THE

PHYSICAL REVIEW

Statistical Mechanics of Dimers on a Plane Lattice. II.
Dimer Correlations and Monomers

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(Received 23 April 1963)

In part I of this paper, exact expressions were obtained for the partition function and thermodynamic properties of an $m \times n$ plane square lattice filled with $\frac{1}{2}mn$ rigid dimers each occupying two adjacent lattice sites. In this part the correlation properties of the model are studied with the aid of a general perturbation theory for Pfaffians. Closed formulas are derived for the changes in the probability of a dimer occupying a given bond that are induced by the proximity of an edge or a corner of the lattice (singlet correlations) and, in the center of the lattice, by the fixed position of another dimer (pair correlations). We show how to calculate the number of configurations of a dimer lattice containing a pair of monomers (or holes) a fixed distance apart. The explicit result when the separation vector is $(p, 0)$ or $(p, 1)$ involves a Toeplitz determinant $|a_{i-j+1}|$ $(i, j = 1, 2, \cdots p)$ defined by

$$\sum_{n=-\infty}^{\infty} a_n e^{in\theta} = \text{sgn}\{\cos\theta\} \exp[-i \cot^{-1}(\tau \cos\theta)],$$

where $\tau = x/y$ and x and y are the activities of x and y dimers. A similar result holds along the diagonals $(p, p \pm 1)$. The relative number of configurations decays to zero with radial separation r as $B/r^{1/2}$.

1. INTRODUCTION

IN a recent paper[1] the statistical mechanics of a plane square lattice fully packed with rigid *dimers*, each of which occupies two nearest neighbor lattice sites to the exclusion of other dimers, was investigated. Exact closed expressions were obtained for the partition function of a finite $m \times n$ lattice and of an infinitely large lattice in terms of the activities x and y of horizontal and vertical dimers. Similar results have been obtained independently by Temperley[2] and, somewhat earlier, by Kasteleyn.[3] The dimer problem is of interest in its own right, as a model of a fluid of hard-core diatomic molecules, but also because of its connection with various other problems in statistical mechanics.[4]

The solution of the dimer problem is obtained by expressing the partition function as a Pfaffian. This is a classical mathematical form derived from the super-diagonal elements of an antisymmetric matrix and is

numerically equal to the square root of the corresponding antisymmetric determinant.[5] Pfaffians were recently introduced into physics by Caianiello and Fubini[6] for problems in field theory involving fermion operators, and by Hurst and Green[7] in connection with the well-known Ising model of ferromagnetism.

The main technical difficulty in the dimer problem is to ensure that all the terms in the expansion of the Pfaffian (each term corresponding to a configuration of dimers on the lattice) appear with the correct (positive) sign. This crucial point was considered in detail by Fisher[1] and by Kasteleyn[3] for the dimer problem on the plane square lattice. More recently, Kasteleyn[8] has shown that this difficulty can be overcome for dimers filling an *arbitrary* planar graph.[9]

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[1] M. E. Fisher, Phys. Rev. **124**, 1664 (1961) (to be denoted here as I).

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

[3] P. W. Kasteleyn, Physica **27**, 1209 (1961).

[4] References to the earlier literature are given in Refs. 1 and 3.

[5] R. F. Scott and G. B. Mathews, *The Theory of Determinants* (Cambridge University Press, New York, 1904), 2nd ed., pp. 92–97; T. Muir, *A Treatise on the Theory of Determinants* (MacMillan and Company, Limited, London, 1882), pp. 196–203. As noted by Montroll *et al.* (in Ref. 15), Pfaffians were used by Kelvin in the study of gyroscopic stability: See W. Thomson and P. G. Tait, *A Treatise on Natural Philosophy* (Cambridge University Press, London, 1879), Part I, Sec. 345 (ix) p. 394.

[6] E. R. Caianiello and S. Fubini, Nuovo Cimento **9**, 1218 (1952); E. R. Caianiello, *ibid.* **14**, Suppl. 1, 177 (1959).

[7] C. A. Hurst and H. S. Green, J. Chem. Phys. **33**, 1059 (1960).

[8] P. W. Kasteleyn, J. Math. Phys. **4**, 287 (1963).

[9] A *planar* graph is any set of *sites* connected together by *bonds*

(Kasteleyn also analyzed the signs for the plane square Ising lattice[10] and Green has since considered the question for more general plane Ising lattices.[11])

All the exact solutions so far obtained refer to a lattice of N sites *completely filled* with $\frac{1}{2}N$ dimers. Of considerable interest is the more general problem in which *monomers* (or holes) are also present so that the lattice is not completely filled by dimers. This problem has been solved exactly only for a one-dimensional lattice (see Ref. 1, for example). For plane lattices series expansions may be derived but they apply only to the case of a weak solution of dimers in a "sea" of monomers[12] (low-density limit). In this paper we consider the complementary but more difficult problem of a few monomers in a dense sea of dimers (high-density limit). In particular, we show how to obtain exact expressions for the incremental free energy of two monomers at an arbitrary fixed distance apart in an otherwise full square lattice. The results (see Sec. 9) are expressed in terms of a Toeplitz determinant whose elements derive from the basic Green's function for the problem. The formulas are very reminiscent of the analogous results for the spin pair correlation functions of the Ising model[13] which were first derived by Kaufman and Onsager.[13–15]

We also investigate the correlations in orientation and position between a pair of dimers in the center of a large lattice filled with dimers. As might be expected, the net correlation oscillates and falls off rather slowly with the distance of separation (see Sec. 7). Similarly, we have calculated explicitly the effect on the dimers of the proximity of an edge and of a corner of the lattice (see Sec. 6). Dimers tend to align parallel to a long edge and the effect decays only as $1/r$.

The technique of calculation (described in Sec. 3) is to reformulate the various problems as perturbations on the standard Pfaffian describing the full lattice. To discuss the lattice with monomers, it is necessary to use Kasteleyn's general theory for planar graphs (Sec. 2). The perturbed Pfaffians are then evaluated in terms of lower order Pfaffians with the aid of a Green's function.[16] The required elements of the Green's function are trigonometric double integrals of a type familiar in lattice problems (see Sec. 4). For the case considered here, of a plane square lattice with different

activities for horizontal and vertical dimers, all these integrals reduce to elementary functions and the thermodynamic and correlation properties of the lattice exhibit no singularities.[1] (Singularities would, of course, correspond to phase transitions.)

Surprisingly, perhaps, the plane square lattice is not typical in this respect since, as shown explicitly by Kasteleyn[8] dimer assemblies on other lattices[17] do exhibit singularities and undergo transitions. The corresponding Green's functions must then be expressed in terms of elliptic integrals which, however, reduce to elementary functions at the transition points. Consequently, the simple square lattice dimer problem is probably best regarded as corresponding to the transition point of the more general checkerboard lattice.[17] The investigation of the correlation properties and the effects of monomers on more general lattices will be reserved, however, for another communication.

2. THE PARTITION FUNCTION AS A PFAFFIAN

In this section we review the various ways of expressing the partition function as a Pfaffian which have been found by the different authors and prove their equivalence. This also serves to introduce our notation (which differs slightly from that in I).

We consider a square lattice of n rows of m sites (m and n were interchanged in I). The Cartesian coordinates of a site are denoted by (r,s) with $r = 1, 2, 3, \cdots m$ and $s = 1, 2, 3, \cdots n$. We suppose the sites are labeled in some order $k = k(r,s) = 1, 2, 3, \cdots nm$.

The configurational grand partition function for monomers and dimers is defined by

$$Z_{mn}(x,y,z) = \sum_{N_x,N_y,N_0} g_{mn}(N_x,N_y,N_0)x^{N_x}y^{N_y}z^{N_0}, \quad (2.1)$$

where $g_{mn}(N_x,N_y,N_0)$ is the number of distinct configurations of N_x horizontal or x dimers, N_y vertical or y dimers, and N_0 monomers or unoccupied sites on an $m \times n$ lattice, and where x, y, and z are the activities of x dimers, y dimers, and monomers, respectively. If x/z^2 and y/z^2 are small, low-density series expansions are readily derived.[12] If $z = 0$, we have the high-density limit for which explicit solutions were obtained previously.[1–3]

Restricting ourselves now to the case $z = 0$, we consider an antisymmetric matrix $\mathbf{D} = [D_{kk'}] = [-D_{k'k}]$ whose $(nm)^2$ elements are labeled by the sites of the lattice. The element $D_{kk'}$ is taken to be zero unless the sites k and k' are connected by a nearest neighbor bond of the lattice. In that case we set

$$D_{kk'} = D(r, s; r+1, s) = \alpha_{rs}x$$

and

$$D_{kk'} = D(r, s; r, s+1) = \beta_{rs}y, \quad (2.2)$$

which can be embedded in a plane with no crossing bonds. The graph divides the plane into disjoint *faces* each enclosed by a polygonal *mesh*.

[10] See also A. N. Dykhne and Yu. B. Rumer, Usp. Fiz. Nauk **75**, 101 (1961) [translation: Soviet Phys.—Usp. **4**, 698 (1962)] who follow Hurst and Green (Ref. 7) more closely.

[11] H. S. Green, Z. Physik **171**, 129 (1963).

[12] M. E. Fisher and H. N. V. Temperley, Rev. Mod. Phys. **32**, 1029 (1960).

[13] B. Kaufman and L. Onsager, Phys. Rev. **76**, 1244 (1949).

[14] R. B. Potts and J. C. Ward, Progr. Theoret. Phys. (Kyoto) **13**, 38 (1955).

[15] E. W. Montroll, R. B. Potts, and J. C. Ward, J. Math. Phys. **4**, 308 (1963).

[16] The method is an extension of that used for determinants by E. W. Montroll and R. B. Potts, Phys. Rev. **102**, 72 (1956), in their study of the vibration of harmonic lattices with defects.

[17] Kasteleyn investigated the honeycomb and the triangular lattices, and the 'checkerboard' lattice in which the activities of the four possible dimers around alternate squares of a square lattice are distinguished.

where α_{rs} and β_{rs} are factors of modulus unity. It is easy to see from the definition of a Pfaffian[1,3,5,6] that the terms in the expansion of $\mathrm{Pf}(\mathbf{D})$ are in one-one correspondence with the configurations of x and y dimers which completely fill the lattice.[1-3] Furthermore, the modulus of each term has the same value as in the partition function; the sign (or, more generally, the argument) of each term, however, depends on the factors α_{rs} and β_{rs} and on the parity of the permutation appropriate to the configuration. The latter depends, in turn, on the labeling of the sites.

It was proved in I that if the sites are labeled in 'zigzag' order i.e., along the first row, *back* along the second, along the third row, and so on, so that

$$k_{\mathrm{I}}(r,s)=r+(s-1)m \qquad (s\ \mathrm{odd})$$
$$=m-r+1+(s-1)m \qquad (s\ \mathrm{even}), \qquad (2.3)$$

and one defines the matrix $\mathbf{D}_{\mathrm{I}}$ with elements $\mathbf{D}_{\mathrm{I}}(r,s;r',s')$ given by (2.2) with

$$\alpha_{\mathrm{I},rs}=\beta_{\mathrm{I},rs}=+1, \qquad (2.4)$$

then $\mathrm{Pf}(\mathbf{D}_{\mathrm{I}})$ counts all the terms with positive sign. Thus, we have

$$Z_{mn}(x,y,0)=\mathrm{Pf}(\mathbf{D}_{\mathrm{I}})=[\mathrm{Det}(\mathbf{D}_{\mathrm{I}})]^{1/2}, \qquad (2.5)$$

from which the partition function may be calculated by diagonalizing $\mathbf{D}_{\mathrm{I}}$ as done in I.

The labeling (2.3) is not very convenient for studying correlations in the center of the lattice. For this purpose the dictionary order

$$k_{\mathrm{II}}(r,s)=r+(s-1)m \quad (\mathrm{all}\ s) \qquad (2.6)$$

is preferable. The appropriate matrix $\mathbf{D}_{\mathrm{II}}$ and, hence, the correct Pfaffian may be found merely by rearranging the rows and columns of $\mathbf{D}_{\mathrm{I}}$ in accordance with (2.6) and remembering the antisymmetry. {These operations leave $[\mathrm{Pf}(\mathbf{D})]^2=\mathrm{Det}(\mathbf{D})$ unaltered and, hence, $\mathrm{Pf}(\mathbf{D})$ can change at most by a factor -1.} One finds immediately that

$$\alpha_{\mathrm{II},rs}=-(-1)^s, \quad \beta_{\mathrm{II},rs}=+1. \qquad (2.7)$$

Alternatively, we may rotate the lattice clockwise through a right angle and use dictionary order about the new origin. In terms of the old coordinates this is the order

$$k_{\mathrm{III}}(r,s)=s+(m-r)n, \qquad (2.8)$$

which yields

$$\alpha_{\mathrm{III},rs}=(-1)^s, \quad \beta_{\mathrm{III},rs}=+1. \qquad (2.9)$$

On going to the new coordinates by $r\to m-s+1$, $s\to r$ and interchanging x and y, α and β, and m and n, we obtain the matrix $\mathbf{D}_{\mathrm{IV}}$ given by the orthodox dictionary order

$$k_{\mathrm{IV}}(r,s)=r+(s-1)m \qquad (2.10)$$

and by (2.2) with

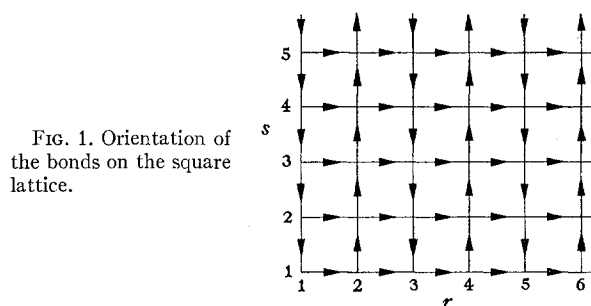$$\alpha_{\mathrm{IV},rs}=+1, \quad \beta_{\mathrm{IV},rs}=(-1)^s. \qquad (2.11)$$

FIG. 1. Orientation of the bonds on the square lattice.

This matrix, which is just a rearrangement of $\mathbf{D}_{\mathrm{I}}$, is identical with that found and proved valid from first principles by Kasteleyn.[3,18] Following Kasteleyn, the signs of the elements may be summarized conveniently by *orienting* the lattice bonds as shown in Fig. 1 and using the following convention[3,8]:

RULE A. *The sign of the element $D_{kk'}$ is positive if the arrow runs from the site k towards the site k' but negative if the arrow points in the opposite sense.*

Notice that the rule automatically ensures that $\mathbf{D}$ is antisymmetric. The correctness of this sign allocation follows generally from Kasteleyn's later theorems[8] which may be stated:

THEOREM. *If the bonds of a planar graph[9] G are oriented so that the number of arrows pointing clockwise around each mesh is odd, which is always possible, and if the signs of the elements of $\mathbf{D}$ are allocated in accordance with Rule A then all dimer configurations on G will be counted by $\mathrm{Pf}(\mathbf{D})$ with a positive sign.*

It is readily verified from Fig. 1 that each primitive square in the lattice has a 'clockwise odd' orientation. Application of the theorem to other lattices merely requires the discovery of a correct and convenient orientation of the bonds. We may reverse the previous train of argument and deduce $\mathbf{D}_{\mathrm{I}}$, $\mathbf{D}_{\mathrm{II}}$, and $\mathbf{D}_{\mathrm{III}}$ from $\mathbf{D}_{\mathrm{IV}}$ by reorienting the bonds in Fig. 1 by rotating the lattice counter clockwise through a right angle and applying Rule A and the appropriate labeling systems (2.3), (2.6), and (2.8).

The matrices $\mathbf{D}_{\mathrm{I}}$ to $\mathbf{D}_{\mathrm{IV}}$ all suffer from the inconvenience that they do not exhibit quite the full symmetry of lattice owing to the alternation of signs (or the zigzag labeling). Wu[19] has shown from first principles that this can be avoided for the plane square lattice by using dictionary labeling

$$k_0(r,s)=r+(s-1)m \qquad (2.12)$$

and the simple choice

$$\alpha_{0,rs}=1, \quad \beta_{0,rs}=i, \qquad (2.13)$$

[18] The correspondence with Kasteleyn's notation in Ref. 3 is $(r,s;r',s')\to(i,j;i',j')$, $x\to z$, $y\to z'$ and $m,n\to m,n$.
[19] T. T. Wu, J. Math. Phys. 3, 1265 (1962).

so that

$$D_0(r, s; r+1, s) = -D_0(r+1, s; r, s) = x,$$

$$D_0(r, s; r, s+1) = -D_0(r, s+1; r, s) = iy, \quad (2.14)$$

$$D_0(r, s; r', s') = 0, \quad \text{otherwise.}$$

It is not difficult to verify that Wu's matrix D_0 can also be derived directly from D_{IV} (and therefore from D_I) by multiplying all those rows of D_{IV} which correspond to sites of odd r by $-i$ and all those corresponding to sites of even r by $+i$. These operations multiply $\text{Det}(D_{IV})$ by $(-i^2)^{\frac{1}{2}mn}$ which is unity since $\frac{1}{2}mn$ must be even if the lattice can be filled with dimers [otherwise $\text{Det}(D) \equiv 0$]. The simple form of the matrix D_0 makes it the most convenient basis for a study of the correlations and we adopt it as the standard form.

3. PERTURBATION THEORY FOR PFAFFIANS

In this section we show how a Pfaffian P which differs only in a few elements from a Pfaffian P_0 can be calculated in terms of P_0 and the elements of suitable Green's function. Thus, suppose

$$P_0 = \text{Pf}(D_0)$$

and

$$P = \text{Pf}(D) = \text{Pf}(D_0+E), \quad (3.1)$$

where D_0, D and E are antisymmetric matrices and only a relatively few elements of E are nonzero.[20] We may suppose D_0 to be a nonsingular matrix (since otherwise P_0 vanishes identically) and so may define the Green's function matrix

$$G = D_0^{-1}. \quad (3.2)$$

Then, since the determinant of a product of matrices equals the product of the determinants

$$P^2 = \text{Det}(D_0+E) = \text{Det}(D_0) \, \text{Det}(I+GE)$$

$$= P_0^2 \, \text{Det}(I+GE), \quad (3.3)$$

where I is a unit matrix of appropriate dimensionality. Now each column of the matrix GE will be identically zero unless the matrix E has a nonzero element in the corresponding column (or, in view of the antisymmetry, in the corresponding row). If the determinant $\Delta = \text{Det}(I+GE)$ is expanded successively by those

columns which are zero in GE it may be reduced to the form

$$(P/P_0)^2 = \Delta = \text{Det}(I'+ge). \quad (3.4)$$

Here the *reduced* Green's function and perturbation matrices g and e, are antisymmetric square matrices formed from G and E by retaining only those rows and columns in which E has nonzero elements. Similarly, I' is a reduced unit matrix of corresponding dimensionality. Note that the rows and columns of g and e need not finally be ordered in the same sequence as in G and E.

The effects of a perturbation on P_0 can thus be found by evaluating the relatively small determinant Δ. In fact, the labor can be reduced further by noting that Δ itself can be expressed as the squares of Pfaffians. To see this, suppose $\text{Det}(e) \neq 0$. This will be true, as shown below, if the nonzero elements $E_{kk'}$ of E have no subscripts in common (i.e., the corresponding bonds[20] do not meet at any site) but need not be true otherwise. We then have from (3.4)[21]

$$\Delta = \text{Det}(e) \, \text{Det}(e^{-1}+g) \quad (3.5)$$

so that, in virtue of the antisymmetry of e, e^{-1} and g, the perturbation factor is

$$\Pi = P/P_0 = \Delta^{1/2} = \text{Pf}(e) \, \text{Pf}(e^{-1}+g). \quad (3.6)$$

We assume here and elsewhere that the sign of the square root is chosen to yield a positive result when the perturbations are small.

A more explicit result can be obtained if we assume definitely that there are only h nonzero elements $E_{kk'}$ of E and that the $2h$ indices k, k' are distinct. If we relabel the indices k_1, k_1', k_2, k_2', $\cdots k_h$, k_h' for use in in the reduced matrices g and e as 1, 2, 3, 4, $\cdots 2h-1$, $2h$ the only nonzero elements of e are

$$e_{12} = -e_{21} = E_{k_1 k_1'} = \epsilon_{12}, \quad e_{34} = -e_{43} = E_{k_2 k_2'} = \epsilon_{34}, \quad \cdots$$

$$\cdots e_{2h-1,2h} = -e_{2h,2h-1} = E_{k_h k_h'} = \epsilon_{2h-1,2h}, \quad (3.7)$$

while the $4h^2$ elements of g are

$$g_{2a-1,2b-1} = G_{k_a k_b}, \quad g_{2a-1,2b} = -g_{2b,2a-1} = G_{k_a k'_b}$$

$$g_{2a,2b} = G_{k'_a k'_b}. \quad (3.8)$$

The matrix e is thus diagonal in 2×2 blocks of the form

$$\begin{bmatrix} 0 & \epsilon_{2i-1,2i} \\ -\epsilon_{2i-1,2i} & 0 \end{bmatrix} \quad \text{each of which has the inverse} \quad \begin{bmatrix} 0 & -1/\epsilon_{2i-1,2i} \\ 1/\epsilon_{2i-1,2i} & 0 \end{bmatrix}.$$

Consequently, $\text{Det}(e) = \prod_{i=1}^{h}(\epsilon_{2i-1,2i})^2 \neq 0$. The antisymmetry of $\text{Det}(e^{-1}+g)$ in (3.5) is preserved if the first row and column are each multiplied by $-\epsilon_{12}$, the third row and column by $-\epsilon_{34}$, $\cdots$ the $(2h-1)$th row and column

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[20] In lattice applications each nonzero element $E_{kk'}$ of E corresponds to a *perturbed bond* between sites k and k'.

[21] This procedure has also been used by Montroll, Potts, and Ward (Ref. 15), but they did not reduce the Pfaffian as far as we do. Nor did they need to consider the case $\text{Det}(e) = 0$.

by $-\epsilon_{2h-1,2h}$.[22] On taking the square root, we obtain the perturbation factor as the single Pfaffian

$$\Pi = P/P_0 = \begin{vmatrix} 1-\epsilon_{12}g_{12} & \epsilon_{12}\epsilon_{34}g_{13} & -\epsilon_{12}g_{14} & \epsilon_{12}\epsilon_{56}g_{15} & -\epsilon_{12}g_{16} \\ & -\epsilon_{34}g_{23} & g_{24} & -\epsilon_{56}g_{25} & g_{26} \\ & & 1-\epsilon_{34}g_{34} & \epsilon_{34}\epsilon_{56}g_{35} & -\epsilon_{34}g_{36} \\ & & & -\epsilon_{56}g_{45} & g_{46} \\ & & & & 1-\epsilon_{56}g_{56} \end{vmatrix} \quad (3.9)$$

where the general coefficient may be written

$$\begin{bmatrix} \pi_{2i-1,2j-1} & \pi_{2i-1,2j} \\ \pi_{2i,2j-1} & \pi_{2i,2j} \end{bmatrix} = \begin{bmatrix} \epsilon_{2j-1,2j}\epsilon_{2i-1,2i}g_{2i-1,2j-1} & (\delta_{ij}-\epsilon_{2i-1,2i}g_{2i-1,2j}) \\ -\epsilon_{2j-1,2j}g_{2i,2j-1} & g_{2i,2j} \end{bmatrix}. \quad (3.10)$$

Particular cases of this result which we will require are, for a single perturbed element in the Pfaffian,

$$\Pi_{12} = 1 - \epsilon_{12}g_{12} = 1 - \epsilon_{12}G_{k_1 k_2} \quad (3.11)$$

and for two altered elements

$$\Pi_{12,34} - \Pi_{12}\Pi_{34} = -\epsilon_{12}\epsilon_{34}(g_{13}g_{24} - g_{14}g_{23}). \quad (3.12)$$

The formula (3.9) has been proved only for the case when the indices of the perturbation elements $E_{kk'}$ are all distinct. Indeed it is easy to see that $\text{Det}(\mathbf{e}) = 0$ if, for example, the only nonzero perturbation elements are $E_{12} = e_{12}$ and $E_{23} = e_{23}$. In such a case the inverse $\mathbf{e}^{-1}$ does not exist and the proof breaks down. By direct verification one discovers, none the less, that (3.9) is still valid even if some of the indices do refer to the same row or column. The reason for this, which lies in the antisymmetry of $\mathbf{E}$ and the vanishing of g_{jj} is indicated in Appendix A. In this way, or directly, one finds, for example, for a 'chain' of two bonds[20]

$$\Pi_{12,23} = 1 - \epsilon_{12}g_{12} - \epsilon_{23}g_{23}, \quad (3.13)$$

and, generally, for a 'star' of h bonds

$$\Pi_{1,2;1,3;\cdots 1,h+1} = 1 - \sum_{i=2}^{h+1} \epsilon_{1i}g_{1i}. \quad (3.14)$$

Similarly for a 'triangle' one finds

$$\Pi_{12,23,31} = 1 - \epsilon_{12}g_{12} - \epsilon_{23}g_{23} - \epsilon_{31}g_{31}. \quad (3.15)$$

4. EVALUATION OF THE GREEN'S FUNCTION

To utilize the perturbation formalism for Pfaffians developed in the previous section, we must calculate the Green's function, i.e., the matrix inverse of the basic counting matrix $\mathbf{D}_0$ defined in Sec. 2. It is straightforward to verify that if $\mathbf{D}_0$ is transformed by the

unitary matrix $\mathbf{U}$ with elements

$$U_{kk'} = U(r,s;r',s')$$

$$= \frac{2i^{r+s+2}}{(m+1)^{1/2}(n+1)^{1/2}} \sin\frac{\pi r r'}{(m+1)} \sin\frac{\pi s s'}{(n+1)}, \quad (4.1)$$

it is reduced to the diagonal form $\mathbf{\Lambda} = \text{diag}\{\lambda_j\}$ where the eigenvalues are

$$\lambda_j = \lambda(p,q) = 2i\left[x\cos\frac{p\pi}{m+1} + iy\cos\frac{q\pi}{n+1}\right]. \quad (4.2)$$

Since $\text{Det}(\mathbf{D}_0) = \Pi_j\lambda_j$, an exact expression for the partition function follows immediately as in I. The inverse $\mathbf{G}$ is now determined by

$$\mathbf{G} = \mathbf{D}_0^{-1} = \mathbf{U}\mathbf{\Lambda}^{-1}\mathbf{U}^\dagger = \left[\sum_{j=1}^{mn} U_{kj}(1/\lambda_j)U^*_{k'j}\right]. \quad (4.3)$$

More explicitly, if we set

$$\theta_p = p\pi/(m+1) \quad \text{and} \quad \phi_q = q\pi/(n+1), \quad (4.4)$$

we have

$$G_{kk'} = G(r,r';s,s') = \frac{2i^{r+s-r'-s'+1}}{(m+1)(n+1)}$$

$$\times \sum_{p=1}^{m}\sum_{q=1}^{n} \frac{\sin r\theta_p \sin r'\theta_p \sin s\phi_q \sin s'\phi_q}{x^2\cos^2\theta_p + y^2\cos^2\phi_q}$$

$$\times (-x\cos\theta_p + iy\cos\theta_q). \quad (4.5)$$

Of great importance for simplifying the subsequent calculations are the symmetry properties of $G(r,r';s,s')$. Consider the transformation of the dummy variable $p \rightarrow m+1-p'$ which results in $\cos\theta_p \rightarrow -\cos\theta_{p'}$ and $\sin r\theta_p \rightarrow (-)^{r+1}\sin r\theta_{p'}$. If we denote the parts of the Green's function proportional to $-x$ and to iy by G_X and G_Y, respectively, we find $G_X = -(-)^{r+r'}G_X$ and $G_Y = (-)^{r+r'}G_Y$. Thus, $G_X \equiv 0$ if $r+r'$ is even, while $G_Y \equiv 0$ if $r+r'$ is odd. Similarly, by considering the transformation $q \rightarrow n+1-q'$, we deduce that $G_Y \equiv 0$ if $s+s'$ is even, while $G_X \equiv 0$ if $s+s'$ is odd. On defining the

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[22] The minus signs are inserted to ensure that the Pfaffian (3.9) is positive for small perturbations. A somewhat more symmetrical looking result can be obtained by transposing the determinant and then multiplying the first pair of rows and columns by $\epsilon_{12}^{1/2}$ the second pair by $\epsilon_{34}^{1/2}$ and so on.

coordinates (t,u) of the separation of the points k and k' by

$$t=r'-r, \quad u=s'-s, \tag{4.6}$$

we thus see that

$G_{kk'}=G(r,s\,;r',s')\equiv0$ if t and u have the
$$\text{same parity.} \tag{4.7}$$

In other words $G_{kk'}$ vanishes unless the sites k and k' are on *different sublattices*. The nonzero elements of $\mathbf{G}$ correspond to $(t+u+1)$ even and are

$$G_{kk'}=G(r,s\,;r',s')=\frac{2(-1)^{\frac{1}{2}(t+u+1)}}{(m+1)(n+1)}$$

$$\times\sum_{p=1}^{m}\sum_{q=1}^{n}\frac{\sin r\theta_p\,\sin r'\theta_p\,\sin s\phi_q\,\sin s'\phi_q}{x^2\cos^2\theta_p+y^2\cos^2\phi_q}$$

$$\times\begin{cases}-x\cos\theta_p, & t\text{ odd, }u\text{ even.}\\ iy\cos\phi_q, & t\text{ even, }u\text{ odd.}\end{cases} \tag{4.8}$$

By interchanging r and r' and s and s', one immediately verifies the generalized antisymmetry relations

$$G(r,s\,;r',s')=(-)^t\,G(r',s\,;r,s')$$
$$=(-)^u\,G(r,s'\,;r',s)=-G(r',s'\,;r,s). \tag{4.9}$$

An important recurrence relation for the Green's function follows by writing out the identities

$$\mathbf{GD}_0=\mathbf{I}=\mathbf{D}_0\mathbf{G} \tag{4.10}$$

in detail. This yields

$$xG(r,s\,;r+t-1,s+u)+iyG(r,s\,;r+t,s+u-1)$$
$$-xG(r,s\,;r+t+1,s+u)-iyG(r,s\,;r+t,s+u+1)$$
$$=\delta_{rr'}\delta_{ss'}=\delta_{0t}\delta_{0u} \tag{4.11}$$

and a similar relation which can be obtained directly by using the antisymmetry of $\mathbf{G}$.

The formula (4.8) gives the Green's function exactly for a finite $m\times n$ lattice. We shall be chiefly interested, however, in very large lattices so that we consider the limit $m\to\infty$, $n\to\infty$ with r, s, r', and s' remaining finite. If we introduce the variables

$$\alpha=\frac{2\pi p}{m+1}-\pi, \quad \beta=\frac{2\pi q}{n+1}-\pi, \tag{4.12}$$

which become continuous in the limit, the sums approach integrals, and we find, after some elementary manipulation, that

$$G(r,s\,;r',s')=\frac{1}{\pi^2}\int_0^\pi\int_0^\pi d\alpha\,d\beta\frac{M(r,s\,|\,t,u\,|\,\alpha,\beta)}{x^2(1-\cos\alpha)+y^2(1-\cos\beta)}, \tag{4.13}$$

where

$$M(r,s\,|\,t,u\,|\,\alpha,\beta)\equiv0 \quad (t,\,u\text{ both odd, both even})$$

$$=\tfrac{1}{2}x\{\cos\tfrac{1}{2}(t+1)\alpha-\cos\tfrac{1}{2}(t-1)\alpha$$
$$+(-)^r\cos[r+\tfrac{1}{2}(t-1)\alpha]$$
$$-(-)^r\cos[r+\tfrac{1}{2}(t+1)\alpha]\}$$
$$\times[\cos\tfrac{1}{2}u\beta-(-)^s\cos(s+\tfrac{1}{2}u)\beta],$$
$$(t\text{ odd, }u\text{ even}), \tag{4.14}$$

$$=-\tfrac{1}{2}iy[\cos\tfrac{1}{2}t\alpha-(-)^r\cos(r+\tfrac{1}{2}t)\alpha]$$
$$\times\{\cos\tfrac{1}{2}(u+1)\beta-\cos\tfrac{1}{2}(u-1)\beta$$
$$+(-)^s\cos[s+\tfrac{1}{2}(u-1)]\beta$$
$$-(-)^s\cos[s+\tfrac{1}{2}(u+1)]\beta\}, \quad (t\text{ even, }u\text{ odd}).$$

In the center of a large lattice we expect $G(r,s\,;r',s')$ to depend only on the distance separating the sites k and k', i.e., only on $t=r'-r$ and $u=s'-s$. Inspection of (4.14) shows that this comes about as r and $s\to\infty$ owing to the increasingly rapid oscillation of the terms depending on r and s. In the center of an infinite lattice we thus find

$$M(t,u\,|\,\alpha,\beta)=0 \quad (t,\,u\text{ both odd, both even})$$

$$=\tfrac{1}{2}x[\cos\tfrac{1}{2}(t+1)\alpha-\cos\tfrac{1}{2}(t-1)\alpha]\cos\tfrac{1}{2}u\beta,$$
$$(t\text{ odd, }u\text{ even})$$
$$=\tfrac{1}{2}iy\cos\tfrac{1}{2}t\alpha[\cos\tfrac{1}{2}(u+1)\beta-\cos\tfrac{1}{2}(u-1)\beta],$$
$$(t\text{ even, }u\text{ odd}). \tag{4.15}$$

In discussing correlations in the center of the lattice, it proves convenient to introduce the abbreviated notation

$$G(r,s\,;r',s')=[t,u]=-[-t,-u], \quad (r,s\to\infty). \tag{4.16}$$

The other symmetry properties of the symbol $[t,u]$ follow from (4.9).

The integrals (4.13) with $M(\alpha,\beta)$ given by (4.14) or (4.15) are of an elementary type for finite r, s, r', and s' and may be evaluated as in I with the aid of well-known standard forms. We quote here only the first few Green's function elements for the center of an infinite lattice.

$$[0,0]=[\pm1,\pm1]=[\pm2,0]=[0,\pm2]=\cdots=0, \tag{4.17}$$
$$[1,0]=-[-1,0]=-(1/\pi x)\tan^{-1}(x/y),$$
$$[0,1]=-[0,-1]=(1/i\pi y)\tan^{-1}(y/x), \tag{4.18}$$

and

$$[1,2]=-[-1,\pm2]=[1,-2]$$
$$=-(1/\pi y)[1-(x/y)\tan^{-1}(x/y)], \tag{4.19}$$
$$[2,1]=-[\pm2,-1]=[-2,1]$$
$$=-(1/i\pi x)[1-(y/x)\tan^{-1}(y/x)].$$

Further results follow immediately with the aid of the recurrence relation (4.11) and the symmetry properties (4.9). All the central elements with $|t|+|u|\leqslant5$ are tabulated in Appendix B for general x and y and for

$x=y$ up to $|t|+|u| \leqslant 11$. Various elements for the edge of a lattice, i.e., for $r \to \infty$, s finite (and vice versa) and for a corner of the lattice, i.e., for r and s finite, are also tabulated in Appendix B.

For large t and u or for large but finite r and s, asymptotic expansions of the Green's function elements may be obtained as inverse power series in t, u, r, or s by integrating by parts repeatedly. The method and various formulas are presented in Appendix C.

5. OCCUPATION PROBABILITIES FOR SINGLE DIMERS

To calculate the probability that a given bond in the lattice is occupied by a dimer and to study the influence of the proximity of an edge or a corner of the lattice on this probability, it is convenient to introduce a set of occupancy variables depending on the configuration Γ of dimers on the lattice. Let $\nu_a = \nu_{kk'}(\Gamma) = 1$ if, in the configuration Γ, the bond a between sites k and k' is occupied by a dimer, but let $\nu_a = \nu_{kk'}(\Gamma) = 0$ if the bond is *not* occupied. It is also useful to define the corresponding vacancy variables $\bar{\nu}_a = 1 - \nu_a$ which take the value zero when a bond is occupied. The probability in thermodynamic equilibrium that the bond l is occupied may now be written

$$P_a = \Pr\{\nu_a = 1\} = \langle \nu_a \rangle = 1 - \langle \bar{\nu}_a \rangle, \quad (5.1)$$

where the angular brackets denote an average over the grand canonical ensemble. If $A(\Gamma)$ is a variable depending on the configuration, this average is defined as usual by

$$\langle A \rangle = (1/Z) \sum_{\Gamma} A(\Gamma) x^{N_x} y^{N_y} z^{N_0}. \quad (5.2)$$

(The activity z is included for generality although in this and the next few sections we shall be concerned only with the high-density limit $z=0$.)

Now consider the average $\langle \bar{\nu}_l \rangle$. The configurations entering the sum in (5.2) will be all possible configurations *except* those in which the bond l is occupied by a dimer. The required configurations will (when $z=0$) be counted by the Pfaffian of $\mathbf{D}_0$ if the matrix is modified by setting equal to zero the elements $D_{kk'}$ and $D_{k'k}$ corresponding to the bond a. In other words, we require to calculate a perturbed Pfaffian where by (2.14), (3.1), and (3.7) the nonzero perturbation elements are

$$E_{k,k+1} = \epsilon_a = -x \quad \text{or} \quad E_{k,k+m} = \epsilon_a = -iy, \quad (5.3)$$

for a horizontal or vertical bond, respectively. Appealing to the results of the Sec. 3, in particular, (3.9) and (3.10), we obtain

$$\langle \bar{\nu}_{k,k+1} \rangle = 1 + x G_{k,k+1} \quad (5.4)$$

and similarly for a vertical or y bond. Finally, by (5.1) the probability of occupation of the horizontal bond

leading from the point $k(r,s)$ to the right is

$$P_X(r,s) = -x G(r, s; r+1, s), \quad (5.5)$$

while for the corresponding vertical bond it is

$$P_Y(r,s) = -iy G(r, s; r, s+1). \quad (5.6)$$

These results together with the expressions (4.8) and (4.13) to (4.15) for the Green's function enable us to study the probability of occupation of any bond in a finite or infinite lattice. In the center of a large (strictly, infinite) lattice we expect P_X and P_Y to become independent of position and to be proportional merely to the over-all densities ρ_x and ρ_y of x and y dimers. These densities were calculated in I in the standard way by differentiating the grand partition function with respect to the activities. In terms of the number of dimers per site this yields

$$\rho_x = (1/\pi) \tan^{-1}(x/y), \quad \rho_y = (1/\pi) \tan^{-1}(y/x) \quad (5.7)$$

so that

$$\rho_x + \rho_y = \tfrac{1}{2}. \quad (5.8)$$

Note that the activities x and y may be eliminated in favor of the densities by setting $xy = 1$ and

$$\tau = x/y = \tan \pi \rho_x = \cot \pi \rho_y. \quad (5.9)$$

By using the expressions (4.18) for the Green's function elements $[1, 0]$ and $[0, 1]$ we, indeed, at once verify that, in the center of the lattice

$$P_X(\infty) = -x[1, 0] = (1/\pi) \tan^{-1}(x/y) = \rho_x \quad (5.10)$$

and similarly for $P_Y(\infty)$. In the symmetric case $x=y$ or $\tau = 1$, the probability of occupation of a central bond is $\tfrac{1}{4}$.

The recurrence relation (4.11) with $t=u=0$ and the antisymmetry of the Green's function imply by (5.5) and (5.6) that

$$P_X(r-1, s) + P_Y(r, s-1) + P_X(r,s) + P_Y(r,s) = 1. \quad (5.11)$$

This merely expresses the "conservation of dimers," i.e., the fact that in the high-density limit all sites must be filled by the end of some dimer.

6. EFFECTS OF AN EDGE AND A CORNER

Near an edge or a corner of the lattice the occupation probabilities will deviate from their central values and, for example, in the symmetric case x dimers might preponderate over y dimers near an edge or vice versa. Consider an edge parallel to the x axis. Far from the corner, r tends to infinity and s measures the distance of a bond inwards from the edge. The Green's function element (5.5) for parallel or x bonds is thus given by (4.13) with

$$M_{11}(s) = \tfrac{1}{2} x (\cos \alpha - 1)[1 - (-)^s \cos \beta]. \quad (6.1)$$

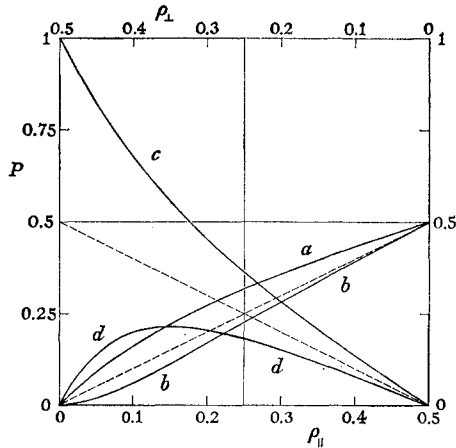On evaluating the integral for $s=1$ (see Appendix B) one finds that the probability of occupation of a bond

FIG. 2. Occupation probabilities of dimers near the edge of the lattice. Variation of (a) $P_{||}(1)$, (b) $P_{||}(2)$, (c) $P_{\perp}(1)$, and (d) $P_{\perp}(2)$ with the densities $\rho_{||}$ and $\rho_{\perp}$.

in the edge is

$$P_{||}(1) = \rho_{||} - \rho_{\perp}\tau^2 + (\tau/\pi), \qquad (6.2)$$

where we have written τ for x/y and $\rho_{||}$ and $\rho_{\perp}$ for the parallel and perpendicular densities ρ_x and ρ_y. In the symmetrical case, therefore,

$$P_{||}(1) = 1/\pi = 0.318\ 3099, \qquad (x=y), \qquad (6.3)$$

rather than $\frac{1}{4}$ as in the center of the lattice. The probability of a parallel dimer is thus appreciably enhanced. Indeed, for small $\rho_{||}$ $(\tau \to 0)$ one has

$$P_{||}(1) = 2\rho_{||} + O(\rho_{||}^2), \qquad (6.4)$$

so that the probability of a dimer lying in the edge of the lattice is doubled relative to parallel dimers in the center.

The probability of occupation of the first perpendicular bond may be found by performing the appropriate integral or, more simply, by using the conservation relation (5.11), which yields

$$P_{\perp}(1) = 2\rho_{\perp}(1+\tau^2) - 2(\tau/\pi). \qquad (6.5)$$

In the symmetric case

$$P_{\perp}(1) = 1 - (2/\pi) = 0.363\ 3802, \qquad (x=y) \qquad (6.6)$$

which is also greater than $\frac{1}{4}$. At first sight, it seems paradoxical that the probabilities at the edge for both parallel and perpendicular dimers are increased. The result is clearly due, however, to the fact that a perpendicular dimer cannot stick out through the edge of the lattice ! This is borne out by the discovery that $P_{\perp}(1)$ approaches 1 as $\rho_{\perp} \to \frac{1}{2}$, whereas $P_{||}(1)$ only approaches $\frac{1}{2}$ as $\rho_{||} \to \frac{1}{2}$. This behavior can be seen in Fig. 2 which is a plot of the occupation probabilities versus the densities. The value (6.6) might be compared most appropriately with $\frac{1}{4} + \frac{1}{4} = \frac{1}{2}$, the total *a priori* probability for perpendicular dimers through a point, rather than with $\frac{1}{4}$.

For the second parallel bond $(s=2)$ we find (see Appendix B)

$$P_{||}(2) = \rho_{||} + \rho_{\perp}\tau^2(2+3\tau^2) - (\tau/\pi)(1+3\tau^2), \qquad (6.7)$$

which shows that the probability of a parallel dimer in the second row is *decreased* somewhat below the central value. In particular, when $x=y$

$$P_{||}(2) = \tfrac{3}{2} - (4/\pi) = 0.226\ 7604, \qquad (x=y) \qquad (6.8)$$

while, when $\rho_{||}$ is small,

$$P_{||}(2) = \pi^2\rho_{||}^2 + O(\rho_{||}^3). \qquad (6.9)$$

As may be anticipated from the factor $(-1)^s$ in (6.1) this effect is the start of a regular alternation which is typical of the repulsive interactions between the rigid dimers. Thus, the probability of occupation of the second perpendicular bond, namely,

$$P_{\perp}(2) = 2(\tau/\pi)(2+3\tau^2) - 6\rho_{\perp}\tau^2(1+\tau^2), \qquad (6.10)$$

also falls below the central value $\rho_{\perp}$. In fact, in the symmetric case

$$P_{\perp}(2) = (10/\pi) - 3 = 0.183\ 0999, \qquad (x=y). \qquad (6.11)$$

These probabilities also are plotted in Fig. 2. One notes that $P_{\perp}(2) \to 0$ as $\rho_{\perp} \to \frac{1}{2}$ $(\rho_{||} \to 0)$ as is to be expected from the remarks above since, when all dimers are perpendicular to the edge, occupied and vacant perpendicular bonds must follow one another in alternation.

The spread of correlations into the lattice in the symmetric case is clearly shown by Table I which gives the first five values of the singlet correlation coefficients

$$c_{||}(s) = P_{||}(s) - P_{||}(\infty), \qquad c_{\perp}(s) = P_{\perp}(s) - P_{\perp}(\infty). \qquad (6.12)$$

In virtue of (5.11) the coefficients satisfy

$$c_{\perp}(s) + 2c_{||}(s) + c_{\perp}(s-1) = 0. \qquad (6.13)$$

In Table I, the coefficients have been normalized by dividing by the densities (corresponding to $s \to \infty$) so that they represent the fractional increase (or decrease) in the occupation probabilities. As noted above, the correlation coefficients alternate regularly in sign and their magnitudes decay to zero. The decay is much more rapid for the parallel bonds than for the perpendicular bonds. In fact, one can derive from (6.1) [and the corresponding expression for $M_{\perp}(s)$] the asymptotic

TABLE I. Values of the normalized singlet correlation coefficients

$$C_{||}(s) = [P_{||}(s) - P_{||}(\infty)]/P_{||}(\infty),$$
$$C_{\perp}(s) = [P_{\perp}(s) - P_{\perp}(\infty)]/P_{\perp}(\infty)$$

for dimers near an edge in the symmetric case $x=y$.

s	$C_{||}(s)$	$C_{\perp}(s)$
1	$(4/\pi) - 1 = 0.273\ 240$	$3 - (8/\pi) = 0.453\ 520$
2	$-(16/\pi) + 5 = -0.092\ 958$	$-13 + (40/\pi) = -0.267\ 605$
3	$(236/3\pi) - 25 = 0.040\ 379$	$63 - (592/3\pi) = 0.186\ 850$
4	$-(1216/3\pi) + 129 = -0.021\ 607$	$-321 + (1008/\pi) = -0.143\ 635$
5	$(32092/15\pi) - 681 = 0.013\ 391$	$1683 - (79304/15\pi) = 0.116\ 853$

formulas

$$c_{||}(s) \approx (-1)^{s+1}/4\pi\tau s^2 + O[s^{-4}] \qquad (6.14)$$

and

$$c_\perp(s) \approx (-1)^{s+1}/2\pi\tau(s+\tfrac{1}{2}) + O[(s+\tfrac{1}{2})^{-3}] \qquad (6.15)$$

(see Appendix C). The inverse power laws of decay, rather than exponential laws might have been expected by analogy with the theory of lattice dynamics with harmonic forces.[23] When $\tau \to 0$ so that $\rho_{||} \to 0$ and all dimers tend to align perpendicular to the edge, the coefficients of $1/s^2$ and $1/(s+\tfrac{1}{2})$ in these formulas diverge. This is due to the onset of the long-range alternating order referred to above which occurs when $\tau = \rho_{||} = 0$. Consequently, the asymptotic behavior is only approached when $s \gg 1/\tau = y/x$. For the symmetric case $\tau = 1$, however, the first term in the expansions are already quite accurate when $s \geqslant 3$ (compare with Table I).

Despite the alternation of signs in the parallel correlation coefficients, there is a net increase in the number of parallel dimers in the vicinity of an edge. To compute the increment $\sigma_{||}$ in the mean number of parallel dimers per site of a long straight edge, we introduce a convergence factor μ with $0 < \mu < 1$ and write

$$\sigma_{||}(\mu) = \sum_{s=1}^{\infty} \mu^s c_{||}(s). \qquad (6.16)$$

From (6.1) and (5.5) we have

$$\sigma_{||}(\mu) = \frac{1}{2\pi^2} \sum_{s=1}^{\infty} (-\mu)^s \int_0^\pi \int_0^\pi \frac{\tau^2(\cos\alpha - 1)\cos s\beta \, d\alpha \, d\beta}{\tau^2(1-\cos\alpha) + (1-\cos\beta)}. \qquad (6.17)$$

The integration with respect to α is readily performed. For $|\mu| < 1$, the summation on s and the second integration may be interchanged which yields

$$\sigma_{||}(\mu) = \frac{1}{4\pi} \int_0^\pi \frac{\sin\tfrac{1}{2}\beta}{[\tau^2 + \sin^2\tfrac{1}{2}\beta]^{1/2}} \left\{ \frac{1-\mu^2}{1+2\mu\cos\beta+\mu^2} - 1 \right\} d\beta. \qquad (6.18)$$

The substitution $w = \cos\tfrac{1}{2}\beta$ reduces the second member to standard form (see Appendix A). For the first member the further substitutions $v = 1/w$ and $\xi^2 = (1-\mu)^2 \times [(1+\tau^2)v^2 - 1]$ are necessary. The limit $\mu \to 1-$ may then be taken, which finally yields

$$\sigma_{||} = \sum_{s=1}^{\infty} c_{||}(s) = \tfrac{1}{4}(1+\tau^2)^{-1/2} - \tfrac{1}{2}\rho_\perp. \qquad (6.19)$$

This expression is positive for all densities of parallel or perpendicular dimers. In the symmetric case $x = y$, one finds that

$$\sigma_{||} = \tfrac{1}{4}(\sqrt{2} - 1) = 0.0517767, \qquad (6.20)$$

_____
[23] See the paper by Montroll and Potts quoted in Ref. 16.

which shows the magnitude of the "attraction" of parallel dimers towards the edge.

The result (6.20) may be found in an alternative way by using the asymptotic expression for the free energy of a large but finite lattice which was obtained in I. The mean total number of x dimers in a finite lattice is found by calculating $x(\partial/\partial x) \log Z_{mn}(x,y)$. The resulting expression contains "bulk" terms proportional to mn and "boundary" terms proportional to m and n separately. The constant of proportionality of the term in m should be equal to $2\sigma_{||}$ (since there are two opposite edges of length m). It is easily verified that this gives the same result as (6.19).

The effects of the corner of a lattice may be found similarly from (5.5) and (5.6) by using the full expressions (4.13) to (4.14) for the Green's function with finite r and s. In fact, one can show that

$$P_X(r,s) = \rho_x + (-)^r x[2r+1, 0] + (-)^s x[1, 2s] - (-)^{r+s} x[2r+1, 2s], \qquad (6.21)$$

which reduces to the previous results for dimers parallel or perpendicular to an edge when r or s approaches infinity. For the corner bond $(r=s=1)$ one finds

$$P_X(1,1) = \rho_x[2 + (1/\tau^2)] - \tau^2\rho_y + (\tau/\pi) - (1/\tau\pi). \qquad (6.22)$$

The expression for $P_Y(1,1)$ follows by symmetry in x and y ($x \leftrightarrow y$, $\tau \leftrightarrow 1/\tau$). In the symmetric case, the first few numerical values are

$$\begin{aligned} P_X(1,1) &= P_Y(1,1) = \tfrac{1}{2}, \\ P_X(2,1) &= P_Y(1,2) = (16/3\pi) - \tfrac{3}{2} = 0.197\,6527, \\ P_X(1,2) &= P_Y(2,1) = 2 - (16/3\pi) = 0.302\,3473, \\ P_X(2,2) &= P_Y(2,2) = (16/3\pi) - \tfrac{3}{2} = 0.197\,6527. \end{aligned} \qquad (6.23)$$

7. INTERACTION OF TWO DIMERS

The effective interaction of a pair of dimers in a close-packed sea of dimers may be studied by calculating the joint occupation probabilities for two bonds a and b. Using occupancy variables as in Sec. 5, the joint occupation probability may be written successively as

$$\begin{aligned} P_{ab} &= \Pr\{\nu_a = 1, \nu_b = 1\} = \langle \nu_a \nu_b \rangle \\ &= 1 - \langle \bar\nu_a \rangle - \langle \bar\nu_b \rangle + \langle \bar\nu_a \bar\nu_b \rangle \\ &= \langle (1-\nu_a) \rangle \langle (1-\bar\nu_b) \rangle + (\langle \bar\nu_a \bar\nu_b \rangle - \langle \bar\nu_a \rangle \langle \bar\nu_b \rangle), \quad (7.1) \end{aligned}$$

so that

$$P_{ab} = P_a P_b + c_{ab}, \qquad (7.2)$$

where P_a and P_b are the singlet occupation probabilities already discussed and c_{ab} is a pair correlation function defined by (7.2) or, more explicitly by

$$c_{ab} = \langle \bar\nu_a \bar\nu_b \rangle - \langle \bar\nu_a \rangle \langle \bar\nu_b \rangle. \qquad (7.3)$$

This function gives a complete description of the interdependence of the probabilities of vacancy and occupation as can be seen for the following formulas
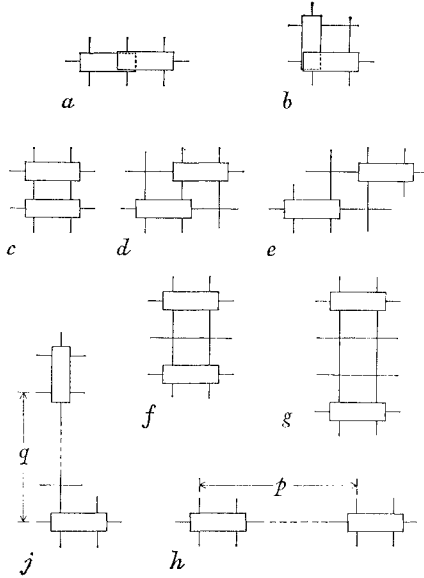
FIG. 3. Various configurations of pairs of dimers in the center of the lattice the probabilities of which are discussed in the text.

which are derived in analogy with (7.3),

$$P_{\bar{a}\bar{b}} = \Pr\{\nu_a = 0,\ \nu_b = 0\} = (1 - P_a)(1 - P_b) + c_{ab},$$
$$P_{a\bar{b}} = \Pr\{\nu_a = 1,\ \nu_b = 0\} = P_a(1 - P_b) - c_{ab}, \qquad (7.4)$$
$$P_{\bar{a}b} = \Pr\{\nu_a = 0,\ \nu_b = 1\} = (1 - P_a)P_b - c_{ab}.$$

To calculate $\langle \bar{\nu}_a \bar{\nu}_b \rangle$ and thence c_{ab} we consider a perturbed Pfaffian corresponding to the deletion of the two lattice bonds a and b. As before the nonzero perturbation elements are $-x$ or $-iy$ depending on whether the bonds are horizontal or vertical. Using the results (3.12) and (5.4) then yields

$$c_{xx}(r_a, s_a; r_b, s_b)$$
$$= -x^2 [G(r_a, s_a; r_b, s_b)G(r_a+1, s_a; r_b+1, s_b)$$
$$\qquad - G(r_a+1, s_a; r_b, s_b)G(r_a, s_a; r_a+1, s_b)] \quad (7.5)$$

for the correlation between two x bonds leading from the points $k_a = k(r_a, s_a)$ and $k_b = k(r_b, s_b)$. Similar expressions hold for c_{xy} and c_{yy}.

In the center of a large lattice, the correlations will depend only on the separation of the bonds (and their relative orientation). If we define

$$p = r_a - r_b, \qquad q = s_a - s_b, \qquad (7.6)$$

then for a pair of parallel horizontal bonds in the center of an infinite lattice

$$c_{xx}(p,q) = -x^2 \{ [p, q]^2 - [p-1, q][p+1, q] \}, \quad (7.7)$$

while for a pair of mutually perpendicular bonds

$$c_{xy}(p,q) = -ixy\{ [p, q][p-1, q+1]$$
$$\qquad - [p, q+1][p-1, q] \}. \quad (7.8)$$

(The symbols $[p, q]$ are the central Green's function elements defined in Sec. 4.) A similar expression holds

for $c_{yy}(p,q)$. The recurrence relation (4.11) for the Green's function implies that the pair correlation functions satisfy

$$c_{xx}(p-1, q) + c_{xy}(p, q-1) + c_{xx}(p,q) + c_{xy}(p,q) = 0, \quad (7.9)$$

which merely restates the conservation of dimers at each site.

Specific results for the center of a lattice follow by substituting the Green's function elements calculated in Appendix B into (7.7) and (7.8). Owing to the sublattice property (4.7) either the first or second term in both (7.7) and (7.8) must vanish. For two horizontal bonds meeting at a point as in Fig. 3(a) one obtains, using (4.18),

$$c_{xx}(1,0) = -\rho_x^2 \qquad (7.10)$$

while for a vertical and horizontal bond meeting at point as in Fig. 3(b)

$$c_{xy}(0,0) = c_{xy}(1,0) = -\rho_x \rho_y. \qquad (7.11)$$

Since the singlet probabilities P_a and P_b are equal to ρ_x or ρ_y the joint occupation probabilities in this case are zero, which simply confirms that two dimers may not overlap at a site.

For a pair of nearest neighbor parallel bonds [Fig. 3(c)] one finds, on the other hand,

$$c_{xx}(0,1) = \tau^2 \rho_y^2. \qquad (7.12)$$

In the symmetric case $x = y$, $\tau = 1$ this yields $c_{xx}(0,1) = \frac{1}{16}$ so that the probability of joint occupation is double that for two independent bonds $(= \frac{1}{4} \times \frac{1}{4})$. This indicates the strong tendency towards orientational ordering produced by the purely repulsive forces between dimers. As we shall find, however, the effect decays to zero with separation and does not lead to long-range ordering.

When $\tau \to 0$ so that $\rho_x \to 0$, the correlation $c_{xx}(0,1)$ varies as $\frac{1}{2}\pi\rho_x$ and tends to zero. On the other hand, when $\rho_y \to 0$ $(\tau \to \infty)$, one finds

$$c_{xx}(0,1) = 1/\pi^2 + \frac{2}{3}\rho_y^2 + O(\rho_y^4) \qquad (7.13)$$

which implies that however small the concentration of y dimers, there is a *strong* correlation between adjacent x dimers. The origin of this correlation can be seen by considering two adjacent rows in a lattice almost full of x dimers. If these rows are straddled by a y dimer then, because of the rigid interactions, the x dimers on either side of the y dimer will be strictly matched in pairs one above the other. Furthermore, this matching will extend indefinitely along the rows. It can only be broken by the intervention of another y dimer which straddles one of the rows but not the other. At low y-dimer densities, this is improbable and the correlation becomes long range. On this interpretation, one would expect a corresponding *reduction* of occupation probabilities for a bond in an adjacent row which is offset by one unit to the right (or left). In fact, one finds for the

TABLE II. Values of the normalized pair correlation coefficients ($\times 10^5$) in the center of the lattice.

q	p'=0'	1'	2'	3'	4'	5'	6'	7'	8'	9'	C_xy(p',q')
q	•	•	•	•	•	•	•	•	•	•	• q'
		404	-363	912	-733	971	-744				7'
7	3491	-3141	2825	-2269	1823	-1397	1071				
		-755	679	-1468	1179	-1397	1071	-1071			6'
6	-163	-163	353	-763	904	-1071	1071	-1071			
		1081	-868	1878	-1320	1564	-1071	1071	-744		5'
5	7161	-5754	4624	-3251	2285	-1564	1071	-744	517		
		-2488	1999	-3251	2285	-2285	1564	-1397	971	-844	4'
4	-864	-864	1405	-2285	2285	-2285	2041	-1823	1585	-1377	
		4216	-2540	2285	-2285	2285	-1320	1179	-733	637	3'
3	20568	-12392	7466	-4131	2285	-1320	763	-474	295	-197	
		-12392	7466	-7466	4131	-3251	1878	-1468	912	-735	2'
2	-7466	-7466	7466	-7466	5875	-4624	3614	-2825	2276	-1834	
		27324	-7466	7466	-2540	1999	-868	679	-363	293	1'
1	100000	-27324	7466	-2540	864	-375	163	-87	47	-29	
		-100000	27324	-12392	4216	-2488	1081	-755	404	-310	0'
0	-100000	-100000	45352	-20568	12136	-7161	5000	-3491	2684	-2063	
C_xx(p,q) p=	0	1	2	3	4	5	6	7	8	9	

configuration of Fig. 3(d)

$$c_{xx}(1,1) = \rho_y[\rho_x - (\tau/\pi)] \qquad (7.14)$$

so that as $\rho_y \to 0$,

$$c_{xx}(1,1) = -1/\pi^2 + \tfrac{1}{2}\rho_y + O(\rho_y^2) \qquad (7.15)$$

as expected. Similarly, with an offset of two units as in Fig. 3(e), one has as $\rho_y \to 0$

$$c_{xx}(2,1) = +1/\pi^2 - \rho_y + O(\rho_y^2). \qquad (7.16)$$

For a pair of parallel next nearest neighbor bonds in the same column [Fig. 3(f)], the correlation coefficient is

$$c_{xx}(0,2) = -[(\tau/\pi) - \tau^2\rho_y]^2, \qquad (7.17)$$

which is always negative indicating a decreased probability of occupation. In the symmetric case $x=y$, one finds $c_{xx}(0,2) = -\tfrac{1}{16}[(4/\pi) - 1]^2 = -0.004666$. For a separation of one further row, as in Fig. 3(g), the result is

$$c_{xx}(0,3) = \tau^2[\rho_y(1+2\tau^2) - 2(\tau/\pi)]^2, \qquad (7.18)$$

which is again positive. Asymptotic analysis of the Green's function elements (see Appendix C) shows that

$$c_{xx}(0,q) \approx +1/\pi^2 q^2 + O[q^{-3}] \quad q \text{ odd},$$
$$\approx -1/\tau^2\pi^2 q^4 + O[q^{-6}] \quad q \text{ even}. \qquad (7.19)$$

Apart from the alternation of signs, it is notable that the asymptotic form is different for q odd or even. This, and the divergence of the coefficient of q^{-4} as $\tau \to 0$ ($\rho_x \to 0$) is due to the same phenomenon discussed above. In this case, when the vast majority of dimers are y dimers, the space between two horizontal dimers will be filled by vertical dimers and, hence, the horizontal dimers must be an odd number of rows apart.

The asymptotic behavior of the correlations between two bonds in the same row as in Fig. 3(h) is given by

$$c_{xx}(p,0) \approx (-)^p \tau^2/\pi^2 p^2 + O[p^{-3}], \qquad (7.20)$$

which exhibits the expected alternation and divergence as $\rho_y \to 0$ ($\tau \to \infty$). For a vertical bond in the same column as an horizontal bond [Fig. 3(j)], one has a more rapid decay since

$$c_{xy}(0,q) = c_{xy}(1,q) \approx -(-1)^q/\tau^2\pi^2 q^3 + O[q^{-4}]. \qquad (7.21)$$

Further details of the spread of the short-range correlations may be seen from Table II where the numerical values of the pair correlation coefficient for the symmetric case $x=y$ are set out for values of p and q in the region $p+q \leqslant 9$. The coefficients which are transcendents of the form $[a - (b/\pi)][c - (d/\pi)]$ with $a, b, c,$ and d positive integers, have been normalized by dividing by $\rho^2 = \rho_x\rho_y = \tfrac{1}{16}$ and multiplying by 10^5. The

entries $-100\,000$ thus indicate the total absence of a second dimer while the entry $100\,000$ indicates an enhancement of the joint occupation probability by 100%. To bring out the alternating and zigzag nature of the correlations, negative coefficients have been printed in italics. It is also evident that the correlations spread most strongly along the lattice axes.

8. DILUTE MONOMERS

For a finite $m\times n$ lattice the partition function $Z_{mn}(x,y,z)$ for monomers and dimers is simply a polynomial. Consequently, we may write, for mn even,

$$Z_{mn}(x,y,z)=Z_{mn}^{(0)}(x,y)+z^2Z_{mn}^{(2)}(x,y)$$
$$+z^4Z_{mn}^{(4)}(x,y)+\cdots, \quad (8.1)$$

where $Z_{mn}^{(0)}$ is the partition function for a lattice full of dimers and has already been evaluated. The coefficient of z^2, namely, $Z_{mn}^{(2)}$, is the partition function of a lattice full of dimers except for a pair of monomers (or holes) which may be anywhere in the lattice. Similarly, $Z_{mn}^{(4)}$ corresponds to a lattice with four monomers. (Only even powers of z appear since, on starting with a lattice full of dimers, two monomers must be inserted for each dimer removed.[24]) If $\Omega_{mn}(x,y;r,s;p,q)$ is the partition function for a lattice with two monomers fixed at the sites (r,s) and $(r+p, s+q)$ but otherwise full of dimers, we clearly have

$$Z_{mn}^{(2)}(x,y)=\sum_{r,s}\sum_{p,q}\Omega_{mn}(x,y;r,s;p,q). \quad (8.2)$$

The increment in the thermodynamic potential per site due to the presence of monomers may now be written

$$-\Delta F/kT=(1/mn)[\ln Z_{mn}(x,y,z)-\ln Z_{mn}^{(0)}(x,y)]$$
$$=\ln[1+Q_{mn}(x,y,z)], \quad (8.3)$$

where for small enough z and finite mn we may expand $Q_{mn}(x,y,z)$ as

$$Q_{mn}(x,y,z)=\frac{z^2}{mn}\sum_{r,s}\sum_{p,q}\omega_{mn}(x,y;r,s;p,q)+O(z^4), \quad (8.4)$$

in which we have introduced the basic monomer pair correlation coefficients

$$\omega_{mn}(x,y;r,s;p,q)=\Omega_{mn}(x,y;r,s;p,q)/Z_{mn}^{(0)}(x,y). \quad (8.5)$$

In the limit $m, n\to\infty$ this correlation coefficient, which measures the ratio of the number of configurations with two fixed holes to the number with no holes, will approach a limit $\omega(x,y;r,s;p,q)$. If r and s are also allowed to become infinite, corresponding to both monomers being far from the edge of the lattice, $\omega(x,y)$ becomes independent of r and s. *Formally* we

then have

$$Q(x,y,z)=\lim_{m,n\to\infty}Q_{mn}(x,y,z)$$
$$=z^2\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\omega(x,y;p,q)+\cdots, \quad (8.6)$$

where we have supposed $\omega(x,y;0,0)\equiv0$.[25]

If the double sum in (8.6) converges, it is an indication that $Q(x,y,z)$ and, hence, the limiting thermodynamic potential, has an expansion in powers of z^2 (possibly asymptotic). If, on the other hand, the sum diverges, its mode of divergence is related to the analytic behavior of $Q(x,y,z)$ at $z=0$ which must then be 'sharper' than z^2. By analogy with the pair spin correlations in the Ising model[13–15] (comparing z with the magnetic field) we might expect the existence of long-range order as evidenced by[26]

$$\lim_{p,q\to\infty}\omega(x,y;p,q)=\omega_\infty(x,y)>0 \quad (8.7)$$

with

$$\chi(x,y)=\sum_{p=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}[\omega(x,y;p,q)-\omega_\infty(x,y)],$$
$$\text{convergent.} \quad (8.8)$$

In this case, the behavior of $Q(x,y,z)$ should be

$$Q(x,y,z)=[\omega_\infty(x,y)]^{1/2}|z|+\chi(x,y)z^2+\cdots. \quad (8.9)$$

In the next section, we show how to calculate $\omega_{mn}(x,y;r,s;p,q)$ for dimers on the plane square lattice and thence the limit $\omega(x,y;p,q)$. We also show that $\omega(x,y;p,q)\to0$ as $p, q\to\infty$ so that the long-range order parameter $\omega_\infty(x,y)$ is identically zero. We have, so far, been unable to decide the convergence of (8.8) rigorously although we believe that this sum is divergent. This would be analogous to the Ising model *at* its transition temperature as pointed out in the introduction. In that case $\omega_\infty\equiv0$, but the sum (8.8), corresponding to the ferromagnetic susceptibility χ, does not converge since the pair correlations only decay as $1/r^{1/4}$.[27] If $\chi(x,y)$ is infinite, the analytic behavior of $Q(z)$ must then be more singular than z^2 but less singular than $|z|$. Even for the Ising model, this aspect of the behavior at T_c is not yet known.

9. INTERACTION OF TWO MONOMERS

In this section, we study the interaction of a pair of monomers in a lattice otherwise full of x and y dimers by computing the monomer pair correlation coefficients

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[24] The techniques described below may be adapted to the case when mn is odd so that the possible number of monomers is one, three, five, etc.

[25] This is consistent with (8.5) since, if mn is even and $p=q=0$ so that the two monomers formally coincide, an *odd* number of sites will be left vacant for the dimers; but then

$$\Omega_{mn}(x,y;r,s;0,0)\equiv0.$$

[26] If the long-range order were direction dependent, the formulas (8.8) and (8.9) would have to be modified appropriately.

[27] See M. E. Fisher, Physica **25**, 521 (1959); C. Domb, Advan. Phys. **9**, 200 (1960) and Ref. 13.
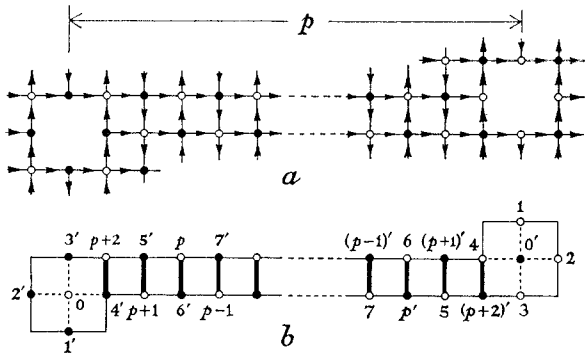
FIG. 4. Lattice with two holes in adjacent rows (a) oriented as in Fig. 1, (b) with modified orientation indicated by bold bonds which are reversed relative to (a).

FIG. 5. Correct reorientations preserving sublattice symmetry for arbitrary position of two holes.

$\omega_{mn}(x,y; r,s; p,q)$ defined by (8.5). The methods employed would also yield quadruple and higher order correlation functions although explicit results would be more complicated. The calculation divides into three sections: firstly, we obtain a Pfaffian and thence a determinant of order $mn-2$ which counts the dimer configurations correctly when the monomers are regarded as holes in the lattice, i.e., as missing sites; secondly, we show how this Pfaffian may be regarded as a perturbation on the basic Pfaffian $\mathrm{Pf}(\mathbf{D}_0)$ for a perfect lattice; lastly, we use perturbation theory and the properties of the Green's function to reduce $\omega(x,y,p,q)$ to a determinant of Toeplitz type, of order depending on the spacing of the monomers.

The square lattice can be divided into two disjoint sublattices such that each site on one sublattice has neighbors on the opposite sublattice. Since any dimer fills one site on each sublattice, it follows (when mn is even) that if there are $2k$ monomers in the lattice, k of them must lie on one sublattice and k on the opposite sublattice. In particular, for two monomers, one at (r,s) and the other at $(r',s') = (r+p, s+q)$, we have $\omega(x,y) \equiv 0$ unless $p+q$ is odd. This result would, of course, come out of the theory but it is more economical and convenient to avoid considering the impossible configurations.

To count the dimer configurations with two monomers we delete the sites (r,s) and (r',s') to yield a modified lattice with two "holes" each consisting of four basic squares of the original lattice. This modified lattice has $(mn-2)$ sites and is to be filled with dimers. It is a planar graph and accordingly by Kasteleyn's theorem (Sec. 2) we may construct a Pfaffian (of Type IV) which counts all configurations with positive sign by suitably orientating the bonds of the lattice. To see how this may be done, suppose, firstly, the two monomers are in adjoining rows so that $q=1$ and p is even. If we retain Kasteleyn's orientation [see Fig. 1 and Eqs. (2.10) and (2.11)] then all meshes have a clockwise odd orientation except the two holes as shown in Fig. 4(a). Consider the first hole: Its orientation parity can be corrected by reversing the arrow of any one of its
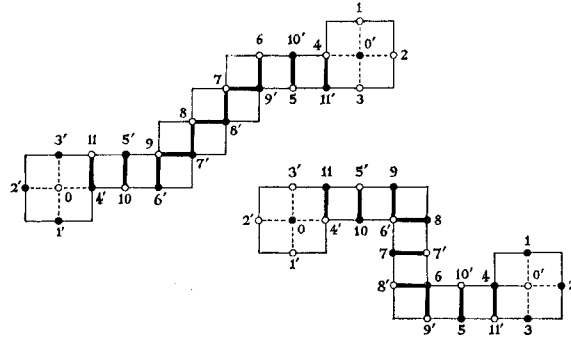
perimeter bonds. Choose that one marked boldly in Fig. 4(b). This reversal, however, spoils the orientation parity of the adjacent square. This, in turn, may be corrected by reversing the opposite bond (second bold bond) which disturbs the parity of the next square. Proceeding to reverse all the bold bonds marked in Fig. 4(b), we eventually arrive at the second hole so that the last reversal leaves all meshes with a clockwise odd orientation parity as required by the theorem. The appropriate Pfaffian of Type IV may now be written down by choosing the factor α_{rs} and β_{rs} of Sec. 2 to be $+1$ or -1 in accordance with the bond orientations.

In Fig. 4(b), the sites on the two sublattices (including the 'missing' site) have been distinguished by open and solid circles and they have been labeled $k=0, 1, 2, \cdots$ $p, p+1, p+2$ on the first sublattice and $k'=0', 1', 2', \cdots$ $p', (p+1)', (p+2)'$ on the second sublattice. It will be seen that there is complete symmetry between the two sublattices (ignoring the edges of the lattice). For the Green's function elements in the center of the lattice, this implies

$$[k_1,k_2'] = -[k_1',k_2] = [k_2,k_1']. \qquad (9.1)$$

This symmetry is not an essential feature of the problem since there are many other correct orientations which are nonsymmetric, but it greatly simplifies the subsequent manipulations. Reference to Fig. 5 shows that more than one similar reorientation of bonds can be found to preserve both the sublattice symmetry and the correct orientation parity for an arbitrary position of the two holes. For two holes in the same row (p odd, $q=0$) a particularly simple reorientation is shown in Fig. 6. This arrangement, however, does not have the full symmetry expressed by (9.1) and leads to a slightly more complicated analysis.

The prescriptions summarized in Figs. 4, 5, and 6 enable the monomer correlation $\omega_{mn}(x,y; r,s; p,q)$ on a
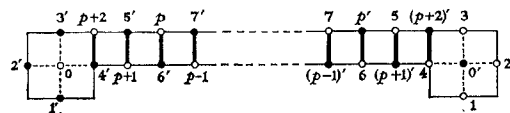

FIG. 6. A simple reorientation of bonds for two holes in the same row.

finite lattice to be expressed exactly as the ratio of two Pfaffians derived from a matrix $\mathbf{D}$ of order $mn-2$ and from $\mathbf{D}_0$ of order mn, respectively. To calculate this ratio by perturbation theory as before, we must augment the order of $\mathbf{D}$ without changing the absolute value of its Pfaffian, and then multiply appropriate rows and columns by $+i$ and $-i$ as in Sec. 2 so that it is comparable to the matrix $\mathbf{D}_0$. To increase the order of $\mathbf{D}$ to mn we reintroduce indices for the deleted sites (r,s) and $(r',s')=(r+p, s+q)$ but set all the new matrix elements involving these sites to zero except for

$$D(r,s; r',s')=1=-D(r',s'; r,s). \qquad (9.2)$$

By rearranging the rows and columns of the determinant of the augmented matrix $\mathbf{D}^*$ we easily see that

$$Pf(\mathbf{D}^*)=[Det(\mathbf{D}^*)]^{1/2}$$

$$= \begin{vmatrix} 0 & \pm 1 & & \\ & & & 0 \\ \mp 1 & 0 & & \\ & & & \\ 0 & & D & \end{vmatrix}^{1/2} \qquad (9.3)$$

$$=[Det(\mathbf{D})]^{1/2}=\pm Pf(\mathbf{D})$$

as required.

The augmented matrix $\mathbf{D}^*$ is of the same order as $\mathbf{D}_0$ and, on multiplying rows of odd r by $-i$ and columns of even r by $+i$, we see that it may be derived directly from $\mathbf{D}_0$ by: (i) Adding elements $(-)^r i$ and $-(-)^r i$ in the places $(r,s; r',s')$ and $(r',s'; r,s)$, respectively; (ii) deleting those elements corresponding to the 'missing' bonds shown dotted in Figs. 3 to 5; and (iii) changing the sign of those elements of $\mathbf{D}_0$ corresponding to the bold bonds in Figs. 4 to 6. Then, arguing as in Sec. 3 [Eq. (3.4)] we have

$$[\omega_{mn}(x,y; r,s; p,q)]^2=Det(\mathbf{I}'+\mathbf{g}\mathbf{e}), \qquad (9.4)$$

where $\mathbf{g}$ and $\mathbf{e}$ are the reduced Green's function and perturbation matrices.

If we now restrict ourselves to $p>q\geqslant 1$ and use the arrangement and labeling of Figs. 4(a) and 5(a), these matrices are of order $2(p+3)$ and the nonzero elements of $\mathbf{e}$ are

$$e_{00'}=(-)^r i=-e_{0'0}, \qquad (9.5)$$

$$e_{01'}=-e_{0'1}=iy=-e_{1'0}=e_{1\ 0'},$$

$$e_{02'}=-e_{0'2}=+x=-e_{2'0}=e_{2\ 0'},$$

$$e_{03'}=-e_{0'3}=-iy=-e_{3'0}=e_{3\ 0'}, \qquad (9.6)$$

$$e_{04'}=-e_{0'4}=-x=-e_{4'0}=e_{4\ 0'},$$

and

$$e_{4,(p+2)'}=-e_{4',(p+2)}=+2iy=-e_{(p+2)',4}=e_{(p+2),4'},$$

$$e_{5,(p+1)'}=-e_{5',(p+1)}=-2iy=-e_{(p+1)',5}=e_{(p+1),5'},$$

$$e_{6,p'}=-e_{6',p}=+2iy=-e_{p',6}=e_{p,6'}$$

$$\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot$$

where further elements equal to $\pm 2x$ occur if $q>1$.

10. REDUCTION OF THE DETERMINANT

The determinant (9.4) could now be reduced to the square of a Pfaffian as in Sec. 3. In the present instance, however, we prefer an alternative procedure which takes advantage of the sublattice symmetries. If the rows and columns of $\mathbf{e}$ and $\mathbf{g}$ are ordered in the sequence $0, 1, 2, \cdots (p+1)(p+2), 0', 1', 2', \cdots (p+1)', (p+2)'$ the matrices may be partitioned in the form

$$\mathbf{e}=\begin{bmatrix} 0 & \mathbf{e}^+ \\ \mathbf{e}^- & 0 \end{bmatrix} \quad \mathbf{g}=\begin{bmatrix} 0 & \mathbf{g}^+ \\ \mathbf{g}^- & 0 \end{bmatrix} \qquad (10.1)$$

since by (9.5)–(9.7) the only nonzero elements of $\mathbf{e}$ are those *between different sublattices* while by (4.7) the same is true of the Green's function $\mathbf{G}$ and hence of $\mathbf{g}$. Because of the antisymmetry of $\mathbf{e}$ and $\mathbf{g}$, we must have

$$\mathbf{e}^-=-(\mathbf{e}^+)^T, \quad \mathbf{g}^-=-(\mathbf{g}^+)^T \qquad (10.2)$$

so that by (9.4)

$$\omega^2=Det\{\mathbf{I}''-\mathbf{g}^+(\mathbf{e}^+)^T\} \ Det\{\mathbf{I}''-(\mathbf{g}^+)^T\mathbf{e}^+\} \qquad (10.3)$$

where $\mathbf{I}''$ is a unit matrix order $(p+3)$.

Now in virtue of the sublattice symmetry of the reorientations or explicitly by (9.5) to (9.7), $\mathbf{e}^+$ is a symmetric matrix. If, at this stage, we restrict ourselves to monomers in the center of a large lattice, it follows from (9.1) that $\mathbf{g}^+$ is also symmetric. Finally, therefore, the monomer correlation function is given by a single determinant of order $(p+3)$, namely,

$$\omega(x,y; p,q)=\pm Det(\mathbf{I}''-\mathbf{g}^+\mathbf{e}^+), \qquad (10.4)$$

where the sign is chosen to make ω positive. (Actually this result can also be proved under more general conditions.)

We now reduce this determinant to a determinant of order p by using the recurrence relation (4.11) which the Green's function obeys by virtue of its definition as a reciprocal. For illustration, we consider in detail only the simplest case $q=1$ (p even) illustrated in Fig. 3. The matrix $\mathbf{g}^+$ may then be written out.[28] The elements in the first two rows are

$$g_{00'}=[p,1], \quad g_{01'}=[0,-1], \quad g_{02'}=[-1,0], \quad g_{03'}=[0,1],$$

$$g_{04'}=[1,0], \quad g_{05'}=[2,1], \quad g_{06'}=[3,0], \quad \cdots g_{0,(p+2)'}=[p-1,0];$$

$$g_{1\ 0'}=[0,-1], \quad g_{1\ 1'}=[-p,-3], \quad g_{1\ 2'}=[-(p+1),-2],$$

$$g_{1\ 3'}=[-p,-1], \quad g_{1\ 4'}=[-(p-1),-2], \quad \cdots g_{1,(p+2)'}=[-1,-2]. \qquad (10.5)$$

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[28] To economize space, we do not display the complete matrix.

By symmetry, these are also the elements of the first two columns. The elements $g_{jk'}$ with $j,k' \geqslant 4$ form a matrix of simple structure with respect to the trailing diagonals. Thus, for example,

$$g_{5,(p+2)'} = g_{6,(p+1)'} = g_{7,p'} = g_{8,p'-1} = \cdots = [1,0],$$

while

$$g_{4,(p+2)'} = g_{6,p'} = \cdots = [0,-1],$$

although

$$g_{5,(p+1)'} = g_{7,(p-1)'} = \cdots = [0,+1]. \tag{10.6}$$

Now form the matrix $\mathbf{I}'' - \mathbf{g}^+\mathbf{e}^+$ and use the recurrence relation (4.11) in the form

$$x[t-1, u] + iy[t, u-1] - x[t+1, u] - iy[t, u+1] = \delta_{0t}\delta_{0u}. \tag{10.7}$$

Without loss of generality we may suppose r in (9.5) is even. By (9.5), (9.6), and (9.12) the elements of 0'th column of $\mathbf{I}'' - \mathbf{g}^+\mathbf{e}^+$ are then

$$1 - i[p,1] - (iy[0,-1] + x[-1,0] - iy[0,1] - x[1,0]) = -i[p,1]$$
$$-i[0,-1] - (iy[-p,-3] + x[-p-1,-2] - iy[-p,-1] - x[-p+1,-2]) = -i[0,-1], \tag{10.8}$$
$$\vdots$$
$$-i[p-1,0] - (iy[-1,-2] + x[-2,-1] - iy[-1,0] - x[0,-1]) = -i[p-1,0].$$

This column is thus simply $-i$ times the 0th row (or column) of $\mathbf{g}^+$. By (9.6) the 1'th, 2'th, and 3'th columns of $\mathbf{g}^+\mathbf{e}^+$ are also proportional to the 0th row of $\mathbf{g}^+$, the appropriate factors being iy, x and $-iy$. Similarly, by (9.6) and (9.7), the 4'th column of $\mathbf{g}^+\mathbf{e}^+$ is $-x$ times the 0th row plus $2iy$ times the $(p+2)$th (or last) row of $\mathbf{g}^+$. All these elements (except those proportional to $2iy$) may be eliminated from $\mathrm{Det}(\mathbf{I}'' - \mathbf{g}^+\mathbf{e}^+)$ by subtracting the appropriate multiple of the 0'th column from the 1'th, 2'th, 3'th, and 4'th columns. The only nonzero elements left in the 1'th, 2'th, and 3'th columns of the determinant are on the diagonal and have the value unity. Expanding the determinant by these columns finally expresses $\omega(x,y,p,1)$ as a $p \times p$ determinant of the form

$$\begin{vmatrix}
-i[p,1] & -2iy[p-1,0] & 2iy[p-2,1] & \cdots & -2iy[1,0] \\
-i[1,0] & 1-2iy[0,-1] & 2iy[-1,0] & \cdots & -2iy[-p+2,-1] \\
-i[2,1] & -2iy[1,0] & 1+2iy[0,1] & \cdots & -2iy[-p+3,0] \\
-i[3,0] & -2iy[2,-1] & 2iy[1,0] & \cdots & -2iy[-p+4,-1] \\
\vdots & \vdots & \vdots & & \vdots \\
-i[p-2,1] & -2iy[p-3,0] & \cdots & & \\
-i[p-1,0] & -2iy[p-2,-1] & 2iy[p-3,0] & \cdots & 1-2iy[0,-1]
\end{vmatrix}. \tag{10.9}$$

The nature of this determinant is made more transparent by permuting the first row through to the bottom (which introduces a factor -1), multiplying the first column by $-2iy$, and using the symmetry relations

$$[2v, -1] = -[2v, 1] = -[-2v, 1], \tag{10.10}$$

which follow from (4.9). Except for an alternation of signs in alternate diagonals the resulting determinant is almost of Toeplitz form (i.e., the elements in any one diagonal are the same.)[29] By multiplying the 1st, 4th, 5th, 8th, 9th, $\cdots$ columns and the 3rd, 4th, 7th, 8th, 11th, 12th, $\cdots$ rows by -1 and transposing, we can finally write $\omega(x,y; p,1)$ as a perfect Toeplitz matrix, namely,[30]

$$\omega(x,y; p,1) = \pm(1/2y)|a_{i-j+1}| \quad (p \text{ even})$$

$$= \frac{\pm 1}{2y}\begin{vmatrix}
a_1 & a_2 & a_3 & \cdots & a_{p-1} & a_p \\
a_0 & a_1 & a_2 & \cdots & \cdots & a_{p-1} \\
a_1 & a_0 & a_1 & \cdots & & \\
\vdots & \vdots & \vdots & & \vdots & \vdots \\
a_{-(p-3)} & \cdots & \cdots & & a_1 & a_2 \\
a_{-(p-2)} & a_{-(p-3)} & \cdots & & a_0 & a_1
\end{vmatrix}, \tag{10.11}$$

[29] U. Grenander and G. Szegö, *Toeplitz Forms and Their Applications* (University of California Press, Berkeley, and Cambridge University Press, Cambridge, 1958).

[30] A Toeplitz determinant is usually written $|c_{i-j}|$. For convenience, we have displaced the zeroth element by one place so that $c_n = a_{n+1}$. Grenander and Szegö (Ref. 28) consider only Hermitian Toeplitz matrices but generalizations of the most important theorems are available for non-Hermitian matrices.

where the sign is chosen to make ω positive and where, on using the symmetry relation,

$$[2v-1, 0] = -[-(2v-1), 0],\tag{10.12}$$

the matrix elements a_n are given by

$$a_0 = 1 + 2iy[0,1],$$

$$a_1 = a_{-1} = -2iy[1,0], \quad a_2 = a_{-2} = -2iy[2,1],$$

$$a_3 = a_{-3} = +2iy[3,0], \quad a_4 = a_{-4} = +2iy[4,1],\tag{10.13}$$

$$\cdots \qquad \cdots \qquad \cdots \qquad \cdots$$

$$a_{2k-1} = a_{-2k+1} = (-)^k 2iy[2k-1, 0], \quad a_{2k} = a_{-2k} = (-)^k 2iy[2k,1].$$

The explicit values of the matrix elements may be found from Appendix B but they are conveniently summarized in the generating function[29]

$$A(\theta) = \sum_{n=-\infty}^{\infty} a_n e^{in\theta},\tag{10.14}$$

from which, by Fourier transformation,

$$a_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} A(\theta) e^{-in\theta} d\theta.\tag{10.15}$$

To find an expression for $A(\theta)$, we can manipulate the expressions (4.13) and (4.15) for the Green's function elements appearing in (10.13), into the form (10.15). Thus,

$$\frac{1}{2iy}\left\{ \begin{matrix} a_{2k-1} \\ a_{2k} - \delta_{0k} \end{matrix} \right\} = \int_{-\pi}^{\pi} \frac{d\alpha}{2\pi} \int_{-\pi}^{\pi} \frac{d\beta}{2\pi} e^{-k\pi i}[\Delta(\alpha,\beta)]^{-1}$$

$$\times \left\{ \begin{matrix} 2x \sin\frac{1}{2}\alpha \sin(k-\frac{1}{2})\alpha \\ iy(1-\cos\beta)\cos k\alpha \end{matrix} \right\},\tag{10.16}$$

where

$$\Delta(\alpha,\beta) = x^2(1-\cos\alpha) + y^2(1-\cos\beta).\tag{10.17}$$

On adding odd functions to the integrals to yield complex exponentials in $-i(k-\frac{1}{2})\alpha$ and $-ik\alpha$ and setting $\alpha+\pi = 2\theta$ we obtain

$$a_n - \delta_{0n} = iy \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{-in\theta} \int_{-\pi}^{\pi} \frac{d\beta}{2\pi} [\Delta(\alpha,\beta)]^{-1}$$

$$\times [-2x\cos\theta + iy(1-\cos\beta)].\tag{10.18}$$

Comparison with (10.15) yields an expression for $A(\theta)$ as a single integral over the angle β. On performing this integral (as in Appendix B) we find

$$A(\theta) = \text{sgn}\{\cos\theta\}\left(\frac{x\cos\theta - iy}{x\cos\theta + iy}\right)^{1/2}.\tag{10.19}$$

The step function $\text{sgn}\{\cos\theta\}$ arises from the necessity of consistently taking the positive root of $\sqrt{\cos^2\theta} = |\cos\theta|$. The complex function $A(\theta)$ is of unit modulus so we may write

$$A(\theta) = \exp[i\delta(\theta)],\tag{10.20}$$

where the real angle $\delta(\theta)$ is given by

$$\delta(\theta) = \frac{1}{2}\pi[1 - \text{sgn}\{\cos\theta\}] - \cot^{-1}(\tau\cos\theta),$$

$$= \frac{1}{2}\pi[1 - \text{sgn}\{\cos\theta\}] - \tan^{-1}(\tan\pi\rho_y \cos\theta),\tag{10.21}$$

and is an even periodic function of θ with step discontinuities at $\theta = \pm\frac{1}{2}\pi$. The formulas (10.11), (10.15), and (10.19) to (10.21) are very similar to expressions obtained by Onsager, and Kaufman, and Onsager[13] in their study of the spin pair correlations of the Ising model.

We note in passing that the result (10.19) can be used with (10.15) to express the matrix elements a_n in terms of the associated Legendre functions $P_{-\frac{1}{2}}^k(\zeta)$ of suitable argument. The resulting formula does not, however, lead to explicit values for general n. The asymptotic behavior of a_n for large n is determined by the discontinuity in $A(\theta)$ and its derivative. Thus, one finds that the coefficient a_{2k} behaves as $(-1)^{k+1}/k^2$ $(k \to \infty)$ and is real, while a_{2k+1} is purely imaginary but goes to zero only as $(-1)^{k+1}/k$. (See also Appendix C.)

The result (10.11) holds only for p even since $\omega(x,y; p,1)$ must be zero when p is odd as mentioned in Sec. 8. Similarly, the correlation coefficient for two monomers in the *same* row, $\omega(x,y; p,0)$ vanishes if p is even. When p is odd, however, it may be calculated along the lines above. It is most natural to use the bond orientations shown in Fig. 6 although these are not quite as symmetric as those of Figs. 4 and 5. Performing the appropriate analysis yields

$$(p \text{ odd}) \quad \omega(x,y; p,0) = \frac{\pm i}{2y} \begin{vmatrix} a_1 & a_2 & a_3 & \cdots & a_p \\ a_0 & a_1 & a_2 & \cdots & a_{p-1} \\ a_{-1} & a_0 & a_1 & & \\ \vdots & \vdots & \vdots & & \vdots \\ a_{-(p-2)} & a_{-(p-3)} & & \cdots & a_1 \end{vmatrix}\tag{10.22}$$

which, apart from the factor i and the order of the determinant, is precisely the same as (10.11). If x and y are interchanged in the definition of the a_n similar formulas, of course, hold for $\omega(x,y; 0,q)$ (q odd) and for $\omega(x, y; \pm1, q)$ (q even).

The formulas (10.11) and (10.22) give expressions for the monomer correlations along the rows and columns of the lattice. By the same methods, one may derive compact expressions for the correlations along the diagonals $(p, p+1)$ and $(p+1, p)$. We find

$$\omega(x, y; p-1, p)=\frac{\pm i}{2x}|b_{i-j+1}|$$

$$(i, j=1, 2, \cdots p), \quad (10.23)$$

where

$$b_0=1+2x[1, 0],$$

$$b_k=-2x[k-1, k],$$

$$b_{-k}=(iy/x)^k+2x[k+1, k], \quad (k=1, 2, 3, \cdots). \quad (10.24)$$

For the symmetric case $x=y$ these elements can be evaluated explicitly for general k as finite sums over the inverse odd integers (see Appendix B).

11. BEHAVIOR OF THE MONOMER CORRELATION COEFFICIENTS

Explicit values for the monomer correlation coefficients for nearby monomers may be found by substituting for the elements a_n from Appendix B and evaluating the appropriate Toeplitz determinants. For two adjacent monomers in the same row one finds

$$\omega(1,0)=(1/x)\rho_x. \quad (11.1)$$

Two such adjacent monomers are quite equivalent to one missing x dimer. The 'dimensional' factor $(1/x)$ corresponds to the removal of this dimer and its replacement by two monomers. The factor ρ_x is simply the known probability of occupation of the linking bond by an x dimer.

For the next nearest possible conjunction of monomers we have

$$\omega(2,1)=(1/x)(2/\pi)\rho_x \quad (11.2)$$

so that for all x and y this configuration has a weight smaller by the factor $2/\pi=0.63\,662$. For the next nearest separation of two monomers in the same row the coefficient is

$$\omega(3,0)=(1/x)\tau^{-2}\rho_x[8\tau^{-1}\rho_x(1+\tau^2)-(4/\pi^2)], \quad (11.3)$$

which varies in a more complex way with $\tau=x/y$.

In the symmetric case $x=y=1$, the first few values along a row, normalized by dividing by $\omega(1,0)=\frac{1}{4}$, are

$$4\omega(1,0)=1,$$

$$4\omega(2,1)=2/\pi,$$

$$4\omega(3,0)=1-(4/\pi^2), \quad (11.4)$$

$$4\omega(4,1)=(8/\pi^2)[1-(4/\pi^2)].$$

TABLE III. Values of the normalized monomer correlation coefficients $\omega_p=\omega(p,0)$ for p even, and $\omega_p=\omega(p,1)$ for p odd for the symmetric case $x=y=1$. The column headed r gives the length of the vector between the monomers, and B_r is an amplitude defined in the text.

p	$4\omega_p$	r	B_r
1	1.000000	1	1.00000
2	0.636620	2.236068	0.95197
3	0.594715	3	1.03008
4	0.482058	4.123106	0.97884
5	0.450629	5	1.00764
6	0.399501	6.082763	0.98530
7	0.377337	7	0.99834
8	0.347721	8.062258	0.98732
9	0.331513	9	0.99454
10	0.311707	10.049876	0.988161
11	0.299327	11	0.992754
12	0.284892	12.041595	0.988605
13	0.275077	13	0.991805

The numerical values for these row coefficients and the succeeding ones up to $\omega(12, 1)$ and $\omega(13, 0)$ are presented in Table III. The magnitude of the coefficients decreases slowly but monotonically with monomer separation so that, in effect, two monomers in a sea of dimers feel a weak but long-range attraction.

The behavior of the correlations for large separations and the possible existence of a long-range correlation may be investigated by means of certain fundamental theorems concerning Toeplitz determinants.[31] We may state these theorems as follows:

If $D_p\{F\}=|f_{i-j}|$ is the Toeplitz determinant of order p generated by the function

$$F(\theta)=\sum_{n=-\infty}^{\infty} f_n e^{in\theta}, \quad (11.5)$$

then

$$G\{F\}=\lim_{p\to\infty}|D_p|^{1/p}=\left|\exp\left\{\frac{1}{2\pi}\int_{-\pi}^{\pi}\ln F(\theta)d\theta\right\}\right|, \quad (11.6)$$

and, further,

$$\lim_{p\to\infty}|D_p|/G^p=\exp\{\sum_{n=1}^{\infty}nk_nk_{-n}\}, \quad (11.7)$$

where

$$k_n=\frac{1}{2\pi}\int_{-\pi}^{\pi}\ln F(\theta)e^{-in\theta}d\theta. \quad (11.8)$$

For the determinant $D_p=|a_{i-j+1}|$ appearing in the formula for $\omega_p=\omega(p,0)$ or $\omega(p,1)$, we have

$$F(\theta)=e^{-i\theta}A(\theta)=e^{i[\delta(\theta)-\theta]}, \quad (-\pi<\theta\leqslant\pi). \quad (11.9)$$

By (10.21) the integral in (11.6) then yields $k_0=-\frac{1}{2}i\pi$ so that $G=1$. This implies that the correlations ω_p do not decrease (or increase) exponentially fast. We may now use (11.7) to determine whether the correlation

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[31] See Grenander and Szegö (Ref. 29), p. 76 and M. Kac, *Probability and Related Topics in Physical Sciences* (Interscience Publishers Inc., New York, 1959), pp. 45–55, from which the generalization to non-Hermitian Toeplitz determinants follows.

has an infinite range. Owing to the discontinuities in the function $[\delta(\theta)-\theta]$ the expression for $\sum n k_n k_{-n}$ contains as a leading term the sum $\sum(-1/n)$ which diverges logarithmically to $-\infty$. This indicates that the correlation coefficients decay to zero i.e.,

$$\lim_{p\to\infty}\omega(p,0)=\lim_{p\to\infty}\omega(p,1)=0 \qquad (11.10)$$

so that, as mentioned in Sec. 8, there is no long-range order.

Since the decay of the correlations is slower than exponential, it is natural to expect an inverse power-law dependence on the separation distance $r=(p^2+q^2)^{1/2}$. This is, in fact, the case for the plane square Ising model at its critical point.[27] Unfortunately, there is apparently no general analytical technique available for estimating the asymptotic behavior of a Toeplitz determinant in higher approximation. Numerical study of the thirteen entries in Table III, however, suggests that (at least in the case $x=y$) an inverse square-root law is obeyed, namely,

$$\omega_p\approx B/4r^{1/2} \quad (r\to\infty). \qquad (11.11)$$

The accuracy of this formula may be gauged from the last column of Table III where values of the amplitude

$$B_r=4r^{1/2}\omega_p \qquad (11.12)$$

are tabulated. These lie within 4% of $B=0.990$ and fall into two sets (p odd and even) which are rapidly approaching a common value. In fact, by plotting the values against $1/r^2$, one discovers that B_r appears to approach its limiting value almost linearly with $1/r^2$. Linear extrapolation of the last few pairs of values to $1/r^2=0$ yields the sequence 0.98993, 0.98892, 0.98965, 0.98914, 0.98961, 0.98941 as estimates for $B_\infty=B$. From these we conclude that the true limiting amplitude in (11.11) lies close to $B=0.98950$ and that for finite r along a row,

$$B_r=B[1+b/r^2+O(1/r^3)], \qquad (11.13)$$

where $b\simeq0.37$ for odd p and $b\simeq-0.12$ for even p. (For the Ising spin correlations the correction terms are of the same relative order.)

We may examine the diagonal correlations in the same way. From (10.21) we have computed the first 22 values of $\omega(p+1,p)$. The corresponding amplitudes B_r are again observed to behave like (11.13) but with $b\simeq-0.26$ and only the term in $1/r^3$ depending on the parity of p. By linear extrapolation of the B_r for the last six even values of p we obtain 0.989499, 0.989497, 0.989494, 0.989492, 0.989491 as estimates for B. This

strongly indicates that

$$B=0.989490, \qquad (11.14)$$

correct to five figures. Within the accuracy obtainable, this is exactly the same as the estimate 0.98950 obtained from the row correlations. This equality suggests that when $x=y$ the monomer correlations decay isotropically (with full angular symmetry).

If (11.11) is correct, as the numerical evidence suggests, the single sums

$$\sum_{k=1}^{\infty}\omega(2k,1),\quad \sum_{k=1}^{\infty}\omega(2k-1,0),\quad\text{and}\quad \sum_{k=1}^{\infty}\omega(k+1,k)$$

are divergent so that the double sum defining $\chi(x,y)$ in (8.8) is certainly divergent. We must conclude that the general partition function $Z(x,y,z)$ for monomers and dimers does not have an expansion about $z=0$ in integral powers of z. As explained before, this conclusion probably does not apply to monomer-dimer mixtures on more general plane lattices.

ACKNOWLEDGMENTS

APPENDIX A: REDUCTION OF A PERTURBED PFAFFIAN

To indicate why the expression (3.9) is valid even when some of the subscripts are not distinct, we consider the case in which two elements have a common index (i.e., two perturbed bonds meet at a site[20]) while the remaining elements have distinct indices. Thus, suppose that the only nonzero perturbation elements are e_{12}, e_{24} and e_{56}, e_{78}. (We reserve the index 3 for later use.) The reduced perturbation matrix e thus has the form

$$\begin{bmatrix} 0 & e_{12} & 0 & & & \\ -e_{12} & 0 & e_{24} & & & \\ 0 & -e_{24} & 0 & & & \\ & & & & & \\ & & & & 0 & e_{56} \\ & & & & -e_{56} & 0 \end{bmatrix},$$

the determinant of which clearly vanishes. The determinant Δ of (3.4) is, therefore,

$$\Delta=\begin{bmatrix} (1-e_{12}g_{12}) & (e_{12}g_{11}-e_{24}g_{14}) & e_{24}g_{12}; & -e_{56}g_{16} & \cdots \\ -e_{12}g_{22} & (1+e_{12}g_{21}-e_{24}g_{24}) & e_{24}g_{22}; & -e_{56}g_{26} & \cdots \\ -e_{12}g_{42} & (e_{12}g_{41}-e_{24}g_{44}) & (1+e_{24}g_{42}); & -e_{56}g_{46} & \cdots \\ & & & & \\ -e_{12}g_{52} & (e_{12}g_{51}-e_{24}g_{54}) & e_{24}g_{52}; & (1-e_{56}g_{56}) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix}.$$

We enlarge this determinant by inserting a row and column of elements between the second and third rows and columns, respectively. By choosing the new diagonal element as unity and the other elements in the row as zero the remaining elements in the new column may be chosen arbitrarily. Thus, we write

$$
\Delta = \Delta' = \begin{bmatrix}
(1-e_{12}g_{12}) & (e_{12}g_{11}-e_{24}g_{14}) & -e_{24}g_{14} & e_{24}g_{12}; & -e_{56}g_{16} & \cdots \\
-e_{12}g_{22} & (1+e_{12}g_{21}-e_{24}g_{24}) & -e_{24}g_{24} & e_{24}g_{22}; & -e_{56}g_{26} & \cdots \\
0 & 0 & 1 & 0 & ; & 0 & \cdots \\
-e_{12}g_{42} & (e_{12}g_{41}-e_{24}g_{44}) & -e_{24}g_{44} & (1+e_{24}g_{42}); & -e_{56}g_{46} & \cdots \\
-e_{12}g_{52} & (e_{12}g_{51}-e_{24}g_{54}) & -e_{24}g_{54} & e_{24}g_{52}; & (1-e_{56}g_{56}) & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots
\end{bmatrix}.
$$

Now subtract the (new) third column from the second column and then add the second row to the third row. On introducing the new index 3 with the understanding that it is equivalent to 2 so that $e_{34}=e_{24}$, $g_{3j}=g_{2j}$ and $g_{j3}=g_{j2}$, we finally obtain

$$
\Delta = \Delta'' = \begin{bmatrix}
1-e_{12}g_{12} & e_{12}g_{11}; & -e_{34}g_{14} & e_{34}g_{13}; & -e_{56}g_{16} & \cdots \\
-e_{12}g_{22} & 1+e_{12}g_{21}; & -e_{34}g_{24} & e_{34}g_{23}; & -e_{56}g_{26} & \cdots \\
-e_{12}g_{32} & e_{12}g_{31}; & 1-e_{34}g_{34} & e_{34}g_{33}; & -e_{56}g_{36} & \cdots \\
-e_{12}g_{42} & e_{12}g_{41}; & -e_{34}g_{44} & 1+e_{34}g_{43}; & -e_{56}g_{46} & \cdots \\
-e_{12}g_{52} & e_{12}g_{51}; & -e_{34}g_{54} & e_{34}g_{53}; & 1-e_{56}g_{56} & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots
\end{bmatrix}.
$$

This determinant may clearly be written as

$$
\Delta = \Delta'' = \mathrm{Det}(\mathbf{I''}+\mathbf{g''e''}),
$$

where $\mathbf{e''}$ and $\mathbf{g''}$ have the standard forms (3.7) and (3.8) corresponding to distinct indices which were assumed in the text. In particular, $\mathrm{Det}(\mathbf{e''})\neq 0$ so the reduction to a Pfaffian may be performed as before, the index 3 being finally set equal to 2 whereupon the matrix element $g_{23}=-g_{32}$ vanishes identically.

APPENDIX B: THE GREEN'S FUNCTION ELEMENTS AND THEIR CALCULATION

The integrals for the Green's function elements given in Sec. 4 may be performed systematically with the aid of the elementary standard forms

$$
\frac{1}{\pi}\int_0^\pi \frac{d\theta}{A-B\cos\theta}=\frac{1}{(A^2-B^2)^{1/2}}, \quad (A>B), \tag{B1}
$$

$$
\int_0^1 \frac{dw}{(a^2-w^2)^{1/2}}=\sin^{-1}(1/a), \quad (a>1), \tag{B2}
$$

$$
\int_0^1 \frac{w^2 dw}{(a^2-w^2)^{1/2}}=-\tfrac{1}{2}(a^2-1)^{1/2}+\tfrac{1}{2}a^2\sin^{-1}(1/a), \tag{B3}
$$

$$
\int_0^1 \frac{w^4 dw}{(a^2-w^2)^{1/2}}=-\tfrac{1}{8}(2+3a^2)(a^2-1)^{1/2}+\tfrac{3}{8}a^4\sin^{-1}(1/a), \tag{B4}
$$

and their extensions (see, for example, Dwight[32]). The procedure is best illustrated by example. Consider the

[32] H. B. Dwight, *Tables of Integrals and Other Mathematical Data* (The Macmillan Company, New York, 1957), 3rd ed.

simplest central Green's function element

$$
[1,0]=\frac{x}{2\pi^2}\int_0^\pi\int_0^\pi (\cos\alpha-1)[\Delta(\alpha,\beta)]^{-1}d\alpha d\beta \tag{B5}
$$

where

$$
\Delta(\alpha,\beta)=x^2+y^2-x^2\cos\alpha-y^2\cos\beta, \tag{B6}
$$

and where we assume that x and y are real and positive. Set $\beta=\theta$ and

$$
A=x^2+y^2-x^2\cos\alpha, \quad B=y^2 \tag{B7}
$$

so that

$$
(A-B)^{1/2}=2^{1/2}x|\sin\tfrac{1}{2}\alpha|,
$$
$$
(A+B)^{1/2}=2^{1/2}(y^2+x^2\sin^2\tfrac{1}{2}\alpha)^{1/2}. \tag{B8}
$$

Performing the θ integral by (B1) and making the substitution

$$
w=\cos\tfrac{1}{2}\alpha, \quad dw=-\tfrac{1}{2}\sin\tfrac{1}{2}\alpha d\alpha \tag{B9}
$$

reduces the integral to the type (B2) with

$$
a^2=(x^2+y^2)/y^2 \tag{B10}
$$

so that, finally,

$$
[1,0]=-(1/\pi x)\sin^{-1}(1/a)
$$
$$
=-(1/\pi x)\tan^{-1}(x/y). \tag{B11}
$$

A typical more complicated case is, for example, given by an element near the edge such as

$$
M_{11}(2)=\tfrac{1}{2}x(\cos\alpha-1)(1-\cos 2\beta), \tag{B12}
$$

[see Eq. (6.1)]. If we rewrite this as

$$
M_{11}(2)=x(\cos\alpha-1)+x(\cos\alpha-1)\cos^2\beta, \tag{B13}
$$

the integral splits into two parts, the first being equal to the element $[1,0]$. Making the substitutions (B7)

and (B8) in the second part yields, on dividing out, and using (B1),

$$\frac{x}{\pi^2}\int_0^\pi (\cos\alpha-1)d\alpha\int_0^\pi d\theta\frac{\cos^2\theta}{A-B\cos\theta}$$

$$=\frac{x}{\pi}\int_0^\pi d\alpha(\cos\alpha-1)\left[-\frac{A}{B^2}+\frac{A^2}{B^2(A^2-B^2)^{1/2}}\right]. \quad (B14)$$

The substitution (B9) gives $A=y^2+2x^2-2x^2w^2$ so that expanding the final term in A^2 leads to integrals of the forms (B2), (B3), and (B4). The other parts merely involve simple trigonometric integrals. Collecting terms yields the result (6.7) quoted in the text.

The labor of calculating the set of Green's function elements tabulated below is much reduced by exploiting the basic recurrence relation (4.11) and the symmetry in x and y.

Green's Function Elements for General x and y

Note that

$$\tau=x/y, \quad \bar\tau=y/x \quad (B15)$$

and

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

$$\rho_y=(1/\pi)\tan^{-1}(y/x)=\tfrac{1}{2}-\rho_x. \quad (B16)$$

$$-x[1,0]=\rho_x,$$
$$-iy[0,1]=\rho_y, \quad (B17)$$

$$-x[1,2]=(\tau/\pi)-\tau^2\rho_y,$$
$$-iy[2,1]=(\bar\tau/\pi)-\bar\tau^2\rho_x. \quad (B18)$$

$$-x[3,0]=\rho_x(1+2\bar\tau^2)-(2/\pi)\bar\tau,$$
$$-iy[0,3]=\rho_y(1+2\tau^2)-(2/\pi)\tau, \quad (B19)$$

$$-x[3,2]=(\bar\tau/\pi)-\bar\tau^2\rho_x,$$
$$-iy[2,3]=(\tau/\pi)-\tau^2\rho_y, \quad (B20)$$

$$-x[1,4]=(\tau/\pi)(1+3\tau^2)-\rho_y\tau^2(2+3\tau^2),$$
$$-iy[4,1]=(\bar\tau/\pi)(1+3\bar\tau^2)-\rho_x\bar\tau^2(2+3\bar\tau^2), \quad (B21)$$

$$-x[5,0]=\rho_x(1+6\bar\tau^2+6\bar\tau^4)-(2/\pi)\bar\tau(2+3\bar\tau^2),$$
$$-iy[0,5]=\rho_y(1+6\tau^2+6\tau^4)-(2/\pi)\tau(2+3\tau^2). \quad (B22)$$

When $x=y$, an explicit general result can be obtained for the diagonal elements $[2s+1, 2s]$ by making the transformation $\alpha'=\tfrac{1}{2}(\alpha+\beta)$, $\beta'=\tfrac{1}{2}(\alpha-\beta)$. The integration over β' may then be performed by using (B1) which yields

$$x[2s+1, 2s]=x[2s-1, 2s]$$

$$=iy[2s, 2s+1]=iy[2s, 2s-1]$$

$$=-(1/4\pi)\int_0^\pi \sin2s\theta[\sec\theta-\tan\theta]d\theta. \quad (B23)$$

TABLE IV. Green's function elements for $x=y$.

$-x[1,0]=-iy[0,1]=$	$(1/4)$			$=0.250\ 000,$
$-x[1,2]=-iy[2,1]=$	$(1/\pi)$	$-$	$(1/4)$	$=0.068\ 310,$
$-x[3,0]=-iy[0,3]=$	$(3/4)$	$-$	$(2/\pi)$	$=0.113\ 380,$
$-x[3,2]=-iy[2,3]=$	$(1/\pi)$	$-$	$(1/4)$	$=0.068\ 310,$
$-x[1,4]=-iy[4,1]=$	$(4/\pi)$	$-$	$(5/4)$	$=0.023\ 240,$
$-x[5,0]=-iy[0,5]=$	$(13/4)$	$-$	$(10/\pi)$	$=0.066\ 901,$
$-x[3,4]=-iy[4,3]=$	$(1/4)$	$-$	$(2/3\pi)$	$=0.037\ 793,$
$-x[5,2]=-iy[2,5]=$	$(17/3\pi)$	$-$	$(7/4)$	$=0.053\ 756,$
$-x[1,6]=-iy[6,1]=$	$(59/3\pi)$	$-$	$(25/4)$	$=0.010\ 094,$
$-x[7,0]=-iy[0,7]=$	$(63/4)$	$-$	$(148/3\pi)$	$=0.046\ 713,$
$-x[5,4]=-iy[4,5]=$	$(1/4)$	$-$	$(2/3\pi)$	$=0.037\ 793,$
$-x[3,6]=-iy[6,3]=$	$(9/4)$	$-$	$(7/\pi)$	$=0.021\ 831,$
$-x[7,2]=-iy[2,7]=$	$(97/3\pi)$	$-$	$(41/4)$	$=0.042\ 020,$
$-x[1,8]=-iy[8,1]=$	$(304/3\pi)$	$-$	$(129/4)$	$=0.005\ 401,$
$-x[9,0]=-iy[0,9]=$	$(321/4)$	$-$	$(252/\pi)$	$=0.035\ 909,$
$-x[5,6]=-iy[6,5]=$	$(13/15\pi)$	$-$	$(1/4)$	$=0.025\ 869,$
$-x[7,4]=-iy[4,7]=$	$(11/4)$	$-$	$(128/15\pi)$	$=0.033\ 756,$
$-x[3,8]=-iy[8,3]=$	$(61/4)$	$-$	$(718/15\pi)$	$=0.013\ 567,$
$-x[9,2]=-iy[2,9]=$	$(2723/15\pi)$	$-$	$(231/4)$	$=0.033\ 855,$
$-x[1,10]=-iy[10,1]=$	$(8023/15\pi)$	$-$	$(681/4)$	$=0.003\ 347,$
$-x[11,0]=-iy[0,11]=$	$(1683/4)$	$-$	$(19\ 826/15\pi)$	$=0.029\ 216.$

After some manipulation one can derive the simple results

$$x[2s+1, 2s]=-(1/4\pi)[\psi(\tfrac{3}{4}+\tfrac{1}{2}s)-\psi(\tfrac{1}{4}+\tfrac{1}{2}s)], \quad (B24)$$

where $\psi(z)$ is the logarithmic derivative of the gamma function, and

$$x[2s+1, 2s]=-(-)^s\left\{\frac{1}{4}+\frac{1}{\pi}\sum_{r=1}^s\frac{(-1)^r}{2r-1}\right\}. \quad (B25)$$

Explicit values for these and other elements when $x=y$ are tabulated in Table IV.

APPENDIX C: ASYMPTOTIC BEHAVIOR OF THE GREEN'S FUNCTION

To obtain the asymptotic behavior of the Green's function elements for large r, s, t, or u from the double integral representation of Sec. 4, the general procedure is to perform the integral not involving the parameter in question and to integrate the second variable by parts repeatedly. The method may be illustrated by deriving the expression (6.15) for the decay of the correlation for a single dimer perpendicular to the edge of the lattice. The dependence on the distance s from the edge is given by the integral

$$c_\perp(s)=\frac{(-)^{s+1}}{(2\pi)^2}\int_{-\pi}^\pi\int_{-\pi}^\pi\tfrac{1}{2}y^2\frac{\cos s\beta-\cos(s+1)\beta}{x^2+y^2-x^2\cos\alpha-y^2\cos\beta}d\alpha d\beta. \quad (C1)$$

Performing the integral on α with the aid of (B1), as in Appendix B, yields

$$c_\perp(s)=\frac{(-)^{s+1}}{2\pi}\int_0^\pi\frac{\sin(s+\tfrac{1}{2})\beta}{(\tau^2+\sin^2\tfrac{1}{2}\beta)^{1/2}}d\beta, \quad (\tau>0). \quad (C2)$$

Integrating by parts between the limits 0 and π yields

$$c_1(s) = \frac{(-)^{s+1}}{2\pi(s+\frac{1}{2})}\left\{\frac{1}{\tau} - \int_0^\pi \frac{\cos(s+\frac{1}{2})\beta \, \sin\frac{1}{2}\beta \, \cos\frac{1}{2}\beta d\beta}{2(\tau^2+\sin^2\frac{1}{2}\beta)^{3/2}}\right\}.$$

$$(C3)$$

On integrating the factor $\cos(s+\frac{1}{2})\beta$ by parts again, a

contribution of order $1/(s+\frac{1}{2})^2$ is obtained, but the integrated term clearly vanishes at both limits. A further integration by parts yields a nonvanishing term of order $1/(s+\frac{1}{2})^3$, thereby confirming the result (6.15) quoted in the text. In a similar way, one may derive all the other asymptotic expressions of the Green's function elements which are quoted.

Nuclear Spin-Lattice Relaxation in Liquids

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(Received 9 July 1963)

The spin-lattice relaxation in liquids has been investigated on the basis of quasicrystalline models for them. Explicit expressions for spin-lattice relaxation time T_1 are derived for the jump-diffusion model and the stochastic model. The theory has been applied to the case of water and the constants used in the calculation are derived from the experimental data on the cold-neutron scattering. The spin-lattice relaxation is found to be quite insensitive to the details of the models.

I. INTRODUCTION

NUCLEAR spin-lattice relaxation involves the exchange of energy between the nuclear-spin system and the "lattice" of the material in which the spins are located. The rate at which the thermal equilibrium is established among the nuclear spin-energy levels is expressed in terms of a parameter T_1, called the spin-lattice relaxation time. Bloembergen, Purcell, and Pound have discussed a general theory of relaxation in liquids and have shown that T_1 can be expressed in terms of the Fourier transforms of the correlation function of the interactions coupling the nuclear spins to the lattice of the liquid.[1,2] In ordinary liquids, the important relaxation mechanisms are the couplings of the nuclear spins to the random translational and rotational motions of the molecules via the magnetic dipolar interaction of the nuclear moments. Recently, cold-neutron spectroscopy has given detailed information about the atomic motions in liquids,[3–5] and has led many workers to propose quasicrystalline models[6–9] for them. The present work is concerned with the in-

terpretation of T_1 measurement for water on the basis of these models, on the lines of approach of Bloembergen, Purcell, and Pound. Sections II and III are devoted to the discussion of the spin-lattice relaxation in liquids on the basis of the jump-diffusion model and the stochastic model, respectively. In Sec. IV, the theory is applied to the case of water and the results are compared with the experiment.

II. JUMP-DIFFUSION MODEL

We shall start with the general expression [1,10] for T_1

$$T_1^{-1} = \frac{3}{2}\gamma^4\hbar^2 I(I+1)[J^{(1)}(\omega_0) + J^{(2)}(2\omega_0)]. \quad (1)$$

Here, γ is the nuclear gyromagnetic ratio, ω_0 the Larmor frequency of nuclei, I the nuclear-spin number and

$$J^{(m)}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}k_m(t)dt; \quad m=1, 2. \quad (2)$$

The correlation function $k_m(t)$ is related to the random functions $F_m(t)$ by the relation

$$k_m(t) = N\langle F_m(t')F_m^*(t'+t)\rangle_{\mathrm{av}(t')}, \quad (3)$$

where N is the number of molecules per cm³. For dipole-dipole interactions

$$F_1(t) = \left(\frac{8\pi}{15}\right)^{1/2}\frac{Y_2^1(\theta,\phi)}{r^3}, \quad F_2(t) = \left(\frac{32\pi}{15}\right)^{1/2}\frac{Y_2^2(\theta,\phi)}{r^3}, \quad (4)$$

where $Y_2^m(\theta,\phi)$ is a spherical harmonic and (r,θ,ϕ) denote the spherical polar coordinates of a spin relative

[1] N. Bloembergen, E. M. Purcell, and R. V. Pound, Phys. Rev. **73**, 679 (1948).

[2] N. Bloembergen, thesis, Leiden, 1948 (Martinus, Nijhoff, The Hague).

[3] B. N. Brockhouse, Suppl. Nuovo Cimento **9**, 45 (1958).

[4] B. N. Brockhouse, Phys. Rev. Letters **2**, 287 (1959).

[5] D. J. Hughes, H. Palevsky, W. Kley, and E. Tunkelo, Phys. Rev. Letters **3**, 91 (1959).

[6] K. S. Singwi and A. Sjölander, Phys. Rev. **119**, 863 (1960).

[7] C. T. Chudley and R. J. Elliott, Proc. Phys. Soc. (London) **77**, 353 (1961).

[8] A. Rahman, K. S. Singwi, and A. Sjölander, Phys. Rev. **122**, 9 (1961).

[9] A. Rahman, K. S. Singwi, and A. Sjölander, Phys. Rev. **126**, 997 (1962).

[10] R. Kubo and K. Tomita, J. Phys. Soc. Japan **9**, 888 (1954).