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Relations between the 'percolation' and 'colouring' problem and other graph-theoretical problems associated with regular planar lattices: some exact results for the 'percolation' problem

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A transfer-matrix approach is introduced to calculate the 'Whitney polynomial' of a planar lattice, which is a generalization of the 'percolation' and 'colouring' problems. This new approach turns out to be equivalent to calculating eigenvalues and traces of Heisenberg type operators on an auxiliary lattice which are very closely related to problems of 'ice' or 'hydrogen-bond' type that have been solved analytically by Lieb (1967*a* to *d*). Solutions for certain limiting cases are already known. The expected numbers of components and circuits can now be calculated for the plane square lattice 'percolation' problem in a special class of cases, namely those for which $p_H + p_V = 1$ where p_H and p_V are, respectively, the probabilities that any given horizontal or vertical bond is present. This class of cases is known, from the work of Sykes & Essam (1964, 1966), to be critical in the sense that a connected path across a large lattice exists with probability effectively unity whenever $p_H + p_V \geqslant 1$. Relations with other problems involving the enumeration of graphs on lattices, such as the tree, Onsager and dimer problems are pointed out. It is found that, for the plane square lattice, the treatment of problems of 'ice' type is very considerably simplified by building up the lattice diagonally, rather than horizontally or vertically.

The two available analytic methods of handling these problems, the Bethe–Húlthen 'ansatz' approach and the Kaufman–Onsager 'spinor' approach are compared.

1. Introduction

A very wide variety of physical and technical problems associated with repeating networks or crystals can be reduced to graph-theoretical form, involving enumerations of arrangements of points and lines on a lattice subject to certain restrictions. Throughout this paper, the word 'lattice' is used in the physical and not in the mathematical sense and we shall use the regular plane square lattice, in which each 'point' or 'node' or 'site' is connected by 'lines' or 'bonds' to four nearest neighbouring points, by way of illustration. (Unless otherwise stated, the word 'line' or 'bond' refers to one connecting a pair of nearest neighbouring points of the lattice.) By a 'graph' we mean a collection of such lines, together with the points that they intersect and any remaining isolated points of the lattice. A 'subgraph' is obtained from a graph by deleting one or more of its lines *without* removing any of the points. A 'component' (of a graph or subgraph) is a maximal connected portion of the

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graph. The words 'circuit' and 'tree' have their usual meanings, a 'forest' is a collection of disconnected trees and isolated points. It will be assumed that the reader is familiar with Euler's notion of independent circuits. The 'cyclomatic number' or 'nullity' of any graph or component is the number of independent circuits in it. We shall often imagine the lattice to be progressively built up row by row, neighbouring points in a row being added one at a time, and we shall then use the expression 'lattice' as an abbreviation for 'the graph consisting of all the points added so far, together with all the nearest neighbour bonds between pairs of these points'. We do not postulate the addition of a line to a graph unless both its end-points have already been added to the lattice.

In some problems we shall be concerned with directed lines and we shall denote these by arrows or by positive or negative signs, but we shall never introduce multiple lines between a pair of points. We shall also recognize the possibility that points on the lattice may be 'coloured' in two or more different ways.

2. Types of problem of physical interest

It is obvious that a very large number of mathematical problems can be posed about arrangements of points and lines on a lattice. In this paper we shall be concerned with relations between four types of problem of physical interest.

A. The enumeration of trees and forests is possible for any lattice, planar or not, the general theory having been laid down by Kirchoff and Sylvester. More complicated problems, however, arise if individual trees are to be weighted according to certain prescriptions. See, for example, Tutte (1954).

B. The enumeration of the number of ways of disposing $\frac{1}{2}$L black points on a plane square lattice of L points with a specified number of nearest-neighbour black pairs was accomplished by Onsager (1944). The results, which are of considerable interest in a number of branches of physics, for example magnetism, metallurgy, theory of solutions, adsorption, have since been extended to virtually all regular planar lattices and have been re-derived by a variety of different methods, but with only marginal improvements on the scope of Onsager's original results. (For example, a little is now known about arrangements involving three or four colours (Betts 1964) and about correlations at various distances (Kaufman & Onsager 1949).)

C. Recently Lieb (1967*a* to *d*) and others have given a unified treatment of a set of physical problems of 'hydrogen-bond' or 'ice' type. The simplest such problem is to ask for the number of ways in which arrows can be assigned to bonds on the lattice, in such a way that exactly two arrows point to every node. This models the situation for hydrogen-bonded molecules. In ice, for example, each hydrogen atom can occupy one of two positions between a pair of oxygen atoms, but, in the neighbourhood of each oxygen there are always the same numbers of hydrogens in the 'near' and 'distant' positions. These numbers are obviously two each if we 'model' ice by putting oxygens on the points of a plane square lattice, the hydrogens each occupying one of the bonds in two possible positions subject to the above. There are

six types of node, 1 to 6 of figure 1, satisfying the above restriction. More sophisticated problems of this type, in which different statistical mechanical probabilities are assigned to the six types of node satisfying the ice condition have also been solved; Lieb (1967*b*, *c*), Sutherland (1967), Sutherland, Yang & Yang (1967), Yang (1967). These serve as models of ferroelectric and antiferroelectric assemblies, with or without an applied electric field.

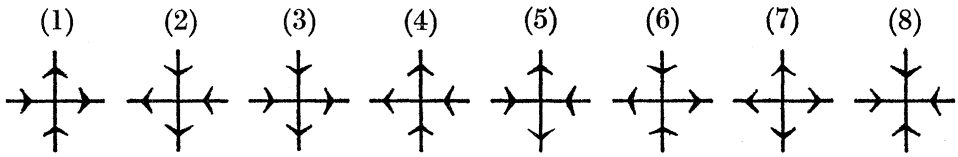

FIGURE 1

D. The problem of the number of ways of colouring the points of a lattice with k colours in such a way that no two neighbouring points are coloured alike was studied and generalized by Whitney (1932). The problem is trivial for $k = 1$ or 2. For $k = 3$ the problem on the plane square lattice is equivalent to the ice problem (Lieb 1967*d*). No other exact result is known at present. Whitney's generalization turned out to be closely related to the 'percolation' problem, which amounts to asking for the expected number of connected components of a random graph, each bond on the lattice having a chance p or $1-p$ of being selected or rejected for inclusion in the graph. This is closely connected with various problems in magnetism and is also of interest in communication and porous medium problems, when we think of each bond as being 'open' or 'blocked' and ask for the probability that a continuous path exists through the whole lattice. Sykes & Essam (1964, 1966) rediscovered a result of Whitney (1932), a dual transformation very similar to that known to exist for the Onsager (1944) problem, and were able, for several lattices, to determine the critical value of p above which a long path through the lattice (or equivalently, a large connected domain of 'open' bonds), might be expected to occur with a probability of effectively unity. This was a very important piece of information, but left outstanding the more general problem, namely that of determining in general the number of ways of choosing M lines which have points in common in such a way as to give rise to N disconnected components. (Obviously there are two different versions of the problem according to whether or not we count an isolated point in the lattice, not intersected by any of the M lines, as a 'component' of the graph.) The related 'dimer' problem (Kasteleyn 1962; Temperley & Fisher 1961), in which we ask for the number of ways of choosing $\frac{1}{2}$L lines from a lattice of L points in such a way that no two of them pass through the same point on the lattice, so that there are no isolated points and $\frac{1}{2}$L components each consisting of one line, can be solved (by a variety of methods) for any regular planar lattice, but it is only for this limiting case that an analytic solution is known at present. (In graph-theoretical terminology this problem amounts to determining the number of 1-factors of a lattice.)

3. General relations between these problems

We shall interest ourselves only in the analytic form of the solutions of these problems in the limiting case where L, the number of points on the lattice, is very large. A very considerable amount of information about all these problems is also available from series expansions of various types, obtained by direct enumeration of configurations involving relatively small numbers of points and lines, followed by attempts to deduce trends for large graphs. In this paper we shall make only one comparison with this approach. We are far from attempting to deny its utility. Indeed, until quite recently, the number of analytic results available was quite small, and it is enough to say that, in all cases where comparison of series and analytic results has been possible, agreement has been very close indeed.

Lieb (1967*a* to *d*) showed that there is a very close analytical connexion between problems of 'generalized ice' type (type C above) and another problem that has an extensive literature, namely a one-dimensional array of 'spins' each interacting with two nearest neighbours with a Heisenberg type interaction. He was able to exploit various known results about this one-dimensional array and to obtain exact solutions for the various 'generalized ice' problems.

In this paper we shall do two things. We shall exhibit the relationships between these types of problem in a new and physically more transparent light. We shall also derive a transfer-matrix approach to Whitney's (1932) problem (generalization of the percolation and chromatic polynomial problems), and we shall show that this problem, too, can be reduced to problems of 'generalized ice' type which might be soluble by similar means. Various relations with Tutte's work (1954) on the Whitney problem and with the Onsager problem (1944) will also be exhibited, and we shall show how to calculate the expected numbers of components and circuits for the critical cases of the 'percolation' problem.

4. Analytic methods available

Much confusion exists in the literature about notation. One can work with Pauli, Fermi, Heisenberg or permutation operators or with creation and annihilation operators. Throughout this paper we shall use Onsager's (1944) definitions and notation. We describe our assembly by a set of 'spin variables', μ_i, each of which assumes only the values ± 1, and for each spin the operators C_i, S_i have the properties: $C_i 1 \to 1$, $C_i \mu_i \to -\mu_i$, $S_i 1 \to \mu_i$, $S_i \mu_i \to 1$. Since $\mu_i^2 = 1$ we are never concerned with powers of μ_i higher than the first, and the two possible 'states' of 'spin' i are represented by $\frac{1}{2}(1+\mu_i)$ and $\frac{1}{2}(1-\mu_i)$. We can represent C_i and S_i as direct products of 2×2 matrices of Pauli type thus

$$C_i = \mathrm{I} \times \mathrm{I} \times \ldots \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \times \mathrm{I} \times \ldots,$$

$$S_i = \mathrm{I} \times \mathrm{I} \times \ldots \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \times \mathrm{I} \times \ldots.$$

The Onsager interaction operator is $\exp(HS_1S_2)$ and it will be seen that it has the effect of multiplying a term like $\frac{1}{4}(1+\mu_1)(1+\mu_2)$ or $\frac{1}{4}(1-\mu_1)(1-\mu_2)$ by e^H, and any term of the form $\frac{1}{4}(1-\mu_1)(1+\mu_2)$ or $\frac{1}{4}(1+\mu_1)(1-\mu_2)$ by e^{-H}, thus distinguishing between pairs of like and unlike neighbours, in the same row.

The Heisenberg interaction operator can be written

$$C_1C_2 - C_1C_2S_1S_2 + \Delta S_1S_2. \tag{1}$$

If two neighbouring spins are alike, it simply multiplies the term $\frac{1}{4}(1+\mu_1)(1+\mu_2)$ or $\frac{1}{4}(1-\mu_1)(1-\mu_2)$ by Δ. If they are unlike it has the effect

$$\tfrac{1}{4}(1+\mu_1)(1-\mu_2) \to \tfrac{1}{2}(1-\mu_1)(1+\mu_2) - \tfrac{1}{4}\Delta(1+\mu_1)(1-\mu_2). \tag{2}$$

For $\Delta = 1$, it can be simply expressed as $2\mathrm{T}_{12}-1$ where T_{12} is the operator that changes μ_1 into μ_2 and vice versa. This is usually known as the isotropic Heisenberg case. (Note that all operators are to act on quantities appearing to their right, never to their left. Therefore we make the convention that BA is to be interpreted as: First operation A, then operation B.)

Although many variants of them exist in the literature there are, in effect, only two basic methods of tackling these problems. We can express Onsager's operators in terms of anti-commuting 'spinors' in various ways, for example

$$\left.\begin{aligned} S_1 &= P_1 & S_1C_1 &= Q_1 \\ S_2C_1 &= P_2 & S_2C_2C_1 &= Q_2, \\ S_3C_1C_2 &= P_3 & S_3C_3C_2C_1 &= Q_3, \end{aligned}\right\} \tag{3}$$

etc.

so that

$$\left.\begin{aligned} C_1 &= P_1Q_1 & S_1S_2 &= -P_2Q_1 & C_1C_2S_1S_2 &= -P_1Q_2, \\ C_2 &= P_2Q_2 & S_2S_3 &= -P_3Q_2 & C_2C_3S_2S_3 &= -P_2Q_3, \\ \dots & & \dots & & \dots & \dots, \end{aligned}\right\} \tag{4}$$

and, for any problem that be expressed as that of finding the trace of a product like

$$\mathrm{tr}\exp(AP_1Q_1)\times\exp(BP_2Q_1)\times\exp(CP_2Q_2)\times\exp(DP_3Q_2)\times\dots, \tag{5}$$

in which we have exponentials of second-order products of these spinors, we can exploit the isomorphism of the spinor and rotation groups (Kaufman & Onsager 1949) to infer the eigenvalues and hence the trace. Various other approaches, using determinants, vacuum to vacuum expectations, Wick's theorem, Pfaffians etc. are all nearly equivalent and apply to the same types of case.

For the 'ice-like' problems, the 'ansatz' method introduced by Bethe (1931) exploits the fact that, while the Heisenberg operators (1) may introduce numerical factors, none of them ever changes the total number of plus or minus spins in a row of spins. At most, it permutes pairs of unlike spins, changing $(+\ -)$ to $(-\ +)$. It is this property of a sum (or product) of Heisenberg operators that makes possible the methods used by Bethe (1931) and Húlthen (1938) and a large number of later workers for electron assemblies and applied by Lieb (1967 *a* to *d*) to the 'ice-like' problems.

5. A transfer matrix for the Whitney and percolation problems

The principle of the transfer-matrix is now well known as a result of Onsager's (1944) and other work. Imagine the lattice built up row by row and point by point. In the Onsager model (1944) the interactions are between nearest neighbours only. Then, if (figure 2) we add to the lattice a point such as D', the spin on it interacts with those on points C' and D, but with no others. At each stage we keep, in terms of the μ's, a record of *all* the possible configurations of the spins on all the 'outside' points (that is to say of $A', B', C', D', E, F, \ldots$, at the stage shown in figure 2) each

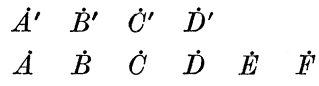

Figure 2

configuration weighted with the appropriate Boltzman factor due to the interactions. (These 'outside' points are nearest neighbours of points that will be added at a later stage. We call all other points such as A, B, C 'inside' points, and we need not specify the configuration of their spins.) In terms of the μ's our generating function will contain two sets of terms one corresponding to μ_D being negative, the other to μ_D being positive. These may be written

$$\phi = \tfrac{1}{2}(1-\mu_D) f(\mu'_A, \mu'_B, \mu'_C, \mu_E, \mu_F) + \tfrac{1}{2}(1+\mu_D)\, g(\mu'_A, \mu'_B, \mu'_C, \mu_E, \mu_F).$$

Apply the operator $\exp(HS_D S'_D)$ which gives a factor e^H for a like pair, e^{-H} for an unlike pair and sum over both configurations ($\mu_D = \pm 1$) of spin D that is now on an 'inside' point. The relation between the generating functions before and after adding point D' and putting in the effect of the interaction $(D - D')$ is

$$\phi'(\mu'_A, \mu'_B, \mu'_C, \mu'_D \ldots) = (e^H + C_D e^{-H})\, \phi(\mu'_A, \mu'_B, \mu'_C, \mu_D, \ldots).$$

The interaction $(C' - D')$ can be taken care of simply by operating with $\exp(HS'_C S'_D)$. No summation is performed, since C' and D' are both still 'outside' points. The total effect of adding point D', summing over both configurations of the spin on point D and then allowing for the factor in the partition function due to the interaction $(C' - D')$ is precisely given by operating on ϕ with

$$\exp(HS'_C S'_D)\,(e^H + C_D e^{-H})$$

and we get a similar pair of factors each time we add a point to the lattice. Operators like C_A, $S_B S_C$ are all expressible as quadratic products of spinors as shown by (3) and (4), hence the Onsager problem is soluble.

These considerations are well known, but we have set them down because they give a clue on how to set up the transfer operator for the Whitney problem. Whitney (1932) defined a polynomial for any lattice (which need not be regular)

$$W(x, y) = \sum_G x^{rG} y^{sG}, \tag{6}$$

where G runs over all subgraphs of the lattice, including the null graph and multi-component subgraphs. r_G and s_G are respectively the rank and nullity of G. The nullity of G is defined as the number of independent circuits in G (independent in Euler's sense). The rank is best defined indirectly. If we add a line to a subgraph G in such a way as to connect two points already joined in G we form a new circuit, and the rank is unchanged. Otherwise it is increased by one by adding a line. Thus r_G+s_G is simply the total number of lines in G, Euler's relation then gives the number of components of G as $\mathrm{L}-r_G$, if we make the convention that each isolated point counts as a 'component' of G.

It must now be shown that the chromatic polynomial and the generating function for the number of disconnected components in a random graph on the lattice are both particular cases of (6). The result for the latter is immediate. For a lattice of L points, the number of disconnected components is $\mathrm{L}-r_G$, and since the total number of lines in G, l_G, is just r_G+s_G, we have

$$\sum_G r_G x^{l_G} = \left[x\frac{\partial}{\partial x}W(x,y)\right]_{y=x}. \tag{6a}$$

Dividing this expression by $W(x,x)$ gives us the expected rank (L minus the expected number of components) of a random graph, if we put $p = x/(1+x)$. This is one of the problems of 'bond' type studied by Sykes & Essam (1964, 1966).

To derive the chromatic polynomial, we use the inclusion–exclusion method, following Whitney (1932). The number of ways of colouring the lattice in k colours without restriction is just k^{L}. From this we subtract the number of ways of colouring it so that at least two nearest neighbours are coloured alike, which is $k^{\mathrm{L}-1}\times$ (the number of lines in the lattice). We have now subtracted twice over the number of ways in which the points on a subgraph of type  are coloured alike which we correct for by adding $k^{\mathrm{L}-2}$ for each subgraph. We make similar corrections for larger subgraphs. When the graph contains circuits the argument becomes more elaborate, and the reader is referred to Whitney's (1932) paper for details, but the final result is

$$p(k) = k^{\mathrm{L}}\mathrm{W}(-1/k, -1). \tag{6b}$$

This asserts that there is a (1–1) correspondence between the terms of the Whitney polynomial and the terms occurring in the subtraction process that we use to eliminate those cases in which one or more neighbouring points are coloured alike.

In order to derive a transfer operator for calculating (6) we (figure 2) consider the effect of adding point D' to the lattice. We may, but need not, add one or both of the lines $D\,D'$ and $C'\,D'$ to each of the subgraphs G. Therefore, we need a record of whether or not C' and D were previously connected by lines in the subgraph G. Later on we shall need similar information about D' and E and so on as we go round the lattice, adding a point to each column in turn. How do we specify the sets into which these 'outside' points are connected up by the lines in each G? We can describe a typical situation by a notation like $\phi = (A\,B)\,(C)\,(D\,F\,G)\,(E)$, which means that A and B are connected C and E are isolated, while D, F and G form a connected group or set.

Consider now the possibilities relating to the line $D\,D'$ (figure 2). If we add this line to any graph G, the point D' will now be connected to just the same 'outside' points as was D by the lines in G, and to no others. The effect is to increase r_G by one. Now suppose that we omit the line $D\,D'$. Point D' will now be unconnected with any of the other 'outside' points and two cases arise. If D was connected to other 'outside' points, we must replace, e.g. $(D\,F\,G)$ by $(D')\,(F\,G)$. If D was isolated, we simply replace (D) by (D'). We describe these three possibilities by the factor $(x+D_D+E_D)$, where D_D corresponds to selecting those graphs in which D was isolated while E_D corresponds to an operation like $(D\,F\,G)\rightarrow(D')\,(F\,G)$, that is to isolating D' if D was *not* previously isolated. Similarly, we can examine the effect of adding the line $C'\,D'$ or omitting it. If we omit it, the rank, nullity and the connectivity situation are all unchanged. If we add this line, there are two possibilities. Either C' and D' were already connected by lines in G, in which case the number of circuits is increased by one, or else C' and D' were not connected by lines in G, in which case the addition of this line will increase the rank by one. Thus we can describe the three possibilities by the factor $(1+yP_{C'D'}+xQ_{C'D'})$ where operator $P_{C'D'}$ selects graphs in which points C' and D' are joined, while the operator $Q_{C'D'}$ selects graphs in which C' and D' are *not* joined, and then joins them.

Thus, we have a pair of operators the product of which takes account, for each subgraph G, of the possible contributions to the Whitney polynomial $\mathrm{W}(x,y)$ of adding, or omitting, the two extra lines incident on a point such as D' (figure 2) and, at the same time, these operators ensure that a proper record of the connectivity of the set of 'outside' points is maintained for all cases. Consider the simple case of a lattice with three points in each row. There are five possibilities: All three points are isolated which we describe by $[(A)\,(B)\,(C)]$. All three points are connected which we describe by $[(A\,B\,C)]$. Two points are connected, but the third is isolated, which we describe by $[(A\,B)\,(C)]$, $[(A\,C)\,(B)]$ or $[(A)\,(B\,C)]$. Plainly there is a 1–1 correspondence between the possible ways in which M points in a row can be 'connected up' and the partitions of these points into sets. The rows and columns of the transfer matrix will correspond with these possible partitions, and the matrix elements of the operators we have just been discussing are readily written down. For example:

$$\left.\begin{aligned}
P_{AB}[(A\,B)\,(C)] &= [(A\,B)\,(C)],\\
Q_{AB}[(A\,B)\,(C)] &= 0,\\
P_{AB}[(A)\,(B\,C)] &= 0,\\
Q_{AB}[(A)\,(B\,C)] &= [(A\,B\,C)],\\
D_A[(A\,B)\,(C)] &= 0,\\
D_A[(A)\,(B\,C)] &= [(A)\,(B\,C)],\\
E_A[(A\,B)\,(C)] &= [(A)\,(B)\,(C)],\\
E_A[(A)\,(B\,C)] &= 0,
\end{aligned}\right\} \qquad (7)$$

correspond to the above definitions of the operators in words. In this representation the P's and D's are wholly diagonal, the E's and Q's are wholly non-diagonal.

We can now verify that the operators described above do take proper account both of the changes in connectivity of the 'outside' set of points and of the weights to be given to each possible subgraph in the Whitney polynomial as we build the lattice up one point at a time. The transfer matrix is thus a product of pairs of such operators. (We make the usual assumption that the lattice is wrapped round a cylinder, so that column M+1 is identical with column 1. For M large, it makes little difference whether we dispose our points on the cylinder in 'screw' fashion or in successive rings, and the difference can easily be investigated in a particular case.)

We impose a further boundary condition (standard in this type of problem) that the initial and final connectivities are to be the same after a large number of lattice points have been added, in other words that if we begin with the connectivity $(A)(B)(C)$ we restrict ourselves to graphs in which the last three points added are also isolated from one another, and similarly for other initial connectivities. This means that we must work with the *trace* of the transfer matrix. As usual, this corresponds simply to identifying the first row of points with the (N+1)th. Since the transfer matrix is effectively the N-th power of an operator corresponding to adding one row, and we are concerned with the case of large N, the problem is also that of finding the largest eigenvalue of the transfer operator for one row, which itself consists of a product of M pairs of operators of the type described above.

6. Abstract properties of the transfer operators

Certain results can be proved from the abstract properties of these operators without use of any representation of them. We have, for example,

$$P_{AB}^2 = P_{AB}, \quad Q_{AB}^2 = 0, \quad P_{AB}Q_{AB} = Q_{AB}, \quad Q_{AB}P_{AB} = 0$$

and analogous properties of the D's and E's. Also

$$D_A P_{AB} = P_{AB} D_A = 0, \quad D_A Q_{AB} = 0, \quad P_{AB} E_A = 0. \tag{8}$$

We notice from (7) that the P's and D's leave the number of parts of any partition the same, every Q reduces the number of parts by one, while every E increases the number of parts by one. Therefore, if any product of such operators is multiplied out, the only terms that can contribute to a trace are those which contain equal numbers of Q's and E's. It follows that the trace of any such operator is unaffected by the transformation

$$Q_{ij} \to \alpha Q_{ij} \quad E_i \to \alpha^{-1} E_i \tag{9}$$

(provided that α is independent of i and j and is a number not an operator). The interpretation of the terms in the transfer matrix that arise solely from products of the Q's and E's is immediate. Consider the product

$$\ldots(1 + x_H Q_{BC})(x_V + E_B)(1 + x_H Q_{AB})(x_V + E_A)\ldots. \tag{10}$$

We have made a distinction between horizontal and vertical lines of the lattices by giving them separate selector variables x_H and x_V but otherwise this operator is

obtained from the product of operators that generates the Whitney polynomial by omitting all the terms involving P's and D's. Which subgraphs does the trace of (10) enumerate?

If we start and finish with all M points in a row connected we enumerate just the trees on the lattice. The absence from (10) of all terms involving the P's means that the graphs involved cannot contain any circuits, while the fact that there are no terms involving D's means that we are concerned only with one-component graphs. (We give in the appendix the straightforward, but rather lengthy, graph-theoretical argument on which the last statement is based. For the plane square lattice, it follows also from the duality relations that we shall prove shortly.) Other matrix elements making up (10) correspond to our starting and finishing with graphs containing more than one component, that is to say with 'forests' of two or more non-overlapping trees. By using relations (8), the operators for the Whitney polynomial can be factorized, and instead of (10), we have, for the whole transfer operator

$$\ldots(1+x_H Q_{BC})\,(1+yP_{BC})\,(x_V+E_B)\,(1+D_B x_V)\ldots. \tag{11}$$

The trace of any product of the Q's and E's either vanishes, or designates a tree (together with the 'forest' generated from it by omitting one or more of the branches in the first and last rows of the lattice). The effect of the factors involving the P's and D's is to weight some of the trees with factors of the type 1, $1+y$ or $1+1/x_V$, the precise number of such factors depending on the particular tree and on the order in which the factors come in (11). Tutte (1954) showed that, if we take all the trees in the lattice and weight each one of them according to a rather complicated prescription based on putting all the lines in the lattice in some sort of dictionary order, looking at each tree and weighting each line in the lattice using, for each, one of these factors 1, $(1+y)$ or $(1+1/x)$, we arrive at what Tutte calls the 'dichromate' of the lattice, which, to a factor, is just the Whitney polynomial (6). It can, in actual cases, be explicitly verified that the process indicated by (11) is equivalent to numbering the lines of the lattice in a particular way and then applying Tutte's prescription (1954) (the result of which he proved to be independent of the numbering convention actually used).

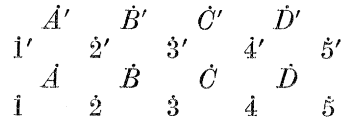

FIGURE 3

To derive the dual relations between these operators let figure 3 represent a small portion of the original lattice denoted by letters. As usual, the dual lattice is built up of points, one for each empty polygon, which are denoted by numbers. Corresponding lines, e.g. $1'\,2'$ and $A\,A'$, or $2\,2'$ and $A\,B$ intersect at right angles. We associate graphs on the original lattice with graphs on the dual lattice according to the following rule. If a line, e.g. $A\,A'$, is present in the original graph its counterpart

$1'\,2'$ is *absent* from the associated graph on the dual lattice and vice versa. In figure 3, we suppose that the dual lattice has been built up as far as the lines $1'\,2'$, $2'\,3'$, $3'\,4'$, etc., so that $1'$, $2'$, $3'$, etc. are 'outside' points and that the original lattice has been built up as far as the lines $A\,A'$, $B\,B'$, $C\,C'$, so that A', B', C' are 'outside' points in the original lattice. (Lines like $A'\,B'$, $B'\,C'$ have not yet been added.) In the dual lattice the operator $P_{2'3'}$ selects just those graphs for which the points $2'$, $3'$ are connected, either directly by the line $2'\,3'$, or else indirectly by paths like $2'\,2\,3\,3'$. The assertion that there is, in the dual lattice, such a direct or indirect path connecting $2'$ and $3'$ is equivalent to saying that, in the original lattice, there is *no* path connecting B' with either A' or C' nor, for that matter, with any of the other 'outside' points like D' in the original lattice. Furthermore any path connecting B' and C' on the original lattice (with the exception of the direct line $B'\,C'$ which has not yet been added to it) must inevitably cross somewhere any path that connects $2'$ and $3'$ on the dual lattice (since we may not use lines like $B'\,C'$).

In other words, if we associate graphs on the original lattice with graphs on the dual lattice by the rule just given, the operator $P_{2'3'}$, selecting graphs in which $2'$ and $3'$ are joined in the dual lattice, is equivalent to the operator $D_{B'}$, which selects graphs on the original lattice for which B' is isolated from all other 'outside' points. Reciprocally, we can infer the equivalence of $D_{3'}$ and $P_{B'C'}$, etc. We can also infer the equivalence of operators like $Q_{2'3'}$ and $E_{B'}$. For $Q_{2'3'}$ selects those graphs in which $2'$ and $3'$ are *not* connected in the dual lattice and then introduces such a connexion, and this is easily seen to be the counterpart of selecting those graphs in which B' is connected to at least one of the outside points $A', C', D', \ldots$, on the original lattice and then isolating B' from all of them.

It is easily verified that this dual relationship between operators has the relationship of Whitney (1932)

$$\mathrm{W_L}(x, y) = x^{rL} y^{nL}\, \mathrm{W_L}\left(\frac{1}{y}, \frac{1}{x}\right) \tag{12}$$

as a particular consequence. Sykes & Essam's (1964) relations between the generating functions for the expected numbers of components of a graph and its dual then follows as a particular case, using $(6a)$.

7. Particular representations of the transfer operators

A fairly obvious principle to try out is to represent the nodes of connexion among the points, $A, B, C \ldots$ as follows:

$$(A) \text{ by } \left(\frac{1+\mu_A}{2}\right), \quad (AB) \text{ by } \left(\frac{1+\mu_A\mu_B}{2}\right), \quad (ABC) \text{ by } \left(\frac{1+\mu_A\mu_B\mu_C}{2}\right), \text{etc.} \tag{13}$$

so that, for example the mode of connexion

$$(A)\,(BCD)\,(EF) \text{ is represented by } \left(\frac{1+\mu_A}{2}\right)\left(\frac{1+\mu_B\mu_C\mu_D}{2}\right)\left(\frac{1+\mu_E\mu_F}{2}\right).$$

It is then easy to obtain related representations of particular combinations of the operators P and Q and of D and E. For example, it is readily verified that D_A+E_A is represented by $\frac{1}{2}(1+S_A)$ because this operator sends

$$\left(\frac{1+\mu_A}{2}\right)\rightarrow\left(\frac{1+\mu_A}{2}\right);\quad\left(\frac{1+\mu_A\mu_B\mu_C}{2}\right)\rightarrow\left(\frac{1+\mu_A}{2}\right)\left(\frac{1+\mu_B\mu_C}{2}\right), \tag{14}$$

i.e. it sends $(A)(BC\ldots)$ into itself and (ABC) into $(A)(BC)$, etc. Moreover, $1+C_AC_B$ can represent $2P_{AB}+Q_{AB}$ because it sends

$$\left(\frac{1+\mu_A}{2}\right)\left(\frac{1+\mu_B}{2}\right)\rightarrow\left(\frac{1+\mu_A\mu_B}{2}\right);\quad\left(\frac{1+\mu_A\mu_B\mu_C}{2}\right)\rightarrow 2\left(\frac{1+\mu_A\mu_B\mu_C}{2}\right). \tag{15}$$

However, these results proved difficult to generalize, the factors of 2 in (15) are very troublesome and a fundamental flaw in this representation was found. We have seen that for $\mathrm{M}=3$ there are five different possible modes of connexion but the above representations of them are *not*, as they should be, linearly independent. For M large, there are too few linearly independent functions of the μ's, 2^{M} in fact, to match the number of possible modes of connexion of a row of M points, which, as we shall see presently, is asymptotically proportional to 4^{M} for a planar lattice.

However, some of the results suggested by (14) and (15) are, in fact, correct. If these representatives were truly linearly independent, the problem of calculating the trace of the corresponding transfer matrix would become equivalent to the solution of the Onsager problem (1944) (after making the transformation of operators $C_r\rightarrow S_r$; $S_r\rightarrow C_r$). In fact Kasteleyn & Fortuin (1969) have shown, by an entirely different method, that the Onsager problem without magnetic field is, in fact, equivalent to the result suggested by (14) and (15), namely to an enumeration of the subgraphs of the lattice according to their numbers of lines, an extra factor of 2 being inserted for every independent circuit in each subgraph. (According to (15) a factor 2 is associated with each P type operator.)

The above suggests that we need 2M spin variables to form the basis of a representation of all the distinct ways in which M points $A, B, C, \ldots$ in an open row can be connected. We first classify those 'modes of connexion' that are possible on a *planar* lattice. (Already, for $\mathrm{M}=4$, we notice that the mode $(AC)(BD)$ is impossible, since it certainly implies some crossing of bonds. We are already aware of quite a number of enumeration problems that become impossible if the lattice is non-planar so we shall be wise to take account of this point.) Point A in the row is either isolated, or is connected to one or more other points in the row. Choose the farthest of these from A, say K, then K cannot be connected to any point to its right but may be connected to any or all of the points between it and A. Because of the existence of the connexion between A and K none of the points between A and K can be connected to points to the right of K without some crossing of bonds. Let $f(n)$ be the number of ways of connecting up n points in a row, subject to the above restriction. Then

$$f(n)=f(n-1)+f(n-2)+f(n-3)f(2)+f(n-4)f3)\ldots. \tag{16}$$

mode (A) mode (AB) mode (AC) mode (AD)

The first term corresponds to point A being isolated. There are then $f(n-1)$ ways of connecting up the remaining points. If A is connected solely to B, there are $f(n-2)$ ways of connecting up the remaining $n-2$ points. If point A is known to be connected, at the farthest, to point C, point C may, or may not, be connected also to point B hence the factor $f(2)$. The factor $f(n-3)$ then describes possible modes of connexion of the $n-3$ points to the right of C. If point A is known to be connected, at the farthest, to point D, point D may, or may not, be also connected to either or both of points B and C, hence the factor $f(3)$ and the factor $f(n-4)$ describes the modes of connexion of $n-4$ points to the right of D, etc. Equations such as (16) occur in a large number of enumeration problems, and the generating function is of a well known type.

Defining

$$g(z) = \sum_{n=1}^{\infty} f(n)\, z^n,$$

we find easily from (16) that

$$g(z) = \frac{1-2z-(1-4z)^{\frac{1}{2}}}{2z}. \tag{17}$$

Equation (17) confirms the statement that the number of possible modes of connexion is ultimately proportional to 4^{M}.

We have already stated that a very large number of sets of objects of mathematical and physical interest are enumerated by (17). For example:

The quantum states of an assembly of 2M electrons, with total spin zero (which implies a magnetic moment of zero).

The number of independent commutators that can be formed of $\mathrm{M}+1$ operators.

The number of 'lattice permutations' (in the mathematical sense) of 2M numbers in an $(\mathrm{M} \times 2)$ Young tableau.

The number of even–odd pairings of 2M points round a circle that can be realized without any crossing of the straight lines joining the M pairs.

The number of one-dimensional random walks of 2M steps, each of which may be to the right or the left, that eventually return to the origin, subject to the condition that no part of the walk ever goes to the left of the origin.

We follow the treatment of the Heisenberg problem used by Húlthen (1938) and others. We study an assembly of 2M spins which we label by numbers and use the bracket notation [1 2] to mean $(\mu_1 \text{–} \mu_2)$, etc. We can show inductively that there is a (1–1) correspondence between their wavefunctions with total spin zero and the possible modes of connexion of an 'outside' row of M points on a planar lattice. Using the classification (16), we begin with [1 2] whenever the first 'outside' point A in the lattice is isolated, we begin with [1 4] whenever the mode of connexion on the lattice is of type $(A\,B)$, with [1 6] whenever the mode of connexion is of type $(A\,C)$, with [1 8] whenever it is of type $(A\,D)$, etc. Proceeding inductively, we can infer from equation (16) a 1–1 correspondence between Húlthen type wavefunctions involving 2M spins and possible modes of connexion involving a row of M points on

a planar lattice given that it exists for smaller values of M. Specifically, we have for

$$\mathrm{M}=2 \quad [1\,2]\,[3\,4]\rightarrow(A)\,(B),\ [1\,4]\,[2,3]\rightarrow(A\,B),$$

and for

$$\left.\begin{aligned}\mathrm{M}=3 \quad & [1\,2]\,[3\,4]\,[5\,6]\rightarrow(A)\,(B)\,(C),\\ & [1\,2]\,[3\,6]\,[4\,5]\rightarrow(A)\,(B\,C),\\ & [1\,4]\,[2\,3]\,[5\,6]\rightarrow(A\,B)\,(C),\\ & [1\,6]\,[2\,3]\,[4\,5]\rightarrow(A\,B\,C),\\ & [1\,6]\,[2\,5]\,[3\,4]\rightarrow(A\,C)\,(B).\end{aligned}\right\} \tag{18}$$

Húltheu (1938) studied the problem of a one-dimensional array of electrons with a nearest-neighbour interaction of Heisenberg type, with $\Delta = 1$ in (1). Such an 'isotropic' Heisenberg interaction can be reduced to a permutation operator $1-\mathrm{T}_{12}$ where T_{12} sends μ_1 and μ_2 into one another. We have, in fact

$$\left.\begin{aligned}(1-\mathrm{T}_{12})\,[1\,2] &= 2[1\,2],\\ (1-\mathrm{T}_{23})\,[1\,2]\,[3\,4] &= [4\,1]\,[2\,3],\\ (1-\mathrm{T}_{23})\,[4\,1]\,[2\,3] &= 2[4\,1]\,[2\,3].\end{aligned}\right\} \tag{19}$$

That is to say that these permutation operators are of just the type we require for discussing connexion problems on a lattice. $(1-\mathrm{T}_{12})$ always has [1 2] as end-result, corresponding, according to (18), to configurations with point A isolated and must therefore represent $2D_A+E_A$. Also, according to (19), $(1-\mathrm{T}_{23})$ will always have [2 3] as end result. Examination of representation (18) shows that [2 3] always means that points A and B on the lattice are connected (and analogous results are true generally) and we conclude that operator $(1-\mathrm{T}_{23})$ represents $2P_{AB}+Q_{AB}$.

Thus, we are saddled with unwanted factors of two of the same type as that which appeared in (15). However, we have got over the fundamental difficulty that vitiated representations of the type (13), since we can now prove formally that the number of independent Húlthen wavefunctions for 2M spins is precisely the same as the number of *admissible* modes of connecting up M points in a row on a planar lattice. (An inductive argument, based on a comparison of expressions (16) and (18), in fact shows how to set up a (1–1) correspondence between these two sets of entities.) We are led to look for transformations of these operators which nevertheless retain the form of the relations (19), but with different numerical coefficients. Such transformations indeed exist, but the transformed operators are complicated.

The most useful type of operator to replace $(1-\mathrm{T}_{12})$ in (19) seems to be the following:

$$U_{12}=\left[\frac{r}{s}+C_1C_2\right]\frac{(1+s_1)\,(1-s_2)}{4}+\left[\frac{s}{r}+C_1C_2\right]\frac{(1-s_1)\,(1+s_2)}{4}, \tag{20}$$

which was found by a systematic study of operators obeying relations like (19). The Húlthen type wavefunction is replaced by

$$[1\,2]=r\,\frac{(1+\mu_1)\,(1-\mu_2)}{4}+s\,\frac{(1-\mu_1)\,(1+\mu_2)}{4}, \tag{20'}$$

which reduces to $\mu_1 - \mu_2$ if $r = -s = 2$ for which case (20) reduces to $(T_{12} - 1)$ and we recover (19). Using these new operators and Húlthen symbols it will be found that, instead of relations (19) we have, for example,

$$\left.\begin{aligned} U_{34}\,[3\,4] &= \left(\frac{r}{s}+\frac{s}{r}\right)[3\,4], \\ U_{34}[2\,3]\,[4\,5] &= [2\,5]\,[3\,4], \\ U_{34}[3\,6]\,[4\,5] &= [3\,4]\,[5\,6], \\ U_{34}[1\,4]\,[2\,3] &= [1\,2]\,[3\,4]. \end{aligned}\right\} \tag{19'}$$

In these relations, we suppose that the 2M electrons are arranged in a ring and are numbered in a line $1, 2, 3, \ldots, n-1, n$. The last three relationships can be represented graphically. They correspond to the three situations that can occur if 3 and 4 are in different brackets. The two points joined to 3 and 4 can be both to the left of 3, both to the right of 4, or 3 can be joined to a point on its left and 4 to a point on its right. These situations are shown graphically in figure 4.

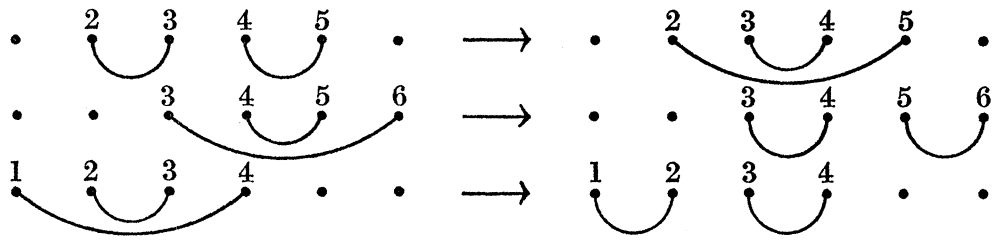

FIGURE 4

This represents the three topologically distinct ways in which electrons 3 and 4 can each be associated with one other electron, without any crossing of lines, that is, excluding functions like [1 4] [2 5]. It is known that sets of wavefunctions such as (18), in which each bracket contains one odd and one even number and 'crossings' are not allowed, form a linearly independent set. In the appendix, we prove that the more general functions formed out of 'generalized Húlthen brackets' like (20′) are also linearly independent. Relations (19′) differ slightly in form from (19) in that in (19′) two numbers in a bracket always appear in their natural cyclic order.

We now suppose that these electron spins are disposed on the *lines* of an auxiliary lattice, which is related to the points on the original lattice (shown in brackets as $(A)\,(B)\,(C)$, etc.) in the manner shown in figure 5. This exhibits a relationship between a row of M points in the original lattice and a set of 2M lines that we group into odd–even pairs, according to Húlthen's formalism. As exemplified in expressions (18), each possible way of grouping the lines into odd–even pairs is associated with a mode of 'connecting up' a row of M points on the original lattice by bonds in this lattice. Thus, the presence of [1 2] means that point (A) is isolated, the presence of [2 3] means that points (A) and (B) are joined, etc. It can be verified that

operators (20) represent the following abstract operators (see the definitions of P_{AB}, Q_{AB}, D_A, E_A in § 5).

$$U_{12} = \left(\frac{r}{s}+\frac{s}{r}\right) D_A + E_A; \quad U_{23} = \left(\frac{r}{s}+\frac{s}{r}\right) P_{AB} + Q_{AB}.$$

The μ's in (20) and (20′) are associated with the *lines* of the auxiliary lattice shown in figure 5.

We shall be interested in finding the trace of a product such as

$$\ldots(1+xU_{45})\,(1+xU_{23})\ldots(1+XU_{34})\,(1+XU_{12})\ldots, \tag{21}$$

where the selector variables x and X are usually different for a problem of 'percolation' or 'chromatic' type. Also in the 'percolation' problem we are interested in the case $r/s+s/r = 1$, i.e. r/s is complex. We shall show presently that, apart from these analytic complications, the finding of the trace of an operator such as (21) is effectively equivalent to solving problems of 'generalized ice' type as effected by Lieb (1967*a* to *d*).

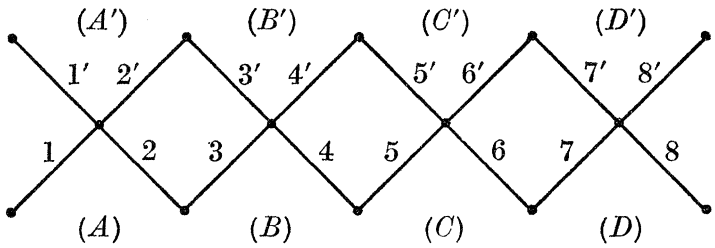

FIGURE 5

Both the mathematical treatment and the interpretation of 'ice-like' problems are very much simplified if we build up our lattice diagonally instead of horizontally or vertically. Lieb (1967*a* to *d*) solved his problems by setting up operator relations between 'arrow configurations' in successive rows of vertical arrows (thus losing the symmetry between vertical and horizontal). Their operator structure is complicated, and their relationships with Heisenberg type problems only become apparent when their eigenfunctions are found. From the new point of view, the relevant Heisenberg-like operators can be written down almost directly, for an 'ice-type' problem or for the problem on the auxiliary lattice that we associate with a 'percolation type problem'.

We use a new method of building up a plane square lattice, line by line this time. We associate a 'spin' variable with each line, according to the direction of its arrow, and we number the lines according to the conventions shown in figures 5 and 6*a*. We turn the plane square lattice anticlockwise through 45° (compare figure 6*b*). Each row of lines is built up, one line at a time, and the lines are added in the order $1\,2\,3\ldots 1'\,2'\,3'\ldots 1''\,2''\,3''$ (figure 6*a*). These remarks apply both to the actual lattice in an 'ice-like' problem or to the auxiliary lattice that we use in a 'percolation' type problem. An arrow (or spin variable) is associated with each of the lines in figure 6*a* or 6*b*.

We restrict ourselves again to arrangements of arrows such that, at each node of the lattice shown in figure 5 there are 0, 2 or 4 arrows in the positive directions. We use the convention that a positive direction of arrow is upwards or to the right (figure 6*b*) and is associated with $\mu = +1$, or with $\frac{1}{2}(1+\mu)$. The result of this restriction is that there are again eight possible types of node (figure 7). If we wish to assign different weights to them, we can do this by means of operators of generalized

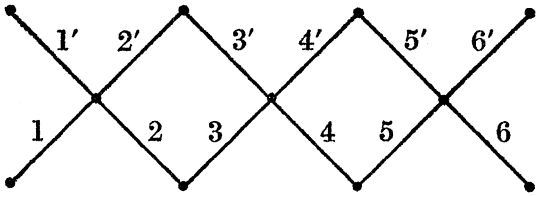

FIGURE 6*a*

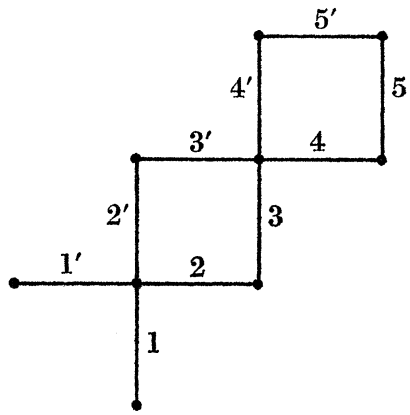

FIGURE 6*b*

(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
+	−	−	+	+	−	+	−
+ · +	− · −	+ · +	− · −	+ · −	− · +	− · +	+ · −
+	−	−	+	−	+	−	+

FIGURE 7

Heisenberg type. Suppose that we have added all the lines forming the row (1 2 3 4 5 ...) in figure 6*a*. The operator describing the possible ways of adding the pair of lines 1′ 2′ can now be written down as a sum of terms, one term corresponding to each permitted type of node. The conventions for distinguishing node types are exhibited in figure 7 in terms of positive and negative signs and will be found to agree with those of figure 1 (which are expressed in terms of arrows).

The form of operator that we now use is associated with a sum of terms, one corresponding to each of these types of node. The operator associated with the node of type (4) is, for example, $C_1C_2(1+S_1)(1-S_2)/4$. In words, we first select from all the possible configurations of the row (1 2 3 4 ...) (figure 6*a*) those corresponding to bond 1 being positive and bond 2 negative, by means of the operator $\frac{1}{4}(1+S_1)(1-S_2)$. The further operator C_1C_2 now changes $\frac{1}{4}(1+\mu_1)(1-\mu_2)$ to $\frac{1}{4}(1-\mu_1')(1+\mu_2')$ in view of the fact that this correctly describes the configuration (1′ negative, 2′ positive) of the two remaining bonds at a node of type (4) (see figures 6*b* and 7). For some types

of node the operator C_1C_2 is absent, for example the operator corresponding to the addition of a node of type (1) is just $\frac{1}{4}(1+S_1)(1+S_2)$ (see figure 7). The effect of restricting ourselves to nodes with even numbers of positive arrows is that operators C_1 and C_2 never appear separately.

Rather than writing down these 'Heisenberg-like' forms of each of the operators corresponding to nodes of types (1) to (8), it is more illuminating to define each of the operators J_1 to J_8 as the effect of adding the corresponding type of node to the lattice in the position (1 2, 1′ 2′) and to express operators such as C_1C_2, S_1S_2, etc. in terms of them.

TABLE 1

$$
\begin{aligned}
I &= J_1+J_2+J_7+J_8\\
S_1S_2 &= J_1+J_2-J_7-J_8\\
S_1 &= J_1-J_2+J_7-J_8\\
S_2 &= J_1-J_2-J_7+J_8\\
C_1C_2 &= J_3+J_4+J_5+J_6\\
C_1C_2S_1S_2 &= -J_3-J_4+J_5+J_6\\
C_1C_2S_1 &= -J_3+J_4+J_5-J_6\\
C_1C_2S_2 &= -J_3-J_4+J_5-J_6
\end{aligned}
$$

For the first four 'diagonal' operators the configurations of the 'initial' pair of bonds (1 2) and the 'final' pair of bonds (1′ 2′) are the same, for the last four 'off-diagonal' operators the signs of bonds 1 and 2 are both reversed.

In the original 'ice' problem we excluded nodes of types 7 and 8 because (see figure 1) they correspond to all arrows pointing respectively away from the node or towards it, which are excluded by the 'ice' condition. All the other types of node from 1 to 6 are permissible and are weighted equally. Therefore, the problem of calculating the entropy of the 'ice' model reduces to that of calculating the trace of the product of operators of the type $[\frac{1}{2}(1+S_1S_2)+C_1C_2]$, one such operator for each node of the lattice. Similarly, for the generalizations of the 'ice' problem studied by Lieb (1967*a* to *d*), the relevant operators are now *weighted* sums of the operators J_1 to J_6, the relative weights given to them being the various Boltzmann factors appropriate to each type of node.

Obviously, the operator forms of these problems are greatly changed by this device of building up the lattice in a diagonal, rather than in a horizontal or vertical direction, and should lead to simpler treatments. We have shown that problems of the 'colouring' or 'percolation' type are also reducible to these 'generalized Heisenberg' problems. We have, however, the additional complication that the addition of one row of nodes 1 to M to the original lattice corresponds to the addition of a row of 2M lines to the auxiliary or 'Heisenberg' lattice shown in figures 5 and 6 and we have further pointed out that such problems will, in general, involve different selector variables for operators of the two types, U_{12}, U_{34}, U_{56}, etc., and U_{23}, U_{45}, U_{67}, etc.

It has been pointed out by Fan & Wu (1970) that symmetry and other relations lead to a very large number of possibilities of transforming these 'ice-like' problems into one another. The device of building up the lattice diagonally rather than horizontally or vertically obviously opens up a whole fresh set of such possibilities.

8. The general Whitney problem in operator form

We set out below the Whitney problem for a plane square lattice, express it in operator form and then convert it into a Heisenberg-like problem on the auxiliary plane square lattice. The problem will then be specialized to the 'percolation' and 'chromatic polynomial' cases.

The full Whitney problem is to evaluate the sum (over all subgraphs G of the lattice containing L points)

$$\sum_G = Z^{C_G} Y^{S_G} x_H^{l_H} x_V^{l_V} \mathrm{W}(x_H, x_V, Z, Y), \tag{22}$$

where $(\mathrm{L}-C_G)$ and S_G are respectively the rank and nullity of G, and l_H, l_V are the numbers of horizontal and vertical bonds in G. Z, Y, x_H, x_V are the corresponding selector variables. Because of the Euler relation.

$$C_G = \mathrm{L} - l_H - l_V + S_G$$

one of these four selector variables is redundant. (We have three independent selector variables compared with Whitney's two because we desire to keep separate records of the vertical and horizontal bonds in G.)

In operator form the evaluation of W is equivalent to finding the trace of the product of the following type

$$\mathrm{W}(x_H, x_V, Z, Y) = \mathrm{tr}\,\Pi\,(x_V + ZD_A + [E_A/\alpha])\,\Pi\,(1 + Yx_H P_{AB} + \alpha x_H Q_{AB}), \tag{23}$$

one factor for each horizontal or vertical bond on the lattice, where, as we have seen from equation (9), α is a parameter that can be chosen arbitrarily without affecting the trace. We can write this relationship slightly more symmetrically thus

$$x_V^{-\mathrm{L}}\,\mathrm{W} = \mathrm{tr}\,\Pi \ldots \left(1 + \frac{Z}{x_V} D_A + \frac{E_A}{\alpha x_V}\right) \Pi\,(1 + Yx_H P_{AB} + \alpha x_H Q_{AB}) \ldots, \tag{24}$$

and the dual transformation can be shown, by applying the argument that led to equation (12), to send

$$x_H^{-1} \to x_V', \quad x_V^{-1} \to x_H', \quad Y^{-1} \to Z', \quad Z^{-1} \to Y', \tag{25}$$

i.e. the dual transformation interchanges horizontal and vertical lines present and absent and also components and independent circuits present and absent. Equation (12) is a particular case of this.

For the theory given above to be applicable, the ratio of the coefficients of D_A and E_A must be the same as the ratio of the coefficients of P_{AB} and Q_{AB}, which implies $\alpha^2 = YZ$. If, in expression (20), we write e^{θ} for r/s and use (19) we conclude that

$$U_{12} \quad \text{represents} \quad 2\cosh\theta D_A + E_A,$$
$$U_{23} \quad \text{represents} \quad 2\cosh\theta P_{AB} + Q_{AB}.$$

With the above choice of α, the selector variables appearing in expression (20), that is in the operator product

$$\ldots(1 + XU_{12})\,(1 + XU_{34}) \ldots (1 + xU_{23})\,(1 + xU_{45}) \ldots \tag{26}$$

are related to the selector variables occurring in the Whitney polynomial (22) as follows

$$X = Z^{\frac{1}{2}}/Y^{\frac{1}{2}}x_V, \quad x = Y^{\frac{1}{2}}x_H/Z^{\frac{1}{2}}, \quad 2\cosh\theta = (YZ)^{\frac{1}{2}}. \tag{27}$$

The chromatic polynomial is, to a factor, the Whitney polynomial for the following special values of these variables: $Z = 1$, $Yx_H = -1$ (a weight of -1 for each line completing a circuit), $x_H = x_V = -1/k$ (a weight of $-1/k$ for each other line) from which we conclude that in (26) $X = -k^{-\frac{1}{2}}$, $Y = k$, $x = -k^{\frac{1}{2}}$, $2\cosh\theta = k^{\frac{1}{2}}$. In terms of the J operators, Table 1 and expression (20) of text, we have

$$U_{12} = J_3 + J_4 + \mathrm{e}^{-\theta}J_7 + \mathrm{e}^{\theta}J_8.$$

For the particular choice of selector variable occurring in the chromatic polynomial the weights given to each type of node by the operator $1 + XU_{12}$ are indicated by

$$1 + XU_{12} = J_1 + J_2 - k^{\frac{1}{2}}J_3 - k^{\frac{1}{2}}J_4 + (1 - k^{\frac{1}{2}}\mathrm{e}^{-\theta})J_7 + (1 - k^{\frac{1}{2}}\mathrm{e}^{\theta})J_8, \tag{28}$$

$1 + xU_{23}$ having an analogous expansion with $k^{\frac{1}{2}}$ replaced by $k^{-\frac{1}{2}}$. [The operators $J_1 \ldots J_8$ are of course different in the two cases operating respectively on $(\mu_1; \mu_2)$ and on $(\mu_2; \mu_3)$.]

We can also formulate the percolation problem as a particular case of the general Whitney problem expressed in operator form in (23) and (26). We are interested mainly in the expected number of disconnected components on the lattice as a function of x_H and x_V. This is given by

$$\bar{C}_G = \left[Z \frac{\partial}{\partial Z} \{\ln \mathrm{W}(x_H, x_V, Z, Y)\} \right]_{Y=Z=1}, \tag{29}$$

or we can calculate the sum of the expected numbers of components and circuits as follows

$$\bar{C}_G + \bar{S}_G = \left[Z \frac{\partial}{\partial Z} \{\ln W(x_H, x_V, Z, Z)\} \right]_{Z=1}, \tag{30}$$

where W is given by (23). The calculation of W itself is trivial for the special case $Y = Z = 1$, for we have simply that any of the L horizontal lines may be present or absent, so may any of the L vertical lines, and the generating function for all the subgraphs is simply

$$\mathrm{W}(x_H, x_V, 1, 1) = (1 + x_H)^{\mathrm{L}}(1 + x_V)^{\mathrm{L}},$$

since $Y = Z = 1$ weights all the subgraphs equally. The percolation problem is equivalent to calculating the differential coefficient with respect to Z, *afterwards* putting Z equal to 1. A more general version of the problem is to calculate W as a function of x_H, x_V and Z.

According to (24) this is the problem of calculating

$$x_V^{-\mathrm{L}}\,\mathrm{W}(x_H, x_V, Z, Z) = \mathrm{tr}\,\Pi \left(1 + \frac{Z}{x_V}D_l + \frac{1}{x_V}E_l\right) \times \Pi\,(1 + Zx_H P_{lm} + x_H Q_{lm}), \tag{31}$$

where we have put the disposable constant α equal to unity.

At present, we can give an exact solution of this problem in only one set of cases, that in which $x_H = 1/x_V = x$ (say). These are known (Sykes & Essam 1964, 1966), to be the critical cases of the percolation problem, for we have p_H, the probability that any given horizontal line is present is $p_H = x_H/(1+x_H)$ with a similar relation for p_V. Thus, for these cases $x_H x_V = 1$ implies $p_H + p_V = 1$, and $p_H + p_V \geqslant 1$ is the critical condition for large connected domains to form.

To evaluate $\mathrm{W}(x, 1/x, Z, Z)$ in the form (24) we want to calculate

$$\mathrm{tr}\,\Pi\,(1+xZP_{lm}+xQ_{lm})\ldots\,\Pi\,(1+xZD_l+xE_l)\ldots.$$

Using the representation (20) we conclude that this is equivalent to calculating

$$\mathrm{tr}\,\Pi\,(1+xU_{23})\ldots\,\Pi\,(1+xU_{12})\ldots, \tag{32}$$

where U_{12} represents $2\cosh\theta D_A + E_A$ and U_{23} represents $2\cosh\theta P_{AB} + Q_{AB}$ as before. For this problem

$$Z = 2\cosh\theta. \tag{33}$$

In terms of the J operators (table 1) we have

$$U_{12} = J_3 + J_4 + e^{-\theta}J_7 + \mathrm{e}^{\theta}J_8$$

with a similar expression for U_{23}. Also using table 1, we see that the operator $1+xU_{12}$ is represented by

$$1+xU_{12} = J_1 + J_2 + xJ_3 + xJ_4 + (1+x\,\mathrm{e}^{-\theta})J_7 + (1+x\,\mathrm{e}^{\theta})J_8, \tag{34}$$

and we suppose that the auxiliary lattice shown in figure 4 to be built up diagonally in the way shown in figure 5*a* and described above in words (p. 266). The addition of the lines (1′, 2′) in figure 5*a* corresponds to the application of the operator $1+xU_{12}$, the addition of the lines (3′, 4′) to the application of the operator $1+xU_{34}$ and so on. Proceeding to the next row of lines, the addition of the pair (2″, 3″) corresponds to applying $(1+xU_{23})$, the addition of the pair (4″, 5″) corresponds to applying $(1+xU_{45})$ and so on. That is to say that the addition of two rows of lines to the auxiliary lattice corresponds precisely to the successive application of the two operator products $\Pi(1+xU_{12})$ and $\Pi(1+xU_{23})$, which, in turn, corresponds to the successive application of the two operator products in (32) that is, to the addition of a row of points, and some or all of the lines incident to them, to the original lattice.

In the special case we are considering, $1/x_V = x_H = x$, the operators $1+xU_{12}$ and $1+xU_{34}$ both assign the following weights to the various types of node in the auxiliary lattice:

TABLE 2

node type	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
weight	1	1	x	x	0	0	$1+x\mathrm{e}^{-\theta}$	$1+x\mathrm{e}^{\theta}$

these weights being the same for both sets of operators. By taking two further steps, we can reduce this to a problem whose solution is known. We revert for a moment from a description of the node types in terms of spin variables (figure 7) to a description in terms of arrows (figure 1). Of the permitted types of node type (8) corresponds to a 'sink' of arrows, type (7) to a 'source' of arrows, all others corresponding to the

specification 'two in and two out'. We can therefore infer that, at all events if we have a 'torus' or 'screw' type of boundary condition so that there are no 'raw edges' of the original or of the auxiliary lattices, the numbers of nodes of types (7) and (8) must be exactly equal. It will, therefore, make no difference to the eigenvalues and traces of our operators if we replace both the weights $(1+x\,\mathrm{e}^{-\theta})$ $(1+x\,\mathrm{e}^{\theta})$ by the square root of their product $(1+x^2+2x\cosh\theta)^{\frac{1}{2}}$. We now apply the transformation corresponding to reversal of all the horizontal arrows in figure 1 which sends $J_1 \leftrightarrow J_4$, $J_2 \leftrightarrow J_3$, $J_5 \leftrightarrow J_7$, $J_6 \leftrightarrow J_8$, and changes the weights from those given in table 2 to those given in table 3 below. These are compared with the weights assigned to a 'generalized ice' problem of which the solution has been given by Sutherland (1967).

TABLE 3

node type	(1)	(2)	(3)	(4)	(5) & (6)	(7) & (8)
weight in transformed problem	x	x	1	1	$(1+x^2+2x\cosh\theta)^{\frac{1}{2}}$	0
weight in Sutherland's problem	$\mathrm{e}^{\delta/2T}$	$\mathrm{e}^{\delta/2T}$	$\mathrm{e}^{-\delta/2T}$	$\mathrm{e}^{-\delta/2T}$	$\mathrm{e}^{\epsilon/T}$	0

Comparison of these makes it evident that the problems are equivalent, if we make the identifications

$$x = \mathrm{e}^{\delta/T}; \quad 1+x^2+2x\cosh\theta = \mathrm{e}^{2\epsilon/T}\,\mathrm{e}^{\delta/T} \tag{35}$$

and introduce a multiplying factor $x^{\frac{1}{2}}$ for each node in the auxiliary lattice.

It is only in the special case $x_H x_V = 1$ that we can, at present, reduce the percolation problem to an 'ice-type' problem whose solution is known. If x_H differs from $1/x_V$ we can still carry through the same steps but we arrive now at what might be called a 'staggered ice' problem. By this we mean that now the auxiliary lattice has to be divided into two interlacing sublattices, with two different sets of weights for the six node types on the two sublattices. (Reference to figure 6*a* shows that the two sublattices in fact correspond to successive rows of nodes of the auxiliary lattice if we follow the plan of building it up diagonally described above.) This 'staggered ice' type of problem is akin to the antiferromagnetic Onsager–Ising problem. It can be handled by a suitable modification of the Bethe–Húlthen ansatz method, but we reserve discussion of this for another paper. For the present, we confine ourselves to deriving some exact results for the percolation problem in the critical cases $x_H x_V = 1$. (It is very reasonable that the critical cases of the percolation problem should correspond to equal weightings of the nodes in the two sublattices that make up the auxiliary lattice. In the Onsager–Ising antiferromagnetic problem the two sublattices become indistinguishable at the critical temperature.)

9. Exact results for the critical case of the percolation problem

Sutherland's (1967) result is that the transfer-matrix problem specified in table 3 has the same eigenfunctions as a Heisenberg type Hamiltonian with anistropy parameter Δ, where $2\Delta = 2\cosh(\delta/T) - \mathrm{e}^{2\epsilon/T}$ which, using (35) and (33), gives

$$\Delta = -\cosh\theta = -\tfrac{1}{2}Z; \ \mathrm{e}^{\delta/T} = x. \tag{36}$$

In using the result given by Sutherland (1967) to evaluate the Whitney polynomial $W(x, 1/x, Z, Z)$ for the limiting case of a large lattice, the following points must be remembered:

(*a*) The auxiliary lattice has twice as many nodes as the original lattice (see figure 5, where letters represent nodes of the original lattice and numbers lines of the auxiliary lattice).

(*b*) The initial factor $x^{\frac{1}{2}}$ for each node of the auxiliary lattice, to allow for the differences between the weighting of the nodes in Sutherland's problem and in the transformed form of our problem. (See the comparison in table 3.)

(*c*) The version of Sutherland's problem which is of interest to us corresponds to an 'ice' type problem with electric field zero. For this, the relevant value of Sutherland's parameter, y, corresponding to the largest eigenvalue of our problem, is zero.

We can now use table 3 and relations (36) to transcribe Sutherland's result to our notation. We find, using (31), (32) and (34):

$$W(x, 1/x, Z, Z) = x^{\frac{1}{2}L} \exp\left[L \int \rho(k)\, dk \ln\left\{\frac{(Z+x)^2 + 1 + 2(Z+x)\cos k}{x + 1/x - 2\cos k}\right\}\right], \quad (37)$$

where $\rho(k)$ is a function related to Δ, that is to say to Z in this problem, by an integral equation (Yang & Yang (1966), equation (6*a*)). For the case $y = 0$ that we are interested in, this integral equation can be solved explicitly by changing the variable from k to α by the transformation

$$e^{ik} = \frac{e^{i\mu} - e^{\alpha}}{e^{\alpha + i\mu} - 1}, \quad (38)$$

where $\cos\mu = -\Delta = \frac{1}{2}Z$. In terms of this new variable, the Yang & Yang integral equation is soluble by Fourier transforms, and we find

$$\rho(k)\, dk = \frac{d\alpha}{4\mu} \operatorname{sech}\left(\frac{\pi\alpha}{2\mu}\right), \quad (39)$$

which is valid for the interesting range of values $-1 < \Delta < 1$ (i.e. Z between 2 and -2). Using (38) and (39) in (37) together with the fact that the integral of $\rho(k)$ is $\frac{1}{2}$ (in conformity with the fact that for $y = 0$ there are just $\frac{1}{2}L$ factors in Sutherland's product expression for the largest eigenvalue of the transfer matrix), we find finally

$$W(x, 1/x, Z, Z) = x^{L} \exp\left[\frac{L}{4\mu} \int_{-\infty}^{\infty} d\alpha \operatorname{sech}\left(\frac{\pi\alpha}{2\mu}\right) \times \ln\left\{\frac{(1 + 2x\cos\mu + x^2)\cosh\alpha - \cos 3\mu - 2x\cos 2\mu - x^2\cos\mu}{(1 + 2x\cos\mu + x^2)\cosh\alpha - (x^2+1)\cos\mu - 2x}\right\}\right], \quad (40)$$

where $\cos\mu = \frac{1}{2}Z = \cosh\theta$.

It is straightforward, but tedious, to verify that, in the special case $Z = 1$, this reduces to the required form $(1+x)^{2L}/x^{L}$. [By the substitution $s = \sinh(\frac{1}{2}\alpha)$ (40) reduces to straightforward contour integrations for this special value of μ.]

For the special case $x = 1$, that is to say with horizontal and vertical bonds each open with a probability $\frac{1}{2}$, the critical value in the symmetric case, (40) simplifies to the following generating function:

$$W(1, 1, Z, Z) = \exp\left[\frac{L}{4\mu}\int_{-\infty}^{+\infty} d\alpha \operatorname{sech}\left(\frac{\pi\alpha}{2\mu}\right) \ln\left(\frac{\cosh\alpha - \cos 2\mu}{\cosh\alpha - 1}\right)\right]. \tag{41}$$

This integral has not yet been evaluated in closed form but its analytic behaviour is known, since it has already appeared in the exact treatment of Rys's F-model of an antiferroelectric (Lieb 1967*b*).

10. Discussion of the properties of generating function (41)

The integral can, in principle, be evaluated whenever μ is a rational multiple of π. The exact values in table 4 are enough to give a general idea of the behaviour of $\ln W$ as a function of μ or Z.

Table 4

μ	Z	$(1/L)\ln W$	
0	2	$4\ln[\Gamma(\frac{1}{4})/2\Gamma(\frac{3}{4})]$	$= 1.56632\ldots$
$\frac{1}{3}\pi$	1	$\ln 4$	$= 1.38629\ldots$
$\frac{1}{2}\pi$	0	$(4/\pi) \times$ Catalan's constant	$= 1.16624\ldots$
$\frac{2}{3}\pi$	-1	$3\ln\frac{4}{3}$	$= 0.86304\ldots$
π	-2	0	

Professor Cooper's results are given in the appendix (table 6). The case $Z = 1$, for which the generating function is trivial, is discussed above. The case $Z = 0$ is the problem of the number of trees on a plane square lattice, and checks with the value obtained from Kirchhoff's determinant (Temperley 1958). For $Z = -1$, table 3 shows that we recover the ice problem, all nodes being weighted equally for $x = 1$.

We infer that the form of $\ln W$ as a function of Z has a radius of convergence of 2. At $Z = 2$ the function has a natural boundary but all derivatives with respect to μ are finite (Lieb 1967*b*). At $Z = -2$, the generating function becomes oscillating, the contributions from even and odd values of $C_G + S_G$ cancelling out.

As already stated, (41), considered as a function of Z, is the generating function for $C_G + S_G$. At critical conditions the expected number of bonds is just L (2L bonds present each with probability $\frac{1}{2}$), so the expected numbers of circuits and components are equal. The integral is awkward to handle numerically, because of the logarithmic singularity at $\alpha = 0$. Professor D. C. Cooper has kindly tabulated the integral for us and estimated the first two derivatives with respect to $\ln Z$ at $Z = 1$, which gives the expected values of $C_G + S_G$ and $(C_G + S_G)^2$ for the percolation problem in the critical case. Unfortunately, the only comparison that is possible at present with series expansion work is with the two types of expansion, 'perimeter' and 'irreducible diagram' given by Sykes & Essam (1964, 1966). The convergence of either type of series *at* the critical probability $\frac{1}{2}$ is a matter for speculation, however, M. F. Sykes & J. W. Essam give (private communication) the following estimate for $\bar{C}_G$ on the

basis of much longer expansions now available. This is compared with the value obtained from (41) (table 5). Agreement can be considered excellent. Information is also available on mean sizes of components, but it is not easy to see how to make a valid comparison with (41), since (41) includes the contribution from isolated points in the subgraph, each isolated point contributing 1 to $\overline{C}_G$.

TABLE 5

Estimates of $\overline{C}_G$, the *expected* number of components for $p = \frac{1}{2}$	
from Professor Cooper's estimate of the derivative of (41)	$\overline{C}_G = \mathrm{L} \times 0.0980_7$
from eleven terms of perimeter series	$\overline{C}_G > \mathrm{L} \times 0.0939_7$
estimated contribution of remaining terms (from extrapolation)	$\mathrm{L} \times 0.004_1$

11. PROSPECT OF FURTHER ANALYTIC TREATMENTS OF INTERESTING PROBLEMS

We still have available only two *basic* analytic methods mentioned above, the Bethe–Húlthen 'ansatz' method and the Kaufman–Onsager 'spinor' method. The Bethe–Húlthen method depends for its success on fulfilment of the 'ice' condition or something equivalent, because, as we build up a lattice row by row, we must be able to assert that the total numbers of up and down spins remain constant from row to row. We have shown that a particular case of the percolation problem can be reduced to a problem of this type. Thus some versions of the Whitney polynomial problem can definitely be solved now for certain ranges of the selector variables. To what extent these ranges can be extended by analytic continuation and transformations of the problem still remains to be seen.

The situation of the Kaufman–Onsager (1949) method is rather different. We might expect to be able to factorize operators such as (20) (into the required form of products of exponentials of quadratic spinors) in special cases only. (We recall that the Onsager (1944) problem has itself only been solved for zero applied magnetic field.) Thus, if we use transformations like (19), we might expect to factorize an operator like (20) only if there were some definite relation between the selector variables, e.g. those for numbers of lines and numbers of circuits. If we consider the percolation operator (34), it can only be so factorized in the limiting case $Z = 0$, which, as has been pointed out above, enumerates trees and forests on the lattice, an already solved problem.

Since the Kaufman–Onsager method does not depend on the 'ice' condition, it is to be expected that it will solve problems outside the scope of the 'ansatz' method. An algebraic criterion determining whether or not an operator of the type occurring in (20) (when U is some linear combination of operators J_1 to J_8) can be so factorized would be very valuable.

Although it does not lead to anything new, it is, from this new point of view, instructive to look at the Onsager model with first and second nearest neighbour interactions. This can also be reduced to a 'generalized Heisenberg' type of problem in the manner of Fan & Wu (1969). Let the spins be arranged on a plane square

lattice. Draw all the bonds on the dual lattice that separate positive and negative spins. These boundaries form closed domains, and 0, 2, or 4 lines therefore pass through every node. Thus we have a problem to which the formalism (21) can be applied. Identifying positive arrows with lines and letting $e^{\pm H_1}$, $e^{\pm H_2}$ be the Boltzmann factors for like/unlike pairs of first/second nearest neighbours, we assign the weights shown in figure 8 to the eight types of node on the dual lattice.

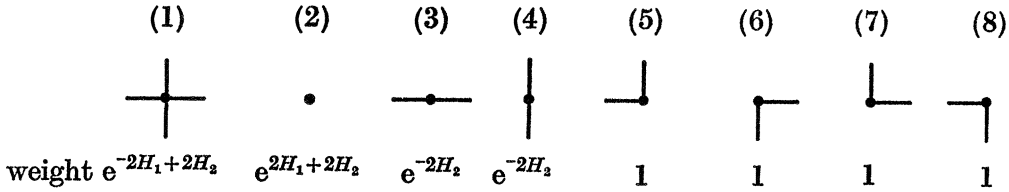

FIGURE 8

(The enumeration of pairs of first and second nearest neighbours is easily checked for each node.) The operator for each node on the dual lattice is easily written out, and it is readily verified that, for these weights, it can be factorized into

$$\tfrac{1}{2}(e^{2H_2}+1)\exp[-\tfrac{1}{2}H_1(S_1+S_2)][1+C_1C_2e^{-2H_2}]$$
$$\times[1+S_1S_2\tanh H_2]\exp[-\tfrac{1}{2}H_1(S_1+S_2)]. \quad (42)$$

The problem cannot be solved by the 'ansatz' method, because all eight types of node are involved. Although the operator *has* factorized, we cannot express *all* of S_1, S_2, C_1C_2, S_1S_2 in the required form as quadratic spinors! In the two limiting cases $H_1 = 0$ or $H_2 = 0$, we are concerned respectively with the smaller sets $C_1C_2, \ldots, S_1S_2$ or with $C_1C_2, \ldots, S_1, S_2, \ldots$, either of which *can* be so expressed. In either of these two cases we recover the Onsager (1944) problem.

It does not seem to be possible to derive the dimer problem *directly* as a limiting case of the Whitney polynomial. This contains terms of the type $Z^{\frac{1}{2}L}x_H^{l_H}x_V^{l_V}$ with $l_H+l_V = \frac{1}{2}L$, but many graphs of different structure also give rise to terms with the same powers of the selector variables. However Lieb (1967*e*), using a slightly different formalism, has shown that the dimer problem can be reduced to the estimation of traces of products of operators like $1+pC_1C_2(1+S_1)(1+S_2)$, which closely resembles the limiting form of (26) when the parameter α becomes large.

The problem of a mixture of monomers and dimers was formulated, though not solved, by Lieb (1967*e*), but only in terms of operators involving the C_r, by themselves, and thus not strictly of 'ice' type. The problem of 'rigid squares' in which a 'molecule' occupies a site on the lattice and the four neighbouring sites can also be formulated in this way, but again only in terms of operators involving odd powers of the C_r, and thus not of the 'ice' type.

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Appendix. Proofs of certain results assumed in the text

We prove the assertion made in the text that, if the operator product (23) is supposed to be expanded into individual products of operators of the type $\ldots D_A Q_{BC} E_C \ldots$ each such operator either vanishes or corresponds to just one possible subgraph on the lattice. Further, there is one D-type factor for every disconnected component of the subgraph. If we take any particular subgraph on the lattice, the rules given in the text tell us, at every step, which term to select out of the three that occur in every factor of the operator product (23). Furthermore, since the only operations described by this operator product are the addition or omission of bonds on the lattice, every term in this product must either vanish, if it calls for an impossible sequence of operations like P_{AB} followed by D_A, or else must correspond to a subgraph built up by such operations, that is to one of the subgraphs of the lattice.

Consider any disconnected component of a subgraph. In it we can define a unique point, which we call the summit, by the following rules:

(*a*) Take all the points that are connected, directly or indirectly by the lines in this component.

(*b*) Take the *highest row* of points in the lattice that has at least one point in set (*a*).

(*c*) Of the points in this row, take the one *furthest to the right* that is still in set (*a*).

This is the summit and there is exactly one summit for each component. Figure 9 represents a typical component of the subgraph. S is the summit of this component.

We claim that, if the operation of adding the point S' to the lattice is described by the operator D_S, then S, the point vertically below S', must be a summit. Consider the situation when the point S' has just been added. The operator D_S implies that: (*a*) S' is isolated after the addition of S' to the lattice *and* that (*b*) S was isolated immediately before S' was added (that is to say immediately after the addition of R'). Unless both these conditions are satisfied, the effect of D_S will produce an impossible operation, and the corresponding term would vanish in the operator product.

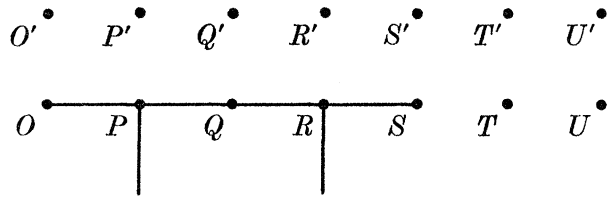

FIGURE 9

Now (*b*) implies that, immediately after the addition of R', S was not connected to R', Q', P' or O', that is S was not connected to any point to its left in the row immediately above it. Nor, since it was isolated, could S be connected to any point to its right, such as T or U in the same row. Further S cannot be connected to S', since the operator D_S in the operator product (23) implies the absence of the line SS', and the two points cannot be connected indirectly since by (*a*) and (*b*) they are both isolated from the set of points O', P', Q', R', T, U through which any such indirect path must pass. Since S is not connected to S', not to T nor to U, etc., it cannot be connected to any of the points T', U', etc., in the same row as and to the right of S' that are later added in the process of building up this row. This row therefore forms a barrier in the sense that no point in it can ever be connected to S. That is, we conclude that S is in the topmost row of the component. That it is the right-hand point follows easily. Suppose not. Then S is connected, via the bonds of the component, with some point, say U in the same row and to the right of S. It would be so connected at the moment of the addition of the point S' and the appropriate operation would then be E_S rather than D_S, because D_S only gives a possible operation if S is isolated. Thus we have a contradiction and can conclude that S *is* the right-hand point in the topmost row of the component.

Thus every summit point corresponds to a D operator. (A particular case of a summit is an isolated point with no lines incident to it.) There is exactly one summit point per component.

It is also necessary to prove linear independence for the 'wavefunctions' used in the text which consist of products of M 'generalized Húlthen brackets'. The generalized Húlthen bracket involves two of the spin-variables μ_i, μ_j.

$$[i,j] = \frac{r(1+\mu_i)(1-\mu_j)+s(1-\mu_i)(1+\mu_j)}{4}, \qquad \text{(A 1)}$$

where r and s are fixed constants. Our generalized 'wavefunctions' are products of M such brackets taken according to the following rules:

(a) In any bracket $i < j$.

(b) Every number between 1 and 2M appears just once.

(c) A pair of brackets $[a\,c][b\,d]$ with $a < b < c < d$ (which would correspond to 'crossing of bonds') never occurs.

We define 'round bracket symbols' $(i\,j)$ by the relation

$$(i\,j) = \frac{(1+\mu_i)(1-\mu_j)}{4} \tag{A 2}$$

and 'basic wave-functions' as products of M of these symbols not necessarily obeying the rules (a), (b), (c) but simply the conditions that there are exactly M positive spins and that each spin is mentioned once.

A generalized wavefunction is uniquely determined if we specify the first numbers in each of the M square brackets. Not all possible choices of these M numbers define possible wavefunctions, but two different generalized wavefunctions can never correspond to the same set of numbers.

Proof. Write the generalized wavefunction in the form

$$[a_1 b_1][a_2 b_2]\ldots[a_{\mathrm{M}} b_{\mathrm{M}}],$$

with $a_1 < a_2 < a_3 \ldots$. (Also $a_i < b_i$ because of (a) above.) Clearly $a_1 = 1$. We make some choice of the other $\mathrm{M}-1$ a's and try to choose the b's so that we have a permissible wavefunction. We must choose $b_{\mathrm{M}} = 1 + a_{\mathrm{M}}$. If we do not we must have a bracket $[a_j, 1+a_{\mathrm{M}}]$ with $a_j < a_{\mathrm{M}}$ and we cannot then choose any other number for b_{M} without violating (c). With the right-hand bracket fixed as $[a_{\mathrm{M}}, 1+a_{\mathrm{M}}]$, a repetition of the same argument shows that the only permissible choice of $b_{\mathrm{M}-1}$ is 'the smallest number above $a_{\mathrm{M}-1}$ that is not a_{M} or b_{M} that is, that has not already been used'. We proceed inductively, filling up the brackets in turn from the right, the choice at every step being determined by the rule: b_j is 'the smallest number greater than a_j that has not already been used'. It is easily shown inductively that rule (c) above is violated if any other choice is made for any of the b_j. On the other hand, it can happen at some stage that *no* b_j can be so chosen, which means that the corresponding choice of a_j's does not correspond to a permissible wave function. Thus, we can label any generalized wavefunction by specifying the particular choice of a_j's that gives rise to it. We can define a binary number by means of the a_j's, by replacing a_j by the power $2^{2\mathrm{M}-j}$. For example, for $\mathrm{M} = 3$, the permitted pairings are ordered in the following way:

$$\left.\begin{aligned}
&[1\,2][3\,4][5\,6] \to 2^5 + 2^3 + 2 = 42,\\
&[1\,2][3\,6][4\,5] \to 2^5 + 2^3 + 2^2 = 44,\\
&[1\,4][2\,3][5\,6] \to 2^5 + 2^4 + 2 = 50,\\
&[1\,6][2\,3][4\,5] \to 2^5 + 2^4 + 2^2 = 52,\\
&[1\,6][2\,5][3\,4] \to 2^5 + 2^4 + 2^3 = 56.
\end{aligned}\right\} \tag{A 3}$$

We call this binary number f and we can use it to label the generalized wavefunctions [square brackets]. We can also label the ϕ's (basic wavefunctions), by picking out

the M positive spins and introducing, as in (A 3), the term 2^{2M-j} whenever spin j is positive.

We now suppose the generalized wavefunctions to be expressed as linear combinations of the basic wavefunctions. Using (A 1) and (A 2) and remembering that the two types of wavefunction are obtained by multiplying the corresponding types of bracket together, we conclude, that if f is any binary number and ψ_f, ϕ_f are the corresponding generalized and basic wavefunctions that

$$\psi_f = r^M \phi_f + \text{other terms.} \tag{A 4}$$

The equality of the binary numbers specifying ψ_f and ϕ_f follows from (A 1) and the methods of constructing the ψ's and ϕ's. Inspection of (A 1) shows that the 'other terms' are obtained from ϕ_f by reversing the signs of the spins within one or more of the brackets in the product of round bracket symbols that make up ϕ_f. Since, for a permitted wavefunction ψ_f, a_j is less than b_j in any bracket, these interchanges will produce from ϕ_f other ϕ's described by a binary number larger than f. This means that the matrix relation between the ψ's and ϕ's is triangular, with the diagonal terms equal to r^M, any non-diagonal terms arising from ϕ's with a larger binary suffix than f.

The linear independence of the ϕ's is obvious. That of the ψ's now follows from (A 4), because, if f runs downwards in turn through the values that lead to a permissible ψ, at every stage we have at least one new ϕ (namely ϕ_f) which has never appeared in the previous equations. Further, it appears with the non-zero coefficient r^M. This proves linear independence, and in particular proves it for the particular case $r = -s$ corresponding to the Húlthen wavefunctions. We can now also infer completeness, because the number of spin-zero wavefunctions for 2M electrons is known to be

$$\frac{1}{M+1}\binom{2M}{M}$$

which also follows from generating function (17) of the text.

TABLE 6. VALUES OF (1/L) ln W CALCULATED BY COOPER FROM (41)

$Z = 2\cos\mu$	(1/L) ln W	$Z = 2\cos\mu$	(1/L) ln W
−2.0	0	0	1.16624_4
−1.8	0.41550_4	0.2	1.21480_9
−1.6	0.57220_7	0.4	1.26077_9
−1.4	0.68757_0	0.6	1.30450_4
−1.2	0.78191_7	0.8	1.34626_5
−1.0	0.86304_6	1.0	1.38629_4
−0.8	0.93492_3	1.2	1.42478_6
−0.6	0.99988_4	1.4	1.46190_6
−0.4	1.05944_3	1.6	1.49779_7
−0.2	1.11464_4	1.8	1.53258_3
0	1.16624_4	2.0	1.56632_0

At $Z = 1$, $\frac{1}{L}\frac{\partial(\ln W)}{\partial Z} = 0.196_2$. $\frac{1}{L}\frac{\partial^2 \ln W}{\partial Z^2} = -0.037_7$.