properties of the plasma are maintained constant. We have discussed the conditions of applicability of the theory as presented and have shown that experiments performed to date should be describable within the approximations employed.

ACKNOWLEDGMENTS

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Statistical Mechanics of Dimers on a Plane Lattice

MICHAEL E. FISHER
Wheatstone Physics Laboratory, King's College, London, England
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This paper considers the statistical mechanics of hard rigid dimers distributed on a lattice (each dimer occupying two nearest neighbor lattice sites). The problem is solved in exact closed form for a finite $m\times n$ plane square lattice with edges which is completely filled with $\frac{1}{2}mn$ dimers (close-packed limit). In terms of the activities x and y of horizontal and vertical dimers, the configurational partition function $Z_{mn}(x,y)$ is given in the limit of a large lattice by

$$\lim_{m,n\to\infty}(mn)^{-1}\ln Z_{mn}(x,y)=\tfrac{1}{2}\ln y+(1/\pi)\int_0^{x/y}(1/v)\tan^{-1}v\,dv.$$

It follows that the free energy and entropy of the system are smooth continuous functions of the densities of horizontal and vertical dimers. The number of ways of filling the lattice with dimers is calculated exactly for $m=n=8$ and is given asymptotically by $[\exp(2G/\pi)]^{\frac{1}{4}mn}=(1.791\,623)^{\frac{1}{4}mn}$. The results are derived with the aid of operator techniques which reduce the partition function to a Pfaffian and hence to a determinant. Some results are also presented for the more general case with monomers present.

1. INTRODUCTION

ONE of the simplest models of a system containing diatomic molecules is that of lattice gas (or solution) of N_d *rigid dimers*, each of which fills two nearest neighbor sites of a space lattice of N sites. The remaining $N-2N_d$ sites of the lattice may be regarded as occupied by N_0 "holes" (or "monomers"). This model has been used by many authors to discuss the thermodynamics of adsorbed films and mixed solutions.[1–5] It is also interesting in connection with the theory of the condensation of gases.[6] All the thermodynamic properties can be derived from the configurational grand partition function and it is the calculation of this which constitutes the main theoretical problem. Since (in the simplest form of the model) there are no interactions other than "hard core" infinite repulsive forces between dimers, the problem reduces to the determination of the number of ways of placing N_d identical dimers on the lattice so that no two overlap. This is an unsolved combinatorial problem of considerable interest in its own right,[7] and is comparable to the well-known topological aspects of the Ising model[8] first elucidated by Kac and Ward.[9,10]

For a one-dimensional lattice (linear chain) the partition function (or generating function) can be evaluated quite easily in closed form[11] (see Sec. 8) but for two- or three-dimensional lattices no exact results are available. (The Bethe approximation and low-density series expansions have been employed in the main.[1–4]) This paper considers the problem on the plane square (or rectangular) lattice and the partition function is evaluated exactly for the case when the dimers completely fill the lattice (close-packed or high-density limit, $N_d=\frac{1}{2}N$). Our results are exact even for a finite $n\times m$ rectangular lattice with edges so that both bulk and boundary terms in the free energy of a large lattice can be determined.

The partition function is calculated with the aid of operator techniques and the argument follows the lines used recently by Hurst and Green[12] in rederiving Onsager's solution of the plane square Ising model.[8] In

[1] R. H. Fowler and G. S. Rushbrooke, Trans. Faraday Soc. **33**, 1272 (1937).
[2] T. S. Chang, Proc. Roy. Soc. (London) **A169**, 512 (1939); Proc. Cambridge Phil. Soc. **35**, 265 (1939).
[3] J. K. Roberts and A. R. Miller, Proc. Cambridge Phil. Soc. **35**, 293 (1939).
[4] G. S. Rushbrooke, H. I. Scoins, and A. J. Wakefield, Discussions Faraday Soc. No. 15, 57 (1953).
[5] H. S. Green and R. Leipnik, Revs. Modern Phys. **32**, 129 (1960); but see reference 11.
[6] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 410 (1952).
[7] F. Harary, "Feynman's simplification of the Kac-Ward treatment of the two-dimensional Ising problem"; (planographed preprint) University of Michigan, June 12, 1958; to appear as a chapter in a book on graph theory.
[8] L. Onsager, Phys. Rev. **65**, 117 (1944).
[9] M. Kac and J. C. Ward, Phys. Rev. **88**, 1332 (1952).
[10] S. Sherman, J. Math. Phys. **1**, 202 (1960).
[11] M. E. Fisher and H. N. V. Temperley, Revs. Modern Phys. **32**, 1029 (1960).
[12] C. A. Hurst and H. S. Green, J. Chem. Phys. **33**, 1059 (1960).

Sec. 2 the configurational grand partition function is expressed as the trace of a product involving anticommuting operators. The basic theorems for reducing such a trace to a Pfaffian and thence to an antisymmetric determinant are presented in the following section. In Sec. 4 the determinant is evaluated with the aid of successive unitary transformations. The exact results for finite lattices are discussed in Sec. 5. Asymptotic formulas for large lattices are derived in Secs. 6 and 7 and compared with Onsager's solution of the Ising problem. The (unsolved) problem of low and intermediate dimer densities is considered briefly in the last section.

The principal results of this work (in particular, the limit for an infinite lattice) were derived independently by Temperley a short time prior to their discovery by the author. A brief preliminary announcement of the results was published conjointly.[13]

After the completion of this paper the author received a preprint of a paper by P. W. Kasteleyn (to be published in Physica) which also treats the dimer problem. Kasteleyn obtains the exact results for a rectangular lattice wrapped on a torus as well as for one with edges. However, his method of approach to the central problem is different from that used here and in some directions his work does not go as far.

2. THE PARTITION FUNCTION AS A TRACE

Consider a plane rectangular lattice of m rows and n columns and $N=mn$ sites. If $g_{mn}(N_x,N_y,N_0)$ is the number of ways of placing N_x horizontal or x-dimers, N_y vertical or y-dimers, and N_0 monomers on the lattice so that no sites are multiply occupied ($2N_x+2N_y+N_0=mn$), then the required configurational grand partition function is the generating function

$$Z_{mn}(x,y,z)=\sum_{N_x,N_y,N_0} g_{mn}(N_x,N_y,N_0)x^{N_x}y^{N_y}z^{N_0}, \quad (1)$$

where, thermodynamically, x, y, and z are the activities of x-dimers, y-dimers, and monomers, respectively. [We remark parenthetically that if each dimer has a magnetic moment μ and a field with components H_x and H_y is present, then the activities x and y have factors $\cosh(\mu H_x/kT)$ and $\cosh(\mu H_y/kT)$, respectively.]

To obtain an explicit expression for Z_{mn} we introduce a set of 4ν anticommuting operators A_i obeying the relations[14]

$$A_iA_j+A_jA_i=2\delta_{ij}, \quad (2)$$

where δ_{ij} is the Kronecker delta function. Consequently,

$$A_i^2=I, \quad (3)$$

where I is the identity operator. These operators are readily represented as direct products of 4ν two-by-two matrices but there is no need to make use of such representations. From (2) and (3) it follows[15] that

$$\mathrm{Tr}\{A_i\}=0, \quad \mathrm{Tr}\{A_iA_j\}=0 \quad (i\neq j), \quad (4)$$

$$\mathrm{Tr}\{A_iA_jA_k\}=0 \quad (i\neq j\neq k), \quad \cdots,$$

$$\mathrm{Tr}\{A_i^2\}=\mathrm{Tr}\{I\}=t, \quad (5)$$

where Tr{ } denotes the trace taken in a representation of dimension t.

Choosing ν so that the number of operators 4ν equals or exceeds the number of bonds, a distinct operator A_i may be associated with each bond. (Some operators might be left over but this does not matter.) If the sites of the lattice are labelled by the parameter $k=1, 2, 3, \cdots mn$, then it is convenient to denote the operator for a bond from site k to site l by A_{kl}. Now consider the trace of the following product of operators taken over the mn sites of the lattice.

$$\prod_{k=1}^{mn} V_k=\prod_{k=1}^{mn}(z_kI+x_{kl_1}{}^{\frac{1}{2}}A_{kl_1}+x_{kl_2}{}^{\frac{1}{2}}A_{kl_2}+y_{kl_3}{}^{\frac{1}{2}}A_{kl_3}+y_{kl_4}{}^{\frac{1}{2}}A_{kl_4}), \quad (6)$$

where l_1 to l_4 denote the nearest neighbor sites of k. The trace of any term in the expansion of this product will vanish unless each operator A_{kl} appears in the term either twice or not at all. Consequently, any nonvanishing term in the trace will have the form

$$(-)^p z_{k_1}z_{k_2}\cdots z_{k_q}x_{k_rl_r}x_{k_sl_s}\cdots y_{k_ul_u}y_{k_vl_v}\cdots y_{k_wl_w}t,$$

and will correspond to a configuration of the lattice in which the sites $k_1, k_2, \cdots k_q$ are occupied by monomers, and neighboring pairs of sites k_r and l_r, k_s and l_s, $\cdots$ are occupied by x-dimers while pairs k_u and l_u, k_v and l_v, $\cdots$, k_w and l_w are occupied by y-dimers. Clearly, to any possible configuration of nonoverlapping dimers and monomers there corresponds a term in the trace and vice versa.

The sign of a term in the expansion of (6) is determined, in virtue of the anticommutation of the operators, by the parity p of the number of interchanges of adjacent operators in the term required to bring like operators together in pairs. *If the parity is even for all terms* then, setting $z_k=z$, $x_{kl}=x$, and $y_{kl}=y$, we have for the partition function

$$Z_{mn}(x,y,z)=t^{-1}\,\mathrm{Tr}\{\prod_{k=1}^{mn} V_k(x,y,z)\}. \quad (7)$$

This is the basic expression for the calculation of Z and a similar relation can evidently be written down for any lattice and arrangement of bonds. Its validity,

[13] H. N. V. Temperley and M. E. Fisher, Phil. Mag. 6, 1061 (1961).

[14] Hurst and Green employ a double set of absorption and creation operators a_i and a_i^* rather than a single set of operators A_i. The present method seems somewhat simpler. In the close-packed limit one may go directly to a Pfaffian (see reference 13 and Kasteleyn's forthcoming paper).

[15] Using the invariance of the trace under cyclic interchange, we have $\mathrm{Tr}\{A_i\}=\mathrm{Tr}\{A_iA_j^2\}=\mathrm{Tr}\{A_jA_iA_j\}=-\mathrm{Tr}\{A_iA_jA_j\}=-\mathrm{Tr}\{A_i\}$, so that $\mathrm{Tr}\{A_i\}=0$. The succeeding results in (4) can be proved by similar devices.

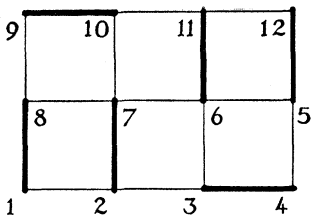

FIG. 1. A close-packed configuration of dimers on a 3×4 plane square-lattice showing the "zig-zag" numbering system.

however, rests on ensuring that the sign of all terms is positive, and herein lies the main difficulty of the problem. We will now show how it is possible to achieve this for the plane square lattice in the close-packed limit $z=0$. In this case each site is occupied either by an x- or a y-dimer. [The result (7) is valid also when $y=0$ for all z but since y-dimers do not then occur the problem is essentially one-dimensional.]

The parity of each term in the expansion of (6) is determined by the order of factors in the product, that is by the numbering sequence of the lattice sites. If, provisionally, the lattice sites are labeled by their Cartesian coordinates (r,s), where $r=0, 1, 2, \cdots, n-2, n-1$ and $s=0, 1, 2, \cdots, m-2, m-1$, then the "obvious method" of numbering points is in dictionary order, namely $k(r,s)=sn+r+1$. By considering examples of small lattices, however, it is easily seen that this is unsatisfactory.[16] Instead we introduce a "zig-zag" dictionary order in which *alternate rows* are numbered *in reverse order* (see Fig. 1). Explicitly, we set

$$\begin{aligned} k(r,s)&=sn+r+1, \quad (s \text{ even}),\\ &=sn+n-r, \quad (r \text{ odd}). \end{aligned} \tag{8}$$

With this numbering procedure all the terms of nonzero trace in the expansion of (6) when $z=0$ have positive sign after pairing of like operators. This is easily verified for particular examples, but its general proof requires more detailed argument. The reader uninterested in the details should omit the remainder of this section. (We remark in passing that the question of signs seems to have been considered incompletely by Hurst and Green[12] in their treatment of the Ising model. Their formulas are presumably valid, however, since they yield the correct limiting answer.)

To prove that the number of interchanges required to bring like pairs of operators together is always even, it is convenient to introduce a graphical representation[17]

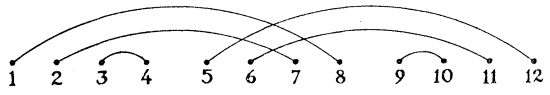

FIG. 2. Graphical representation of the ordered product of anticommuting operators corresponding to the configuration shown in Fig. 1.

[16] H. N. V. Temperley (private communication, to be published) has solved this problem by affixing minus signs to some of the y_{kl} in (6), and Kasteleyn effectively adopts the same course.

[17] This has been employed by C. A. Hurst (private communication).

of the product of operators corresponding to a given lattice configuration. The N ordered operators, one for each of the N lattice sites, are represented by an ordered linear array of points. Those points corresponding to like operators are joined by a line lying above the points (see Fig. 2). Any such line represents an x- or a y-dimer lying on the bond joining corresponding lattice sites (see Fig. 2). In the case $z=0$ every point will be the termination of a line since all the lattice sites are occupied by bonds. (In the general case, points corresponding to monomer occupation may be omitted since the identity operator commutes with all A_i.)

The lines in a graph representing a given product will in general intersect one another. Let f be the total number of (simple) intersections in the graph (f may be zero). The parity of f is an invariant of the product representing the graph since however the lines are distorted, new intersections are always created in pairs and existing ones destroyed in pairs. Interchange of the order of a pair of adjacent unlike operators corresponds to a similar interchange of points. This necessarily changes the parity of f since a single new intersection must be created or a single old intersection destroyed; e.g., consider the interchange of points 6 and 7 or 7 and 8 in Fig. 2. (More generally, if the lines are appreciably distorted, an odd number of intersections greater than unity might be created or destroyed on interchange.)

When all the operators are paired, the graph can clearly be drawn with no intersections and in this case f is even. Thus any graph obtainable from the fully paired graph by an even number of interchanges will have f even, and vice versa. Consequently, the parity of f for a given graph is equal to p and indicates directly the sign of the product after pairing. This reduces the problem to proving that f is even for any allowable configuration on the square lattice when the numbering system (8) is used.

To simplify the language of the following argument, we will assume that the lines of the graph are always drawn so as to minimize the number of intersections (as in Figs. 2 and 3). Otherwise, for a statement such as "two lines do not intersect" read "can be drawn in such a way as not to intersect." Any x-dimer corresponds to a line (an x-line) between consecutive points. Consequently, no x-line intersects another x-line or intersects a y-line (see Fig. 3). In virtue of the zig-zag numbering, y-lines between rows s and $s+1$ do not intersect one another. In fact, the only intersections are between y-lines to successive rows, i.e., $y(s-1, s)$ with $y(s, s+1)$ (see Fig. 3). Consequently, if we consider all x-lines and all those y-lines between alternate pairs of rows, namely, between rows $2u$ and $2u+1$ ($u=0, 1, 2, \cdots$), there are no intersections (see solid lines in Fig. 3). This proves that f is equal to the total number of intersections made by those y-lines between complementary alternate pairs of rows, namely, rows $2u-1$ and $2u$ ($u=1, 2, 3, \cdots$) (see broken lines in

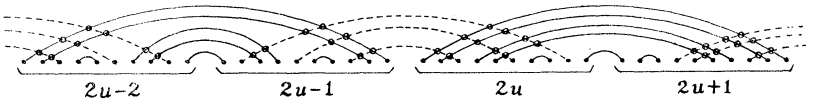

FIG. 3. Part of a graph for a product representing a configuration on a general plane square lattice.

Fig. 3). Hence, if it can be shown that no y-line between row $2u-1$ and row $2u$ intersects an odd number of lines, it follows that f must be even as required. [These arguments serve also to prove the validity of (7) for all z when $y=0$ or when y-dimers can only be placed between alternate pairs of rows.]

To prove that a y-line between the point $2un+1+r$ in row $2u$ and the point $2un-r$ in row $2u-1$ intersects other y-lines an even number of times, consider the number of intermediate points "spanned" by the y-line. No line not terminating on one of these points intersects the y-line. There are $2r$ intermediate points and each one must be the termination of either (a) an x-line in row $2u$ or $2u-1$, (b) an "internal" y-line from row $2u$ to $2u-1$ or (c) an "external" y-line either from row $2u$ to $2u+1$ or from row $2u-1$ to $2u-2$ (see Fig. 3). But each x-line (a) and internal y-line (b) accounts for two of the intermediate points so that if the number of these lines is w, the number of external y-lines (c) must be $2r-2w$ and so is even. Each external y-line, however, intersects the original y-line once (and only once) and hence the total number of intersections is always even.

This completes the proof of the validity of (6), (7), and (8) when $z=0$. The argument breaks down when $z\neq 0$ since, if an odd number of monomers occupies the intermediate points (or sites), the number of external y-lines is odd and the term has a negative sign. A very simple configuration for which this arises is shown in Fig. 4. When $z=0$ the proof applies to the plane honeycomb lattice (in "brick form")[18] but not to the triangular lattice formed by adding one set of diagonals to the square lattice. In this latter case the number of intermediate points may be odd, as can be seen from the example in Fig. 5. Similar difficulties arise in the case of multilayer and three-dimensional lattices.

3. REDUCTION OF A TRACE TO A PFAFFIAN

By Eq. (7) the partition function is expressed as the product of a number of factors, each of which is an inhomogeneous linear combination of anticommuting operators. As pointed out by Hurst and Green,[12] such an expression may be reduced to a Pfaffian. A Pfaffian of order $2h$ is a triangular array of $h(2h-1)$ elements (r,s):

$$P=\diagdown(r,s)|=|\,(1,2)(1,3)(1,4)\cdots(1,2h)\;(2,3)(2,4)\cdots(2,2h)\;(3,4)\cdots(3,2h)\;\cdots\;(2h-1,2h)|, \tag{9}$$

which may be expanded by its first row in the same way as a determinant, except that the minor of an element (r,s) is a Pfaffian of order $2(h-1)$ obtained from P by deleting *both* the rth row and column *and* the sth row and column.[19–21] By iterating this relation the complete expansion is found to be

$$P=\sum(-)^p(l_1,l_2)(l_3,l_4)\cdots(l_{2h-1},l_{2h}), \tag{10}$$

where the sum is over the $(2h-1)!!\equiv(2h-1)(2h-3)\cdots\times5\times3\times1$ permutations $(l_1,l_2,\cdots l_{2h})$ satisfying $l_1<l_2$, $l_3<l_4,\cdots$, $l_{2h-1}<l_{2h}$ and $l_1<l_3<l_5<\cdots<l_{2h-1}$, and p is the parity of the permutation.[21,22] For the present purpose the most important property of a Pfaffian is that its square is equal to an antisymmetric determinant. In fact[19,20]

$$P^2=D=|d_{rs}|, \tag{11}$$

where

$$d_{rr}=0,\quad d_{rs}=(r,s)=-d_{sr},\quad r<s. \tag{12}$$

The basic theorem relating a Pfaffian to the trace of a product of operators is

$$t^{-1}\,\mathrm{Tr}\{\prod_{r=1}^{2h}V_r\}=\diagdown(v_{r0}v_{s0}-\sum_{i=1}^{4\nu}(-)^{r+s}v_{ri}v_{si})|, \tag{13}$$

where

$$V_r=v_{r0}I+\sum_{i=1}^{4\nu}v_{ri}A_i, \tag{14}$$

and where the A_i obey the anticommutation relations (2). (This theorem is more general than that used by

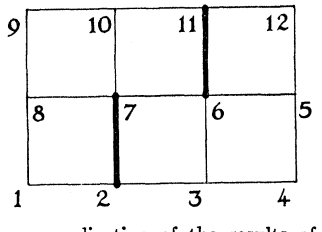

FIG. 4. A simple configuration of intermediate dimer density which is enumerated with incorrect sign.

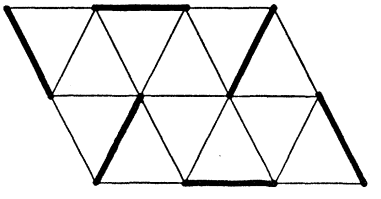

FIG. 5. Example of a close-packed configuration on the triangular lattice enumerated with a wrong sign.

[18] It is hoped to publish the generalization of the results of this paper to other lattices including the plane honeycomb.

[19] R. F. Scott and G. B. Mathews, *The Theory of Determinants* (Cambridge University Press, New York, 1904), 2nd ed., pp. 92–97.

[20] T. Muir, *A Treatise on the Theory of Determinants* (MacMillan and Company, Ltd., London, 1882), pp. 196–203.

[21] E. R. Caianiello and S. Fubini, Nuovo cimento **9**, 1218 (1952).

[22] E. R. Caianiello, Nuovo cimento **10**, 1634 (1953).

Hurst and Green which applied to a product of *homogeneous* linear factors, i.e., $v_{r0}=0$ for all r.) The assumption that the product has an even number of terms is no restriction since a factor $V_{2h}=I$ does not alter the product. This theorem may be proved by a slight extension of the argument used by Caianiello and Fubini[21] for the case in which the A_i were Dirac's γ matrices. For the sake of completeness and to give insight into the structure of the theory we present the proof. The reader prepared to accept the result may, however, omit the remainder of the section.

The first step is to reduce the product of inhomogeneous linear factors to one of homogeneous linear factors. We introduce a complementary set of operators defined by

$$B_0=\prod_{j=1}^{4\nu} A_j, \tag{15}$$

and

$$B_j=iA_jB_0=-iB_0A_j, \quad (i^2=-1). \tag{16}$$

It is then easy to verify the commutation relation

$$B_iB_j+B_jB_i=2\delta_{ij}, \quad (i=0, 1, 2, \cdots 4\nu) \tag{17}$$

with, in particular,

$$B_0^2=I. \tag{18}$$

Following Caianiello and Fubini, we now write the product as

$$\prod_{r=1}^{2h} V_r=(V_1B_0)(B_0V_2)(V_3B_0)(B_0V_4)\cdots(B_0V_{2h})$$

$$=\prod_{r=1}^{2h} Q_r, \tag{19}$$

where

$$Q_r=\sum_{j=0}^{4\nu} q_{rj}B_j \tag{20}$$

is a homogeneous linear combination of the B_i. By (14) and (19) the coefficients in Q_r are simply

$$q_{r0}=t_{r0}, \quad q_{rj}=(-)^r it_{rj}. \tag{21}$$

By virtue of (17), the operators Q_r obey the commutation relations

$$Q_rQ_s+Q_sQ_r=2(r,s), \quad (r,s)=\sum_{j=1}^{4\nu} q_{rj}q_{sj}. \tag{22}$$

Using these to shift Q_1 successively to the right, we have

$$\begin{aligned}
&Q_1Q_2Q_3\cdots Q_{2h}\\
&\quad=-Q_2Q_1Q_3Q_4\cdots Q_{2h}+2(1,2)Q_3Q_4\cdots Q_{2h}\\
&\quad=(-)^2Q_2Q_3Q_1Q_4Q_5\cdots Q_{2h}-2(1,3)Q_2Q_4\cdots Q_{2h}\\
&\qquad\qquad+2(1,2)Q_3Q_4\cdots Q_{2h}\\
&\qquad\cdots\cdots\cdots\cdots\\
&\quad=(-)^{2m+1}Q_2Q_3Q_4\cdots Q_{2h}Q_1\\
&\qquad+2\sum_{k=2}^{2h}(-)^k(1,k)Q_2\cdots Q_{k-1}Q_{k+1}\cdots Q_{2h}.
\end{aligned} \tag{23}$$

On recalling that the trace is invariant under cyclic interchange, this implies

$$\mathrm{Tr}\{\prod_{r=1}^{2h} Q_r\}=\sum_{k=2}^{2h}(-)^k(1,k)\ \mathrm{Tr}\{Q_2\cdots Q_{k-1}Q_{k+1}\cdots Q_{2h}\}, \tag{24}$$

which is essentially the rule for expanding a Pfaffian by its first row. If (24) is iterated, we arrive at an expression like the left-hand side of (10) but multiplied by $\mathrm{Tr}\{I\}$ and so conclude that

$$t^{-1}\,\mathrm{Tr}\{\prod_{r=1}^{2h} Q_r\}=P=\diagdown(r,s)|, \tag{25}$$

where (r,s) is the commutator of Q_r and Q_s defined in (22). Substitution of (21) and (22) in (25) proves the theorem (13).

4. EVALUATION OF THE DETERMINANT

By the results of the previous sections [Eqs. (6), (7), (13), and (14)] we may now express the partition function as Pfaffian of order mn, the elements being labeled in accordance with the numbering of the lattice points.[23] Thus when $z=0$

$$Z_{mn}(x,y,0)=P=\diagdown(k,l)|, \tag{26}$$

where

$$(k,l)=x\xi_{kl}+y\eta_{kl}, \tag{27}$$

in which $\eta_{kl}=1$ or 0 according as the lattice points k and l are or are not connected by a horizontal bond and $\eta_{kl}=1$ or 0 according as they are or are not connected by a vertical bond.

For the case when $y=0$ we note similarly

$$Z_{mn}(x,0,z)=\diagdown(z+x\xi_{kl})|. \tag{28}$$

We will not consider this case further until Sec. 8, so that from here on we assume $z=0$.

On squaring (26) we have (dropping the explicit dependence on z)

$$Z_{mn}^2(x,y)=D_{mn}=|\mathbf{D}|, \tag{29}$$

where $\mathbf{D}$ is an $m\times m$ antisymmetric block matrix

$$\mathbf{D}=\begin{pmatrix}
\mathbf{X} & \mathbf{Y} & & & & \cdot & \\
-\mathbf{Y} & \mathbf{X} & \mathbf{Y} & & & 0 & \\
 & -\mathbf{Y} & \mathbf{X} & \mathbf{Y} & & & \\
 & & \cdot & \cdot & \cdot & \cdot & \\
 & & & \cdot & \cdot & \cdot & \\
 & 0 & & -\mathbf{Y} & \mathbf{X} & \mathbf{Y} & \\
 & & & & -\mathbf{Y} & \mathbf{X} &
\end{pmatrix}, \tag{30}$$

[23] Strictly we should impose the condition mn even, since otherwise the Pfaffian is not defined. This could be avoided by introducing an extra dummy lattice site which would lead to the result we finally obtain.

in which $\mathbf{X}$ and $\mathbf{Y}$ are $n\times n$ matrices of the simple forms

$$\mathbf{X}=\begin{bmatrix} 0 & x & & & & & \\ -x & 0 & x & & & 0 & \\ & -x & 0 & x & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & 0 & & & -x & 0 & x \\ & & & & & -x & 0 \end{bmatrix}, \tag{31}$$

$$\mathbf{Y}=\begin{bmatrix} & & & & y \\ & 0 & & y & \\ & & y & & \\ & \cdot & & & \\ & \cdot & & & \\ y & & 0 & & \\ y & & & & \end{bmatrix}. \tag{32}$$

The matrix $\mathbf{D}$ may be (block) diagonalized with the aid of its eigenvectors which can be derived from the difference equation

$$Yu_{l+1}+Xu_l-Yu_{l-1}=\lambda u_l, \tag{33}$$

with boundary conditions

$$u_0=u_{m+1}=0. \tag{34}$$

Equation (33) has solutions of the form $\exp(i\theta l)$ and $\exp[i(\pi-\theta)l]$, with $\lambda=X+2iY\sin\theta$. The boundary conditions can only be satisfied by

$$\theta=\theta_q=\tfrac{1}{2}\pi+\pi q/(m+1),\quad (q=1, 2, 3, \cdots m-1, m) \tag{35}$$

with corresponding eigenvalues

$$\lambda_q=X+2iY\sin\theta_q, \tag{36}$$

and normalized eigenvectors

$$u_{lq}=2^{\frac{1}{2}}(m+1)^{-\frac{1}{2}}i^{l+1}\sin[\pi ql/(m+1)]. \tag{37}$$

Consequently $\mathbf{D}$ is diagonalized by the unitary (block) matrix $[u_{kq}\mathbf{I}]$ and this yields

$$Z_{mn}{}^2=D_{mn}=\prod_{q=1}^{m}|\mathbf{D}_q|, \tag{38}$$

where

$$\mathbf{D}_q=\mathbf{X}+2i\sin\theta_q\mathbf{Y} \tag{39}$$

is an $n\times n$ matrix. Now by a similar argument the eigenvectors of $\mathbf{X}$ are

$$u_{kr}=2^{\frac{1}{2}}(n+1)^{-\frac{1}{2}}i^{k+1}\sin[\pi rk/(n+1)],\quad (r=1, 2, 3, \cdots, n-1, n). \tag{40}$$

Transformation of $\mathbf{D}_q$ by the corresponding unitary transformation yields the "cruciform" matrix,

$$\begin{bmatrix} 2ix\sin\phi_1 & & & & (-)^{n-1}2i^ny\sin\theta_q \\ & 2ix\sin\phi_2 & & (-)^{n-2}2i^ny\sin\theta_q & \\ & & \cdot & \cdot & \\ & & \cdot & \cdot & \\ & & \cdot & \cdot & \\ & & -2i^ny\sin\theta_q & 2ix\sin\phi_{n-1} & \\ +2i^ny\sin\theta_q & & & & 2ix\sin\phi_n \end{bmatrix}, \tag{41}$$

where

$$\phi_r=\tfrac{1}{2}\pi+\pi r/(n+1). \tag{42}$$

By successive expansion by the first row and final row, the determinant of such a cruciform matrix is easily evaluated as a product of $[\frac{1}{2}(n+1)]$ factors[24] of the type $(d_{11}d_{nn}-d_{1n}d_{n1})$. On noting that $\sin\theta_q=\sin\theta_{n+1-q}$, each term in the product factorizes, and after rearrangement and substitution in (38) we obtain the final result:

$$Z_{mn}{}^2=(-)^{m[\frac{1}{2}n]}2^{mn}\prod_{q=1}^{m}\prod_{r=1}^{n}\left(x\cos\frac{\pi r}{n+1}+iy\cos\frac{\pi q}{m+1}\right). \tag{43}$$

5. FINITE LATTICES

The formula (43) expresses the partition function of a finite $m\times n$ lattice exactly as a product of mn complex terms. If both m and n are odd, then the term for $r=\frac{1}{2}(n+1)$, $q=\frac{1}{2}(m+1)$ vanishes identically so that $Z_{mn}=0$. This reflects correctly the fact that a lattice with an odd number of sites cannot be completely filled with dimers.[23] For a linear chain $m=1$ (or $n=1$) the partition function reduces to

$$Z_{n,1}{}^2=(-)^{[\frac{1}{2}n]}x^n2^n\prod_{r=1}^{n}\cos\frac{\pi r}{n+1}. \tag{44}$$

The product of cosines may be evaluated with the aid of the identity

$$\frac{\sin l\gamma}{\sin\gamma}=2^n\prod_{r=1}^{l-1}[\cos\gamma+\cos(\pi r/l)] \tag{45}$$

[which is easily proved by factorizing $\exp(2l\theta)-1$], and this yields, correctly,

$$Z_{n,1}=x^{\frac{1}{2}n},\quad n \text{ even}$$
$$=0,\quad n \text{ odd}.$$

The identity (45) may obviously be used to perform the product over r in (43) but the resulting expression is a little cumbersome. Instead, if we assume (neglecting the cases when Z_{mn} vanishes) that n is even, we easily

[24] The notation $[x]$ denotes the greatest integer contained in x. If preferred, $\mathbf{D}_q$ may be completely diagonalized by applying further transformations.

obtain from (43) the more convenient expression for the partition function itself:

$$Z_{mn}(x,y)=2^{\frac{1}{2}n[\frac{1}{2}m]}\prod_{q=1}^{[\frac{1}{2}m]}\prod_{r=1}^{\frac{1}{2}n}\left(x^2+y^2+x^2\cos\frac{2\pi r}{n+1}+y^2\cos\frac{2\pi q}{m+1}\right)\begin{cases}\times 1 & \text{for } m \text{ even}\\ \times x^{\frac{1}{2}n} & \text{for } m \text{ odd.}\end{cases} \tag{46}$$

This is manifestly symmetric in m and n and x and y as it should be. For small m and n, the result (46) is readily verified by direct lattice counting; for example,

$$Z_{2,2}=x^2+y^2, \quad Z_{3,2}=x^3+2xy^2.$$

Owing to the vast number of configurations, however, this soon becomes difficult. Thus the total number of configurations ($x=y=1$) for a 4×4 lattice is 36, but for an 8×8 lattice

$$Z_{8,8}(1,1)=12\,988\,816=2^4\times(901)^2. \tag{47}$$

This number represents the number of different ways of placing 32 dominoes on a chess board, each domino covering two squares. $Z_{8,8}$ is expressed by (46) as a product of ten distinct trigonometric factors which may all be expressed in terms of

$$s=\sin(\pi/18)=\sin10^\circ=0.173\,648\,177\,7,$$

and hence calculated numerically. Alternatively, since the expression must be an integer, one may multiply the factors out symbolically and repeatedly use the trigonometric identity $6s-8s^3=1$.

6. INFINITE LATTICES

For a large lattice the limiting behavior of the partition function is

$$Z_{mn}(x,y)\sim[Z(x,y)]^{mn}, \tag{48}$$

where

$$\ln Z(x,y)=\lim_{m,n\to\infty}(mn)^{-1}\ln Z_{mn}(x,y) \tag{49}$$

is essentially the free energy per site of the lattice (divided by $-kT$). This limit is easily found from (46) by taking logarithms, whereupon the products become sums which may be converted directly into integrals. Thus (assuming for simplicity that m is even)

$$\ln Z(x,y)=\tfrac{1}{4}\ln2+(2\pi)^{-2}\times\int_0^\pi\int_0^\pi\ln(x^2+y^2+x^2\cos\alpha+y^2\cos\beta)\,d\alpha\,d\beta. \tag{50}$$

The integral in this formula bears a striking resemblance to Onsager's original expression for the partition function of the rectangular lattice Ising model.[8] The integrand becomes singular at $\alpha=\beta=\pi$ for all x and y (although the integral is always finite). This corresponds to the Ising model *at* its critical temperature $T=T_c$. In fact (50) may be identified with Onsager's result by writing (in Onsager's notation)

$$x/y=(\sinh2H/\sinh2H')^{\frac{1}{2}}=\sinh2H, \tag{51}$$

whence

$$\ln Z(x,y)=\tfrac{1}{4}\ln2y+\tfrac{1}{2}\ln\tfrac{1}{2}\lambda(H,H^*). \tag{52}$$

The density of x-dimers (mean number of x-dimers per lattice site) is given by the general formula

$$\rho_x=x(\partial/\partial x)\ln Z(x,y), \tag{53}$$

and similarly for ρ_y. Differentiation under the integral sign in (50) at once verifies the relation

$$\rho_x+\rho_y=\tfrac{1}{2}, \tag{54}$$

which corresponds to the close packing of the dimers. The integrals for ρ_x may be performed with the aid of the elementary standard forms:

$$\int_0^\pi\frac{d\beta}{a+\cos\beta}=\pi(a^2-1)^{-\frac{1}{2}}, \quad (a>1)$$

and, with $u=\cos\frac{1}{2}\alpha$,

$$\int_0^1\frac{du}{(b^2-u^2)^{\frac{1}{2}}}=\sin^{-1}(1/b), \quad (b>0) \tag{55}$$

yielding the very simple relation

$$\rho_x=(1/\pi)\tan^{-1}(x/y), \tag{56}$$

and similarly for ρ_y. Integrating (53) with the obvious initial value $\ln Z(0,y)=\frac{1}{2}\ln y$ leads to an expression for the partition function as a single integral:

$$\ln Z(x,y)=(1/\pi)\int_0^{x/y}(1/v)\tan^{-1}v\,dv+\tfrac{1}{2}\ln y, \tag{57}$$

with the series expansion

$$\ln Z(x,y)=(1/\pi)\sum_{l=0}^{\infty}(-)^l\frac{(x/y)^{2l+1}}{(2l+1)^2}+\tfrac{1}{2}\ln y. \tag{58}$$

This series converges for $|x|\leqslant|y|$. When $|y|\leqslant|x|$ the formula remains valid if x and y are interchanged. (This is a reflection of the symmetry between x- and y-dimers.) Simple formulas corresponding to (57) and (58) may similarly be derived for the Ising model partition function at the critical point.

In the symmetric case $x=y=1$ we obtain from (58)

$$\ln Z(1,1)=G/\pi=0.291\,560\,904, \tag{59}$$

where

$$G=1-3^{-2}+5^{-2}-7^{-2}+\cdots=0.915\,965\,594 \tag{60}$$

is Catalan's constant. Thus the number of ways of

filling a lattice with $\frac{1}{2}mn$ dimers is asymptotically

$$Z_{mn}(1,1)\sim\mu^{\frac{1}{2}mn}, \tag{61}$$

where

$$\mu=e^{2G/\pi}=1.791\,623. \tag{62}$$

It is interesting that by numerical extrapolation of the first few ratios $Z_{m,n}/Z_{m,n-2}$, etc., one would estimate $\mu=1.75\pm5$. Indeed, Fowler and Rushbrooke[1] extrapolated the exact results for strips and cylinders of width up to $n=8$ $(m=\infty)$ and concluded that μ was "near 1.8." Reexamination of their data on a $(1/n)$ plot indicates $\mu=1.79\pm3$, which is surprisingly accurate. The Bethe approximation (calculated by Chang[2]) yields $\mu\simeq27/16=1.6875$ and so is in error by 6%.

If the activities x and y are normalized by setting $xy=1$ and we write

$$\tau=x/y=\tan\pi\rho_x, \tag{63}$$

the results may be expressed directly in terms of the density of x-dimers as

$$\ln Z(\rho_x)=\tfrac{1}{4}\ln\cot\pi\rho_x+(1/\pi)\int_0^\tau(1/v)\tan^{-1}v\,dv, \tag{64}$$

with the expansion

$$\ln Z=G/\pi+(1-\tau)^2/4\pi+O[(1-\tau)^4] \tag{65}$$

about the symmetric point $\rho_x=\rho_y=\frac{1}{4}$, $\tau=1$. The entropy of the lattice may be written, using the usual thermodynamic relations, as

$$S/k=\ln Z(\tau)-(\ln\tau)\tau(\partial/\partial\tau)\ln Z(\tau), \tag{66}$$

so that

$$S/k=\rho_x\ln\cot\pi\rho_x+(1/\pi)\int_0^\tau(1/v)\tan^{-1}v\,dv. \tag{67}$$

This has the expansion

$$S/k=G/\pi-(1-\tau)^2/4\pi+O[(1-\tau)^4]. \tag{68}$$

From these relations it follows that the entropy is a smooth continuous function of the densities with a maximum at $\rho_x=\rho_y=\frac{1}{2}$.

7. ASYMPTOTIC EXPANSIONS

The limiting formulas of the previous section represent the leading terms in the asymptotic expansion of the exact result (46) for large m and n. Higher order terms can be obtained by a closer analysis. Taking the logarithm of (46) and assuming for simplicity that m is even, we have $(m=2k, n=2l)$

$$\ln Z_{mn}=kl\ln2+\sum_{q=1}^{k}\sum_{r=1}^{l}\ln(x^2+y^2+x^2\cos\alpha_r+y^2\cos\beta_q), \tag{69}$$

$$\alpha_r=2\pi r/(2l+1),\quad \beta_q=2\pi q/(2k+1).$$

By extending the limits of the sum and inserting missing terms, we may write

$$\ln Z_{mn}=kl\ln2+\tfrac{1}{4}\sum_{q=0}^{2k}\sum_{r=0}^{2l}\ln(x^2+y^2+x^2\cos\alpha_r+y^2\cos\beta_q)$$
$$-\tfrac{1}{4}\sum_{q=0}^{2k}\ln(2x^2+y^2+y^2\cos\beta_q)$$
$$-\tfrac{1}{4}\sum_{r=0}^{2l}\ln(2y^2+x^2+x^2\cos\alpha_r)+\tfrac{1}{4}\ln(2y^2+2x^2). \tag{70}$$

Now the summands of the three sums are periodic functions of their arguments α and β (regarded as continuous variables) and the equispaced points of summation cover the complete periods. Furthermore, the summands are analytic functions of α and β except for a singularity in the first summand at $\alpha=\beta=\pi$. Consequently, we may write

$$\ln Z_{mn}=kl\ln2+(2\pi)^{-2}(k+\tfrac{1}{2})(l+\tfrac{1}{2})$$
$$\times\int_0^{2\pi}\int_0^{2\pi}\ln(x^2+y^2+x^2\cos\alpha+y^2\cos\beta)\,d\alpha\,d\beta$$
$$-(1/4\pi)(k+\tfrac{1}{2})\int_0^{2\pi}\ln(2x^2+y^2+y^2\cos\beta)\,d\beta$$
$$-(1/4\pi)(l+\tfrac{1}{2})\int_0^{2\pi}\ln(2y^2+x^2+x^2\cos\alpha)\,d\alpha$$
$$+\tfrac{1}{4}\ln(2y^2+2x^2)+\epsilon_{mn}, \tag{71}$$

where the truncation error ϵ_{mn} arises almost entirely from the approximation of the first integral in the region of the singularity. (The errors from the remaining regions and from the single integrals fall off exponentially fast with m and n and are thus asymptotically negligible.) Performing the second and third integrals in (71) yields the terms

$$-(k+\tfrac{1}{2})\{\ln[x+(x^2+y^2)^{\frac{1}{2}}]-\tfrac{1}{2}\ln2\},$$
$$-(l+\tfrac{1}{2})\{\ln[y+(x^2+y^2)^{\frac{1}{2}}]-\tfrac{1}{2}\ln2\},$$

which represent contributions to the free energy from the boundary (or edge) of the lattice.

Specializing the results to the symmetric case $x=y=1$, we find

$$\ln Z_{mn}(1,1)\approx mn(G/\pi)-(m+n)[\tfrac{1}{2}\ln(1+2^{\frac{1}{2}})-(G/\pi)]+C_{mn}, \tag{81}$$

where

$$C_{mn}=\epsilon_{mn}+\tfrac{3}{4}\ln2+(G/\pi)-\ln(1+2^{\frac{1}{2}}). \tag{82}$$

The excess contribution to the free energy (divided by kT) per boundary site is thus

$$\tfrac{1}{4}\ln(1+2^{\frac{1}{2}})-(G/2\pi)=0.074\,563\,0. \tag{83}$$

This is positive because the steric hindrance of the boundary reduces the number of allowed configurations.

It is not difficult to see that the truncation error ϵ_{mn}

is bounded and tends to a positive limit dependent only on the ratio m/n. Its actual value is most readily estimated by comparing the numerical values of the sum and integral for small m and n and extrapolating to the limit $m, n \to \infty$. For $m=n$ the error behaves approximately as

$$\epsilon_{nn} \simeq 0.170+0.046/n. \tag{83}$$

By symmetry one can see that the dependence on m/n is quadratic in $[(m/n)-1]$ near $m=n$. Consequently, for most practical purposes the limiting value is sufficiently accurate and C_{mn} in (82) may be taken as 0.100.

8. INTERMEDIATE DENSITIES

In the previous part of the paper the dimer problem has been solved only in the close-packed limit $z=0$. In the absence of y-dimers, on the other hand, the theory of Secs. 2 and 3 is valid for all z and the limiting result per site is then

$$\ln Z(x,0,z) = (1/2\pi)\int_0^\pi \ln(z^2+2x+2x\cos\omega)d\omega$$
$$= \ln\tfrac{1}{2}[z+(z^2+4x)^{\frac{1}{2}}]. \tag{84}$$

The last form of this result is easily verified by generating function techniques[11] since it corresponds to the result for a one-dimensional linear chain. It may also be derived independently from the exact close-packed result (43) or (46) by considering a lattice of only two rows. Each y-dimer can then be identified with a monomer and each x-dimer will be "paired." Consequently, replacement of x and y by $x^{\frac{1}{2}}$ and z, respectively, yields (84) directly.

For comparison with the close-packed formula (50) (in which $z=0$), we may recast (84) in the form

$$\ln Z(x,0,z) = \tfrac{1}{4}\ln 2+(2\pi)^{-2}$$
$$\times\int_0^\pi\int_0^\pi \ln[x^2+2z^2x+\tfrac{1}{2}z^4+x^2\cos\alpha]d\alpha d\beta. \tag{85}$$

Comparison of (85) and (50) suggests various possibilities for the complete result $Z(x,y,z)$ but none of the obvious conjectures generate the exact low-density expansion.[11]

In fact the complete partition function can be expanded as a series in y, namely,

$$\ln Z(x,y,z) = \ln\tfrac{1}{2}[z+(z^2+4x)^{\frac{1}{2}}]+y/(z^2+4x)+O(y^2). \tag{86}$$

The surprisingly simple first-order term in this expansion has been derived by the generating function method applied to an infinite two-row lattice. A few further terms might be found by examining three- and four-row lattices. The result (86) could also have been derived via a Pfaffian from the general theory of Secs. 2 and 3 applied to a lattice with y-dimers between alternate rows only. Real progress towards a complete closed expression for $Z(x,y,z)$ seems, however, to need a further innovation in technique.

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