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The Statistics of Dimers on a Three-Dimensional Lattice. I. An Exactly Solvable Model

V. B. Priezzhev[1]

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A three-dimensional lattice model is proposed for which the constant λ occurring in the dimer problem can be evaluated exactly.

KEY WORDS: Dimers; closed paths; lattice graph; principle of inclusion and exclusion.

1. INTRODUCTION

The three-dimensional dimer problem, one of the classical unsolved problems of lattice statistics, can be formulated as follows. An N-brick is a three-dimensional parallelopiped of volume N with sides whose lengths l_1, l_2, l_3, are integers. A dimer is a 2-brick. The problem is to determine the number of ways of dissecting an N-brick into dimers. Denote this number by f_l, where $l = (l_1, l_2, l_3)$. It is known[1] that if $l_i \to \infty$ $(i = 1, 2, 3)$, then $N^{-1} \ln f_l$ tends to a finite limit λ. The exact value of λ is not known.

The early paper by Fowler and Rushbrooke[2] gave the estimate $\lambda = 0.43$ together with the rigorous bounds

$$0 \leqslant \lambda \leqslant \tfrac{1}{2} \ln 3 \tag{1}$$

Since the number of ways of dissecting an N-brick is a nondecreasing function of the dimensionality, the exact solution of the two-dimensional dimer problem[3,4] yields

$$G/\pi \leqslant \lambda \tag{2}$$

where $G = 0.915965\ldots$ (Catalan's constant).

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[1] Joint Institute for Nuclear Research, Laboratory of Theoretical Physics, Dubna.

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In 1968 Hammersley[5] obtained the lower bound

$$\frac{1}{4\pi^3}\int_0^\pi d\theta_1\int_0^\pi d\theta_2\int_0^\pi d\theta_3 \ln\left(\sum_{i=1}^{3}\sin^2\theta_i\right) \leqslant \lambda \tag{3}$$

In 1978 Minc[6] improved the Fowler–Rushbrooke upper bound (1):

$$\lambda \leqslant \tfrac{1}{12}\ln 6! \tag{4}$$

Thus, from (3) and (4) we have

$$0.418347 \leqslant \lambda \leqslant 0.548270$$

In this paper the three-dimensional lattice model is proposed for which the exact value of λ is equal to the Hammersley lower bound. In the next paper (Part II) we shall use the proposed model to obtain an improved lower bound for the three-dimensional dimer problem.

2. MODEL

The N-brick is the union of N unit cubes; let L be the lattice consisting of centers of these cubes. We denote the lattice points by (x_1, x_2, x_3), $0 \leqslant x_i \leqslant l_i$ $(i = 1,2,3)$. By reduced coordinates of the point (x_1, x_2, x_3) we understand the integers $[k_1, k_2, k_3]$ defined by

$$k_i = x_i \ (\mathrm{mod}\ 2) \qquad (i = 1,2,3) \tag{5}$$

We say that the set of lattice points having reduced coordinates $[0,0,0]$ is a sublattice A_0, and the set of lattice points having reduced coordinates $[1,1,1]$ is a sublattice B_0. Consider an arbitrary dissection of the N-brick. Let p_1 and p_2 be a pair of neighboring points of the sublattice A_0. We say that for any pair $p_1 p_2$ a given dissection generates a path from p_1 to p_2 if the dimer containing p_1 adjoins the unit cube containing p_2. A collection of paths of the form $p_1p_2, p_2p_3, \ldots, p_{n-1}p_n$ is a path from p_1 to p_n.

If in the collection of paths $p_1p_2, p_2p_3, \ldots, p_{n-1}p_n$ the point p_1 coincides with the point p_n, the path p_1p_n is closed. Similarly, we define a path on the sublattice B_0.

Now, we can define our model as follows. Consider all dissections of the N-brick generating no closed path on the sublattices A_0 and B_0. Denote the number of such dissections by f_l^*. The problem consists in finding a limit

$$\lambda^* = \lim_{l_i\to\infty}\frac{1}{N}\ln f_l^* \qquad (i = 1,2,3) \tag{6}$$

In the next section we show that in order to evaluate λ^*, it is sufficient to enumerate dimer configurations containing points of one sublattice only. In Section 4 we shall reduce this problem to the solved problem concerning a number of random walks returning to the original point.

3. FACTORIZATION OF f_l^*

The sublattices A_0 and B_0 contain $N/4$ points of the lattice L. We divide the remainder of lattice points ($3N/4$ points) into two sets A_1 and B_1. A sublattice A_1 is the set of points with reduced coordinates [1,0,0] or [0,1,0] or [0,0,1]; a sublattice B_1 is the set of points with reduced coordinates [1,1,0] or [1,0,1] or [0,1,1].

In every dissection of the N-brick there exist dimers of three sorts: (i) dimers containing points of the set A_0; (ii) dimers containing points of the set B_0; (iii) dimers containing none of the points of the sets A_0 and B_0.

Let us try to dissect the N-brick into dimers in the following manner. First we eliminate from the N-brick the dimers of the sort (i) until in the N-brick there remain no points of the sublattice A_0. Then we eliminate the dimers of the sort (ii) until in the N-brick there remain no points of the sublattice B_0. These procedures are independent because any dimer of the sort (i) intersects none of dimers of the sort (ii). The question arises whether one can always dissect the remaining volume into dimers. The situation here is described by the following theorem.

Theorem 1. Let $D(A_0)$ and $D(B_0)$ be configurations of dimers of the sort (i) and (ii) that contain all points of the sublattices A_0 and B_0 and do not generate a single closed path. Then, the volume resulting from elimination of all dimers belonging to $D(A_0)$ and $D(B_0)$ out of the N-brick can be dissected into dimers in the unique manner.

Before proceeding to prove Theorem 1 we shall point out its corollary.

The numbers of all possible configurations $D(A_0)$ and $D(B_0)$ are obviously equal. Denote them by φ_l. It follows from Theorem 1 that the required number of dissections of the N-brick is

$$f_l^* = (\varphi_l)^2 \tag{7}$$

Let $D(A_0)$ and $D(B_0)$ be two arbitrary dimer configurations satisfying the requirements of Theorem 1. Consider a volume V resulting from the elimination of all dimers belonging to $D(A_0)$ and $D(B_0)$ out of the N-brick. Denote by L_V the subset of the lattice points belonging to V. We denote by G the graph whose vertices are the elements L_V and whose arcs are the unit segments that join all adjacent vertices. As usual, we call the number of arcs incident to the given vertex p the degree of this vertex (denoted by $\deg p$). Every vertex of G belongs to the sublattice A_1 or to the sublattice B_1. Nearest neighbors of a vertex belonging to A_1 (B_1) are vertices belonging to B_1 (A_1).

Let $a_1 \in A_1$ be a vertex of G. If $\deg a_1 > 2$, eliminate from G all arcs incident to a_1 except for two arbitrarily chosen arcs r_1 and r_1'. From the remaining graph choose the connected component $G(a_1; r_1, r_1')$ containing the vertex a_1. Further, let $a_2 \in A_1$ be some vertex of $G(a_1; r_1, r_1')$ having a common adjacent vertex $b \in B_1$ with a_1. If $\deg a_2 > 2$, choose again two arcs r_2 and r_2' from arcs incident to a_2 and eliminate remaining ones. The connected component of the resulting graph containing a_1, a_2 is the graph $G(a_1; r_1, r_1' \mid a_2; r_2, r_2')$. Proceeding with this procedure and choosing at an ith step a vertex $a_i \in A_1$ having a common adjacent vertex with at least one of the sites $a_1, a_2, \ldots, a_{i-1}$, we obtain the subgraph $G(a_1; r_1, r_1' | \cdots | a_k; r_k, r_k')$ of the graph G containing none of the vertices $a_j \in A_1$ with $\deg a_j > 2$. We say that this subgraph is an A_1 subgraph. If G has no vertices $a_j \in A_1$ with $\deg a_j > 2$, it coincides with its A_1 subgraph.

Similarly, we construct a B_1 subgraph. The proof of Theorem 1 is based on the following lemma:

Lemma. Every A_1 subgraph of G contains at least one vertex $a \in A_1$ with $\deg a = 1$ and every B_1 subgraph of G contains at least one vertex $b \in B_l$ with $\deg b = 1$.

Proof. Suppose the contrary, i.e., there exists an A_1 subgraph of G such that all its vertices a_i belonging to A_1 have $\deg a_i = 2$. For every vertex $b_i \in B_1$ of this A_1 subgraph we build a 2×2 square (plaquette) with the center in b_i and the vertices belonging to the sublattice A_0 (except those which do not belong to the N brick). A side of each plaquette either is occupied by the vertex a_j of the A_1 subgraph ($a_j \in A_1$, $\deg a_j = 2$) or is free, i.e., does not contain vertices of the A_1 subgraph. In the first case this side is common for two or more adjacent plaquettes.

A collection of plaquettes cannot encompass any part V' of volume V since otherwise the configuration $D(B_0)$ generates paths enclosed in V'. These paths have no end points (only one path emanates from every point of sublattice B_0 enclosed in V') and therefore contain at least one return point. We arrive at a contradiction with the condition of Theorem 1.

If the collection of plaquettes does not encompass a closed volume, there exists at least one free closed boundary, i.e., a sequence of plaquette sides not containing points of the A_1 subgraph and forming a closed contour Γ.

A side of a plaquette cannot be occupied by a vertex belonging to G and not belonging to the A_1 subgraph. Indeed by definition of G there would be an arc connecting this vertex with the center of the plaquette and, by construction of the A_1 subgraph, only those arcs are eliminated from G which are incident to the vertices of the A_1 subgraph.

Let $\gamma_1, \gamma_2, \ldots, \gamma_{2n-1}, \gamma_{2n}$ be a sequence of lattice points belonging to Γ such that any two successive points in the sequence are neighbors. The first and last points of this sequence are neighbors, too. If point γ_i belongs to the sublattice A_0 (A_1), then the point γ_{i+1} belongs to the sublattice A_1

(A_0). The pairs of elementary cubes corresponding to the pairs (γ_1, γ_2), $(\gamma_3, \gamma_4), \ldots, (\gamma_{2n-1}, \gamma_{2n})$ form the sequence of dimers. These dimers belong to the configuration $D(A_0)$ and generate a closed path, which is a contradiction.

If Γ does not entirely belong to the N-brick, its points belonging to the sublattice A_1 exceed in number those for the sublattice A_0. Then the part of Γ lying inside of the N-brick cannot be formed by $D(A_0)$, which is also a contradiction.

Similarly, we prove the existence of vertex $b \in B_1$ with $\deg b = 1$ in every B_1 subgraph.

Corollary. The graph G contains at least one vertex $a \in A_1$ with $\deg a = 1$ and one vertex $b \in B_1$ with $\deg b = 1$.

Note that every dissection of the volume V into dimers corresponds to a dissection of the graph G into nonintersecting pairs of adjacent vertices. For the proof of Theorem 1 it is sufficient to find such a way of successive elimination of adjacent vertices and arcs from G that after each step a remaining graph obeys the conditions of Theorem 1. Indeed, then every remaining graph has at least two vertices a and b such that $a \in A_1$, $b \in B_1$, $\deg a = 1$, $\deg b = 1$, and we can take as the next pair the vertex a together with its neighbor. At the end, there remains a unique pair of adjacent vertices $a_i \in A_1$, and $b_i \in B_1$ which corresponds to the last dimer.

Proof of Theorem 1. Let Lemma 1 be valid for the connected graph $G^{(n)}$ obtained from the graph G by elimination of n pairs of adjacent vertices (the generalization to the case of several connected components is straightforward). Consider an arbitrarily chosen vertex a_0 of the graph G such that $a_0 \in A_1$, $\deg a_0 = 1$ and a vertex $b_0 \in B_1$ belonging to G and adjacent to a_0. Let $\deg b_0 > 1$ (in case $\deg b_0 = 1$ $G^{(n)}$ is a pair of adjacent vertices $a_0 b_0$ and dissection of the graph G is completed).

Eliminate the pair $a_0 b_0$ from $G^{(n)}$ together with arcs incident to them. We obtain a graph $G^{(n+1)}$. Every B_1 subgraph of $G^{(n+1)}$ contains at least one vertex $b \in B_1$ with $\deg b = 1$ since such a vertex is in every B_1 subgraph of $G^{(n)}$ and elimination of the pair $a_0 b_0$ does not reduce the number of vertices b_i of the sublattice B_1 with $\deg b_i = 1$.

Now we shall prove the existence of the vertex a ($a \in A_1$, $\deg a = 1$) in every A_1 subgraph of $G^{(n+1)}$. In the graph $G^{(n)}$ $\deg b_0 > 1$, so besides a_0 there are not less than one (and not more than three) vertices of A_1 sublattice adjacent to b_0. Denote them by a_k ($1 \leqslant k \leqslant 3$). Note that in the graph $G^{(n)}$ $\deg a_k > 1$ for all a_k. Indeed, in case $\deg a_k = 1$ the B_1 subgraph (with vertices a_k, b_0, a_0 and arcs $a_k b_0, a_0 b_0$) has to exist which has no vertices $b_i \in B_1$ with $\deg b_i = 1$.

If in the graph $G^{(n)}$ $\deg a_k = n_k$, then in the graph $G^{(n+1)}$ $\deg a_k = n_k - 1$, so it is sufficient to consider the case $n_k > 2$ $(1 \leqslant k \leqslant 3)$. In this case one can consider every A_1 subgraph of $G^{(n+1)}$ as the A_1 subgraph of $G^{(n)}$ without arcs $a_k b_0$ $(k = 1, 2, 3)$. But every A_1 subgraph of $G^{(n)}$ has at least one vertex $a \in A_1$ with $\deg a = 1$, therefore such a vertex is in every A_1 subgraph of $G^{(n+1)}$. The theorem is proved. ∎

4. CALCULATION OF φ_l

In the previous section we have defined φ_l as the number of dimer configurations of sort (i) which do not generate a single closed path on the sublattice A_0. Let us formulate in slightly different terms the problem necessary to solve for determining φ_l.

Let $\mathcal{L}$ be a simple cubic lattice of $\mathfrak{N}$ sites. We introduce a new system of graphs. Denote by $\mathcal{G}$ the graph whose vertices are all sites of $\mathcal{L}$. Let $\mathcal{G}$ be an oriented graph such that for every pair of vertices s and s' joined by the edge $D_{ss'}$ directed from s to s' there is an edge $D_{ss'}$ directed from s' to s. An oriented route is defined as a succession of oriented edges (arcs) such that the beginning of the next arc coincides with the end of the preceding one: $D_{i_1 i_2} D_{i_2 i_3} \cdots D_{i_{k-1} i_k}$. To shorten the expressions, we label all pairs $(D_{ss'} D_{s's})$ of oppositely oriented arcs and denote one of the arcs of pair i (it is immaterial, which) by the symbol D_i^+ and the other by D_i^-. Where confusion cannot arise, we shall omit the symbols $\pm$.

In an oriented route the beginning and the end may coincide and it is then said to be cyclic. Any circular permutation of edges of a cyclic route leads to the same route. An oriented route for which there exists a representation in the form $(D_{i_1} D_{i_2} \cdots D_{i_k})^m$, where $m > 1$ is integer, is called a periodic cyclic oriented route. Nonperiodic cyclic oriented routes will simply be called cycles. An elementary cycle is a cycle in which all the vertices are passed through once. We define an elementary subgraph $g \in \mathcal{G}$ as a graph consisting of one or a set of elementary cycles that do not have common vertices.

Now let the lattice $\mathcal{L}$ coincide with the sublattice A_0 so that $\mathfrak{N} = N/8$. In accordance with the above definition φ_l is the number of all subgraphs $g_l \in \mathcal{G}$ which obey the following conditions: (a) g_l contains all vertices of $\mathcal{L}$; (b) every vertex of g_l has one arc leaving it; (c) g_l does not contain single elementary cycles.

The idea of the solution is to enumerate all elementary subgraphs in such a way that each elementary cycle enters into the sum with the "minus" sign. Then, using the inclusion–exclusion combinatorial principle, we can enumerate all subgraphs that do not contain a single elementary cycle.

We introduce a weighted cycle. Ascribe to both arcs D_i^+ and D_i^- the weight $w(i)$ and assume that $w(i) = Z_k$ if arc i is oriented along the axis $e_k (k = 1, 2, 3)$. Define the weight $W(p)$ of the cycle $p = D_{i_1}, D_{i_2}, \ldots, D_{i_k}$ as the product $(-1)w(i_1)w(i_2) \cdots w(i_k)$. Accordingly, the weight of a subgraph g consisting of the elementary cycles $p_1, p_2, \ldots, p_n$ is defined as the product

$$\chi(g) = \prod_{i=1}^{n} W(p_i)$$

We ascribe the weight 1 to the empty subgraph. In Ref. 7 the following theorem was proved:

Theorem 2. The product $\prod_p [1 + W(p)]$ over all possible cycles of the graph $\mathcal{G}$ is equal to the sum $\sum_{g \in \mathcal{G}} \chi(g)$ over all elementary subgraphs of $\mathcal{G}$, including the empty subgraph,

$$\prod_p \left[1 + W(p) \right] = \sum_{g \in \mathcal{G}} \chi(g) \tag{8}$$

To evaluate the right-hand side of (8) we shall use the periodic boundary conditions, i.e., we shall consider the lattice obtained by identifying and joining opposite faces of the original lattice. Equivalence of the two types of the boundary conditions was discussed in Ref. 5.

On the basis of (8), we have

$$\begin{aligned}
\ln \sum_{g \in \mathcal{G}} \chi(g) &= \ln \prod_p \left[1 + W(p) \right] = \ln \prod_p \left\{ 1 - \left[-W(p) \right] \right\} \\
&= -\sum_p \left[\sum_{j=0}^{\infty} \frac{\left[-W(p) \right]^j}{j} \right] \\
&= -\mathfrak{N} \sum_{N_1 + N_2 + N_3 \geqslant 2} \frac{S(N_1, N_2, N_3) Z_1^{N_1} Z_2^{N_2} Z_3^{N_3}}{N_1 + N_2 + N_3}
\end{aligned} \tag{9}$$

where $S(N_1, N_2, N_3)$ is the number of all possible closed paths without restrictions to the periodicity which have N_k arcs oriented along the axis e_k. The last sum in Eq. (9) is multiplied by $\mathfrak{N}$, since a closed path can begin at any site of the lattice $\mathcal{L}$; the denominator $N_1 + N_2 + N_3$ in this sum has arisen because the closed path of length $N_1 + N_2 + N_3$ may have any of the sites contained in it as the first one.

Let $\beta(m_1, m_2, m_3; r_1, r_2, r_3)$ be the sum over all possible paths on the three-dimensional integer lattice $\mathcal{L}$ from the site with coordinates $(0, 0, 0)$ to the site with coordinates (m_1, m_2, m_3), and every path contains r_k steps along e_k. Let $\beta(m_1, m_2, m_3; 0, 0, 0) = \delta_{m_1 0} \delta_{m_2 0} \delta_{m_3 0}$. By definition $S(r_1, r_2, r_3)$

$= \beta(0,0,0;r_1,r_2,r_3)$. The sum $\beta(m_1,m_2,m_3;r_1,r_2,r_3)$ satisfies the recursion relation

$$\begin{aligned}\beta(m_1,m_2,m_3;r_1,r_2,r_3) = \beta(m_1-1,m_2,m_3;r_1-1,r_2,r_3)\\ +\beta(m_1+1,m_2,m_3;r_1-1,r_2,r_3)\\ +\beta(m_1,m_2-1,m_3;r_1,r_2-1,r_3)\\ +\beta(m_1,m_2+1,m_3;r_1,r_2-1,r_3)\\ +\beta(m_1,m_2,m_3-1;r_1,r_2,r_3-1)\\ +\beta(m_1,m_2,m_3+1;r_1,r_2,r_3-1)\end{aligned} \tag{10}$$

We define the Fourier transform of $\beta(m_1,m_2,m_3;r_1,r_2,r_3)$ by the equations

$$\begin{aligned} B(\mathbf{a};\mathbf{r}) &= \frac{1}{\mathfrak{N}}\sum_{m_1=0}^{l_1/2-1}\sum_{m_2=0}^{l_2/2-1}\sum_{m_3=0}^{l_3/2-1}\beta(\mathbf{m};\mathbf{r})\exp\left[-2\pi i\left(\sum_{j=1}^{3}\frac{2a_jm_j}{l_j}\right)\right]\\ \beta(\mathbf{m};\mathbf{r}) &= \sum_{m_1=0}^{l_1/2-1}\sum_{m_2=0}^{l_2/2-1}\sum_{m_3=0}^{l_3/2-1}B(\mathbf{a},\mathbf{r})\exp\left[2\pi i\left(\sum_{j=1}^{3}\frac{2a_jm_j}{l_j}\right)\right]\end{aligned} \tag{11}$$

Introduce the generating functions

$$\begin{aligned} F(\mathbf{a};\mathbf{z}) &= \sum_{r_1\geqslant 0}\sum_{r_2\geqslant 0}\sum_{r_3\geqslant 0}B(\mathbf{a};\mathbf{r})Z_1^{r_1}Z_2^{r_2}Z_3^{r_3}\\ f(\mathbf{m};\mathbf{z}) &= \sum_{r_1\geqslant 0}\sum_{r_2\geqslant 0}\sum_{r_3\geqslant 0}\beta(\mathbf{m};\mathbf{r})Z_1^{r_1}Z_2^{r_2}Z_3^{r_3}\end{aligned} \tag{12}$$

Then on the basis of (10)

$$\begin{aligned} f(m_1,m_2,m_3;Z_1,Z_2,Z_3) = \delta_{m_10}\delta_{m_20}\delta_{m_30} + Z_1 f(m_1-1,m_2,m_3;Z_1,Z_2,Z_3)\\ +Z_1 f(m_1+1,m_2,m_3;Z_1,Z_2,Z_3)\\ +Z_2 f(m_1,m_2-1,m_3;Z_1,Z_2,Z_3)\\ +Z_2 f(m_1,m_2+1,m_3;Z_1,Z_2,Z_3)\\ +Z_3 f(m_1,m_2,m_3-1;Z_1,Z_2,Z_3)\\ +Z_3 f(m_1,m_2,m_3+1;Z_1,Z_2,Z_3)\end{aligned} \tag{13}$$

$$\begin{aligned} F(\mathbf{a},\mathbf{z}) = \frac{1}{\mathfrak{N}} + F(\mathbf{a},\mathbf{z})\bigg[& Z_1\exp\left(-\frac{4\pi i a_1}{l_1}\right) + Z_1\exp\left(\frac{4\pi i a_1}{l_1}\right)\\ & + Z_2\exp\left(-\frac{4\pi i a_2}{l_2}\right) + Z_2\exp\left(\frac{4\pi i a_2}{l_2}\right)\\ & + Z_3\exp\left(-\frac{4\pi i a_3}{l_3}\right) + Z_3\exp\left(\frac{4\pi i a_3}{l_3}\right)\bigg]\end{aligned} \tag{14}$$

whence

$$F(\mathbf{a};\mathbf{z}) = \frac{1/\mathfrak{N}}{1 - R(\mathbf{z})} = \frac{1}{\mathfrak{N}} \sum_{j=0}^{\infty} R^j(\mathbf{z}) \tag{15}$$

where

$$R(\mathbf{z}) = 2 \sum_{j=1}^{3} Z_j \cos \frac{4\pi a_j}{l_j} \tag{16}$$

From Eq. (15) in accordance with (12) we readily obtain

$$\sum_{\substack{r_1, r_2, r_3 \geqslant 0 \\ r_1 + r_2 + r_3 \geqslant 1}} \frac{B(\mathbf{a}, \mathbf{r}) Z_1^{r_1} Z_2^{r_2} Z_3^{r_3}}{r_1 + r_2 + r_3} = \frac{1}{\mathfrak{N}} \sum_{j=0}^{\infty} \frac{R^j(\mathbf{z})}{j} = \frac{1}{\mathfrak{N}} \ln[1 - R(\mathbf{z})] \tag{17}$$

or, using the transformations (11)

$$\sum_{\substack{r_1, r_2, r_3 \geqslant 0 \\ r_1 + r_2 + r_3 \geqslant 1}} \frac{\beta(\mathbf{m}; \mathbf{r}) Z_1^{r_1} Z_2^{r_2} Z_3^{r_3}}{r_1 + r_2 + r_3}$$
$$= -\frac{1}{\mathfrak{N}} \sum_{a_1=0}^{l_1/2-1} \sum_{a_2=0}^{l_2/2-1} \sum_{a_3=0}^{l_3/2-1} \exp\left\{ 2\pi i \left(\sum_{j=1}^{3} \frac{m_j a_j}{l_j} \right) \ln[1 - R(Z)] \right\} \tag{18}$$

For the case of interest to us of a walk returning to the original point, we have

$$\sum_{\substack{r_1, r_2, r_3 \geqslant 0 \\ r_1 + r_2 + r_3 \geqslant 1}} \frac{\beta(\mathbf{0}; \mathbf{r}) Z_1^{r_1} Z_2^{r_2} Z_3^{r_3}}{r_1 + r_2 + r_3} = -\frac{1}{\mathfrak{N}} \sum_{a_1=0}^{l_1/2-1} \sum_{a_2=0}^{l_2/2-1} \sum_{a_3=0}^{l_3/2-1} \ln[1 - R(\mathbf{z})] \tag{19}$$

Taking into account Eq. (9) and the definition of $S(r_1, r_2, r_3)$ we obtain for the sum over all weighted elementary subgraphs $g \in G$ the expression

$$\ln \sum_{g \in \mathcal{G}} \chi(g) = \mathfrak{N} \sum_{r_1 + r_2 + r_3 \geqslant 0} \frac{S(r_1, r_2, r_3) Z_1^{r_1} Z_2^{r_2} Z_3^{r_3}}{r_1 + r_2 + r_3}$$
$$= \sum_{a_1=0}^{l_1/2-1} \sum_{a_2=0}^{l_2/2-1} \sum_{a_3=0}^{l_3/2-1} \ln[1 - R(\mathbf{z})] \tag{20}$$

Consider all subgraphs of $\mathcal{G}$ satisfying the conditions (a) and (b) mentioned above. The total number of such subgraphs containing r_1, r_2, r_3 arcs oriented along e_1, e_2, e_3 is equal to the coefficient of $Z_1^{r_1} Z_2^{r_2} Z_3^{r_3}$ in the expansion of the generating function

$$\psi(Z_1, Z_2, Z_3) = (2Z_1 + 2Z_2 + 2Z_3)^{\mathfrak{N}} \tag{21}$$

To determine φ_l, it is necessary to eliminate from this set the subgraphs containing at least one elementary cycle. Using Eq. (20) we can find an expression for the sum $N(r_1, r_2, r_3)$ of subgraphs that completely consist of cycles. These subgraphs contain r_k arcs oriented along e_k and each subgraph enters into $N(r_1, r_2, r_3)$ with factor $(-1)^m$, where m is the number of elementary cycles in the given graphs. We write Eq. (20) in the form

$$\sum_{g \in \mathcal{G}} \chi(g) = \prod_{a_1=0}^{l_1/2-1} \prod_{a_2=0}^{l_2/2-1} \prod_{a_3=0}^{l_3/2-1} \left[1 + \sum_{j=1}^{3} (Z_j e^{\alpha_j} + Z_j e^{-\alpha_j}) \right] \tag{22}$$

where $\alpha_j = 4\pi i a_j / l_j$; $(1 \leqslant j \leqslant 3)$. It follows from the definition of $\chi(g)$ that the sum $N(r_1, r_2, r_3)$ is equal to the coefficient of $Z_1^{r_1} Z_2^{r_2} Z_3^{r_3}$ in the expansion of the right-hand side of Eq. (22).

Combine (21) and (22) into the form

$$\prod_{a_1=0}^{l_1/2-1} \prod_{a_2=0}^{l_2/2-1} \prod_{a_3=0}^{l_3/2-1} \sum_{j=1}^{3} (2\tilde{Z}_j + Z_j e^{\alpha_j} + Z_j e^{-\alpha_j}) \tag{23}$$

and consider the coefficient of the term $(\tilde{Z}_1^{r_1'} \tilde{Z}_2^{r_2'} \tilde{Z}_3^{r_3'}) \times (Z_1^{r_1} Z_2^{r_2} Z_3^{r_3})$ where $r_1 + r_1' = R_1$, $r_2 + r_2' = R_2$, $r_3 + r_3' = R_3$, $R_1 + R_2 + R_3 = \mathfrak{N}$. This coefficient is equal to the sum $N(r_1, r_2, r_3 | r_1', r_2', r_3')$ over all graphs in which $r_1 + r_2 + r_3$ arcs are combined into cycles, each of them entering into the sum with the factor (-1), and the remaining $r_1 + r_2' + r_3'$ arcs are arranged arbitrarily. Then the coefficient of $Z_1^{R_1} Z_2^{R_2} Z_3^{R_3}$ in the expansion of the expression

$$\prod_{a_1=0}^{l_1/2-1} \prod_{a_2=0}^{l_2/2-1} \prod_{a_3=0}^{l_3/2-1} \sum_{j=1}^{3} (2Z_j + Z_j e^{\alpha_j} + Z_j e^{-\alpha_j}) \tag{24}$$

is equal to

$$\sum_{r_1 \geqslant 0}^{R_1} \sum_{r_2 \geqslant 0}^{R_2} \sum_{r_3 \geqslant 0}^{R_3} N(r_1, r_2, r_3 | R_1 - r_1, R_2 - r_2, R_3 - r_3) \tag{25}$$

We now have the necessary material that enables us, using the inclusion–exclusion principle, to obtain an expression for φ_l. Suppose there are N elements and a certain number of properties $p(1), p(2), \ldots, p(n)$. Suppose further that N_i is the number of elements with property $P(i)$ and, generally, $N_{i_1 i_2 \ldots i_r}$ is the number of elements with properties $p(i_1), p(i_2), \ldots, p(i_r)$. Then the number of elements $N(0)$ that have none of these properties is given by

$$N(0) = N - \sum_i N_i + \sum_{i_1 < i_2} N_{i_1 i_2} - \cdots + (-1)^s \sum_{i_1 < i_2 < \cdots < i_s} N_{i_1 i_2 \cdots i_s} + \cdots + (-1)^n N_{12 \cdots n} \tag{26}$$

To solve the problem, we label by $1, 2, \ldots, n$ all possible elementary cycles on the lattice under consideration. Consider subgraphs $\mathcal{G}_{R_1R_2R_3} \in \mathcal{G}$ such that from every point of the lattice $\mathcal{L}$ one arc emanates, the number of arcs oriented along e_i is R_i ($R_1 + R_2 + R_3 = \mathfrak{N}$). We shall assume that $\mathcal{G}_{R_1R_2R_3}$ has the property $p(i)$ if the elementary cycle i is its subgraph. Let $N_{i_1i_2\ldots i_r}$ be the number of graphs $\mathcal{G}_{R_1R_2R_3}$ whose subgraphs are the cycles i_1, $i_2, \ldots, i_r$. Then the total number of graphs $\mathcal{G}_{R_1R_2R_3}$ not containing any cycle is determined by the right-hand side of Eq. (26). But in accordance with the definition the sum (25) is exactly equal to the right-hand side of (26) since it contains all terms $N_{i_1i_2\cdots i_r}$ with the correct signs.

Therefore the partition function for the subgraphs $\mathcal{G}_{R_1R_2R_3}$ not containing any elementary cycle is

$$\begin{aligned}\varphi_l(Z_1, Z_2, Z_3) &= \sum_{R_1\geqslant 0}\sum_{R_2\geqslant 0}\sum_{R_3\geqslant 0} Z_1^{R_1}Z_2^{R_2}Z_3^{R_3} \\ &\quad\times \sum_{r_1\geqslant 0}\sum_{r_2\geqslant 0}\sum_{r_3\geqslant 0} N(r_1, r_2, r_3 \,|\, R_1 - r_1, R_2 - r_2, R_3 - r_3) \\ &= \prod_{a_1=0}^{l_1/2-1}\prod_{a_2=0}^{l_2/2-1}\prod_{a_3=0}^{l_3/2-1}\sum_{j=1}^{3}\left(2Z_j + 2Z_j\cos\frac{4\pi a_j}{l_j}\right) \end{aligned} \tag{27}$$

The required quantity φ_l is

$$\varphi_l = \varphi_l(1,1,1) = \exp\left[\sum_{a_1=0}^{l_1/2-1}\sum_{a_2=0}^{l_2/2-1}\sum_{a_3=0}^{l_3/2-1}\ln\left(4\sum_{j=1}^{3}\sin^2\frac{2\pi a_j}{l_j}\right)\right] \tag{28}$$

when $l_1, l_2, l_3 \to \infty$. The right-hand side of (28) tends to the triple integral, and using Eqs. (6) and (7) we get

$$\lambda^* = \lim_{l_i\to\infty}\frac{1}{N}\ln\varphi_l^2 = \frac{1}{4\pi^3}\int_0^{\pi}d\theta_1\int_0^{\pi}d\theta_2\int_0^{\pi}d\theta_3\ln\left(4\sum_{j=1}^{3}\sin^2\theta_j\right) \tag{29}$$

Thus, the three-dimensional dimer problem becomes solvable if we add to the standard dimer-problem requirements the additional one that there be no elementary cycles on the sublattices of the original lattice.

The comparison of the value $\lambda^* = 0.418$ with the series-expansion estimate $\lambda = 0.446$[8] shows that the contribution to λ from the forbidden configuration is relatively small. In the next paper a part of this contribution will be taken into account to improve the lower bound for the three-dimensional dimer problem.

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