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PROOF OF THE GENERALIZED EXPRESSIONS FOR THE NUMBER OF PERFECT MATCHINGS OF POLYCUBE GRAPHS

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Abstract

The number of perfect matchings for the linear $2 \times 2 \times n$ cubic lattice was analytically derived by diagonalizing the skew-symmetric $4n \times 4n$ determinant, whose non-zero off-diagonal elements are either ± 1 or $\pm i$ (pure imaginary number). The basic formulation involving the matrix manipulation follows that of Kasteleyn, but the result obtained in this paper is the first example of the analytical solution for a special case of the three-dimensional Ising model.

1. Introduction

A Kekulé structure for a given unsaturated hydrocarbon molecule is in graph theory called a perfect matching pattern for the graph corresponding to the carbon atom skeleton of that molecule [1]. All the component N $(=2m)$ vertices of the graph are spanned by a set of m disjoint edges in a perfect matching pattern. Both the adsorption of dimer molecules as oxygen on metal surfaces composed of two-dimensional periodic arrays of metal atoms (dimer statistics) and the nearest-neighbor spin interaction in antiferromagnetic crystals (Ising model) lead to identical counting problems of maximum matching for a given graph for deriving the partition function [2]. Thus, an efficient algorithm for obtaining the maximum matching number can contribute to various fields of science in addition to its mathematical importance.

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In 1961, Kasteleyn [3] and Temperley [4] independently derived the rigorous expression (1) for the number of perfect matchings on the $m \times n$ square lattice by the use of skew-symmetric matrices and a combinatorial technique:

$$K(2m \times 2n) = 2^{2mn} \prod_{k=1}^{m} \prod_{l=1}^{n} \left[\cos^2\left(\frac{k\pi}{2m+1}\right) + \cos^2\left(\frac{l\pi}{2n+1}\right)\right], \tag{1}$$

where the symbol K signifies the perfect matching number [5–8]. One of the present authors (HH) derived recursion formulas for the number of perfect matchings for several series of polyomino graphs [1,2] by using an operator technique [9] such as

$$K(2 \times 2 \times n) = K_n = 3K_{n-1} + 3K_{n-2} - K_{n-3}, \tag{2}$$

and

$$K(2 \times 3 \times n) = K_n = 6K_{n-1} + 21K_{n-2} - 42K_{n-3} - 89K_{n-4} + 68K_{n-5}$$
$$+ 89K_{n-6} - 42K_{n-7} - 21K_{n-8} + 6K_{n-9} + K_{n-10}. \tag{3}$$

Equation (2) was later confirmed by Hock and McQuistan [10]. For the former series of graphs, the following expression was found to hold from trial-and-error calculations [1]:

$$K(2 \times 2 \times n) = \prod_{k=1}^{n} 2^2 \left[\cos^2\left(\frac{\pi}{3}\right) + \cos^2\left(\frac{\pi}{3}\right) + \cos^2\left(\frac{k\pi}{n+1}\right)\right]. \tag{4}$$

The aim of the present paper is to derive eq. (4) with the use of skew-symmetric matrices and also to show the validity of eq. (2). The final goal of this line of study is to derive in closed form, as in eq. (4), the number of perfect matchings for the network of the $l \times m \times n$ simple cubic lattice. A number of related problems are also discussed.

2. Theory

Before going into our analysis of the three-dimensional cubic lattice, a brief summary of the method established in the two-dimensional dimer problem is presented [3,4,11,12]. Suppose we have a square lattice with $m \times n$ (with even m) points and the assigned coordinates (j, k) as given in fig. 1. The numbering p of the lattice point (j, k) can be chosen as

$$(j, k) \leftrightarrow p = m(k-1) + j. \tag{5}$$

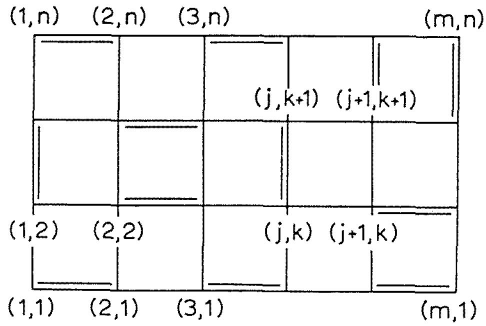

Fig. 1. Coordinates (j, k) of the lattice points in the $m \times n$ square lattice with even m. The set of double bonds represents a perfect matching or a Kekulé pattern.

Any of the allowed configurations C of placing dimers on the lattice lines of Kekulé patterns can be expressed as

$$C = |p_1; p_2|p_3; p_4|p_5; p_6| \dots |p_{mn-1}; p_{mn}|$$

with the following restrictions (canonical ordering):

$$p_1 < p_2; p_3 < p_4; \dots p_{mn-1} < p_{mn};$$
$$p_1 < p_3 < p_5 < \dots < p_{mn-1} \,. \tag{6}$$

It is shown that if we define the following assignment to the triangular array of elements $D(p; p')$, the Pfaffian $Pf(D)$ gives the exact number of the perfect matchings of the given lattice:

$$\begin{aligned} &D(j,k; j+1,k) = 1 && \text{for } 1 \leqslant j \leqslant m-1,\ 1 \leqslant k \leqslant n \\ &D(j,k; j,k+1) = (-1)^j && \text{for } 1 \leqslant j \leqslant m, \quad 1 \leqslant k \leqslant n-1 \\ &D(j,k; j',k') = 0 && \text{otherwise (for non-bonding pair } j < j', k < k') \end{aligned} \tag{7}$$

Next, let us expand the Pfaffian D into a skew-symmetric matrix with elements

$$D(j,k; j',k') = -D(j',k'; j,k) \quad \text{and} \quad D(j,k; j,k) = 0. \tag{8}$$

Then the determinant of D becomes equal to the square of $Pf(D)$, namely

$$\det(D) = Pf^2(D). \tag{9}$$

Note that, in order for $Pf(D)$ to represent the exact value of the perfect matching number K, the product of the matrix elements of D for any square $p_j p_k p_l p_m$ should be equal to -1, or

$$D(p_j; p_k)D(p_j; p_l)D(p_k; p_m)D(p_l; p_m) = -1. \tag{10}$$

The result (1) can be obtained by diagonalizing $\det(D)$.

3. Polycube lattices

The three-dimensional polycube lattice $(2 \times 2 \times n)$ turns out to be a planar graph, and thus we can use the relation $K = Pf(D)$. The lattice point is denoted by (j, k, l) and numbered according to

$$(j, k, l) \leftrightarrow p = j + 2(k-1) + 4(l-1),$$

as in fig. 2. Following the two-dimensional case, the matrix elements of this lattice can be chosen as

$$\begin{cases} D(j, k, l; j+1, k, l) = x \\ D(j, k, l; j, k+1, 1) = (-1)^j y \qquad (j, k = 1, 2;\ l = 1 \sim n) \\ D(j, k, l; j, k, l+1) = z\,. \end{cases} \tag{11}$$

We need to follow the restriction (10) for any square in the lattice. This can be done by setting

$$x = 1, \quad y = 1, \quad \text{and} \quad z = i\,, \tag{12}$$

as

$$x^2 y(-y) = x^2 z^2 = y^2 z^2 = (-y)^2 z^2 = -1\,.$$

Now, by using the three kinds of matrices E, F, and Q as chosen by Kasteleyn [3], the skew-symmetric interaction matrix D for the $2 \times 2 \times n$ lattice can be expressed in terms of their direct product sum as

$$D_{2,2,n} = x\, Q_2 \times E_2 \times E_n + y\, F_2 \times Q_2 \times E_n + z\, E_2 \times E_2 \times Q_n\,, \tag{13}$$

with

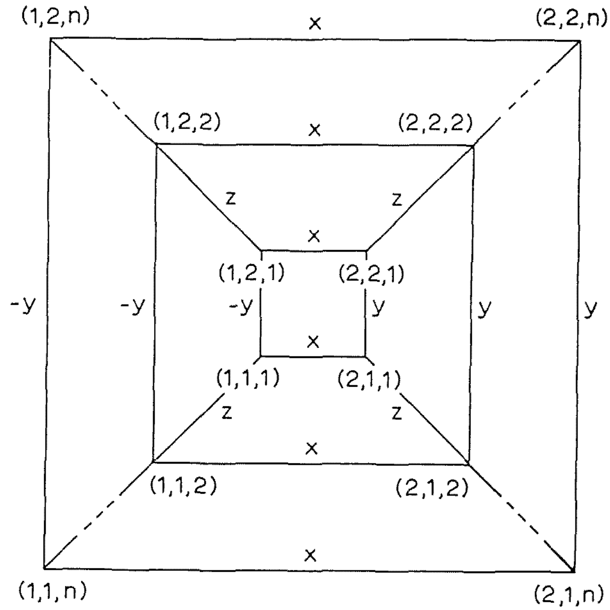

Fig. 2. Coordinates (j, k, l) of the lattice points in the $2 \times 2 \times n$ cubic lattice and the properly assigned skew-symmetric matrix elements for each line as in eq. (11). Note that these numbers refer to the off-diagonal term corresponding to (p_a, p_b), with $p_a < p_b$.

$$E_n = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \\ \cdots & & & & \cdots \\ \cdots & & & & 1 \end{pmatrix} \quad F_n = \begin{pmatrix} -1 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & -1 & 0 & \cdots \\ \cdots & & & & \cdots \\ \cdots & & & & (-1)^n \end{pmatrix}$$

$$Q_n = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ -1 & 0 & 1 & 0 & \cdots \\ 0 & -1 & 0 & 1 & \cdots \\ \cdots & & & & \cdots \\ \cdots & & & & 0 \end{pmatrix}. \qquad (14)$$

In the appendix, an example of the D matrix is given for the case where $n = 3$. The $4n \times 4n$ matrix can be nearly diagonalized by the use of unitary matrix U_n and its inverse U_n^{-1} as

$$\begin{aligned}\widetilde{D}_{2,2,n} &= U_2^{-1} \times U_2^{-1} \times U_n^{-1} D_{2,2,n} U_2 \times U_2 \times U_n \\ &= x U_2^{-1} Q_2 U_2 \times U_2^{-1} E_2 U_2 \times U_n^{-1} E_n U_n \\ &+ y U_2^{-1} F_2 U_2 \times U_2^{-1} Q_2 U_2 \times U_n^{-1} E_n U_n \\ &+ z U_2^{-1} E_2 U_2 \times U_2^{-1} E_2 U_2 \times U_n^{-1} Q_n U_n,\end{aligned} \tag{15}$$

with

$$\begin{aligned}U_n(j,k) &= \sqrt{\frac{2}{n+1}}\; i^j \sin \frac{jk\pi}{n+1} \\ U_n^{-1}(j,k) &= \sqrt{\frac{2}{n+1}}\; (-i)^k \sin \frac{jk\pi}{n+1} \;.\end{aligned} \tag{16}$$

In fact, the D matrix is factorized into $2n$ 2×2 matrices since

$$\det(\widetilde{D}_{2,2,n}) = \left[\prod_{k=1}^{n} (N_k^2 - L_1^2 - M_1^2) \right]^2 , \tag{17}$$

where

$$\begin{aligned}L_1 &= x\lambda_1 = 2x \cos(\pi/3) \\ M_1 &= y\mu_1 = 2y \cos(\pi/3) \\ N_k &= z\nu_k = 2z \cos(k\pi/(n+1)).\end{aligned} \tag{18}$$

An example is given in the appendix for the case where $n = 3$. Here, λ_1, μ_1, and ν_k are, respectively, the solutions of the first, second, and third terms of eq. (15). In particular, ν_k is the kth solution of the characteristic polynomial of the path graph, or linear polyene with n. λ_k and μ_k are the solutions for the special case where $n = 2$, and in deriving eq. (17), the relations $\lambda_1 = -\lambda_2$ and $\mu_1 = -\mu_2$ were used.

Now we have

$$K(2\times 2\times n) = [\det(\widetilde{D}_{2,2,n})]^{1/2}$$

$$= \prod_{k=1}^{n} 2^2[-z^2\cos^2\left(\frac{k\pi}{n+1}\right) + x^2\cos^2(\pi/3) + y^2\cos^2(\pi/3)]\ . \qquad (19)$$

By setting $x = y = 1$ and $z = i$, we obtain the final result,

$$K(2\times 2\times n) = 2^n \prod_{k=1}^{n}\left[1 + 2\cos^2 \frac{k\pi}{n+1}\right]. \qquad (20)$$

Next, we show that eq. (20) satisfies the recursion formula (2). Equation (20) can be converted to

$$K_n = \prod_{k=1}^{n} [4 + 2\cos(2k\pi/(n+1))]\ . \qquad (21)$$

By using the formula of finite product of trigonometric functions [13], we can convert eq. (21) into the following expression [10]:

$$K_n = \prod_{k=1}^{n} [u^2 + v^2 - 2uv\cos(2k\pi/(n+1))]$$

$$= [u^{2(n+1)} - 2u^{n+1}v^{n+1} + v^{2(n+1)}]/(u-v)^2$$

$$= (u^{n+1} - v^{n+1})^2/(u-v)^2, \qquad (22)$$

with

$$u^2 + v^2 = 4 \quad \text{and} \quad uv = -1\,.$$

By using the last expression of eq. (22), it is straightforward to derive the recursion formula (2).

We have thus shown the general expression of the perfect matching number of a special case of the three-dimensional rectangular lattice. One of the break-throughs shown to be useful in this paper is the use of pure imaginary numbers for assigning the weights of particular edges of a graph in decomposing the determinant. This is potentially relevant for the derivation of the matching polynomial of a graph by decomposing the determinant of the associated edge-weighted graph [14].

Although Little [15] proved that we can generalize Kasteleyn's theorem even to non-planar graphs, he did not give any general expressions. Our next aim is to derive the general expressions of the perfect matchings of $2 \times 3 \times n$ and larger lattices.

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Appendix

(1) Example of D matrix for the $2 \times 2 \times 3$ lattice ($x = y = 1$, $z = i$).

$$
D_{2,2,3} = \left[\begin{array}{cccc|cccc|cccc}
0 & x & -y & 0 & z & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-x & 0 & 0 & y & 0 & z & 0 & 0 & 0 & 0 & 0 & 0 \\
y & 0 & 0 & x & 0 & 0 & z & 0 & 0 & 0 & 0 & 0 \\
0 & -y & -x & 0 & 0 & 0 & 0 & z & 0 & 0 & 0 & 0 \\
\hline
-z & 0 & 0 & 0 & 0 & x & -y & 0 & z & 0 & 0 & 0 \\
0 & -z & 0 & 0 & -x & 0 & 0 & y & 0 & z & 0 & 0 \\
0 & 0 & -z & 0 & y & 0 & 0 & x & 0 & 0 & z & 0 \\
0 & 0 & 0 & -z & 0 & -y & -x & 0 & 0 & 0 & 0 & z \\
\hline
0 & 0 & 0 & 0 & -z & 0 & 0 & 0 & 0 & x & -y & 0 \\
0 & 0 & 0 & 0 & 0 & -z & 0 & 0 & -x & 0 & 0 & y \\
0 & 0 & 0 & 0 & 0 & 0 & -z & 0 & y & 0 & 0 & x \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -z & 0 & -y & -x & 0
\end{array}\right]
$$

(2) Example of the nearly diagonalized D matrix for the $2 \times 2 \times 3$ lattice. Note that N_i is imaginary.

$$
\widetilde{D}_{2,2,3} = \left[\begin{array}{cc|cc|cc|cc|cc}
L_1+N_1 & M_1 & & & & & & & & \\
M_1 & L_2+N_1 & & & & & 0 & & & \\
\hline
 & & L_1+N_1 & M_2 & & & & & & \\
 & & M_2 & L_2+N_1 & & & & & & \\
\hline
 & & & & L_1+N_2 & M_1 & & & & \\
 & & & & M_1 & L_2+N_2 & & & & \\
\hline
 & & & & & & L_1+N_2 & M_2 & & \\
 & & 0 & & & & M_2 & L_2+N_2 & & \\
\hline
 & & & & & & & & L_1+N_3 & \dots \\
 & & & & & & & & M_1 & \dots \\
\hline
 & & & & & & & & & \dots
\end{array}\right]
$$