METHODOLOGICAL NOTES

The dimer problem and the Kirchhoff theorem

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Application of the Kirchhoff theorem to lattice statistics leads to solution of the two-dimensional dimer problem, earlier obtained by the Pfaffian method. It is shown that the relation between the theory of network of linear resistors and the dimer problem is particularly useful in the three-dimensional case. A number of dimer configurations on a decorated diamond lattice is found by calculating spanning trees on the corresponding lattice. The Kirchhoff theorem is proved in the spirit of the combinatorical solution of the Ising model.

CONTENTS

INTRODUCTION

Two notable theoretical results, the Kirchhoff matrix theorem[1] and the equation for the partition function of the two-dimensional dimer problem[2,3], were obtained in totally different areas of physics, separated by over a century, and, at first glance, have nothing in common. In fact, these results are so closely related, that in some cases the latter is a simple consequence of the former. We attempt to clarify this connection, and provide some new consequences concerning dimer statistics.

In the first section we provide a short introduction to dimers. We confine ourselves to the simplest statement of the problem, and to explaining the method of its primary solution. A more detailed solution and application of dimers to other problems of statistical physics are discussed in two thorough reviews by Montroll (both translated into Russian[4]).

The second section contains the required definitions of the theory of graphs and the Kirchhoff theorem.

Despite the fact that the theory of linear electrical circuits has become classical a long time ago, in the pedagogical literature it is difficult to find the "electric" and "graphic" parts of this theory in a unified form. Therefore the exposition of the matrix theorem is preceded by a derivation of equations for the resistance of a finite system of conductors.

In the third section we demonstrate the relation between the Kirchhoff theorem and the dimer problem on a two-dimensional square lattice.

In the last section it is shown how the established relation makes it possible to solve the dimer problem on a certain three-dimensional structure of the diamond lattice type.

1. DIMERS

The dimer problem belongs to the extensive class of lattice gas models.[5,6] The lattice gas differs from an ordinary continual gas in that its molecules do not occupy arbitrary positions in space, but are located in sites of a periodic lattice. As a rule, it is assumed that due to strong repulsion at small distances not more than a single molecule can reside in one site. The configuration integral over particle coordinates transforms in this approximation into a lattice sum, which is calculated exactly in several simple cases.

Most often one considers a gas, whose molecules have a spherical shape, and each of them occupies a single site. In this case the molecule is assumed to be a point, coinciding with the lattice site, and is called a monomer. If the molecule has a dumbbell shape, in the lattice gas model it occupies two adjacent sites and is represented in the form of two neighboring points, joined by a lattice edge. A mixture of molecules of two kinds forms a system of monomers and dimers. An example of a typical monomer-dimer mixture is a benzene solution of several hydrocarbons: diphenyl, diphenylmethane, and dibenzyl, where the monomers can be assumed to be C_6H_6 groups.[7]

Besides repulsion at a single site it is also necessary to take into account the interaction between different sites. In a gas consisting of identical monomers one usually considers interactions between nearest lattice sites. This model is equi-

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valent to the Ising model. If the gas has molecules of more complex structure than monomers, this relatively weak interaction is not always accounted for, since even without it the quite important and interesting problem arises of calculating the entropy of a mixture of different molecules.[8,9]

In the general statement this problem is very difficult. In 1960 Green and Leipnik published its solution,[10] but their result turned out to be erroneous.[11] After some time it became clear that the monomer and dimer problem is equivalent to the Ising model in a magnetic field,[12] which so far also has no exact solution.

The only case, in which the entropy can be calculated exactly, is the limit of vanishing monomer density. In this case the lattice is totally covered by dimers, so that each site is occupied by one, and only one, dimer (it is ultimately assumed that the number of sites is even). The problem consists of enumerating the ways of dense packing, i.e., all methods of arranging $(n/2)$ dimers on a lattice with n sites. Sometimes the limit of vanishing monomer density is called the pure dimer problem, but we retain for it the title of the general problem, since in the following we will handle only this case.

The high interest in the enumeration of dense packing of dimers in statistical physics is explained by the fact that numerous lattice models reduce to this problem. A more accurate statement is: any two-dimensional model from the class of "free fermions" can be represented as a dimer problem on some lattice.[13] The basic and most studied representative of the class of "free fermions" is the two-dimensional Ising model in a vanishing magnetic field.

A graphical representation in the form of a set of closed polygons is well-known for states of a spin system with an Ising Hamiltonian.[14] This implies that the solution of the Ising model can be reduced to enumeration of all graphs for which each site is associated with an even number of edges. In the case of a square lattice 0, 2, or 4 edges can meet in a site. All these possibilities are illustrated in Fig. 1. Considering now a lattice with a more complex elementary unit cell (Fig. 2), it can be noted that the different methods of filling elementary unit cells by dimers correspond uniquely to the possible edge locations in a site of a square lattice. Therefore, solution of the dimer problem on a complex lattice after assigning required weights to the edges provides the partition function of the two-dimensional Ising model on a square lattice.

The dimer problem is most simply formulated as follows. Let there be given a square lattice, consisting of M columns and N rows, folded into a torus for the creation of

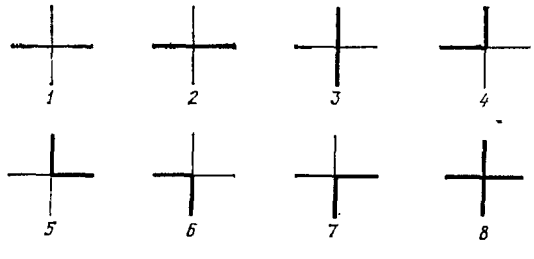

FIG. 1. Graphic representation of the Ising model.

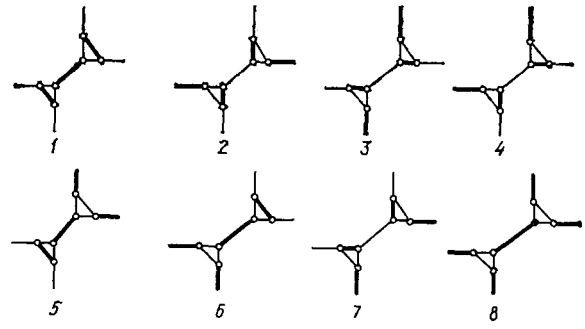

FIG. 2. Dimer coverages of the elementary unit cells, uniquely corresponding to the sites of Fig. 1.

periodic boundary conditions. We denote by $d(m,n)$ the number of ways of totally covering this lattice by m horizontal and n vertical dimers under the condition that $m+n=MN/2$. The partition function or the generating function of dimer configurations is then written in the form

$$\Lambda(x, y) = \sum_{\substack{m,n \\ (m+n=MN/2)}} d(m, n)\, x^m y^n, \tag{1.1}$$

where x,y are parameters or weights, which can be assigned a statistical meaning by expressing them in terms of the reciprocal temperature β and the chemical potentials μ_x, μ_y of horizontal and vertical dimers: $x=\exp(\beta\mu_x,)y=\exp(\beta\mu_y)$.

The total number of dimer coverages F is obtained by putting $x=y=1$:

$$F = \Lambda(1, 1). \tag{1.2}$$

One is usually interested in the system properties for large M and N:

$$\lambda(x, y) = \lim_{M,N\to\infty} \frac{1}{MN} \ln \Lambda(x, y). \tag{1.3}$$

The fundamental quantity characterizing dimer coverages is the molecular freedom of a dimer in dense packing

$$\varphi = e^{2\lambda(1,1)}, \tag{1.4}$$

so that the number of dense packings equals

$$F = \varphi^{MN/2}. \tag{1.5}$$

It is clear from physical considerations that $\Lambda(x,y)$ increases exponentially with increasing lattice size (this fact was rigorously proved in Ref. 15). It is also easy to give a crude estimate of the quantity φ: it must be larger than unity, and cannot exceed the 4-coordination lattice number. The surprisingly accurate estimate $\varphi=1.786$ was obtained by Fowler and Rushbrooke in one of the first dimer studies.[9]

In 1961 Kasteleyn[2] and simultaneously Temperley and Fisher[3] found the exact solution of the dimer problem, and showed that

$$\varphi = e^{2G/\pi} = 1.791623..., \tag{1.6}$$

where $G=1^{-2}-3^{-2}+5^{-2}-7^{-2}+...=0.915965...$ is the Catalan constant. They also obtained the general expression for the partition function in the limit of large M,N:

$$\Lambda(x, y) = \exp\left\{\frac{MN}{(2\pi)^2}\int_0^{\pi}\int \ln 2\left[(x^2+y^2)-x^2\cos\theta_1 - y^2\cos\theta_2\right] d\theta_1\, d\theta_2\right\}. \tag{1.7}$$

The derivation of this equation fits in, generally speaking, among the ideas leading to the solution of the two-dimensional Ising model. Thus, for example, in 1967 Lieb[16] obtained Eq. (1.7) by means of a transition matrix, a method close to the initial Onsager solution. A new technical approach, used in Refs. 2, 3, was the introduction of a Pfaffian,[6] substantially simplifying the matrix approach of the preceding solutions.

The Pfaffian of an antisymmetric matrix of even order $2NA = \{a(p,p')\}$ is defined as:

$$Pf(A) = \sum_P{}' \delta_p a(p_1, p_2)\, a(p_3, p_4) \ldots a(p_{2N-1}, p_{2N}), \quad (1.8)$$

where the summation is carried out over all permutations $P = (p_1, p_2, \ldots, p_{2N})$ of the numbers $(1,2,\ldots,2N)$, satisfying the condition

$$p_1 < p_2;\ p_3 < p_4,\ p_5 < p_6,\ \ldots,\ p_{2N-1} < p_{2N};$$
$$p_1 < p_3 < \ldots < p_{2N-1}, \quad (1.9)$$

and the factor δ_p equals to 1 for even and -1 for odd permutations. It is easily understood why this matrix object is convenient for enumerating the dimer configurations. Consider a square lattice with dimers located on it (Fig. 3). We number all lattice sites row by row. Each site is represented by the number pair (p,p'). The whole dimer configuration can be represented in the form

$$(p_1, p_2)(p_3, p_4) \ldots (p_{2N-1}, p_{2N}), \quad (1.10)$$

ordering the dimers from left to right and from bottom to top. For the configurations shown in Fig. 3 the following representation is obtained:

$$(1, 7)(2, 3)(4, 10)(5, 6)(8, 9)(11, 17) \ldots (23, 24). \quad (1.11)$$

In this description the permutation $(p_1, p_2, \ldots, p_{24})$ of the numbers $(1,2,\ldots,24)$ obeys the same conditions (1.9), as do the matrix subscripts in the definition of a Pfaffian, while the number of ways of satisfying inequalities (1.9) coincides with the number of dimer configurations. In the matrix $A = \{a(p,p')\}$, defined by the conditions

$$a(p, p') = \begin{cases} x, & \text{if } p \text{ and } p' \text{ are horizontally adjacent,} \\ y, & \text{if } p \text{ and } p' \text{ are vertically adjacent,} \\ 0, & \text{if } p \text{ and } p' \text{ are not adjacent,} \end{cases} \quad (1.12)$$

to each nonvanishing matrix element $a(p,p')$ can be associated a dimer (p,p') with its weight factor. From the above consideration it follows that

$$\mathrm{Pf}(A) \sim \Lambda(x, y) \quad (1.13)$$

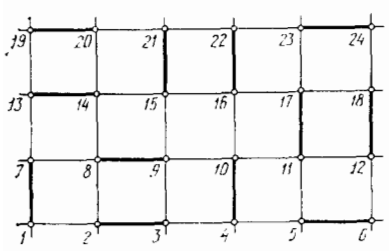

FIG. 3. Dense packing of dimers.

accurately up to the signs in front of the terms of the expansion of the left hand side, which are negative in half the cases.

Despite this successful representation of the partition function, all difficulties are still ahead of us, since we must make the remaining terms of the expansion of the Pfaffian positive and evaluate it. To overcome these difficulties one introduces the concept of superposition polygons, proves the Kasteleyn theorem, constructs the cyclic matrix, and, finally, uses the simple (but nontrivial) equation

$$\mathrm{Det}\, A = (\mathrm{Pf}\, A)^2, \quad (1.14)$$

relating the determinant and the Pfaffian of the antisymmetrix matrix. All these steps are described in great detail in Montroll's reviews mentioned above, and we will not dwell on them, but postpone the derivation of Eq. (1.7) to section 3, where it is obtained as a consequence of the Kirchhoff theorem.

2. THE KIRCHHOFF THEOREM

Consider an interconnected electric circuit, consisting of the points $1,2,\ldots,N$, arbitrarily connected by conductors. The reciprocal resistance of the conductor combining the points i and j is denoted by x_{ij}. At the points k and l let us connect to the circuit a source of current I. We denote by v_i the potential generated at the point i. Ohm's law, in conjunction with the first Kirchhoff law, gives:

$$\left.\begin{aligned} &\sum_{j\neq k} x_{kj}(v_k - v_j) = I; \\ &\sum_{j\neq i} x_{ij}(v_i - v_j) = 0, \quad i \neq k,\ l, \\ &\sum_{j\neq k} x_{lj}(v_l - v_j) = -I, \end{aligned}\right\} \quad (2.1)$$

or in more compact matrix form

$$I_i = \sum_{j=1}^{N} T_{ij} v_j, \quad i = 1, 2, \ldots, N, \quad (2.2)$$

where $I_i = I(\delta_{ik} - \delta_{il})$, and

$$T_{ij} = \begin{cases} \sum_{m\neq i} x_{im}, & i = j, \\ -x_{ij}, & i \neq j. \end{cases} \quad (2.3)$$

To determine the potential difference $v_k - v_l$ it is sufficient to consider $N-1$ independent equations. Taking into account that by the definition of the matrix T

$$\sum_{j\neq l} T_{ij} = -T_{il}, \quad (2.4)$$

we rewrite the first $N-1$ equations (2.2) in the form

$$I\delta_{ik} = \sum_{j=1}^{N} T_{ij}(v_j - v_l), \quad i,\ j \neq l. \quad (2.5)$$

This system has the solution

$$v_k - v_l = I\,\frac{|T^{(k,l)}|}{|T^{(l)}|}; \quad (2.6)$$

where $T^{(l)}$ is the determinant of the matrix obtained from T by deleting the rows and columns with subscript l, and the determinant $T^{(l,k)}$ —by deleting the two rows and columns k and l. From equation (2.6) immediately follows an expression for the resistance R_{kl} between points k and l of the given circuit:

$$R_{kl}=\frac{|T^{(k,\,l)}|}{|T^{(l)}|}. \tag{2.7}$$

The equation obtained is a consequence of Kirchhoff's laws. The Kirchhoff matrix theorem provides this equation with a geometric meaning.

To formulate the matrix theorem consider our electric circuit as a graph G with N marked (enumerated) vertices. The vertices i and j are joined by an edge, and are considered to be adjacent if the circuit contains a conductor connecting the points i and j. The graph G can be set in correspondence with an $(N\times N)$-matrix A, called the adjacency matrix. In this matrix $a_{ij}=1$ if the vertex i is adjacent to the vertex j, and $a_{ij}=0$ otherwise. It is natural to require that the circuit contain no closed loops, exiting and entering a single point; the diagonal elements of A vanish in this case.

A cycle in the graph G is the name given to an alternating sequence of vertices and edges, in which the initial and final vertices coincide. A connected graph is called a tree if it contains no cycles. We say that the subgraph H of the graph G covers G if each vertex of G is a vertex of H. A core of the graph G is a tree covering it. Figure 4 shows a graph with all its cores.

Let M be the matrix obtained from $(-A)$ by replacing each ith element of the principal diagonal by the number of vertices adjacent to i. This number is usually denoted by deg i, and is called the vertex degree.

Kirchhoff showed[1] that the following statement is valid:

2.1. Matrix theorem on trees

Let G be a connected marked graph with the adjacency matrix A. Then all algebraic complements of the matrix M are equal to each other, and their general value is the number of cores of the graph M.

For the graph illustrated in Fig. 4 we have

$$A=\begin{pmatrix}0&1&1&1\\1&0&0&1\\1&0&0&1\\1&1&1&0\end{pmatrix},\quad M=\begin{pmatrix}3&-1&-1&-1\\-1&2&0&-1\\-1&0&2&-1\\-1&-1&-1&3\end{pmatrix}. \tag{2.8}$$

All algebraic complements of the matrix M are equal to 8, i.e., the number of cores of this graph.

In combinatorical calculations it is more convenient to deal not with the number of graphs of a given form, but with their generating functions. We assign to each edge, joining the vertices i and j, the weight x_{ij}. The core of the graph is uniquely determined by the product of weights of the edges appearing in it. The sum of these products over all possible cores is called the core generating function $S(\{x\})$, where by $\{x\}$ we denote the set of all weights of the graph. We put the weight of each edge x_{ij} equal to the conductivity of the circuit portion appearing in the definition (2.3) of the matrix T. In these terms the Kirchhoff theorem acquires the following form:

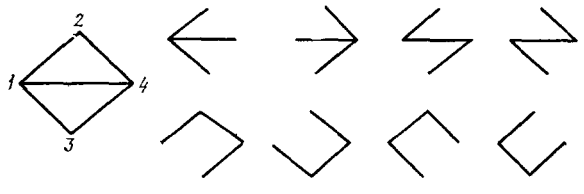

FIG. 4. A graph and all its cores. The first four cores contain edge (14).

For a connected graph G all algebraic complements of the matrix T are identical, and are equal to the core generating function $S(\{x\})$. To understand the connection between the two statements of the theorem it is sufficient to note that the matrices M and T coincide if all $x_{ij}=1$, and the number of cores is simply $S(\{1\})$.

We return now to Eq. (2.7) for the resistance. According to the matrix theorem, the denominator $|T^{(l)}|$ is the generating function of the core trees $S(\{x\})$. The numerator $|T^{(k,l)}|$ is equal to the coefficient of x_{ij} in the expansion of $S(\{x\})$, i.e.,

$$|T^{(k,\,l)}|=\frac{\partial}{\partial x_{kl}}S(\{x\}). \tag{2.9}$$

This implies that $|T^{(k,l)}|$ for $x_{ij}=1$ equals to the number of all cores containing the edge kl. Then from Eq. (2.7) and from the Kirchhoff theorem follows an intersetting prescription for calculating the resistance of a system of one-ohm conductors: for a given circuit it is necessary to find the number of core trees containing the edge kl, and divide it by the number of all cores. It is seen from Fig. 4 that the first number for the edge (1,4) equals 4, and the second is 8. The resistance between the points 1 and 4 is $R_{1,4}=\frac{1}{2}$. If the resistances are not all equal to unity, to calculate R_{kl} it is necessary to find the appropriate generating function.

The following problem can arise: what to do if the points k and l are not joined by a conductor? In this case it is simplest to proceed as follows: add to the circuit a known conductor between the points k and l, find the resistance of the resultant circuit, and then determine R_{kl} of the original circuit by the equation for a parallel connection of conductors.

In the classical study[1] the matrix theorem was obtained implicitly. The formulation given above was taken from F. Harary's book.[17] This book also contains a modern proof of the theorem. Despite its briefness, it is far from elementary. Therefore we provide another proof, intended for the reader more familiar with the Ising model than with the literature on graph theory.

2.2. Proof of the matrix theorem

The first part of the proof consists of a simplified variant of the combinatorical solution of the Ising model.[14]

Consider a connected graph G with N vertices, enumerated by the numbers 1,2, ..., N. As above, we assign the edge joining vertices i and j the weight x_{ij}. We denote by p the closed non-self-intersecting path, passing some sequence of vertices and edges of G, in which all vertices are different. We define the weight $W(p)$ of the path p as the product of all the weights of the edges contained in it taken with a minus sign. Consider the set Γ of closed nonintersecting paths on the graph G. The weight of this set is defined as

$$\chi(\Gamma)=\prod_{p}W(p), \tag{2.10}$$

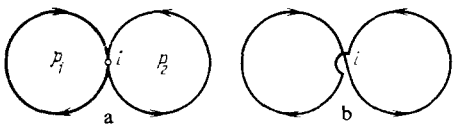

FIG. 5. a) Two paths intersecting at point i; b) one self-intersecting path.

where the product is carried out over all paths of the set Γ.

We denote by $\mathscr{P}$ an arbitrary closed path on G without the restriction on self-intersection. Its weight $W(\mathscr{P})$ is defined similarly to $W(p)$. The following equality is valid

$$\prod_{\mathscr{P}}(1+W(\mathscr{P}))=\sum_{\Gamma}\chi(\Gamma), \tag{2.11}$$

in which the product is carried out over all possible paths on the graph, while the sum is carried out over the whole set of closed nonintersecting paths. To confirm the validity of this equality we expand the product on the left hand side and note that each term of the series obtained corresponds to some set of closed paths. If the set has no intersecting and self-intersecting paths, this term provides a contribution to the right hand side. If the two paths p_1 and p_2 intersect at the point i, as shown in Fig. 5a, then a term can be found, corresponding to one path self-intersecting at the point i, traversing both routes (Fig. 5b). The weight of the pair of paths equals $W(p_1)W(p_2)$ and is positive, the weight of the single path is—$W(p_1)W(p_2)$. Thus, the contribution of all intersecting and self-intersecting paths vanishes, and the required sum remains in the left hand side.

We take the logarithm of both sides of equality (2.11), and, similarly to the way it is done in deriving the partition function of the Ising model,[14] we write:

$$\ln\sum_{\Gamma}\chi(\Gamma)=\sum_{\mathscr{P}}\ln[1+W(\mathscr{P})]=\sum_{\mathscr{P}}[1-(-W(\mathscr{P}))]-$$

$$=-\sum_{\mathscr{P}}\sum_{j=1}^{\infty}\frac{(-W(\mathscr{P}))^j}{j}=-\sum_{r=1}^{\infty}\sum_{i=1}^{N}\frac{W_r(i)}{r}, \tag{2.12}$$

where by $W_r(i)$ we denote the sum of weights of all possible closed paths of r steps, starting and ending at the point i. The weight of these paths is again equal to the product of weights of the traversed edges, but taken with the positive sign.

Continuing the analogy, we note that the sum of the weights of all paths from point i to point j taking r steps $W_r(i,j)$ obeys the following recurrence relation:

$$W_{r+1}(i,\ j)=\sum_{k}\Lambda(j,\ k)\,W_r(i,\ k), \tag{2.13}$$

with the $N\times N$ transition matrix Λ. The elements $\Lambda(i,j)$ of this matrix are equal to the edge weight x_{ij} if the vertices i and j are adjacent, and zero otherwise. The transition of length r is determined by the matrix Λ^r, for which the diagonal elements correspond to return of the path to the original point. Therefore,

$$\operatorname{Tr}\Lambda^r=\sum_{i=1}^{N}W_r(i). \tag{2.14}$$

Denoting by λ_n the eigenvalues of the matrix Λ and taking into account equality (2.12), one can write down:

$$\sum_{\Gamma}\chi(\Gamma)=\exp\Big(-\sum_{r=1}^{\infty}\frac{1}{r}\sum_{n=1}^{N}\lambda_n^r\Big)$$

$$=\exp\Big[\sum_{n=1}^{N}\ln(1-\lambda_n)\Big]=\prod_{n=1}^{N}(1-\lambda_n)=|I-\Lambda|, \tag{2.15}$$

where I is the unit matrix of order N.

Having obtained the expression for the sum $\Sigma\chi(\Gamma)$, we can construct a more useful object—the "partition function" for the closed paths taking into account the vertex weights. For this we assign to each vertex i a weight v_i $(i=1,2,\ldots,N)$. Let the set of closed paths Γ leave unoccupied a part of the graph vertices: $i_1,i_2,\ldots,i_k$. We introduce the product

$$\bar{\chi}(\Gamma)=v_{i_1}v_{i_2}\ldots v_{i_k}\chi(\Gamma) \tag{2.16}$$

and define the function

$$Z(\mathbf{v},\ \{x\})=\sum_{\Gamma}\bar{\chi}(\Gamma), \tag{2.17}$$

summing again over all sets of closed paths. The expression for $Z(\mathbf{v},\{x\})$ is easily obtained, multiplying $\Sigma\chi(\Gamma)$ by Πv_i and replacing the weight of each edge x_{ij} by x_{ij}/v_i. In each set all the v_i will cancel out in vertices occupied by paths, and the required expression will be obtained for $\bar{\varkappa}(\Gamma)$. The factor Πv_i can be introduced by multiplying the row numbered i of the matrix $(1-\Lambda)$ by v_i. We then obtain

$$Z(\mathbf{v},\ \{x\})=\det(v_i\delta_{ij}-\Lambda(i,\ j)). \tag{2.18}$$

Here we reach the end of the analogy with the derivation of the partition function of the Ising model. We have found a "partition function", which is, in some sense, the opposite of the one required. Indeed, the generating function Z enumerates (with minus sign) all possible cycles on the graph, while we seek the cores generating function, i.e., the subgraphs in which there is not a single cycle. The inversion of the problem is carried out by means of the well-known combinatorical inclusion-exclusion principle.

2.3. The inclusion-exclusion principle

Let there be N elements and a certain number of properties $p(1), p(2), \ldots, p(n)$. Let, further, N_i be the number of elements with property $p(i)$, and, generally, let $N_{i_1i_2\ldots i_r}$ be the number of elements with properties $p(i_1), p(i_2), \ldots, p(i_r)$. Then the number of elements $N(0)$ not possessing any of these properties is given by the equation (see, for example, Ref. 18):

$$N(0)=N-\sum_{i}N_i+\sum_{i_1<i_2}N_{i_1i_2}+\ldots+(-1)^s$$

$$\times\sum_{i_1<i_2<\ldots<i_s}+N_{i_1i_2\ldots i_s}\ldots+(-1)^nN_{12\ldots n}. \tag{2.19}$$

To use this equation we note that the arguments $v_1,\ldots,v_N$ of the function $Z(\mathbf{v},\{x\})$ do not appear in the definition of the generating function $S(\{x\})$, and are, in fact, free parameters.

We set

$$v_i = \sum_{j \neq i} x_{ij}, \quad i = 1, 2, \ldots, N, \tag{2.20}$$

and consider Z term by term as the sum (2.17) over all sets of closed paths. The first term arises when the set Γ is empty. We write it down explicitly:

$$\prod_{i=1}^{N} v_i = \prod_{i=1}^{N} \left(\sum_{j \neq i} x_{ij} \right). \tag{2.21}$$

This expression can be regarded as the generating function of transitions between sites under the condition that from each site there emerges a single path to one of the adjacent sites of the graph. We denote by p_{ij} the path from site i into the adjacent site j. The sequence $p_{i_1 i_2} p_{i_2 i_3} \ldots p_{i_{n-1} i_n}$ is the path from site i_1 to site i_n. If i_1 and i_n coincide, the path is closed. In the generating function (2.21) there appear no self-intersecting paths, since only one path emerges from each vertex.

Let all possible combinations of paths obtained by those N elements, which we had in mind in formulating the inclusion-exclusion principle. Then the first term of $Z(\mathbf{v},\{x\})$ corresponds to the first term in the right hand side of Eq. (2.19).

The properties $p(1)$, $p(2)$, ... will be assumed to be closed paths, enumerated in an arbitrary order. The second term of Z is the sum over the sets Γ, consisting of a single closed path, and, by definition, the weight of the path is negative. Consequently, this term of Z corresponds to the second term in Eq. (2.19). The third term of Z is the sum over the sets Γ of two closed paths, and has a positive sign. Continuing this argument, we obtain a full correspondence between Z and the left hand side of Eq. (2.19)—the sum over all path combinations not including a single closed path.

From the result obtained it immediately follows that after substitution of (2.20) we obtain

$$Z(\mathbf{v}, \{x\}) = \det \left(\sum_{j \neq i} x_{ij} - \Lambda(i, j) \right) = |T| = 0, \tag{2.22}$$

since it is impossible to construct a system of paths, emerging from each vertex of the graph, not forming a single closed cycle. We consider now some algebraic complement of T, say $|T^{(1)}|$. In the matrix $T^{(1)}$ the first column and the first row have been deleted, implying that in the generating function of $|T^{(1)}|$ paths passing through vertex 1 are not taken into account. We allow only transitions to vertex 1 from the adjacent vertices $i_1, i_2, \ldots$ due to the diagonal elements $T_{i_1 i_1}$, $T_{i_2 i_2}$, ... Thus, vertex 1 turns out to be a sink for all paths on the graph G. The system of paths passes through each vertex and contains no closed cycles, therefore it is a core. Consequently, we have

$$|T^{(1)}| = S(\{x\}). \tag{2.23}$$

As a sink one can choose any vertex of G, therefore all $|T^{(i)}|$ $(i = 1,2, \ldots, N)$ are equal. Moreover, from the vanishing of the sum of the elements in each row and column of the matrix T it follows that the remaining algebraic complements are also all equal. The theorem is thus proved.

3. DIMERS AND CORES

Consider the problem of dimers on a plane square lattice, formulated in Sec. 1. We intend to show that any dense packing of dimers on this lattice can be represented as a core tree on a certain auxiliary lattice, and thereby identify this dimer partition function $\Lambda(x,y)$ with the core generating function $S(\{x\})$. The expression for $\Lambda(x,y)$ will then follow from the Kirchhoff theorem.

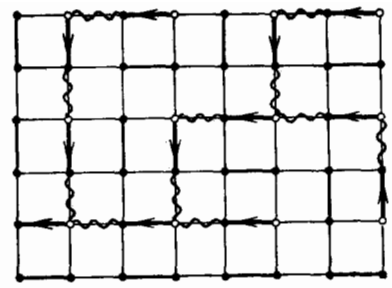

FIG. 6. Dense dimer packing. The light circles are sublattice points. Dimers are marked by arrows, and the wavy lines form a core on the sublattice sites.

For simplicity we assume that both numbers M and N, determining the lattice sizes, are even. The site coordinates are denoted by the pair of integers (k_1,k_2), $1 \leqslant k_1 \leqslant M$, $1 \leqslant k_2 \leqslant N$. The set of sites, whose coordinates take on the values

$$\begin{aligned} k_1 &= 2m, \quad m = 1, 2, \ldots, \frac{M}{2}, \\ k_2 &= 2n, \quad n = 1, 2, \ldots, \frac{N}{2}, \end{aligned} \tag{3.1}$$

together with the edges connecting these sites, are called a sublattice L of the basic lattice. In Fig. 6 the sites of the sublattice L are denoted by light circles, and the remaining sites—by dark ones.

Consider an arbitrary dense dimer packing on the basic lattice. Part of the dimers falls on the sublattice L (see Fig. 6). We provide each of these dimers by an arrow, directed from the end located on a site of L to the other end. From each site of L we draw a path to an adjacent site of L, indicated by the arrow. A simple observation, making it possible to apply the Kirchhoff theorem to the dimer problem, consists of the fact that the set of constructed paths forms a core tree on L.

Indeed, the graph formed by the paths contains all sites of the sublattice L, and, by definition, covers it. The exclusion of cycle formation is generated by the fact that any closed contour on the sites of L covers an odd number of points of the basic lattice, and these cannot be covered by dimers. This is simplest to verify by induction: the elementary square on L consists of one point of the basic lattice, while the connection to the available contour of the following square increases the number of spanned points by 2, 4, or 6, depending on the connection method. Consequently, the graph formed by the paths is a core.

To establish the mutually unique correspondence between the cores of L and dense packings it is necessary to verify that any core, in turn, produces a unique dimer configuration. For this consider all points of the basic lattice, not belonging to the given core. We combine by edges all pairs of adjacent vertices. The graph obtained is also a tree, while each of its branches from a free end to a connection point to

the following one has an even length. Therefore, we can consecutively cover by dimers all vertices of the tree, and thus assign to each core in L a dimer packing on the basic lattice. The uniqueness of this covering follows from the construction.

Let now A be the matrix of the adjacencies of the sublattice L, and M—its corresponding matrix with diagonal elements deg i. Then, according to the matrix theorem, the number of dimer coverages, determined in Sec. 1, is given by the equation:

$$F = |M'|, \tag{3.2}$$

where M is an arbitrary algebraic complement of the matrix M.

Before calculating F explicitly we obtain an expression for the generating function $\Lambda(x,y)$. We recall that x is the weight of a horizontal and y—that of a vertical dimer. In addition to establishing a correspondence between the cores of L and dense packings, we show a more refined property of dimer coverages.

In the given dense dimer packing let m_L horizontal and n_L vertical dimers be placed on the sites of the L sublattice. The packing then contains m_L horizontal and n_L vertical dimers, so that their total number is

$$2m_L + 2n_L = \frac{MN}{2}. \tag{3.3}$$

To prove this we define the reduced site coordinates:

$$\begin{aligned} K_1 &= k_1 \pmod 2, \\ K_2 &= k_2 \pmod 2. \end{aligned} \tag{3.4}$$

Equalities (3.4) imply that K_1 and K_2 equal 0 or 1, depending on whether the numbers $k_1/2$ and $k_2/2$ are even or odd. Consider the square $ABCD$ with reduced coordinates $[K_1,K_2]$, shown in Fig. 7. To each dimer on the basic lattice corresponds a dimer on the square. For example, to a horizontal dimer on a site of sublattice L there corresponds a dimer on the edge CD, and to a vertical on the edge AC. Since all sites of the basic lattice are occupied, the number of dimers covering the points A, B, C, D are equal. If the edge AC has n_L, and the edge CD — m_L dimers, the only way of adding equal numbers of dimers to the vertices of the square is to add n_L dimers to the edge BD and m_L dimers to the edge AB. Hence follows the property mentioned above.

From the set of weights $\{x\}$ appearing in the definition of the core generating function $S(\{x\})$ it is convenient to retain, as in the case of dimers, only two: the weight of a horizontal edge x and of a vertical one y. Let $g(m,n)$ be the number of cores of the sublattice L with m horizontal and n vertical edges. In the new notation the core generating function acquires the form:

$$S(x,\ y) = \sum_{m,\ n} g(m,\ n)\, x^m y^n. \tag{3.5}$$

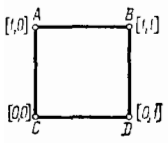

FIG. 7. Representation of a square lattice in reduced coordinates.

Each edge of the core passes through a dimer lying on a site of L. If the core has m edges with weight x and n edges with weight y, then, according to the property proved, in the dense packing connected to this core there are $2m$ horizontal and $2n$ vertical dimers. The number of packings and cores coincide, therefore we obtain for the dimer generating function $\Lambda(x,y)$

$$\Lambda(x,\ y) = \sum_{m,\ n} g(m,\ n)\, x^{2m} y^{2n} = S(x^2,\ y^2). \tag{3.6}$$

The elements of the matrix T, defined by conditions (2.3), are for our choice of weights

$$T_{ij} = \begin{cases} 2x + 2y, & i = j, \\ -x, & i,\ j \quad \text{horizontally adjacent}, \\ -y, & i,\ j \quad \text{vertically adjacent}, \\ 0, & i,\ j \quad \text{not adjacent}. \end{cases} \tag{3.7}$$

By the Kirchhoff theorem $S(x,y)$ is equal to the algebraical complement of the matrix T, and an expression for $\Lambda(x,y)$ follows directly from equality (3.6).

We turn now to derive Eq. (1.7). We must diagonalize the matrix T, for which purpose we use one its properties referred to as cyclic behavior (see, for example, Ref. 4).

A matrix A of order n is called cyclic if its elements $a(i,j)$ depend only on the difference i-j, and satisfy the condition $a(i+n) = a(i)$. A cyclic matrix is diagonalized by means of the orthogonal transformation

$$B = R^{-1}AR, \tag{3.8}$$

where R is a matrix with elements

$$R(k,\ l) = n^{-1/2} e^{-(2\pi i/n)\, kl}. \tag{3.9}$$

Substituting expression (3.9) into Eq. (3.8), we have

$$\begin{aligned} B(j,\ k) &= \sum_{l,\ s=1}^{n} R^{-1}(j,\ l)\, a(s-l)\, R(s,\ k) \\ &= \frac{1}{n} \sum_{l=1}^{n} e^{(2\pi i/n)(k-j)\, l} \sum_{s=1}^{n} a(s-l)\, e^{(2\pi i/n)(s-l)\, k} \\ &= \delta_{jk} \lambda\left(\frac{2\pi j}{n}\right). \end{aligned} \tag{3.10}$$

Due to the periodicity of $a(k)$ the summation over s is independent of l. Therefore

$$\lambda(\varphi) = \sum_{s=1}^{n} a(s)\, e^{is\varphi}. \tag{3.11}$$

For the determinant of the matrix A we obtain:

$$\det A = \det B = \prod_{j=1}^{n} \lambda\left(\frac{2\pi j}{n}\right). \tag{3.12}$$

The matrices being considered depend on the positions of the points i, j, which, in turn, are given by the pair of coordinates (k_1,k_2). In this case the cyclic condition implies that

$$\begin{aligned} a(\mathbf{j},\ \mathbf{k}) &= a(\mathbf{k} - \mathbf{j}), \\ a(\mathbf{k} + \mathbf{n}) &= a(\mathbf{k}). \end{aligned} \tag{3.13}$$

The components of the vector $\mathbf{n}$ are the lattice dimensions. Eqs. (3.9)–(3.11) take on the form

$$R(\mathbf{k}, \mathbf{l}) = (n_1 n_2)^{-1/2} e^{(2\pi i/n_1)(k_1 l_1)} e^{(2\pi i/n_2)(k_2 l_2)}, \quad (3.14)$$

$$B(\mathbf{j}, \mathbf{k}) = \delta_{j_1 k_1} \delta_{j_2 k_2} \lambda\left(\frac{2\pi j_1}{n_1}, \frac{2\pi j_2}{n_2}\right), \quad (3.15)$$

and

$$\lambda(\varphi) = \sum_{\mathbf{s}} a(\mathbf{s}) e^{i\mathbf{s}\varphi}. \quad (3.16)$$

These are exact expressions for the diagonal matrix elements for vectors φ and $\mathbf{s}$ of any dimensionality. The expression for the determinant of A is, similarly to (3.12):

$$\det A = \prod_{j_1=1}^{n_1} \prod_{j_2=1}^{n_2} \lambda(\varphi_1, \varphi_2). \quad (3.17)$$

In the limit of large n_1, n_2 one can put $\varphi_1 = 2\pi j_1/n_1, \varphi_2 = 2\pi j_2/n_2$ and $d\varphi_1 = 2\pi/n_1, d\varphi_2 = 2\pi/n_2$. The following asymptotic equation is then obtained for $\det A$

$$\frac{1}{n_1 n_2} \ln \det A$$

$$= \frac{1}{n_1 n_2} \sum_{j_1=1}^{n_1} \sum_{j_2=1}^{n_2} \ln \lambda(\varphi_1, \varphi_2)$$

$$= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int \ln \lambda(\varphi_1, \varphi_2)\, d\varphi_1\, d\varphi_2. \quad (3.18)$$

These general prescriptions of the theory of cyclic matrices are sufficient for obtaining Eq. (1.7). Firstly, the matrix T is indeed cyclic due to the periodic boundary conditions. Secondly, the only five nonvanishing elements of $T(\mathbf{s})$ have the following vectors $\mathbf{s}$: (0,0),(1,0),(−1,0),(0,1),(0,−1). We substitute them into expression (3.16) for $\lambda(\varphi_1,\varphi_2)$:

$$\lambda(\varphi_1, \varphi_2) = T(0, 0) + T(1, 0) e^{i\varphi_1} + T(-1, 0) e^{-i\varphi_1} + T(0, 1) e^{i\varphi_2} + T(0, -1) e^{-i\varphi_2}, \quad (3.19)$$

or, taking (3.7) into account

$$\lambda(\varphi_1, \varphi_2) = 2x + 2y - xe^{i\varphi_1} - xe^{-i\varphi_1} - ye^{i\varphi_2} - ye^{-i\varphi_2}. \quad (3.20)$$

Recalling that the sublattice dimensions are $n_1 = M/2$ and $n_2 = N/2$, and using Eq. (3.18), we obtain[19]:

$$\ln \det T = \frac{MN}{4} \frac{1}{(2\pi)^2} \int_0^{2\pi} \int \ln (2x + 2y - 2x \cos \varphi_1 - 2y \cos \varphi_2)\, d\varphi_1\, d\varphi_2. \quad (3.21)$$

The asymptotic expressions for large M and N coincide for the determinant and the algebraic complement, therefore expression (3.21) gives $S(x,y)$. Relationship (3.6) is then transformed to the final result (1.7):

$$\ln \Lambda(x, y) = \frac{MN}{4\pi^2} \int_0^{\pi} \int \ln 2 (x^2 + y^2 - x^2 \cos \varphi_1 - y^2 \cos \varphi_2)\, d\varphi_1\, d\varphi_2. \quad (3.22)$$

The number of dimer coverages F is obtained from equality (1.2).

Thus, in the case of a square lattice we have verified that the solution of the dimer problem follows directly from the Kirchhoff theorem. One can find several more lattices with the same simple connection between dimer coverages and cores. One must not, however, overstate the universality of the method: for example, for the lattice illustrated in Fig. 2 the construction described is no longer possible. The advantages of reducing the dimer problem to core enumeration are fully apparent only in the three-dimensional case, to whose treatment we now turn.

4. DIMERS ON THREE-DIMENSIONAL LATTICES

The idea of applying the Kirchhoff theorem to the three-dimensional dimer problem is clear: the validity of the equations for the number of cores is independent of the dimensionality, and if we find cores which uniquely determine dense packing, their enumeration encounters no difficulty. The question consists only of whether there exist such cores for three-dimensional lattices. The answer to it is not clear in advance, since the simple arguments of the preceding Section are substantially based on the lattice being plane. We show below that there exists at least one lattice, close to the diamond structure, for which the matrix theorem gives a generating function of dense packing.

Consider a simple cubic lattice, contained within a parallelepiped with dimensions $N_1 \times N_2 \times N_3$. The lattice is formed by points with integer coordinates (k_1,k_2,k_3), taking on the values $1 \leqslant k_i \leqslant N_i, i = 1,2,3$. The reduced coordinates of the points are denoted by $[K_1,K_2,K_3]$, defined as in Sec. 3:

$$K_i = k_i \pmod 2, \quad i = 1, 2, 3. \quad (4.1)$$

We call the set of points with the reduced coordinates [0,0,0] sublattice A, and the set of points with coordinates [1,1,1]—sublattice B. Choose again an arbitrary dense packing of dimers. We provide each of the dimers situated on the sites of sublattice A or B with an arrow, directed from the end situated on a site of the sublattice towards the other end. From each site of sublattice A we trace a path to an adjacent site of A, indicated by the arrow. The same is done in sublattice B.

Two systems of directed paths, G_a and G_b, have been generated on the sublattices A and B. Unlike the two-dimensional case, we cannot state that all G_a and G_b are dimers, since in the three-dimensional case there are no geometric restrictions on cycle formation. In what follows we shall find a way of getting rid of cycles, and for the time being consider only such G_a and G_b, which form core trees on the sublattices A and B. Two such cores occupy half the sites of the original lattice. The question arises, how many methods exist of covering the remaining points by dimers? The answer to this question can appear to be somewhat unexpected. For any core configurations there is exactly one method of bringing the lattice up to dense packing. The full proof of this fact was given in Ref. 20. Here we give only its outline.

For two given cores on sublattices A and B we determine a new graph G, whose vertices are points not belonging to cores, and whose edges are connections between adjacent points. We construct a square area of size 2×2 with sites at points of sublattice A. If the site at the center of the area is occupied by a core, we paint it dark. An area with a free center is considered white. Consider the set of all white areas. These areas cannot delimit a closed volume, since then

there would be a cutoff portion of the core B, which is by definition connected. Then the set of white areas has a boundary, a set of lines traced over all sides of the white areas adjacent to three dark ones. On this boundary there must be found at least one point of G with degree unity. If the degree of the point is higher than unity, then the side on which this point is found does not belong to the boundary. If the degree of all points on the boundary is zero, the whole boundary belongs to the core B. The white areas, however, form a nonclosed region, therefore one can trace a closed line along its boundary, which contradicts the definition of a core.

We have proved that in the graph G there is at least one point with degree unity. This and a point adjacent to it can be covered uniquely by a dimer. There remains a graph G', which for the same reasons contains at least one point with degree unity. Continuing this construction, we uniquely cover the whole graph G by dimers.

An important consequence immediately follows from the fact that has been proved. Let f be the number of all cores on sublattice A (equal, by symmetry, to the number of cores on sublattice B). Obviously, the points belonging to cores are uniquely covered by dimers. The points not belonging to cores are also uniquely covered. The cores on the sublattices A and B are independent. Therefore, the following inequality is valid for the number of all possible dimer coverages F

$$F \geqslant f^2. \tag{4.2}$$

Unaccounted remain those dimer packings for which at least one closed path is generated on the sublattices A and B. The estimate (4.2) gives the lower bound on molecular freedom of a dimer on a cubic lattice. We proceed to find its numerical value.

The matrix T for sublattices A and B differs from the matrix (3.7) only in that there appear the additional elements $T_{ij} = -z$ for points i and j adjacent in the direction of the z-axis, while the diagonal elements are replaced by $(2x + 2y + 2z)$. We substitute the values of the nonvanishing matrix elements in Eq. (3.16):

$$\lambda(\varphi_1, \varphi_2, \varphi_3) = 2x + 2y + 2z - 2x\cos\varphi_1 - 2y\cos\varphi_2 - 2z\cos\varphi_3. \tag{4.3}$$

Arguing exactly as in the two-dimensional case, we hence obtain an expression for the core generating function

$$S(x, y, z) = \exp\left[\frac{N_1N_2N_3}{8\pi^3}\int_0^{\pi}\int\int \ln 2(x + y + z - x\cos\varphi_1 - y\cos\varphi_2 - z\cos\varphi_3)\,d\varphi_1\,d\varphi_2\,d\varphi_3\right]. \tag{4.4}$$

Recalling that

$$f = S(1, 1, 1), \tag{4.5}$$

we obtain from inequality (4.2) and from the definition of the molecular freedom (1.5):

$$\frac{1}{2}\ln\varphi \geqslant \frac{1}{4\pi^3}\int_0^{\pi}\int\int d\varphi_1\,d\varphi_2\,d\varphi_3 \ln\left(4\sum_{j=1}^{3}\sin^2\varphi_j\right) = 0.418347\ldots \tag{4.6}$$

This is the well-known Hammersley estimate.[21] It is quite close to the presently accepted more reliable value of .446, calculated by a series method.[22] The high accuracy of the estimate shows, by the way, that the contribution of dimer coverages with closed paths on the sublattices is relatively small.

We turn now to the main purpose of this section, the derivation of equations for the partition function of dimers on a three-dimensional lattice. We already saw above that on a cubic lattice there is no natural prohibition on formation of cycles on the sublattices A and B. We introduce this restriction as follows.

We alter the system of dimer weights on a cubic lattice. If the dimer has a weight x (or y), is located on a site of the sublattice A, and is oriented relative to this site in the positive direction of the x (or y) axis, we replace this weight by x' (or y'). If the dimer has a weight x (or y), is located on a site of sublattice B, and is oriented relative to it in the negative direction of the x (or y) axis, we also replace this weight by x' (or y'). The remaining weights remain unchanged. We now set $x' = y' = 0$, i.e., in other words, we remove from the lattice all edges emerging from A sites in the negative direction of the x and y axes, and all edges emerging from B sites in the positive x and y directions. The elementary unit cell of the lattice obtained is illustrated in Fig. 8. The white circles denote sites of sublattice A, and the dark ones—sites of sublattice B. The dashes denote the discarded edges of the original cubic lattice. A lattice of the diamond type (more accurately, a lattice topologically equivalent to it with coordination number 4) is obtained if in addition to the discarded edges we remove from each elementary unit cell the edges (2,7), (3.7), (4,6), and (4,8). In such cases we say that the diamond lattice is decorated by additional edges.

We now examine how the paths appear on the sublattices A and B. Any path from an A site has four possible extensions, and contains not a single portion, directed in the positive direction of the x and y axes. Consequently, the path system on the sublattice does not contain a single closed cycle, and is a core tree. For the same reason there are no cycles on the B sublattice. The cores on the new lattice are a part of the set of all cores on a cubic lattice, and therefore, for points not belonging to cores there exists, according to the property proved, a unique dimer coverage. The dimer partition function is then obtained from the generating function of the cores.

If the sites of sublattices A and B have n_x, n_y, and n_z dimers with weights x, y, and z, arguments entirely similar to the discussion in Sec. 3 show that there exist additional n_x, n_y, and n_z dimers with corresponding weights.

We denote by $S_D(x,y,z)$ the core generating function on one of the sublattices of the decorated diamond lattice. It follows from the discussion above that the dimer partition function on this lattice $\lambda_D(x,y,z)$ is

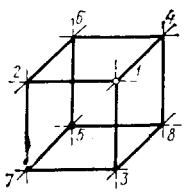

FIG. 8. Decorated diamond lattice. The light circle is a site of sublattice A, and the dark one—a site of sublattice B. The dashed lines denote discarded edges of the cubic lattice.

$$\Lambda_D(x, y, z) = S_D^3(x^2, y^2, z^2). \quad (4.7)$$

To calculate $S_D(x,y,z)$ we find the matrix T on sublattice A. It is clear from the construction that the nonvanishing elements are the following elements $T(\mathbf{s})$ of this cyclic matrix: $T(0,0,0) = x + y + 2z$, $T(-1,0,0) = x$, $T(0,-1,0) = y$, $T(0,0,1) = z$, and $T(0,0,-1) = z$. Substituting them into Eq. (3.16) gives

$$\lambda(\varphi_1, \varphi_2, \varphi_3) = x + y + 2z - xe^{-i\varphi_1} - ye^{-i\varphi_2} - 2z\cos\varphi_3, \quad (4.8)$$

whence, performing standard operations, we obtain

$$S(x, y, z) = \exp\left[\frac{N_1N_2N_3}{8\pi^3}\int_0^{\pi}\int\int \ln(x + y + 2z - xe^{-i\varphi_1} - ye^{-i\varphi_2} - 2z\cos\varphi_3)\, d\varphi_1\, d\varphi_2\, d\varphi_3\right]. \quad (4.9)$$

The final form of the partition function follows from relation (4.7):

$$\Lambda_D(x, y, z) = \exp\left[\frac{N_1N_2N_3}{4\pi^3}\int_0^{\pi}\int\int \ln R(\varphi_1, \varphi_2, \varphi_3)\, d\varphi_1\, d\varphi_2\, d\varphi_3\right], \quad (4.10)$$

where

$$\begin{aligned} R(\varphi_1, \varphi_2, \varphi_3) = {} & 2x^4(1 + \cos\varphi_1) + 2y^4(1 + \cos\varphi_2) + 4z^4(1 + \cos\varphi_3)^2 \\ & + 2x^2y^2(1 + \cos\varphi_1 + \cos\varphi_2 + \cos(\varphi_1 - \varphi_2)) \\ & + 2x^2z^2(1 + \cos\varphi_1)(1 + \cos\varphi_3) \\ & + 4yz(1 + \cos\varphi_2)(1 + \cos\varphi_3). \end{aligned} \quad (4.11)$$

Setting $x = y = z = 1$, we find the value of the molecular freedom φ from Eqs. (4.10) and (1.5). Numerical integration in (4.10) gives:

$$\varphi = 1.97526. \quad (4.12)$$

In the Bethe approximation[12] for a cubic lattice $\varphi = 2.41$, while for the diamond lattice $\varphi = 1.68$. As could be expected, the molecular freedom of the decorated diamond lattice lies between these values.

It remains to consider the important problem of phase transitions in dimer models. Both partition functions (1.7) and (4.10) obtained above are analytic for all positive values of their arguments, and, consequently, give no phase transition. It can be noted that the expressions under the logarithm sign in the integrals (1.7) and (4.10) always vanish at the minimum point in the variable of integration, unlike, say, in the Ising model, in which this occurs only at the critical point. This comment motivated Kasteleyn[23] to state that the model of dimers on a square lattice is equivalent to the Ising model at the critical point. This statement is, possibly, also valid in the three-dimensional case.

The absence of phase transitions in the models considered implies that ordering of dimers takes place continuously. What must be changed in the model, so that phase transitions occur in it? There exists so far no general answer to this question, but comparison of the different known models

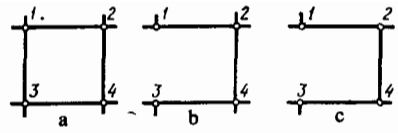

FIG. 9 a) Square lattice, b) decorated hexagonal lattice, c) hexagonal lattice.

makes it possible to draw some conclusions. The first example of a dimer model with a phase transition is the lattice in Fig. 2, equivalent to the Ising model. As is well known, the model has a logarithmic divergence of the specific heat at the critical point. Figure 9 shows four sites of a square (a), decorated hexagonal (b), and hexagonal (c) lattices. The partition function of the dimer models in all three lattices is calculated by the Pfaffian method, and it seems that in the first two models there are no phase transitions, while the third partition function gives a critical point with a root singularity in the specific heat. It is seen from these examples that a phase transition occurs when the lattice becomes sufficiently dilute, or, which is the same, when the molecular freedom of the dimer is sufficiently small.

In just the same manner in the three-dimensional case the decorated diamond lattice has no phase transition, while the discarding of excessive edges and its coversion to a pure diamond lattice lead to a phase transition. Its existence can be proved by using, for example, the Peierls contour method,[24] though in this case the nature of the singularity at the critical point remains unclear.

The dimer problem on the three-dimensional lattice shown in Fig. 10 was recently considered in a number of papers.[25–27] In Ref. 25 an expression was found for the partition function with a specific heat jump at the critical point, and it was stated that this result was exact. However, it was shown in Ref. 26 that the specific heat jump occurred as a result of an approximation, similar to the Bethe approximation, and a logarithmic singularity of the specific heat was predicted[27] for this model. If this assumption will be verified, the dimer problem will be the first model with short-range action, for which critical behavior is exactly known in the three-dimensional case.

CONCLUSIONS

The discussion given above must not be perceived as an attempt of dating the solution of the dimer problem to the

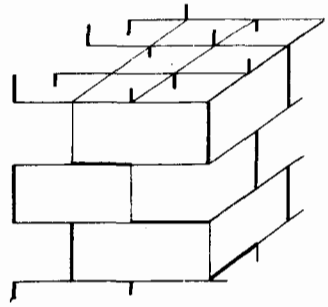

FIG. 10. Three-dimensional dimer model with a phase transition.

nineteenth century. In this connection the moral suggests itself that each result has its own time. From the point of view of pre-Gibbs physics the dimer problem is no more than an amusing puzzle. Moreover, its solution by means of Pfaffians led to the creation of a beautiful and general method, making it possible to solve any plane dimer problem, not necessarily reducible to core enumeration.

It is of greater significance that the Kirchhoff theorem allows to make headway in solving three-dimensional problems, where the Pfaffian method does not work, or, at least, it is not clear how to apply it. Here it is necessary to note that the usefulness of these calculations is strongly reduced due to the analyticity of the core generating function, which leads to absence of a phase transition in all models thus solved. The only practical application of the exact results obtained remains the checking with their aid of the various approximate methods and computational algorithms in the three-dimensional case.

It is currently difficult to predict which of the three-dimensional dimer models is most promising for further study. Some optimism is evoked by the success in the study of phase transitions in the model mentioned at the end of Sec. 4. This model is also interesting in that the structure of the excited ground state in it recalls the vortex structure in superfluid He^4, while attempts of a rigorous proof of the logarithmic singularity at the critical point[28] have additional physical justification.

Besides the dimer problem, the Kirchhoff theorem is naturally applicable to the theory of branching polymers,[19] if the lattice pattern is used, and the polymer is identified with the core of the given lattice. Less obvious is the connection between the Kirchhoff theorem and the limit $n \to 0$ in the n-component Potts model, as was established in Ref. 29 (see also the review of Ref. 30).

The examples provided show that the Kirchhoff theorem is a strong combinatorical statement, which in many cases is equivalent to complicated computational methods of contemporary statistical physics.

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