

In order to simplify the model, put $x = y$ and $u = v$, and then using equations (3.2) and (3.11), we obtain

$$\det(1-kA(r)) = (1+x^2)^2\,(1+u^2)^2 + 16x^2u(1-u^2)$$
$$+ x(1-x^2)(4u^2 - (1-u^2)^2)(\omega^r + \omega^{-r} + \omega^{mr} + \omega^{-mr})$$

$$- u(1-x^2)(1-u^2)(\omega^{(m+1)r} + \omega^{-(m+1)r} + \omega^{(1-m)r} + \omega^{-(1-m)r})$$

If we let the size of the lattice tend to infinity, we obtain for eq. (5.1)

$$\frac{1}{N} \log Z^2 = \frac{1}{(2\pi)^2} \iint_0^{2\pi} d\theta d\phi \log D(\theta,\phi) \qquad (5.2)$$

where $D(\theta,\phi) = (1+x^2)^2 (1+u^2)^2 + 16x^2 u (1-u^2)$

$$+ 2x(1-x^2) (4u^2 - (1-u^2)^2) (\cos\theta + \cos\phi)$$

$$- 2u(1-x^2) (1-u^2) (\cos(\theta+\phi) + \cos(\theta-\phi))$$

The integral in eq. (5.2) is not necessarily analytic since the integrand is singular in the range of integration. The determination of the singularity of such integrals has been discussed by Hurst[17], who shows that the following equations will determine the position of the singularity.

$$D(\theta,\phi) = 0 \qquad (5.3)$$

$$\frac{\partial D(\theta,\phi)}{\partial\theta} = \frac{\partial D(\theta,\phi)}{\partial\phi} = 0 \qquad (5.4)$$

The solutions of eq. (5.4) are θ and ϕ equal to either 0 or 2π. Hence eq. (5.3) becomes

$$1 - 2x - 2u - x^2 - u^2 - 4xu + 2xu^2 + 2x^2 u + x^2 u^2 = 0$$

or

$$1 + 2x - 2u - x^2 - u^2 + 4xu - 2xu^2 + 2x^2 u + x^2 u^2 = 0$$

These two equations were solved numerically and the results are plotted in Figures 13 and 14. The ratio of the diagonal to the horizontal interaction strength (K_3/K_1), is plotted against the transition temperature divided by the transition temperature of the square lattice $(Tc/Tc,s)$. The results are compared to those obtained by Domb and Potts[56], who used high and low temperature extrapolation techniques. The results show the same trend in the case of the ferro-magnetic model, but disagree for the antiferro-magnetic model, where the present calculations indicate a double and triple phase transition. The correct behaviour is not known at this stage, but we should indicate that double phase transitions are not uncommon in antiferro-magnetic systems. Lee and Yang[57] have given a thermodynamic proof that ferro-magnetic systems can only have one possible phase transition point, but this proof does not hold for antiferro-magnetic systems. That it is possible for antiferro-magnetic systems to have multiple phase transitions has been shown firstly by Vaks and Larkin[58], who have solved exactly a two dimensional Ising model which exhibits similar multiple transition points for antiferro-magnetic interactions. Secondly, Bienstock[59] has shown that the antiferro-magnetic three-dimensional Ising model can have a double transition point in a magnetic field.

FERROMAGNETIC CASE

Domb and Potts (- - -)

First Order Approximation (——)

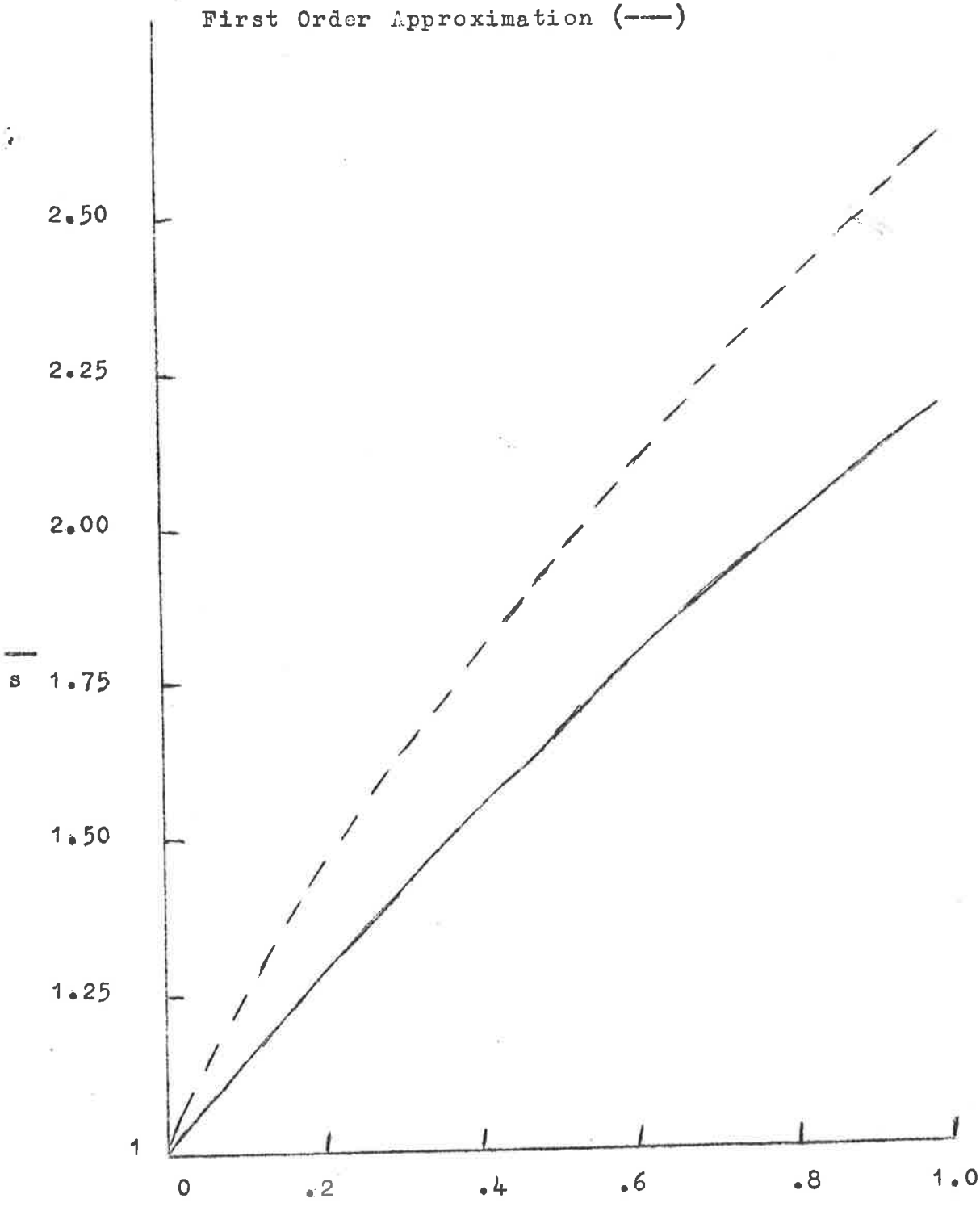


Fig. 13

ANTI-FERROMAGNETIC CASE

Domb and Potts (- - -)

First Order Approximation (——)

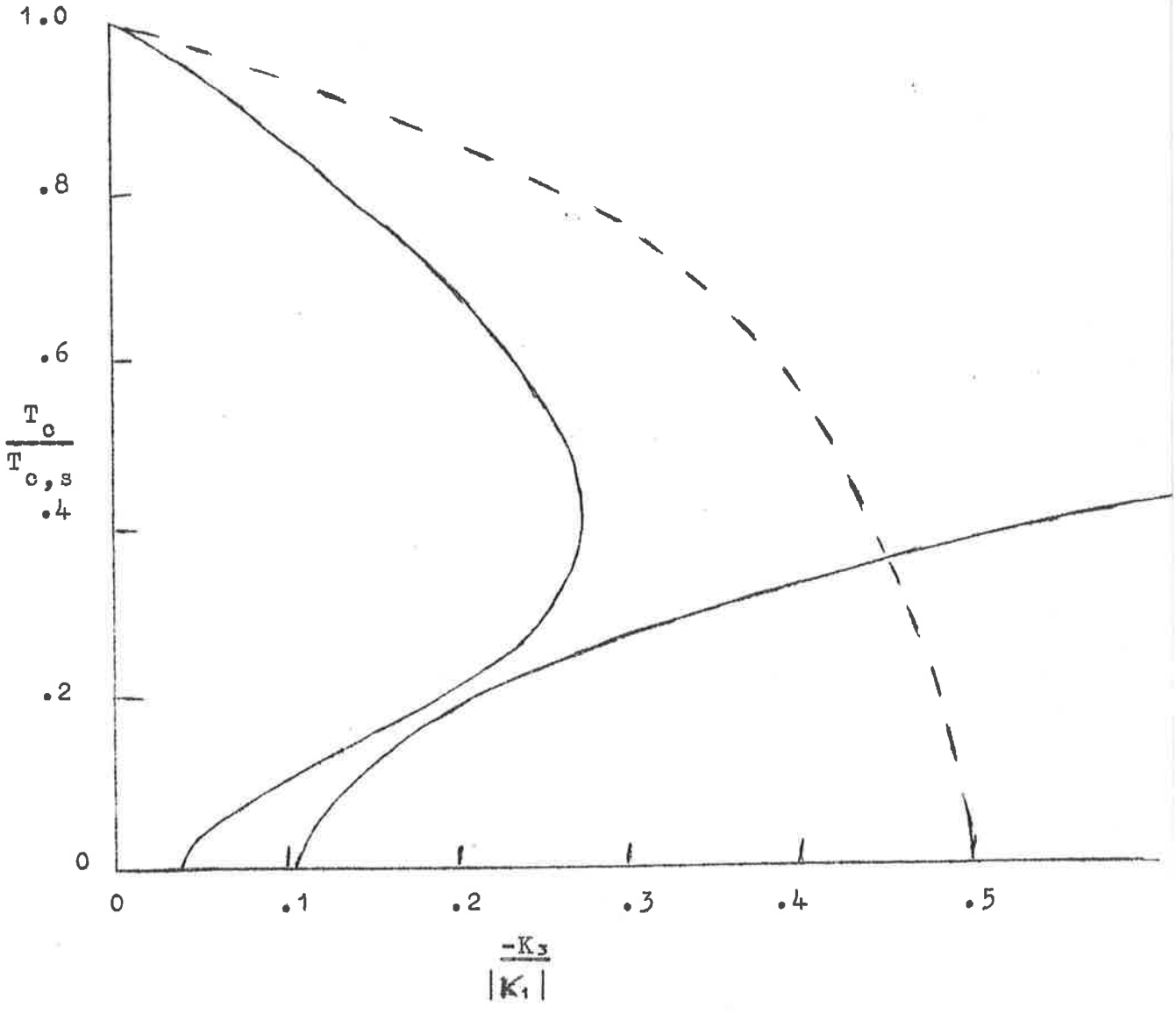


Fig. 14

Finally, double phase transitions occur experimentally, as, for example, in the ferro-electric crystal Rochelle Salt. However, to determine whether a multiple phase transition does occur in the next-nearest neighbour Ising model, one would have to do more extensive study into the high and low temperature expansions, and also look at the singularities of the higher order terms of our perturbation expansion.

5.2 The Critical Indices α, α' .

The critical indices α, α' are determined by the asymptotic behaviour of the specific heat, C, near the critical point temperature, Tc, and are defined by

$$C \sim a\,\epsilon^{-\alpha} + b \qquad T < Tc$$

$$\sim a'\,|\epsilon|^{-\alpha'} + b' \qquad T > Tc$$

where $\epsilon = (T - Tc)/Tc$

From the equation

$$\bar{E} = -\frac{1}{N}\,\frac{\partial}{\partial\beta}\,\log Z$$

we obtain

$$\bar{E} = -\frac{\partial I}{\partial\alpha}\cdot\frac{\partial\alpha}{\partial\beta} - \frac{\partial I}{\partial\gamma}\cdot\frac{\partial\gamma}{\partial\beta} - \frac{\partial I}{\partial\delta}\cdot\frac{\partial\delta}{\partial\beta}$$

where, using the first approximation for the partition function, eq. (5.2) can be written as

$$\frac{\text{Log } Z}{N} = I = \tfrac{1}{2} \cdot \frac{1}{(2\pi)^2} \iint d\theta d\phi \log \left[\alpha + 2\gamma(\cos\theta + \cos\phi) + 2\delta\cos\theta \cos\phi\right]$$

The derivatives of the general expression I, have been evaluated by Green and Hurst[60] in terms of the complete elliptic integrals of the first and third kinds. Using these results, the average energy, $\bar{E}$, can be written as

$$\bar{E}(T) = \bar{E}(Tc) + A(T-Tc) \log |T-Tc| + \ldots$$

for T close to Tc, where the $\log|T-Tc|$ arises from the elliptic integral K(k). Thus the average energy per spin is continuous at the critical point, and the specific heat has a logarithmic singularity at T = Tc. This determines α and α', since, by convention, a logarithmic singularity is denoted by $\alpha = o$; $\alpha' = o$.

5.3 Critical Index β.

A formal expression can be written for the correlation functions of the next-nearest neighbour Ising model, which is analogous to the expression derived in section 4.2 for the square lattice model. We obtain

$$\langle s_1 s_{k+1} \rangle = \langle o | T \exp \left(\sum_{j=1}^{k} H'(j) + \sum_{j=1}^{N} H_o(j) + H_1(j) \right) | o \rangle . Z^{-1}. \quad (5.5)$$

where $H_o(j)$ and $H_1(j)$ are given by eqs. (3.2) and (2.11) and $H'(j)$, for the correlation functions in the x direction, is

defined by

$$H'(j) = \sum_{p,q=1}^{12} \tfrac{1}{2} k'_{p,q} \Lambda^p(j) \Lambda^q(j) \left(\frac{1}{x^2} - 1 \right)$$

where k' is the 12 x 12 matrix

$$k' = \begin{pmatrix} k_1 & 0 \\ 0 & 0 \end{pmatrix}$$

and $k_1 =$

$$\begin{pmatrix} 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

A perturbation expansion can be obtained for eq. (5.5) in the usual way, the first term of which will be

$$\langle s_1 s_{k+1} \rangle = \langle o | T \exp\left(\sum_{j=1}^{k} H'(j) + \sum_{j=1}^{N} H_o(j) \right) | o \rangle \, Z_o^{-1} \qquad (5.6)$$

where Z_o^{-1} is the expression for the partition function, obtained by neglecting the quartic term $H_1(j)$. The expression in eq. (5.6) can be evaluated exactly, using the same technique that was developed in section 4.2 A similar result is obtained, which for the magnetization becomes

$$M^2 = \text{Trace } \log(1-P + Pf(e^{i\theta})) \qquad (5.7)$$

where, using a notation originally used by Green[50]

$$f(z) = (1-\Lambda z)^{\frac{1}{2}} (1-Bz^{-1})^{\frac{1}{2}} (1-Bz)^{\frac{-1}{2}} (1-\Lambda z^{-1})^{-\frac{1}{2}}$$

$$A = \frac{S_1 C_1 C_2^2 + 2 S_1 C_1 S_2 - G}{C_1 - 1 - S_2^2 (C_1 + 1)}$$

$$B = \frac{S_1 C_1 C_2^2 + 2 S_1 C_1 S_2 - G}{C_1 + 1 - S_2^2 (C_1 - 1)}$$

$$G^2 = [C_1^2 C_2^2 + 2 S_1^2 S_2]^2 - (1+2 S_1^2) (1-S_2^2)^2$$

$$C_1 = \frac{1+x^2}{1-x^2} \qquad S_1 = \frac{2x}{1-x^2}$$

$$C_2 = \frac{1+u^2}{1-u^2} \qquad S_2 = \frac{2u}{1-u^2}$$

Equation (5.7) is similar to eq. (4.8) and can be evaluated in an identical way to give

$$M^8 = \frac{(1-A^2)(1-B^2)}{(1-\Lambda B)^2} \qquad T < T_c$$

Like the square lattice case, $\Lambda = 1$ when $T = Tc$.

The critical index β is defined by

$$M \approx a(Tc - T)^{\beta} \qquad T < Tc.$$

and hence

$$\beta = \lim_{T \to Tc} \frac{\log M}{\log(Tc-T)}$$

Substituting the results for M given above, we get

$$\beta = \lim_{T \to Tc} \frac{1}{8} \frac{\log(1-\Lambda)}{\log(Tc-T)}$$

since the other terms are zero in the limit T→Tc. A Taylor's series expansion of Λ about T = Tc gives

$$1 - \Lambda(T) = 1 - \Lambda(Tc) + (T-Tc)\,\Lambda'(Tc) + \ldots.$$

$$= 0 + (T-Tc)\,\Lambda'(Tc) + \ldots.$$

One can verify that $\Lambda'(Tc)$ is non-zero and hence $\beta = \frac{1}{8}$.

The above results for the critical indices α, α', β have been obtained from the first-order expression for the partition function, namely

$$Z = \langle o | T \exp\left(\sum_j H_o(j)\right) | o \rangle$$

which is equivalent to the general Ising problem discussed by Green[50]. This first-order expression was discussed in section 2.2, where it was shown that it counts all the Ising model graphs, but those with an odd number of crossed bonds have a negative weight associated with them. To obtain the correct partition function the quartic term must be introduced. However, it appears from the results obtained above that the analytical behaviour of the partition function is not affected by the incorrect counting of some of these graphs. As mentioned earlier in this chapter, there are, in other fields of physics, precedents for assuming that

the partial summations of the graphs will contain the correct analytical behaviour. However, one would like to have more rigorous criteria for defining when the neglected terms do not contribute. An investigation into this point would involve the calculation of the higher-order terms. For this model the calculation is very tedious, although straightforward; the Green's function requires the inversion of the 12 x 12 matrix $(A^{-1}(r) - k)$ and the subsequent terms are long and involved. Because of this, the calculations for the higher-order terms will be performed on a simpler model, the ferro-electric model, where we will also be able to make a comparison with an exact solution recently found by Lieb.

The setting up of a perturbation series for the three dimensional Ising model has proved unsuccessful, which is no doubt due to that fact that the perturbing hamiltonian, $\mathfrak{H}_1(j)$, contains correction terms of the order of N^2, whereas the 2 dimensional models contain only N correction terms. (See section 2.3). Hence, one would not necessarily expect the first order approximation to count a significant number of graphs correctly. This indeed appears to be the case, for the calculation of the specific heat using the first-order approximation does not contain a singularity at all. An alternative form of partial summation of diagrams must therefore be found before the three-dimensional Ising model can be treated successfully.

CHAPTER 6. DIAGONALIZATION OF THE HAMILTONIAN

In the quantum field theory approach to many-fermion problems, a great many techniques rely on transformations of the fermi-operators. One of the most common transformations is the Fourier transformation to momentum space (or spin waves for magnetism), whereby the summing of the Feynman diagrams is greatly simplified. Other transformations, such as the Bogoluibov canonical transformation are particularly useful in diagonalizing a quadratic expression. Such transformations often result in the useful concept of quasi-particles.

In this chapter, the possibility of applying a transformation to the many-fermion expression for the Ising model is investigated. With an expression such as $\sum_{j=1}^{N} k_{p,q} \Lambda^p(j)\Lambda^q(j)$, the obvious suggestion is to make a Fourier transformation such as

$$a_j^{1*} = \frac{1}{\sqrt{N}} \sum_{k=1}^{N} \exp(2\pi i \; j \; k/_N) \; b_k^{1*}$$

However, if such a transformation is inserted into

$$\langle o| \; T \exp(\Sigma_j \; H_o(j) \;) \; |o\rangle$$

the creation and annihilation operators loose their j dependence, and the operator T becomes meaningless. Thus, in general this transformation cannot be applied directly to the above expression. However, for the particular examples that

arise in the lattice problems, there is an extra property which enables us to overcome this difficulty. Looking at all the possible time-ordered products of operators arising from the pairs of operators in $H_0(j)$, we notice that for every pair of creation and annihilation operators, the creation operator, a_j^{p*}, stands to the right of its corresponding annihilation operator a_j^p. Since we are taking the vacuum to vacuum expectation value, only the products in which all the operators appear in pairs will have non-zero contributions, and hence when the time-ordering is carried out, all the creation operators will appear to the right of their annihilation operator. This was the original reason for needing the time-ordering operator, T, as pointed out in Chapter 2. As an example, consider the operators arising from the square graph shown in Fig. 15, which are

$$T(\Lambda^4(j)\Lambda^3(j)\Lambda^3(j+m)\Lambda^2(j+m)\Lambda^4(j+1)\Lambda^1(j+1)\Lambda^2(j+m+1)\Lambda^1(j+m+1))$$

$$= \Lambda^2(j+m+1)\Lambda^1(j+m+1)\Lambda^3(j+m)\Lambda^2(j+m)\Lambda^4(j+1)\Lambda^1(j+1)\Lambda^4(j)\Lambda^3(j)$$

$$= a^2_{j+1}\ a^1_{j+m}\ a^{1*}_{j+m}\ a^2_j\ a^{2*}_{j+1}\ a^1_j\ a^{2*}_j\ a^{1*}_j\ x^2y^2$$

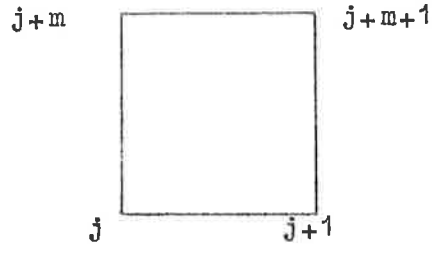


Fig. 15

In field theory the normal order of a product of operators is defined as the creation operators appearing to the left of the annihilation operators. Hence, defining the anti-normal order as the reverse to normal order, it can be seen that the operation of time-ordering on our products of operators puts the operators in an almost anti-normal order.

Define an anti-normal ordering operator $\bar{N}$ such that

$$\bar{N}\ (a_j\ a_k^*\ a_l\ a_m^*\ \cdots\ ) = (-1)^p\ (a_j\ a_l\ \cdots\ a_k^*\ a_m^*)$$

where p is the number of permutations required to rearrange the operators. Then from the previous discussion it follows that T(product of pairs of operators) and $\bar{N}$ (product of pairs of operators) are expressions which can be proved to be equivalent, by rearranging the order of the operators and using the anticommutation relations (2.4). Thus, we can verify for the lattice problems that

$$T\ (\text{product of } a_j) = \bar{N}\ (\text{product of } a_j)$$

and hence

$$\langle o|T\ \exp(\Sigma_j\ H(j))\ |o\rangle = \langle o|\bar{N}\ \exp(\Sigma_j\ H(j))\ |o\rangle$$

since the vacuum to vacuum expectation value of the exponential can be expanded into a series of products of pairs of operators.

This is a very useful result, for the Fourier transformation suggested earlier can now be used, since the operator $\bar{N}$ orders the transformed operators, b_k, in the same way as the original operators a_j.

The Fourier transformation and its inverse are defined as

$$a_j^{1*} = \frac{1}{\sqrt{2N}} \sum_{k=-N}^{N} \omega^{jk} \, b_k^{1*}$$

$$a_j^{1} = \frac{1}{\sqrt{2N}} \sum_{k=-N}^{N} \omega^{-jk} \, b_k^{1}$$

$$b_k^{1*} = \frac{1}{\sqrt{2N}} \sum_{j=-N}^{N} \omega^{-jk} \, a_j^{1*}$$

$$b_k^{1} = \frac{1}{\sqrt{2N}} \sum_{j=-N}^{N} \omega^{jk} \, a_j^{1} \qquad (6.1)$$

where $\omega = \exp(2\pi i/N)$.

Since the lattice has cyclic boundary conditions the operator a_{-i}^{1*}, $o \leq i \leq N$ corresponds to a_{N-i}^{1*}.

The b_k^{1*}, b_k^{2*}, are creation operators, and the b_k^{1}, b_k^{2} are annihilation operators, and they act on the vacuum state accordingly, which can be seen as follows.

$$b_k^{i} \, |o\rangle = \frac{1}{\sqrt{2N}} \sum_{j=-N}^{N} \omega^{+jk} \, a_j^{i} \, |o\rangle = 0$$

$$\langle o| \, b_k^{i*} = \frac{1}{\sqrt{2N}} \sum_{j=-N}^{N} \omega^{-jk} \, \langle o| \, a_j^{i*} = 0$$

The commutation relations of the b_k^{1*}, b_k^1 can be evaluated as follows.

$$\left[b_k^q, b_{k'}^p \right]_+ = \frac{1}{2N} \Sigma_j \Sigma_{j'} \omega^{(jk+j'k')} \left[a_j^q, a_{j'}^p \right]_+$$

$$= 0$$

Similarly $$\left[b_k^{p*}, b_{k'}^{q*} \right]_+ = 0$$

$$\left[b_k^p, b_{k'}^{q*} \right]_+ = \frac{1}{2N} \Sigma_j \Sigma_{j'} \omega^{(jk-j'k')} \left[a_j^p, a_{j'}^{q*} \right]_+$$

$$= \frac{1}{2N} \Sigma_j \Sigma_{j'} \omega^{(jk-j'k')} \delta_{j,j'} \delta_{p,q}$$

$$= \frac{1}{2N} \Sigma_{j=-N}^{N} \omega^{j(k-k')} \delta_{p,q} = \delta_{k,k'} \delta_{p,q}$$

where δ is the kroneker delta symbol.

Thus the new operators, b_k, obey fermion commutation rules.

Inserting the transformation, eq. (6.1) into expressions such as $\Sigma_j a_j^{2*} a_j^{1*}$ we obtain

$$\Sigma_j a_j^{2*} a_j^{1*} = \frac{1}{2N} \Sigma_j \Sigma_k \Sigma_{k'} \omega^{j(k+k')} b_k^{2*} b_{k'}^{1*}$$

$$= \frac{1}{2} \sum_{k=-N}^{N} b_k^{2*} b_{-k}^{1*}$$

$$= \frac{1}{2} \sum_{k=1}^{N} (b_k^{2*} b_{-k}^{1*} + b_{-k}^{2*} b_k^{1*})$$

Also,

$$\Sigma_j a_j^{2*} a_{j-m}^2 = \frac{1}{2N} \Sigma_j \Sigma_k \Sigma_{k'} \omega^{j(k-k')+mk'} b_k^{2*} b_{k'}^2$$

$$= \frac{1}{2} \sum_{k=1}^{N} (b_k^{2*} b_k^2 \omega^{mk} + b_{-k}^{2*} b_{-k}^2 \omega^{-mk})$$

From these calculations we find that under the Fourier transformation, $\Sigma_j H_0(j)$ transforms into $\frac{1}{2}\Sigma_k H_0(k)$ where for the square lattice

$$H_0(k) = xy(b_k^{2*} b_{-k}^{1*} + b_{-k}^{2*} b_k^{1*}) + y(b_k^{2*} b_k^2 \omega^{mk} + b_{-k}^{2*} b_{-k}^2 \omega^{-mk})$$
$$+ y(b_k^{2*} b_k^1 \omega^k + b_{-k}^{2*} b_{-k}^1 \omega^{-k}) + x(b_k^{1*} b_k^2 \omega^{mk} + b_{-k}^{1*} b_{-k}^2 \omega^{-mk})$$
$$+ x(b_k^{1*} b_k^1 \omega^k + b_{-k}^{1*} b_{-k}^1 \omega^{-k}) + (b_k^2 b_{-k}^1 \omega^{(m-1)k} + b_{-k}^2 b_k^1 \omega^{-(m-1)k}) \qquad (6.2)$$

The partition function for the square lattice can now be written as

$$Z = \langle o | \bar{N} \exp(\tfrac{1}{2}\Sigma_k H_0(k)) | o \rangle \qquad (6.3)$$

where the anti-normal operator $\bar{N}$, now acts on the b_k^*, b_k and puts them into anti-normal order. The advantage of the expression we have obtained by transforming the operators is that $H_0(k)$ is diagonalized with respect to the variable (k). This is useful, since using the commutation relations for the operators b_k, it can be seen that the $H_0(k)$ commute for different values of k

$$H_0(k)\, H_0(k') = H_0(k')\, H_0(k) \qquad k \neq k'$$

Thus we can write eq. (6.3) as

$$Z^2 = \prod_{k=1}^{N} \langle o | \bar{N} \exp(H_0(k)) | o \rangle \qquad (6.4)$$

This expression can be evaluated by expanding the exponential and counting all non-zero terms. As there are only four different kinds of operators, all fifth and higher order terms in the series are zero since they do not obey fermi-statistics. Hence we can write eq. (6.4) as

$$Z^2 = \prod_{k=1}^{N} \langle o|\bar{N}\ (1+H_o(k) + \frac{1}{2!}\ (H_o(k))^2 + \frac{1}{3!}\ (H_o(k))^3 + \frac{1}{4!}\ (H_o(k))^4\ )|o\rangle \qquad (6.5)$$

The evaluation of these terms is comparatively simple, where, for example, the only terms contributing to $\langle o|\bar{N}\ H_o(k)\ |o\rangle$ are

$$\langle o|\bar{N}\ (y\ \omega^{mk}\ b_k^{2*}\ b_k^2 + y\omega^{-mk}\ b_{-k}^{2*}\ b_{-k}^2 + x\omega^{k}\ b_k^{1*}\ b_k^1 + x\omega^{-k}\ b_{-k}^{1*}\ b_{-k}^1\ )\ |o\rangle$$

which on putting the terms in anti-normal order and evaluating gives

$$-y(\omega^{mk} + \omega^{-mk}) - x(\omega^{k} + \omega^{-k})$$

Evaluating all the terms in expression (6.5) yields the expected result

$$Z^2 = \prod_{k=1}^{N} (\ (1+x^2)\ (1+y^2)\ - y(1-x^2)\ (\omega^{mk}+\omega^{-mk}) - x(1-y^2)\ (\omega^{k}+\omega^{-k})\ )\ .$$

A Green's function can be defined in terms of these operators in the usual manner, and as would be expected from the analogous procedure in field theory, this Green's function is equivalent to the Fourier transform of the Green's function which was defined in terms of the original operators, a_j^*.

So far we have showed that the Fourier transformation diagonalizes a quadratic Hamiltonian with respect to its 'time' coordinate j. If we look now at the quartic term $a_j^{6*}\ a_j^{5*}\ a_{j-m+1}^4\ a_{j-m}^3$ which occurs in the next nearest neighbour problem, and use a similar transformation, we get

$$2\sum_j a_j^{6*}\ a_j^{5*}\ a_{j-m+1}^4\ a_{j-m}^3 = H_1(j) =$$

$$\frac{1}{2N^2}\sum_j \Sigma_{k_1,\,k_2,\,k_3,\,k_4}\ \omega^{j(k_1+k_2-k_3-k_4)+(m-1)k_3+mk_4} \times$$

$$b_{k_1}^{6*}\ b_{k_2}^{5*}\ b_{k_3}^4\ b_{k_4}^3$$

$$= \frac{1}{2N}\ \Sigma_{k_1\ k_2\ k_3\ k_4}\ \delta(k_1+k_2-k_3-k_4)\ \omega^{(m-1)k_3+mk_4}\, b_{k_1}^{6*} b_{k_2}^{5*} b_{k_3}^4 b_{k_4}^3$$

Now this Hamiltonian is no longer diagonalized with respect to the variable $|k|$, and has the familiar form of the many-fermion Hamiltonian with an interaction. This result enables us to use the many forms of approximations that can be performed on such expressions. The appropriate approximation, however, will have to be justified by physical arguments, and these are not well established yet. Since the

phase transition in superconductivity can be predicted theoretically with a "reduced" Hamiltonian, one is tempted to reduce the above Hamiltonian so that it too becomes a soluble problem, and hope that those terms and diagrams which are neglected do not make an important contribution to the analytic behaviour of the partition function near the transition point. By approximating the Hamiltonian H_1 with the expression

$$H_1' = \frac{1}{2N} \sum_{k_1,k_2} \omega^{(m-1)k_1+mk_2} b^{6*}_{k_1} b^{5*}_{k_2} b^{4}_{k_1} b^{3}_{k_2}$$

the partition function can be evaluated exactly, where we use a technique which is closely related to the Bogoluibov, Zubarev and Tserkovnikov[61] theory for superconductivity. The final result is the same as that obtained by neglecting $H_1(j)$ (eq. (4.1)) except that u and v are replaced by $u - \frac{1}{2}\rho$, $v - \frac{1}{2}\mu$, where ρ, μ are the solutions of an integral equation, similar to that encountered in superconductivity. Thus the inclusion of the "reduced" Hamiltonian gives rise to a change in the interaction strengths of the diagonal bonds, which resembles mass renormalization in field theory[46]. The details of this calculation are given for the ferroelectric problem in section 7.3. To look at the consequences of using such a Hamiltonian on the nature of the interactions and graphs of the Ising model, we express H_1' in terms of

the original operators, a_j, by taking the inverse Fourier transform. We obtain

$$H_1' = \frac{1}{2N} \Sigma^{N}_{j_1, j_2=1} \; a^{6*}_{j_1} \; a^{5*}_{j_2} \; a^{4}_{j_1-m+1} \; a^{3}_{j_2-m}$$

As $N \to \infty$, the weight associated with the quartic terms, $\frac{1}{2N}$, goes to zero. Hence, we have an infinite number of terms of zero weight, and whose total effect is non-zero and finite. The only terms in this hamiltonian which correspond to Ising graphs with crossed bonds are those when $j_1 = j_2$, and these terms are a small proportion of the total number of quartic terms. This reduced hamiltonian model then, though exactly soluble is not very interesting physically. Nevertheless it is interesting to be able to write the partition function in a form which so closely resembles the many-fermion problem.

CHAPTER 7. TWO DIMENSIONAL FERRO-ELECTRICS

7.1 Slater's Model of K.D.P.

Ferro-electrics are materials which possess a spontaneous electric polarization, which can be reversed by apply-
electric field E. Ferro-electricity has been
e electrical analogue of ferromagnetism, as is
he similarity in their names. The analogous
these phenomena are respectively the spon-
ization and magnetism; the dielectric constant
ity; and both have a transition temperature
polarization and magnetization respectively

enon of ferromagnetism has been studied both
nd theoretically in great detail and is now
stood, whereas ferro-electricity was first
e crystal Rochelle salt only in 1921, and
s a rigorous theoretical explanation. Of
e explanations, the thermodynamical theory[62],
of Landau[63] yields many of the experimentally observed results. However, this approach suffers from the drawback that it does not take into consideration any of the microscopic properties of the system. A second, more recent approach, given by Cochran[64] explains ferro-electricity on the basis of lattice vibrations. However, this theory

fails to account for the ferro-electricity in the substance $K H_2PO_4$. The reason is that different mechanisms can produce this phenomenon, and the $K H_2 PO_4$ crystal belongs to a class of ferro-electrics in which the hydrogen bonds play a more important role than the lattice vibrations. One of the first and most widely accepted theories which made use of the hydrogen bonds was due to Slater[25] in 1941 and his model has been successful in predicting some of the ferro-electric properties of $K H_2 PO_4$.

There has been a considerable revival of interest in Slater's model, which until very recently could only be tackled with approximate methods, e.g. mean field method (Slater), high and low temperature series expansions(Nagle[27]). However, due to Lieb's recent exact solution, Slater's model has become the second model of co-operative phenomena to have an exact treatment, which exhibits a phase transition. In this chapter, we shall show how the techniques that were developed earlier for the Ising model can be applied to Slater's model, giving an exact solution for temperatures below the critical point and good approximations for higher temperatures. However, these results have been rather foreshadowed by the arrival of Lieb's exact solution, and so we are now more concerned with using this model as a check for the approximate solutions which are based on our field-theoretical formalism.

In the remainder cf this section, the partition function is expressed as a vacuum to vacuum expectation value. In section 7.2 the thermodynamic quantities are defined in terms of Green's functions, which are calculated exactly for temperatures below the critical temperature. In section 7.3 several high temperature approximations are considered. These give the correct critical behaviour for the specific heat, but fail to exhibit a latent heat. Section 7.4 contains a discussion of the Rys antiferro-electric problem and in the last section Lieb's exact solution is considered.

The $K H_2 PO_4$ crystal contains phosphate groups (PO_4) linked to four neighbouring groups by hydrogen bonds. Slater assumed that the hydrogen atoms are capable of occupying one of two different positions on the hydrogen bond. The different possible arrangements of the hydrogen atoms result in different orientations of the $(H_2 PO_4)^-$ dipoles. The dipoles are assumed to have lowest energy when pointing in the same direction, causing a tendency towards spontaneous polarization at low temperatures, while at high temperatures the dipoles take up a random orientation. There must always be two hydrogen atoms near every (PO_4) group since ($H PO_4$) and ($H_3 PO_4$) are not favoured energetically.

Slater's model of K.D.P. in two-dimensions assumes that the phosphate groups are situated on the lattice sites of a square lattice. The hydrogen atoms are situated on the bonds

between two phosphate groups and can take up two positions as shown

These configurations can be conveniently represented by arrows on the bonds of the lattice as shown

There are only two hydrogen atoms near each (PO_4) group, and this restricts the model to six possible configurations at each vertex, which are labelled and represented as shown in Fig. (16).

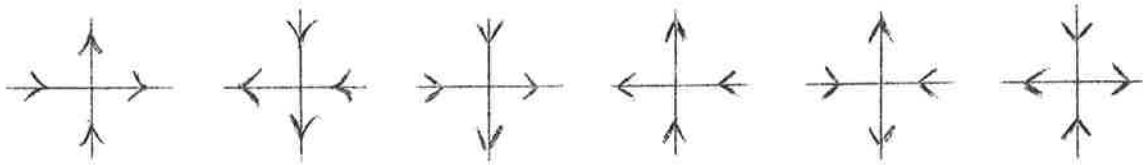


Fig. 16.

Each vertex configuration has an energy associated with it and for the crystal $K H_2 PO_4$, Slater has chosen the energies $\epsilon_1 = \epsilon_2 = 0$: $\epsilon_3 = \epsilon_4 = \epsilon_5 = \epsilon_6 = \epsilon$. For a model of an antiferro-electric substance Rys has defined a different set of interaction energies. We shall also consider the case

when a vertical electric field $\underline{E}$ is present. The dipole moment for two vertical arrows is d, and hence the energies, v_i, due to the electric field are $v_1 = v_4 = -dE$; $v_2 = v_3 = dE$; $v_5 = v_6 = 0$.

The partition function for the model is

$$Z = \sum_{\underline{s}} \exp(-\beta E(s))$$

where the sum is over all possible configurations of the model and E(s) is the energy of the configuration. The sum over all configurations can be replaced by a summation over a class of graphs drawn on the lattice as follows.

The standard configuration of the model is defined by the configuration drawn in Fig. (17).

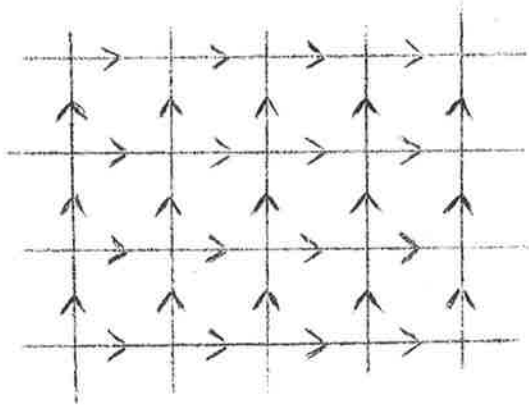


Fig. 17.

Any other configuration can be obtained from the standard configuration by reversing the direction of pairs of arrows at a lattice point. If we represent the reversed spins as lines on the lattice, then the standard configuration is

represented by no lines drawn on the lattice, and the non-standard configurations correspond to closed graphs on the lattice. The possible vertices which represent the allowable reversals of spins on the standard configuration are

An example of a single closed loop is given in Fig. (18).

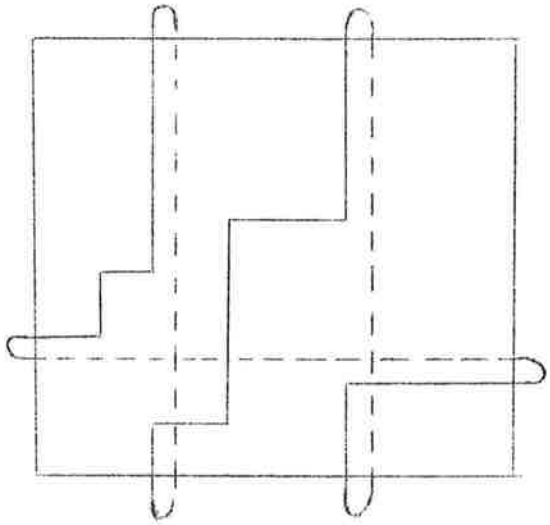


Fig. 18.

We note that every graph must cross the boundary of the lattice and so it will be necessary to discuss the boundary conditions of the lattice. We also see that the graphs are typical Ising graphs where no bond may be repeated, and the graphs are closed loops. An important difference is that there are only six possible vertices whereas the Ising model contains eight. The weights to be associated with these

vertices, after factorizing out a term $\exp(\beta\ E\ d\ N)$, where $-E\ d\ N$ is the energy of the standard configuration are

1	$\exp(-2\beta Ed)$	$\exp(-2\beta Ed-\beta\epsilon)$	$\exp(-\beta\epsilon)$	$\exp(-\beta Ed-\beta\epsilon)$	$\exp(-\beta Ed-\beta\epsilon)$
1	y^2	y^2x	x	yx	yx

where $y = \exp(-\beta Ed)$ $\quad x = \exp(-\beta\epsilon)$

It can now be shown, using the methods of Chapter 2, that

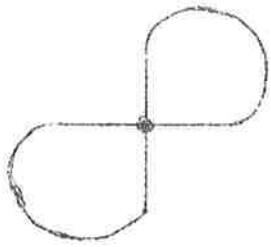
$$Z = y^{-N} \langle o |\ T \exp\Big(\sum_j H_0(j) + H_1(j)\Big)\ | o \rangle \qquad (7.1)$$

where $H_0(j) = a_j^{2*}\ a_{j-m}^2\ y^2x + a_j^{1*}\ a_{j-1}^1\ x + a_j^{1*}\ a_{j-m}^2\ xy$

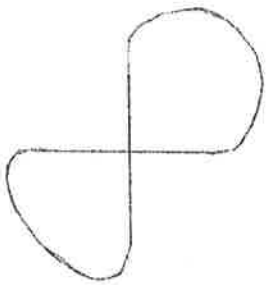
$$+ a_j^{2*}\ a_{j-1}^1\ xy$$

$$H_1(j) = a_j^{2*}\ a_j^{1*}\ a_{j-m}^2\ a_{j-1}^1\ y^2 \qquad (7.2)$$

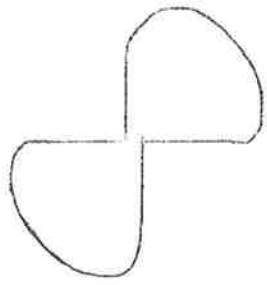
An important difference between this and the Ising model is the appearance of a quartic term, even though there are no crossed bonds. The reason is that when evaluating eq. (7.1) by means of the Feynman graph technique such configurations as



will be counted twice, appearing as



and



(a) (b)

Since (a) has one more crossed bond than (b), and the weights associated with the graphs are the same, the sum of their contributions is zero. As graphs with such a vertex configuration must be included in the sum, a quartic term is added to the hamiltonian to count these graphs. By expanding the exponential of the quartic term, as we have already done for the Ising model in section 2.2, we can prove that these graphs are counted correctly.

As we have already indicated, each graph of the ferro-electric problem must cross the boundaries of the lattice. A bond joining the edges of the lattice is equivalent to a long-range bond and can give rise to crossed-bonds and hence graphs that are weighted with a minus sign. It was

shown by Potts and Ward[67] and Green and Hurst[68], that for the Ising model the graphs which crossed the boundaries and were counted incorrectly gave a neglible contribution. However, this is not necessarily so for the ferro-electric problem, since all the graphs must cross the boundaries. In Fig. 19 the typical crossed bonds arising from helical boundary conditions are shown.

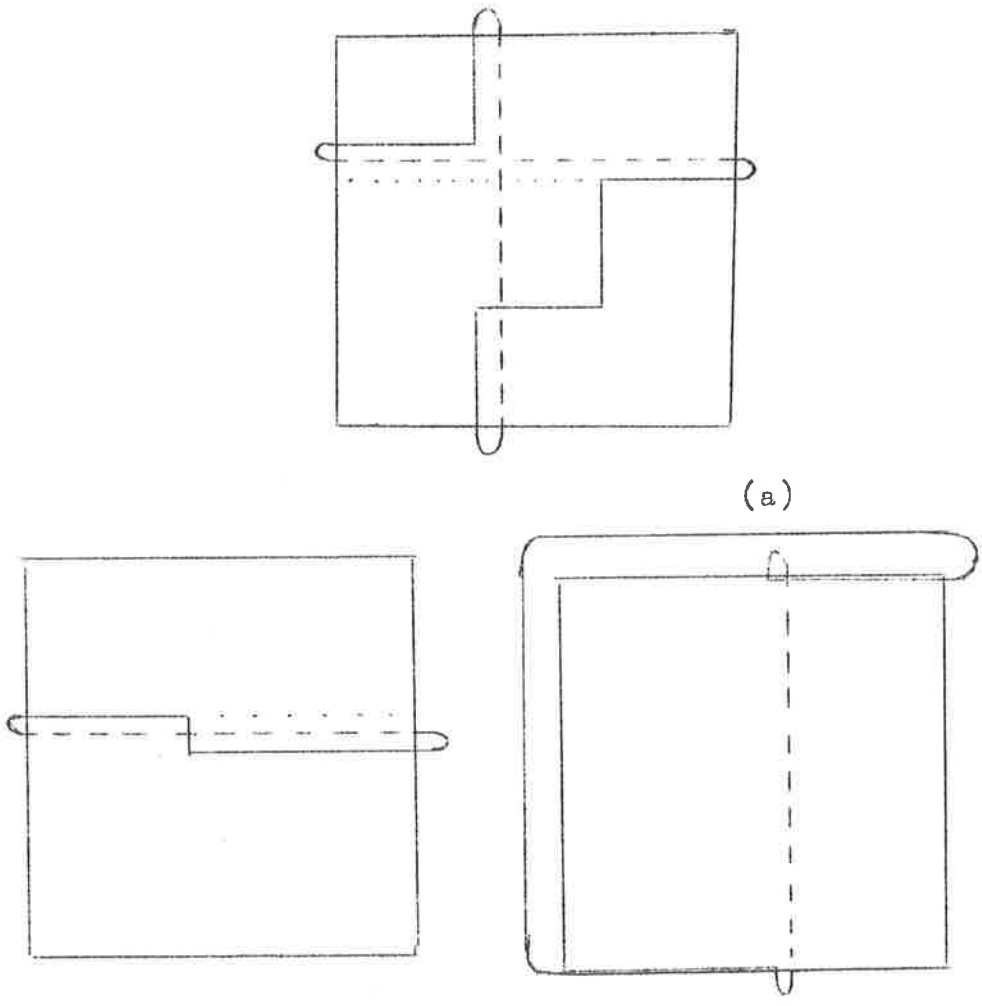


Fig. 19.

The graph in Fig 19(a) has an even number of crossed bonds and is counted correctly while those in Figs. 19(b), (c), have an odd number of crossed bonds and are counted incorrectly. However, graphs (b) and (c) contain a vertex ⅂, which is not an allowable vertex for the ferro-electric problem. By extending the above arguments it can be shown that all the graphs for the ferro-electric model will contain an even number of crossed bonds with helical boundary conditions, and hence the expression (7.1) will count them correctly. However, with toroidal boundary conditions, there are graphs with an odd number of crossed bonds, and an example is given in Fig. (20).

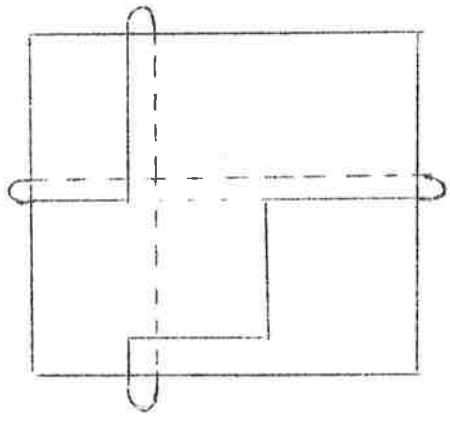


Fig. 20.

Hence, an extra quartic term is required in our hamiltonian if we are to consider a toroidal lattice. However, Lieb has solved the toroidal lattice case, and a simple generalization enables his transfer matrix approach to solve the helical lattice problem. The solutions are identical in the limit $N \to \infty$, and so

we can conclude that the boundary conditions do not affect the thermodynamical properties. Hence, the expression (7.1) is correct, regardless of the boundary conditions, as $N \to \infty$.

Recently, Wu has considered a model of a ferro-electric which is equivalent to replacing the quartic term in eq. (7.1) by zero. He solved this problem using the pfaffian method. We have shown that eq. (7.1) is the correct expression for the partition function of the ferro-electric problem, and that the appearance of the quartic term is why the pfaffian approach has failed.

7.2 Exact Solution for T < Tc.

The partition function has been expressed in terms of a vacuum to vacuum expectation value of a time-ordered product of exponentials. We can now consider the expressions for the average energy per vertex, the spontaneous polarization and correlations in terms of the Green's functions. If we define

$$A^1(j) = a^1_{j-1} \qquad A^2(j) = y a^2_{j-m} \qquad A^3(j) = x a^{1\,*}_{j}$$

$$A^4(j) = xy a^{2\,*}_{j}$$

and

$$k = \begin{pmatrix} 0 & 0 & -1 & -1 \\ 0 & 0 & -1 & -1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

then the eq. (7.2) can be rewritten as

$$H_0(j) = \frac{1}{2} \sum_{p,q} k_{p,q} \Lambda^p(j) \Lambda^q(j)$$

$$H_1(j) = \frac{1}{x^2} \Lambda^4(j) \Lambda^3(j) \Lambda^2(j) \Lambda^1(j) \qquad (7.3)$$

With this notation, the exact Green's functions $G^{pq}(j-k)$ and the free Green's functions $G_0{}^{p,q}(j-k)$ are defined by equations (3.4) and (3.3). The propagator or commutator defined by eq. (3.10a) can be evaluated, giving

$$A(r) = \begin{pmatrix} 0 & 0 & x\omega^{-r} & 0 \\ 0 & 0 & 0 & xy^2\omega^{-mr} \\ -x\omega^{r} & 0 & 0 & 0 \\ 0 & -xy^2\omega^{mr} & 0 & 0 \end{pmatrix}$$

The free Green's function, given by eq. (3.13)

$$G_0{}^{-1}(r) = A^{-1}(r) - k$$

can now be evaluated explicitly. We obtain

$$G_0(r) = \begin{pmatrix} 0 & \Lambda \\ -\Lambda^* & 0 \end{pmatrix}$$

where Λ is a 2 x 2 matrix, and Λ^* the complex conjugate.

$$\Lambda = \frac{1}{\Delta(r)} \begin{pmatrix} \omega^{mr} x^{-1} y^{-2} - 1 & 1 \\ 1 & \omega^{r} x^{-1} - 1 \end{pmatrix} \qquad (7.4)$$

where $\Delta(r) = \dfrac{\omega^{(m+1)r}}{x^2y^2} - \dfrac{\omega^{r}}{x} - \dfrac{\omega^{mr}}{xy^2}$

The free Green's functions, in the co-ordinate representation, $G_0(j-k)$, can be evaluated exactly in the limit of an infinitely large lattice. We consider first

$$G_0{}^{14}(o) = \frac{1}{N}\sum_{r=1}^{N} G_0{}^{14}(r)$$

and replacing the sum by an integral, we obtain

$$G_0{}^{14}(o) = \frac{1}{(2\pi)^2}\iint_0^{2\pi} d\theta d\phi \left(\frac{e^{i(\theta+\phi)}}{x^2y^2} - \frac{e^{i\theta}}{x} - \frac{e^{i\phi}}{xy^2}\right)^{-1}$$

$$= \frac{1}{(2\pi)^2}\iint_0^{2\pi} d\theta d\phi \; \frac{x^2y^2e^{-i(\theta+\phi)}}{\left(1 - \dfrac{xy^2e^{-i\phi}}{1-xe^{-i\theta}}\right)(1-xe^{-i\theta})} \qquad (7.5)$$

The denominator can be expanded as a power series in $e^{-i\phi}$, provided that

$$\left|\frac{xy^2}{1-xe^{-i\theta}}\right| < 1 \qquad (7.6)$$

or $$\cos\theta < \frac{1 + x^2 - x^2y^4}{2x}$$

There are two cases to consider. If $x < \dfrac{1}{1+y^2}$, then the relation in eq. (7.6) holds for all θ, and hence

$$G_0{}^{14}(o) = \frac{1}{(2\pi)^2}\iint_0^{2\pi} d\theta d\phi \; \frac{x^2y^2e^{-i(\theta+\phi)}}{1-xe^{-i\theta}}\left[1 - \frac{xy^2}{1-xe^{-i\theta}}e^{-i\phi} + \ldots\right]$$

$$= 0$$

as the integration with respect to ϕ makes each term in the expansion zero.

If $x > \frac{1}{1+y^2}$, then the relation in eq. (7.6) holds for all $Q < \theta < 2\pi - Q$ where $Q = \arccos\left(\frac{1+x^2-x^2y^4}{2x}\right)$. For θ inside this interval, the integral is zero after integrating with respect to ϕ. When θ is outside this range, we write the integral for $G_o^{14}(o)$ as

$$G_o^{14}(o) = \frac{1}{(2\pi)^2} \iint_o^{2\pi} \frac{-x^2y^2 e^{-i(\theta+\phi)}}{\left(1 - \frac{(1-xe^{-i\theta})e^{i\phi}}{xy^2}\right) xy^2 e^{-i\phi}} d\theta d\phi$$

The denominator can now be expanded as a power series, giving

$$\frac{1}{(2\pi)^2} \int_{-Q}^{Q} \int_o^{2\pi} -xe^{-i\theta} \left(1 - \frac{(1-xe^{-i\theta})e^{i\phi}}{xy^2} + \ldots\right) d\theta d\phi$$

$$= \frac{1}{2\pi} \int_{-Q}^{Q} -xe^{-i\theta} d\theta = -\frac{x}{\pi} \sin Q .$$

A similar integration technique for all the Green's function elements yields the following results

$$G_o^{14}(o) = G_o^{23}(o) = -G_o^{41}(o) = -G_o^{32}(o) =$$

$$\begin{cases} o & x \leq (1+y^2)^{-1} \\ -\frac{x}{\pi} \sin Q & x > (1+y^2)^{-1} \end{cases}$$

$$G_o^{13}(o) = -G_o^{31}(o) = \begin{cases} o & x \leq (1+y^2)^{-1} \\ -\frac{P}{\pi} + \frac{x}{\pi y^2} \sin Q & x > (1+y^2)^{-1} \end{cases}$$

$$G_o^{24}(o) = -G_o^{42}(o) = \begin{cases} o & x \leq (1+y^2)^{-1} \\ -\frac{Q}{\pi} + \frac{x}{\pi} \sin Q & x > (1+y^2)^{-1} \end{cases}$$

where $$Q = \arccos\left(\frac{1+x^2-x^2y^4}{2x}\right)$$

$$P = \arccos\left(\frac{y^4x^2+1-x^2}{2y^2x}\right) \qquad (7.7)$$

The remaining Green's function elements are zero for all x.

A further, very useful result is that

$$G_o(j-k) = 0 \qquad x \leq (1+y^2)^{-1}$$

since we can now determine the exact Green's function for the range of temperatures $x \leq (1+y^2)^{-1}$. The exact Green's function has been shown to be given by

$$G^{-1}(j-k) = G_o^{-1}(j-k) + \Lambda(j-k)$$

where $\Lambda(j-k)$ is the sum of all the irreducible graphs. As the weights associated with these irreducible diagrams are given by $G_o(j-k)$, $\Lambda(j-k)$ will be zero for all $x \leq (1+y^2)^{-1}$. Thus

$$G(j-k) = G_o(j-k) = 0 \qquad x \leq (1+y^2)^{-1}$$

The above evaluation of the exact Green's function enables us to calculate the thermodynamic quantities for all $x \leq (1+y^2)^{-1}$. The internal energy per vertex, $\bar{E}$, is given by

$$\bar{E} = -\frac{1}{N} \cdot \frac{1}{Z} \frac{\partial Z}{\partial \beta}$$

$$= -\frac{1}{N} \frac{\partial x}{\partial \beta} \frac{1}{Z} \cdot \frac{\partial Z}{\partial x} - \frac{1}{N} \cdot \frac{1}{Z} \frac{\partial y}{\partial \beta} \frac{\partial Z}{\partial y}$$

Substituting in eq. (7.1) and using the definition of the Green's function, we obtain

$$\bar{E} = \epsilon(G^{32}(o) + G^{31}(o) + G^{42}(o) + G^{41}(o)) + dE +$$

$$dE(2G^{42}(o) + G^{41}(o) + G^{32}(o) + \frac{2}{x^2}(G^{41}(o)G^{32}(o) - G^{42}(o)G^{31}(o)))$$

$$= dE \text{ for all } x \leq (1+y^2)^{-1} \qquad (7.8)$$

The spontaneous polarization, P, is defined by

$$P = \frac{1}{\beta N} \frac{\partial}{\partial E} \log Z = \frac{1}{\beta N} \frac{\partial Z}{\partial y} \cdot \frac{1}{Z} \cdot \frac{\partial y}{\partial E}$$

$$= d - 2dG^{42}(o) - 2dG^{41}(o) - \frac{2d}{x^2}(G^{41}(o)^2 - G^{42}(o)G^{31}(o))$$

$$= d \qquad x \leq (1+y^2)^{-1}$$

The correlation functions can be expressed in terms of Green's functions as follows. Let <m,n> denote the probability that the horizontal arrows at the sites m and n are both pointing to the right. Then <m,n> is the sum of all configurations weighted with the Boltzman factor, $\exp(-\beta E_s)$, with the arrows

at m and n pointing to the right, divided by the sum of all the configurations (the partition function). To calculate the sum of these configurations we use an expression similar to the one derived for the partition function, except that those terms which represent a reversal of the horizontal arrows at the m^{th} and n^{th} lattice sites are subtracted from the Hamiltonian. Hence,

$$<m,n> = <o|\ T\ \exp(-\Lambda^3(m)\Lambda^1(m) - \Lambda^3(m)\Lambda^2(m) -$$

$$\frac{1}{x^2}\Lambda^4(m)\Lambda^3(m)\Lambda^2(m)\Lambda^1(m) - \Lambda^3(n)\Lambda^1(n) - \Lambda^3(n)\Lambda^2(n) - \frac{1}{x^2}\Lambda^4(n)\Lambda^3(n)$$
$$\Lambda^2(n)\Lambda^1(n))$$

$$\times \exp(\Sigma_{j=1}^{N} H_o(j) + H_1(j)\ )\ |o> \cdot Z^{-1}$$

Expanding the exponential, and omitting terms containing a given operator more than once we obtain

$$<m,n> = <o|\ T\ (1-\Lambda^3(m)\Lambda^1(m) - \Lambda^3(m)\Lambda^2(m) -$$

$$\frac{1}{x^2}\Lambda^4(m)\Lambda^3(m)\Lambda^2(m)\Lambda^1(m)\ )\ (1-\Lambda^3(n)\Lambda^1(n) - \Lambda^3(n)\Lambda^2(n) -$$

$$\frac{1}{x^2}\Lambda^4(n)\Lambda^3(n)\Lambda^2(n)\Lambda^1(n)\ )\ \exp\ (\Sigma_j\ H_o(j) + H_1(j)\ )\ |o> \cdot\ Z^{-1}$$

$$= (1-G^{31}(o) - G^{32}(o) - \frac{1}{x^2}\ G^{41}(o)\ G^{32}(o) + \frac{1}{x^2}\ G^{42}(o)G^{31}(o)\ )^2$$

+ higher order terms, up to $\frac{1}{x^4}\ G^{42}(m-n)G^{31}(m-n)G^{24}(m-n)\times$ $G^{13}(m-n)$.

Hence, for $x < (1+y^2)^{-1}$

$$\langle m,n \rangle = 1 \quad \text{all } m,n.$$

We have calculated the thermodynamic quantities for the case $x < (1+y^2)^{-1}$, obtaining

$$\bar{E} = Ed$$
$$P = d$$
$$\langle m,n \rangle = 1$$

These results show that the model remains in the standard state for all $T \leq Tc$, a result which was known from Nagle's series expansions, and confirmed by Lieb. However, the dependence of the critical temperature on the electric field is a new result. We have that

$$x_c = (1+y^2)^{-1} \qquad (7.9)$$

When $E = 0$, $x_c = \frac{1}{2}$ and thus $Tc = \frac{\epsilon}{k \log 2}$. As $E \to \infty$, $x_c \to 1$ and hence $Tc \to \infty$. This behaviour corresponds to the physically observed behaviour in ferro-electric crystals.

Lieb (private communication) has since shown that his own solution also predicts that the critical temperature is given by the eq. (7.9). Strictly, we have shown only that the critical temperature is given by $x_c \geq (1+y^2)^{-1}$. To obtain the equality it is necessary to show that

$$\bar{E} > Ed \quad \text{for} \quad x > (1+y^2)^{-1}$$

This means that the sum of the Green's functions in eq. (7.8) should not be zero for $x > (1+y^2)^{-1}$. The exact Green's functions are not known exactly in this range, but the zero, first and second order approximations indicate that they are non-zero and thus the above inequality is satisfied.

7.3 Approximate Solutions for T > Tc

For temperatures above the critical point, the free Green's function has been evaluated (eq. (7.7)), but the exact Green's function is insoluble. Thus it is necessary to make approximations for the Green's functions, in order to look at the thermodynamic quantities. It will be shown that the first-order approximation gives the correct asymptotic behaviour of the specific heat, but does not exhibit a latent heat. Higher order approximations are considered and these give the same results.

The first approximation is to neglect the quartic term. This is equivalent to neglecting the second vertex in Fig. 16, and hence reduces to the model considered by Wu. The average energy is given by eq. (7.8) and substituting the values of the free Green's function, we obtain, for the case when the electric field, E, is zero

$$\bar{E} = \frac{2\epsilon}{\pi} \arccos \frac{1}{2x}$$

$\bar{E}$ has a branch point at $x = \frac{1}{2}$ and

$\bar{E} \to 0 \pm 4\epsilon n$ as $x \to \frac{1}{2}$.

The only possible physical value for $\bar{E}$ is 0, and hence $\bar{E}$ is continuous at the transition point. The specific heat, C, is given by

$$C = \frac{\partial \bar{E}}{\partial T} = \frac{2\epsilon^2}{\pi k T^2} \left[4x^2 - 1 \right]^{-\frac{1}{2}}$$

Thus the specific heat diverges at T = Tc. The behaviour of x near $x = \frac{1}{2}$ is determined by the Taylor series

$$\begin{aligned} x &= x_c + (T - Tc) \left.\frac{\partial x}{\partial T}\right|_{T=Tc} + \cdots \\ &= x_c + (T - Tc)\, \epsilon\, x_c \Big/ kT_c^2 \\ &= \tfrac{1}{2} + \Lambda\delta \end{aligned} \qquad (7.10)$$

where $\delta = \left(\frac{T}{Tc} - 1\right)$

Substituting in above we obtain

$$C \approx \frac{2}{\pi k T_c^2}\, \epsilon^2 (1 + 4\Lambda\delta - 1)^{-\frac{1}{2}}$$

and hence the critical index α', defined in Chapter 5, is equal to $\frac{1}{2}$.

We shall now consider higher order approximations in order to verify that the asymptotic behaviour of the specific heat as given by the first order approximation is correct, and to look for an approximation which contains a latent heat. We have considered three kinds of approximations. The first is the

usual perturbation expansion about the quartic terms in the Hamiltonian. The second is the first-order approximation to the Green's function using Dyson's equation, and the third is the "reduced" Hamiltonian approximation which is used in superconductivity theory. All these approximations confirm the above asymptotic behaviour of the specific heat, but there is no latent heat present.

The perturbation expansion for the partition function is

$$Z = \langle o | T \sum_{n=o}^{\infty} \frac{1}{n!} \; (\Sigma_j \, H_1(j)^n \exp(\Sigma_j \, H_o(j) \;) \; | o \rangle$$

We can use the well-known linked-cluster expansion to obtain

$$\text{Log } Z = \log Z_o + \langle \sum_{n=1}^{\infty} \; (\Sigma_j \, H_1(j) \;)^n \rangle_c \qquad (7.11)$$

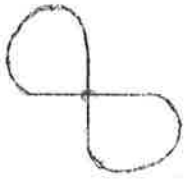
where $\langle \ldots\ldots \rangle_c$ denotes the sum over connected diagrams and

$$Z_o = \langle o | \; T \exp(\Sigma_j \, H_o(j) \;) \; | o \rangle$$

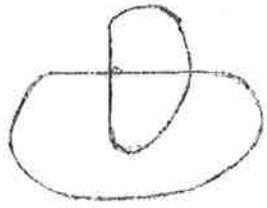
Log Z_o can be calculated using the free Green's function, and the average energy and specific heat arising from this term is identical to the first approximation considered above. The second term of eq. (7.11) is

$$\langle o | T \; \Sigma_j \, \frac{1}{x^2} \; A^4(j) A^3(j) A^2(j) A^1(j) \exp(\Sigma_j \, H_o(j) \;) \; | o \rangle \text{ connected.}$$

The connected diagrams are represented as



and



where the lines represent the free Green's functions. Thus, the first correction to log Z is

$$\Sigma_j \frac{1}{x^2} \left(G_0^{41}(o)\, G_0^{32}(o) - G_0^{42}(o)\, G_0^{31}(o) \right)$$

$$= \frac{N}{\pi^2} \left(\frac{2\, Q \sin Q}{x} - \frac{Q^2}{x^2} \right)$$

where $Q = \arccos (2x)^{-1}$ when $E = 0$.

The average energy, $\bar{E}'$, arising from this term is

$$\bar{E}' = -\frac{1}{N} \frac{\partial}{\partial \beta} \cdot \frac{N}{\pi^2} \left(\frac{2\, Q \sin Q}{x} - \frac{Q^2}{x^2} \right)$$

$$= \frac{\epsilon x}{\pi^2} \left(-\frac{2\, Q \sin Q}{x^2} + \frac{2Q^2}{x^3} + \frac{2 \sin Q}{x} \frac{\partial Q}{\partial x} + \frac{2Q \cdot \cos Q}{x} \frac{\partial Q}{\partial x} - \frac{2Q}{x^2} \frac{\partial Q}{\partial x} \right)$$

Near and above the critical point

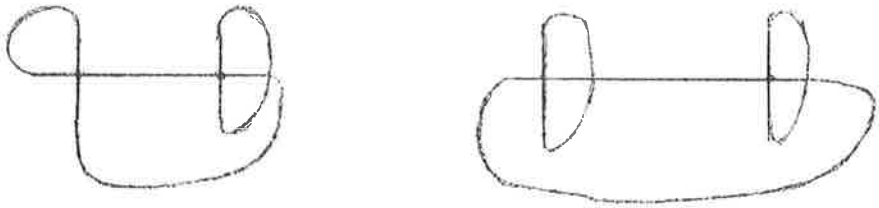
$$Q \approx 2(A\delta)^{\frac{1}{2}} \qquad \sin Q \approx 2(A\delta)^{\frac{1}{2}} \qquad \frac{\partial Q}{\partial x} \approx (A\delta)^{-\frac{1}{2}}$$

where A and δ are defined in eq. (7.10).

Hence, $\bar{E}' \approx \frac{32 \cdot A \cdot \delta \cdot \epsilon}{2\pi^2}$

This correction to the average energy, $\bar{E}$, tends to zero as $T \to T_c$, and hence does not produce a discontinuity in $\bar{E}$.

The next highest order correction consists of terms resulting from graphs with two four-point vertices. There are many possible graphs to be constructed, but we shall look at only one such graph; that shown in Fig. 21(b).



(a) (b)

Fig. 21.

The contribution from this graph is

$$\sum_{j,j'} \frac{1}{x^4} G^{42}(o)\, G^{42}(o)\, G^{31}(j-j')\, G^{13}(j-j')$$

$$= - \sum_{j,j'} \frac{1}{x^4} [G^{42}(o)]^2 \; [G^{31}(j-j')]^2$$

$$= - N \Sigma_j \frac{1}{x^4} [G^{42}(o)]^2 \left[\frac{1}{2\pi} \int_{-Q}^{Q} d\phi \; x^{-j} (1-xe^{i\phi})^{j+1} \right]^2$$

$$= - N \frac{1}{x^4} \left(- \frac{Q}{\pi} + \frac{x \sin Q}{\pi} \right)^2 \left[\frac{1}{2\pi} \int_{-Q}^{Q} d\phi \; x^{-1} (1-xe^{i\phi})^2 \right]^2 +$$

higher terms. (7.12)

$$= - N x^{-4} \left(- \frac{Q}{\pi} + \frac{x \sin Q}{\pi} \right)^2 \left[\frac{x^{-1}}{\pi} Q - \frac{2}{\pi} \sin Q + \frac{x}{2\pi} \sin 2Q \right]^2 + \ldots$$

$$\approx \delta^2 \quad \text{for} \quad T \approx T_c .$$

The neglected terms in eq. (7.12) are also of the order of δ^2. Thus, $\bar{E} \approx \delta$ and $C \approx$ constant, and so this term does not alter the asymptotic behaviour of the average energy.

The prece ding approximations are based on the straightforward perturbation expansion. We shall now consider an

alternative procedure which is an infinite partial summation of graphs, obtained by approximating the Green's function. Dyson's equation for Green's functions, which was derived in Chapter 3 is used.

$$G^{-1}(r) = G_o^{-1}(r) - \Lambda(r)$$

$$\Lambda(r) = \Sigma_j \, \omega^{-rj} \, \Lambda(j) \qquad (7.13)$$

The simplest diagrams for the irreducible vertex part $\Lambda(j-j')$ are those shown in Fig. 22.

Fig. 22.

Defining this first approximation as $\Lambda_o(j-j')$, we note that $\Lambda_o(j-j')$ is zero unless $j = j'$, due to the special structure of the diagrams, and hence

$$\Lambda_o(r) = \Lambda_o(o)$$

From the diagrams in Fig. 22 it can be seen that

$$\Lambda_o^{32}(r) = G_o^{41}(r) \qquad \Lambda_o^{31}(r) = -G_o^{42}(o)$$

$$\Lambda_o^{41}(r) = G_o^{32}(o) \qquad \Lambda_o^{42}(r) = -G_o^{31}(o)$$

Substituting these results into eq. (7.13) gives

$$G(r) = \begin{pmatrix} 0 & M \\ -M^* & 0 \end{pmatrix}$$

where M* is the complex conjugate of the 2x2 matrix M.

$$M = \frac{1}{\Delta'(r)} \begin{pmatrix} \frac{\omega^{mr}}{x} - 1 + A & B + 1 \\ B + 1 & \frac{\omega^{r}}{x} - 1 + A \end{pmatrix}$$

where $A = \frac{Q}{\pi} - \frac{x \sin Q}{\pi}$ $\qquad B = \frac{x}{\pi} \sin Q$

$$\Delta'(r) = \left(\frac{\omega^{mr}}{x} - 1 + A\right)\left(\frac{\omega^{r}}{x} - 1 + A\right) - (B+1)^2$$

The expression (7.8) for $\bar{E}$ becomes, when E = 0

$$\bar{E} = 2\epsilon \left(G^{31}(o) + G^{32}(o)\right)$$

which, on substituting the above approximation is

$$\bar{E} = 2\epsilon \frac{1}{(2\pi)^2} \iint_o^{2\pi} d\theta d\phi \frac{- e^{i\phi}.x^{-1} - Q.\pi^{-1}}{\alpha+\beta(e^{i\theta}+e^{i\phi}) + \gamma e^{i(\theta+\phi)}} \qquad (7.14)$$

where $\alpha = A^2 - B^2 - 2(A+B)$ $\qquad \beta = Ax^{-1} - x^{-1}$

$$\gamma = x^{-2}$$

The asymptotic forms for these functions are for $x \approx \frac{1}{2}$

$$\alpha \approx -\frac{4}{\pi}(\delta)^{\frac{1}{2}} \qquad \beta \approx -2 + \frac{2}{\pi}(\delta)^{\frac{1}{2}} \qquad \gamma \approx 4 - 16\delta$$

The integral in eq. (7.14) can be evaluated in a similar manner to that of eq. (7.5). The result is that for $x>\frac{1}{2}$

$$\bar{E} = \frac{\epsilon}{\pi} \frac{1}{\alpha^2-\beta^2} \arctan \frac{\alpha-\beta}{\alpha+\beta} \left(\frac{2\beta+\gamma+\alpha}{2\beta-\gamma-\alpha}\right)^{\frac{1}{2}} \cdot \times$$

$$\left[4\left(\frac{\beta}{x} - \frac{\alpha}{\pi}\right) + 2(\alpha^2+\beta^2)\left(\frac{1}{\beta x} + \frac{Q}{\pi\alpha}\right)\right]$$

$$- \frac{\epsilon}{\pi}\left(\frac{1}{x\beta} + \frac{Q}{\pi\alpha}\right) \arccos\left(\frac{\gamma \pm \alpha}{-2\beta}\right)$$

Using the asymptotic forms for α, β, γ, we obtain the result that $\bar{E} \approx (\delta)^{\frac{1}{2}}$, which agrees with the previous approximations.

The last approximation which we shall consider is to reduce the Hamiltonian, so as to enable the problem to be solved exactly. One way of doing this, as we have shown, is to eliminate the quartic term. However, a more satisfactory modification is to neglect only some of the quartic terms, which can be done when the Hamiltonian is written in terms of the fourier transformed operators b_k^1, b_k^{1*}. This approach was first used in the theory of superconductivity by Bogoliubov, Zubarev and Tserkovnikov[61]. Apart from its importance for the theory of superconductivity, the Bogoliubov theory is one of the few exact theories in statistical mechanics. Much of the work done in what follows is based on the clear account of the Bogoliubov approach given by Blatt[65].

We have used the fourier transform discussed in Chapter 5 to obtain the following results from eq. (7.2)

$$\sum_{j=1}^{N} H_0(j) = \frac{1}{2}\sum_{k=-N}^{N} H_0(k) = \frac{1}{2}\sum_{k=-N}^{N} x\omega^{k}\, b_k^{1*}\, b_k^{1} +$$

$$x\omega^{mk}\, b_k^{2*}\, b_k^{2} + x\omega^{k}\, b_k^{2*}\, b_k^{1} + x\omega^{mk}\, b_k^{1*}\, b_k^{2}$$

$$\sum_{j=1}^{N} H_1(j) = \frac{1}{4N} \sum_{k_1,k_2,k_3,k_4} \delta(k_1+k_2-k_3-k_4)\,\omega^{mk_3+k_4}\, b_{k_1}^{2*} b_{k_2}^{1*} b_{k_3}^{2} b_{k_4}^{1}$$

To make the problem exactly soluble by the Bogoliubov method, it is necessary to replace $\Sigma_j H_1(j)$ by the "reduced" Hamiltonian H_1.

$$H_1 = \frac{1}{4N} \sum_{k_1,k_2} \omega^{mk_2+k_1}\, b_{k_2}^{2*}\, b_{k_1}^{1*}\, b_{k_2}^{2} b_{k_1}^{1}$$

$$= -\frac{1}{4N} \sum_{k_1,k_2} C_{k_1}\, D_{k_2}$$

where $\quad C_k = \omega^{k}\, b_k^{1*}\, b_k^{1} \qquad D_k = \omega^{mk}\, b_k^{2*}\, b_k^{2}$

Bogoliubov's method consists in making a displacement of the operators C_k, D_k; that is, we introduce a set of real constants μ_k and ρ_k and new operators γ_k and δ_k by

$$C_k = \gamma_k + \mu_k \qquad D_k = \delta_k + \rho_k \tag{7.15}$$

The "reduced"Hamiltonian can now be written in terms of these new quantities.

$$H_1 = \frac{-1}{4N} \sum_{k_1,k_2} \mu_{k_1}\,\rho_{k_2} + \mu_{k_1}\,\delta_{k_2} + \gamma_{k_1}\,\rho_{k_2} + \gamma_{k_1}\,\delta_{k_2} \tag{7.16}$$

If the last term in eq. (7.16) is ignored, the resulting Hamiltonian is quadratic and can be solved exactly. The aim of the Bogoliubov method is to adjust the constants μ_k and ρ_k in such a way that the correction, arising from the neglected terms $\gamma_{k_1}\ \delta_{k_2}$, becomes completely negligible. Let us define

$$\mu = \frac{1}{N}\ \Sigma_k\ \mu_k \qquad\qquad \rho = \frac{1}{N}\ \Sigma_k\ \rho_k \tag{7.17}$$

The expression for the partition function, Z_1, based on the reduced Hamiltonian, then becomes

$$Z_1^2 = \langle o|\ \overline{N}\ \exp\Big(\sum_k H_o(k) - \frac{1}{2}\ \gamma_k\ \rho - \frac{1}{2}\ \delta_k\ \mu\Big)\ |o\rangle\ \times$$

$$\exp\Big(-\frac{N}{2}\ \mu\ \rho\Big)$$

Using equations (7.15) we get

$$Z_1^2 = \langle o|\ \overline{N}\ \exp\Big(\Sigma_k\ H_o(k) - \frac{1}{2}\ \rho\ C_k - \frac{1}{2}\ \mu\ D_k\Big)\ |o\rangle\ \exp\ \Big(\frac{N}{2}\ \mu\ \rho\Big)$$

$$= \langle o|\ \overline{N}\ \ \exp\Big(\Sigma_k\ H^1(k)\ \Big)\ |o\rangle\ \exp\Big(\frac{N}{2}\ \mu\ \rho\Big)$$

where $H^1(k) = b_k^{1*}\ b_k^1\ \omega^k\ \Big(x - \frac{1}{2}\ \rho\Big) + b_k^{2*}\ b_k^2\ \omega^{mk}\ \Big(x - \frac{1}{2}\ \mu\Big)$

$$+ x b_k^{1*}\ b_k^2\ \omega^{mk} + x b_k^{2*}\ b_k^1\ \omega^k\ .$$

Z_1 can be evaluated by the same technique as was used to calculate a similar quadratic expression in Chapter 4. The result is

$$Z_1^2 = \prod_{r=1}^{N} \Big\{1 - \omega^r\Big(x-\tfrac{1}{2}\rho\Big) - \omega^{mr}\ \Big(x-\tfrac{1}{2}\mu\Big) +$$

$$\omega^{(m+1)r}\ \Big(-\frac{x}{2}\ (\rho+\mu) + \frac{1}{4}\ \rho\mu\Big)\Big\}^2 \tag{7.18}$$

The effect of the term $-\frac{1}{4N}\sum_{k_1,k_2}\gamma_{k_1}\delta_{k_2}$, which was neglected in this calculation, now has to be made as small as possible. To do this, we impose the following condition on γ_k and δ_k, which also determines the values of the constants ρ_k, μ_k.

$$\langle o|\ \bar{N}\,\gamma_k \exp\left(\Sigma_k H^1(k)\right)\ |o\rangle = 0$$

$$\langle o|\ \bar{N}\,\delta_k \exp\left(\Sigma_k H^1(k)\right)\ |o\rangle = 0$$

This condition is equivalent to the one used by Bogoliubov, Zubarev and Tserkovnikov in their approach to superconductivity. With such a condition satisfied, they showed that the extra contribution arising from the neglected terms is completely neglible in the limit of infinite volume. A heuristic proof of this for the case considered here is given. The neglected terms are regarded as a perturbation, and expanding about these, we obtain the following perturbation series.

$$\langle o|\ \bar{N}\left[1 + \sum_{n=1}^{\infty}\frac{1}{n!}\left(-\frac{1}{4N}\sum_{k_1,k_2}\gamma_{k_1}\delta_{k_2}\right)^n\right]\exp\left(\Sigma_k H^1(k)\right)|o\rangle \qquad (7.20)$$

The first term in this series has been calculated. The second term is

$$-\frac{1}{4N}\sum_{k_1,k_2}\langle o|\ \bar{N}\,\gamma_{k_1}\delta_{k_2}\exp\left(\Sigma_k H^1(k)\right)\ |o\rangle$$

which can be written, since $H^1(k)$ is diagonal with respect to k

$$- \frac{1}{4\bar{N}} \sum_{k_1,k_2} \langle o|\, \bar{N}\, \gamma_{k_1}\, \exp(H^1(k))\, |o\rangle \langle o|\bar{N}\, \delta_{k_2}\, \exp(H^1(k_2)|o\rangle \times$$

$$\prod_{k\neq k_1,k_2} \langle o|\, \bar{N}\, \exp(H^1(k))\, |o\rangle$$

$= 0$ because of eq. (7.19). The only non-zero contribution is when $k_1 = k_2$, which gives

$$- \frac{1}{4\bar{N}} \sum_{k_1} \langle o|\, \bar{N}\, \gamma_{k_1}\, \delta_{k_1}\, \exp(H^1(k_1)|o\rangle \prod_{k\neq k_1} \langle o|\, \bar{N}\, \exp(H^1(k))|o\rangle$$

The sum over k_1 in the above gives a contribution of the order of N, and this cancels the $\frac{1}{N}$ in front. Thus, the correction term is independent of $\bar{N}$. An extension of this argument shows that all the terms in expression (7.20) are independent of N, and hence, if the series converges, its limit is also independent of N. Thus the correction to the free energy, $F = N^{-1} \log Z$, will be neglible as $N\to\infty$. Hence, eq. (7.18) is exact if ρ and μ are given by the relations (7.19).

Using eqs. (7.19) and (7.15), and the fact that $H^1(k)$ is diagonal with respect to k, we obtain

$$\mu_k = \frac{\langle o|\bar{N}\, \omega^k\, b_k^{1*}\, b_k^1\, \exp(H^1(k))|o\rangle}{\langle o|\bar{N}\, \exp(H^1(k))|o\rangle}$$

$$= [-\omega^k + \omega^{k(m+1)(x-\frac{1}{2}\mu)}].\ \Delta^{-1}(k)$$

where this last result follows from expanding the exponential

and $\Delta(k) = 1-\omega^{k}(x-\frac{1}{2}\rho)-\omega^{mk}(x-\frac{1}{2}\mu) + \omega^{(m+1)k}\ (\frac{1}{2}\rho\mu - \frac{1}{2}x(\rho+\mu))$

Similarly,

$$\rho_k = \frac{\langle o|\bar{N}\ \omega^{mk}\ b_k^{2\,*}\ b_k^2\ \exp(H^1(k))|o\rangle}{\langle o|\bar{N}\ \exp(H^1(k))|o\rangle}$$

$$= [\ -\omega^{mk} + \omega^{(m+1)k}\ (x-\tfrac{1}{2}\rho)]\ \Delta^{-1}(k)$$

Hence, to evaluate ρ and μ from eq. (7.17), we need to solve the coupled integral equations

$$\mu = \frac{1}{N}\sum_k [\ -\omega^{k} + \omega^{(m+1)k}\ (x-\tfrac{1}{2}\mu)]\ \Delta^{-1}(k)$$

$$\rho = \frac{1}{N}\sum_k [\ -\omega^{mk} + \omega^{(m+1)k}\ (x-\tfrac{1}{2}\rho)]\ \Delta^{-1}(k)$$

In the limit as the size of the lattice tends to infinity, the summation can be replaced by integrals, and the above equations become

$$\mu = \frac{1}{(2\pi)^2}\iint_0^{2\pi} d\theta d\phi\ (-e^{i\theta} + e^{i(\theta+\phi)}(x-\tfrac{1}{2}\mu))\ \times$$
$$(1 - (e^{i\theta}+e^{i\phi})\ (x-\tfrac{1}{2}\mu) + e^{i(\theta+\phi)}(\frac{\mu^2}{4} - x\mu))^{-1} \qquad (7.21)$$

where we have chosen the obvious solution $\mu = \rho$. For $x \leq \frac{1}{2}$, it can be seen that $\mu = o$ is a solution as expected. Hence, there is no correction to the expressions already obtained for $T \leq T_c$. For $T > T_c$, we evaluate the integral using similar methods to those used in evaluating eq. (7.5). The results which concern us are firstly that $\mu \geq o$. This is not sur-

prising since the definition of μ is a Green's function, which are related to the correlation functions which are always positive. Secondly, the integral on the R.H.S. of eq. (7.21) is zero if $\mu \geq 2-4x$. Hence, for $x > \frac{1}{2}$, there will be an inconsistency in the integral eq. (7.21) unless $\mu < 2-4x$. Therefore $0 \leq \mu < 2-4x$, and so μ is a continuous function with a singularity at $x = \frac{1}{2}$. It can be shown, by considering the expression for the average energy per vertex, $\bar{E}$, that if μ is continuous at $x = \frac{1}{2}$, then $\bar{E}$ is also continuous. Hence this "reduced" Hamiltonian approximation also fails to exhibit a latent heat.

In the case of superconductivity, there are good physical arguments showing that the "reduced" Hamiltonian contains the important interaction terms when the system is in the superconducting state. Unfortunately, for the ferro-electric problem we can equally argue that the "reduced" Hamiltonian does not contain the dominant terms. However, as this "reduced" model is exactly soluble, it is worthy of some study.

From the previous approximations, we have been unable to obtain a latent heat, or discontinuity in the average energy. The probable reason for this is that in the approximations which we have considered, too much wieght is attached to the graphs which occur in Wu's model, which does not possess a latent heat, and not enough weight to the graphs which arise from the quartic term in the Hamiltonian.

7.4 Rys Antiferro-electric Model

The F-model proposed by Rys[26] to explain the antiferro-electric properties of the crystal $NH_4\ H_2\ PO_4$ has an identical structure to the ferro-electric model discussed in the previous section, but the interaction energies are modified in order to give it antiferro-electric properties. They become, in the absence of an electric field

$$\epsilon_1 = \epsilon_2 = \epsilon_3 = \epsilon_4 = \epsilon \qquad \epsilon_5 = \epsilon_6 = 0.$$

Hence, the partition function can be written as

$$Z = x^N \langle o | T \exp(\Sigma_j H_0(j) + H_1(j)) | o \rangle$$

where $H_0(j) = a_j^{1*} a_{j-1}^1 + a_j^{2*} a_{j-m}^2 + x^{-1} a_j^{2*} a_{j-1}^1 + x^{-1} a_j^{1*} a_{j-m}^2$

$$H_1(j) = (2 - x^{-2})\ a_j^{2*} a_j^{1*} a_{j-m}^2 a_{j-1}^1 \qquad (7.22)$$

This expression, again, cannot be solved exactly, but it does possess some interesting features. We note that $H_1(j) = 0$ when $x = 2^{-\frac{1}{2}}$. Thus at this temperature the model can be solved exactly, and we obtain

$$Z^2 = x^{2N} \prod_{j=1}^{N} \text{determinant } (1 - k\Lambda(r))$$

where

$$k = \begin{pmatrix} 0 & 0 & -1 & -x^{-1} \\ 0 & 0 & -x^{-1} & -1 \\ 1 & x^{-1} & 0 & 0 \\ x^{-1} & 1 & 0 & 0 \end{pmatrix}$$

and

$$A(r) = \begin{pmatrix} 0 & 0 & \omega^{-r} & 0 \\ 0 & 0 & 0 & \omega^{-mr} \\ -\omega^{r} & 0 & 0 & 0 \\ 0 & -\omega^{mr} & 0 & 0 \end{pmatrix}$$

Thus,

$$Z^2 = x^{2N} \prod_{r=1}^{N} (1 - x^{-2} - \omega^r - \omega^{mr} + \omega^{(m+1)r})$$

and/in the limit of a large lattice

$$N^{-1} \log Z = \frac{1}{8\pi^2} \iint_0^{2\pi} d\theta d\phi \; (x^2 - 1 - x^2 e^{i\theta} - x^2 e^{i\phi} + x^2 e^{i(\theta+\phi)})$$

This result has since been confirmed by Wu[66].

The free Green's function is non-zero except when T = 0, and so we cannot obtain an exact solution for a given temperature range as with the Slater model. However, the free Green's function does contain a singular point at $x = \frac{1}{2}$, which indicates that the transition temperature is given by $x_c = \frac{1}{2}$. This was later confirmed by the results of Lieb, which indicates that this simple approximation may have a wider range of validity than it apparently should.

7.5 Lieb's Solution

Lieb has solved the ferro-electric problem by using the transfer matrix approach, which had been previously used by Schultz, Mattis and Lieb to solve the Ising model. There is a similarity in the formalisms since both problems can be expressed as

$$Z = \text{Trace } V^m = \Sigma_i \; \lambda_i^m$$

where λ_i are the eigenvalues of the transfer matrix V. However, the structure of V differs significantly for the

two problems. For all soluble Ising models V can be expressed in terms of Fermi operators, and has an analogous form to soluble many-body problems, which can be solved by diagonalization of a qua dratic form. In principle, all the eigenvalues of V (or the trace of V^m, see for example Thompson[70]) can be evaluated exactly. For the ferro-electric problem, V has a more complex structure, which is similar to that of a system of interacting fermions, and hence cannot be treated exactly. However, Lieb has found that the maximum eigenvalue of V can be calculated. The calculation relies on the remarkable fact that the eigenstate of V corresponding to the maximum eigenvalue is the same as the ground state of one of the few soluble interacting fermion systems, the linear antiferromagnetic Heisenberg chain. Thus using the solution of this latter problem, Lieb is able to obtain an exact solution for an apparently unrelated problem.

In this section we shall consider some interesting aspects of Lieb's solution, without going into any of the mathematical details which have already been well considered by Lieb[71]. The first point which we mention is that the exact solutions of the ice, ferro-electric and antiferro-electric problems all take the form

$$Z = \int_{-Q}^{Q} d\theta \; \rho(\theta) \log D(\theta) \qquad (7.23)$$

where, for example, in the ferro-electric problem

$$Q = \arccos (2x)^{-1}$$

$$D(\theta) = 1 - e^{i\theta} x^{-1}$$

The first-order approximations for these models which can be obtained from the combinatorial method by neglecting the quartic term in eqs. (7.1) or (7.22) are

$$Z = \frac{1}{(2\pi)^2} \iint_0^{2\pi} d\theta d\phi \log D'(\theta,\phi)$$

$$= \frac{1}{2\pi} \int_{-Q}^{Q} d\theta \log D(\theta) \qquad (7.24)$$

Comparing eq. (7.23) and (7.24) we can conclude that our first approximation corresponds to putting $\rho(\theta) = \frac{1}{2\pi}$. Lieb regards $\rho(\theta)$ as a density function, and thus this approximation is equivalent to regarding the distribution of the θ as being uniform. It now becomes apparent that the first order approximation predicts the analytical behaviour of the model correctly because of the close similarity of the approximate solution to the exact solution. The $\rho(\theta)$ does not affect the analytical behaviour of the integral in eq. (7.23), except in that it gives rise to the latent heat.

The second point of interest is that the approximations to the ferro-electric model and the linear Heisenberg chain are very similar. The Hamiltonian of the Heisenberg chain, when expressed in terms of fermi creation and annihilation operators contains a quartic term, and hence cannot be solved exactly, although the ground state has been obtained by

Bethe[72] and Hulthen[73]. Lieb, Schultz and Mattis[74] proposed a soluble model of an antiferromagnetic chain, by truncating the full Hamiltonian so that the quartic term became equal to zero. This is called the X-Y model, and its analogue in the ferro-electric problem is Wu's model, where in the field theoretical formalism, the quartic term is also equal to zero. Thus, in both the ferro-electric problem and the antiferromagnetic chain, by truncating the Hamiltonian, we obtain the Wu and X-Y models. They both have many features of the exact models, but are now linear problems and are completely soluble. In both models, it is found that the neglect of the quartic term is equivalent to replacing the $\rho(0)$ in the exact solution by $(2\pi)^{-1}$.

The last poiht, which should be mentioned, is that Lieb was able to obtain his solution from the fact that the graphs with N/2 vertical bonds contain the dominant contributions. Lieb carries out, essentially, a partial summation of these graphs, since his approach has not yet been able to successfully sum all the graphs. On summing all the graphs with N/2 vertical bonds, he then proves that in the limit $N\to\infty$, all the omitted graphs give rise to a negligible contribution. It was the partial summation of graphs in association with lattice statistical problems which led to the development of the present field theory techniques. However, we have not been able to perform the particular partial summation required

for this model with the formalism developed in this Chapter, apart from using essentially the same method as that used by Lieb.

CHAPTER 8. THE DIMER PROBLEM

Some of the combinatorial methods used for solving lattice statistical problems are based on the use of pfaffians. For the dimer problem this is the best known solution, and for the Ising model the use of pfaffians was the first rigorous combinatorial approach. An alternative technique for the Ising model has been considered. This is related to other quantum mechanical problems of statistical mechanics, and consists of representing such quantities at the partition function by $\langle o|\ T \exp(\Sigma_j H_o(j))\ |o\rangle$. The partition function for the dimer problem can also be written as a vacuum to vacuum expectation value and hence can be evaluated by the techniques developed in previous chapters.

Briefly, the dimer problem is to determine $g(p,q)$, the number of ways of arranging p horizontal dimers and q vertical dimers on a rectangular lattice of m columns and n rows, so that every lattice point is covered by one and only one dimer. The usual quantity computed is the partition function, Z, defined by

$$Z = \sum_{p,q} g(p,q)\, x^p y^q$$

The evaluation of the partition function can be cast as one of counting closed graphs on a lattice, by showing that there is a one-to-one correspondence between the graphs and the dimer configurations. This is demonstrated by joining

the points on the dimer lattice in pairs as shown in Fig. 23.

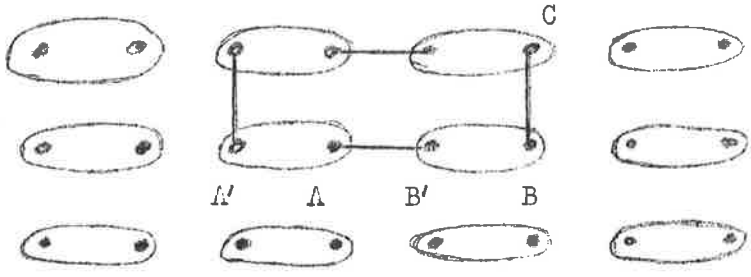


Fig. 23.

These "double" points will be regarded as a single-point for the lattice on which the graphs will be drawn. The standard dimer configuration, in which all the dimers are horizontal between the pairs of points shown, corresponds to no graph drawn on the lattice. For a different dimer configuration, we replace the dimer joining A to A′ by one joining A to B′ say. This then leaves the point B to be covered by a dimer joining B and C. This process is carried out until a dimer covers A′. Then a new dimer configuration will have been produced, to which there corresponds a closed loop on the lattice. It is now easy to see that there is a one-to-one correspondence between dimer configurations and graphs drawn between the "double" lattice points. Kasteleyn[18] used a graph approach to the dimer problem, but his method is not suitable here.

Hence we need to sum all the graphs on the lattice which (1) do not have repeated bonds and (2) do not have more than two bonds joining any one lattice point. There are nine

possible kinds of vertex for this lattice and these are shown in Fig. 24.

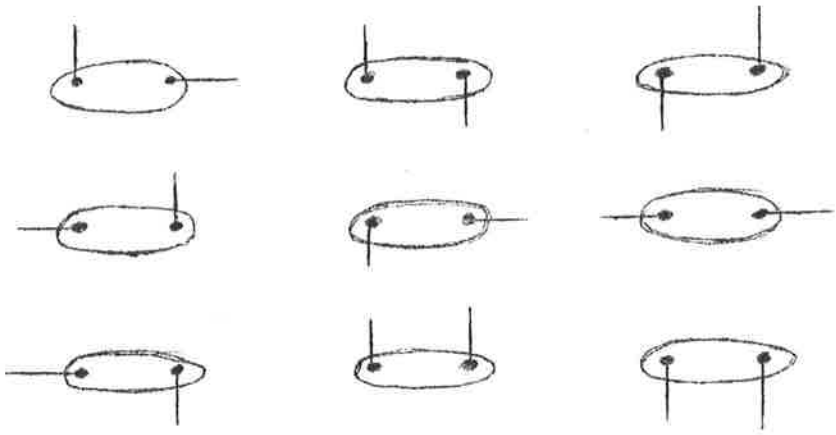


Fig. 24.

The procedure is now identical to the Ising model case. We write the expectation value $\langle o|\ T \exp(\Sigma_j H_o(j))\ |o\rangle$ and show that the sum of all Feynman graphs arising from this expression is equal to the sum of all the Dimer graphs. We associate fermion operators to the bonds as shown in Fig. 25.

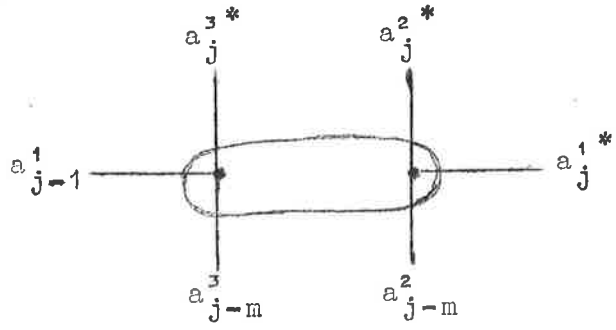


Fig. 25.

Then it can be shown that the expression for H(j) will be

$$H(j) = \frac{xv}{u}\, a_j^{3*}\, a_j^{1*} + \frac{y}{u}\, a_j^{3*}\, a_{j-m}^{2} + \frac{y}{u}\, a_j^{2*}\, a_{j-m}^{3}$$

$$+ \frac{y}{u}\, a_j^{2*}\, a_{j-1}^{1} + \frac{x}{u}\, a_j^{1*}\, a_{j-m}^{3} + \frac{x}{u}\, a_j^{1*}\, a_{j-1}^{1}$$

$$+ \frac{1}{u}\, a_{j-m}^{2}\, a_{j-1}^{1} + \frac{yv}{u}\, a_j^{3*}\, a_j^{2*} + \frac{1}{u}\, a_{j-m}^{2}\, a_{j-m}^{3} \qquad (8.1)$$

The bond weights have been generalized so that vertical dimers in the odd numbered columns have weights v and those in the even numbered columns weight y. Similarly there are two weights u, x for the horizontal dimers as shown in Fig.26.

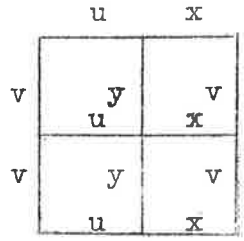


Fig. 26.

The quadratic pairs of operators in the expression H(j) correspond to the vertices drawn in Fig. 18. Hence, it can be seen that all the Feynman diagrams associated with expanding $\langle o|\ T \exp(\Sigma_j H_\bullet(j))\ |o\rangle$ contain all the possible dimer graphs with the correct weight factors. We will now show that the sum of all the Feynman diagrams which are not Dimer diagrams is zero. Firstly, graphs with re peated bonds sum to zero as in the case of the Ising model. Secondly, graphs

four lines to a point sum to give a zero contribution since each vertex can occur in two ways, with opposite signs, as shown in Fig. 27.

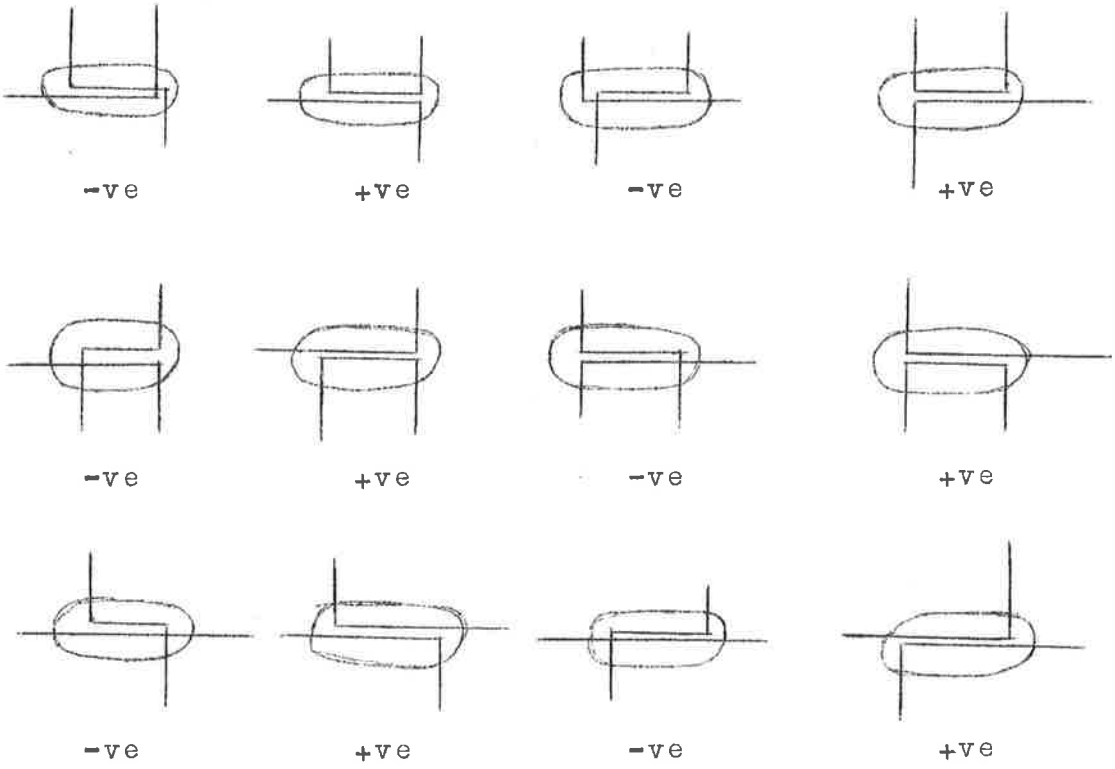
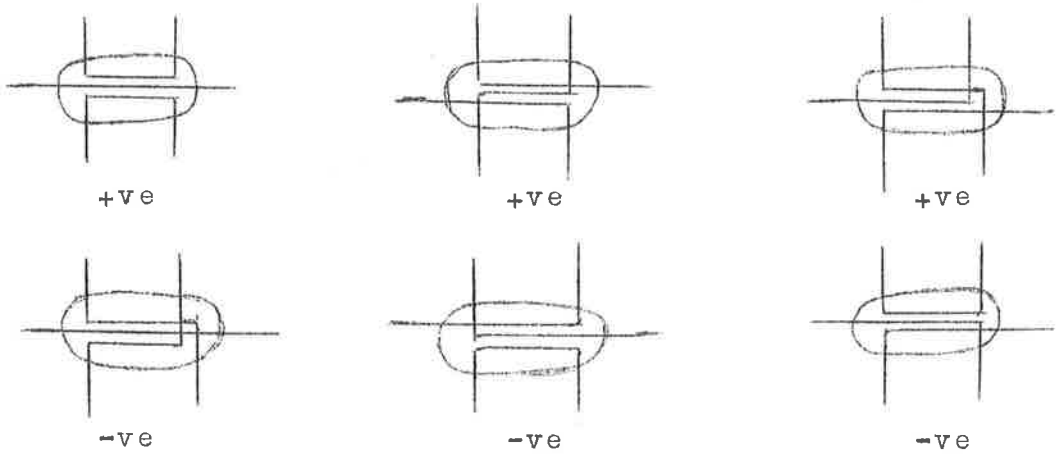


Fig. 27.

and similarly for six bonds at a point



The proof that each graph has the correct sign is the same as that given in Section 2.1 for the Ising model and will not be dealt with again.

Let us define

$$A^1(j) = a^1_{j-1} \qquad A^2(j) = a^3_{j-m} \qquad A^3(j) = a^2_{j-m}$$

$$A^4(j) = x a^{1\,*}_j \qquad A^5(j) = y a^{2\,*}_j \qquad A^6(j) = v a^{3\,*}_j$$

and then H(j), given by eq. (8.1) becomes

$$H(j) = \frac{1}{u} \sum_{p,q} \tfrac{1}{2} k_{p,q} A^p(j) A^q(j)$$

where k is the 6x6 matrix

$$\begin{pmatrix} 0 & 0 & -1 & -1 & -1 & 0 \\ 0 & 0 & -1 & -1 & -1 & 0 \\ 1 & 1 & 0 & 0 & 0 & -1 \\ 1 & 1 & 0 & 0 & 0 & -1 \\ 1 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 1 & 1 & 0 \end{pmatrix}$$

The commutator A(r) can be evaluated in the normal way giving

$$A(r) = \begin{pmatrix} 0 & 0 & 0 & x\omega^{-r} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & v\omega^{-mr} \\ 0 & 0 & 0 & 0 & y\omega^{-mr} & 0 \\ -x\omega^{r} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -v\omega^{mr} & 0 & 0 & 0 \\ 0 & -y\omega^{mr} & 0 & 0 & 0 & 0 \end{pmatrix}$$

Using the results of section 4.1, we obtain

$$Z^2 = u^N \prod_{r=1}^{N/2} \det (1-k\, A(r) / u)$$

$$= \prod_{r=1}^{N/2} \left\{ (u-x\omega^r)\,(u-x\omega^{-r}) + (y\omega^{-mr} - v\omega^{mr})\,(y\omega^{mr} - v\omega^{-mr}) \right\}$$

and letting the size of the lattice tend to infinity gives

$$\text{Log } \mathbf{Z} = \frac{1}{4} \frac{1}{(2\pi)^2} \iint_0^{2\pi} d\theta d\phi \log \left[(u-xe^{i\theta})(u-xe^{-i\theta}) + (ye^{-i\phi} - ve^{i\phi})(ye^{i\phi} - ze^{-i\phi}) \right] \qquad (8.2)$$

This solution of the generalized dimer lattice was given first by Stephenson [69] using the pfaffian approach. For the case when $u = x$, $y = v$ eq. (8.2) reduces to the standard form

$$\text{Log } Z = \frac{1}{4} \frac{1}{(2\pi)^2} \iint_0^{2\pi} d\theta d\phi \log \left[x^2 (1-e^{i\theta})(1-e^{-i\theta}) + y^2 (1-e^{2i\phi})(1-e^{-2i\phi}) \right]$$

As with the Ising model, a Green's function can be defined by the relations given in Chapter 3. This Green's function can be used to obtain the occupation probability of a single dimer, and the joint occupation probability of two dimers. The results obtained are the same as those given by Fisher and Stephenson [20] and will not be repeated. The main concern in including this section is to show that the field-theoretical technique developed in this thesis is a systematic unified

treatment of tackling all known lattice problems; that the partition function for all planar lattice statistical problems can be written as $\langle o|\ T \exp(\Sigma_j H(j))\ |o\rangle$ and that the thermodynamic functions are readily calculated from the Green's functions.

CHAPTER 9. CONCLUSION

The formalism presented in this thesis is based on the combinatorial approach to lattice problems, but it uses the relatively simple properties of fermi operators rather than an explicit representation by unwieldy determinants or pfaffians. This enables the thermodynamic quantities of the soluble two-dimensional nearest-neighbour Ising models and dimer problem to be evaluated simply in terms of the Green's functions. This formalism also has wider applications than other combinatorial methods since lattice problems which cannot normally be expressed in terms of determinants or pfaffians (such as the ferro-electric problem and the next-nearest neighbour Ising model) can be expressed in terms of the fermion operators. The resulting expressions, though it may not always be possible to evaluate them exactly, are at least amenable to the many approximation techniques used in quantum field theory and many fermion theory.

From the view-point of new results, the ferro-electric problem in the presence of an electric field has been the most rewarding. Previously, combinatorial methods were unable to handle this problem, but from the approach developed in this thesis, the exact critical temperature and thermodynamic properties below the critical temperature have been obtained.

For problems which can be formulated in terms of an S-matrix, but which cannot be evaluated exactly, the concept of summing the dominant terms, or the graphs with the dominant contributions, is a possible approach. Various methods of infinite partial summations of graphs have been given in this thesis. In all cases, these approximations have been carried out because of their use in other fields, and lack a simple physical motivation based on the properties of the lattice problem. Despite this, these approximations have been shown to reproduce much of the exact critical phenomena of the models. These results indicate that this new approach may be a useful formalism for partially solving unsolved lattice problems.

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