An expression for the perfect matching number of cubic $2 \times m \times n$ lattices and their asymptotic values

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A general expression of the perfect matching number is derived for the $2 \times m \times n$ cubic lattices for the first time and is examined for infinitely large systems. The results are compared with those obtained from Kasteleyn's expression. The agreement of one of the special solutions of the present expression with that obtained by Kasteleyn demonstrates the correctness of the present approach.

1. Introduction

The concept of perfect matching has been used for explaining the chemical stability of unsaturated hydrocarbons, especially for the case where a comparison of the number $K(G)$ of the Kekulé structures, i.e. the perfect matching number, is meaningful.

The problems of the adsorption of dimer molecules on metal surfaces and of the nearest-neighbor spin interaction in antiferromagnetic metals have close relationship with each other through perfect matching numbers. It is also well known that calculations of the Ising model and the perfect matching number are closely related [1].

Kasteleyn obtained a rigorous analytical expression for the perfect matching number of the $m \times n$ square lattice [1,4]. Temperley and Fisher solved the same problem independently and derived the configurational ground partition function for the infinitely large lattice [2,3]. Hock and McQutstan derived the recursion formula for the perfect matching number of the $2 \times 2 \times n$ lattices [5]. Hosoya, Ohkami and Motoyama developed the operator technique with which recursion formulas of the perfect matching number can easily be derived [6,7].

An analytical expression for the perfect matching number of the $2 \times 2 \times n$ cubic lattices was then derived [8] and a general expression for that of the cylindrical $m \times n$ lattice was predicted [9] by the recursion formula. While these lattices are planar, the $2 \times 3 \times n$ lattices ($n \geqslant 3$) are the simplest non-planar ones among the 3-dimensional rectangular lattices. An analytical expression for the perfect matching number of the latter lattice was obtained by the same method [10].

In this paper an analytical expression for the perfect matching number of the $2 \times m \times n$ rectangular lattice is proposed. A special solution of the present equation is shown to be equal to that obtained by Kasteleyn [1]. This guarantees that the supposed equation is correct.

Because the result obtained here may give some clue for solving the 3-dimensional Ising model, it is desirable to derive a rigorous analytical expression for the perfect matching number of larger 3-dimensional lattices, such as $2 \times 4 \times n$ and $2 \times 5 \times n$, in order to certify the assumed equation.

2. Perfect matching number of finite lattices

2.1. THE CASE OF $2 \times 3 \times n$ LATTICES

It was proved [10] that the perfect matching number of the $2 \times 3 \times n$ lattice is expressed as

$$K(2 \times 3 \times n) = K_n = \sum_{j=1}^{5} a_j (\det \tilde{D}_{n,j})^{1/4} / f(n) , \tag{1}$$

where $a_j = \text{constant}$,

$$f(n) \equiv \prod_{k=1}^{n} (x^2 - 4z^2 \cos^2[k\pi/(n+1)])^{1/4} . \tag{2}$$

The matrix $\tilde{D}_{n,j}$ is obtained by diagonalizing the following matrix:

$$\begin{aligned} D_{n,j} &= xQ_2 \otimes E_3 \otimes E_n + y_j F_2 \otimes Q_3 \otimes E_n \\ &\quad + zE_2 \otimes E_3 \otimes Q_n , \quad j = 1, 2, \ldots, 5 , \end{aligned} \tag{3}$$

where

$$x^2 = 1 , \quad y_j = \text{constant} , \quad \text{and} \quad z^2 = -1 ,$$

the symbol $\otimes$ stands for a direct product of matrices. Matrices Q_n, E_n and F_n are just what were used by Kasteleyn et al. [1,8–10].

2.2. THE CASE OF $2 \times m \times n$ LATTICES

According to the expression for the perfect matching numbers of the $2 \times 3 \times n$ lattice the one for the $2 \times m \times n$ lattice is supposed to be

$$K(2 \times m \times n) = \sum_{b=1}^{b'} \sum_{c=1}^{c'} k_{bc} (\det \tilde{D}_{2,m,n,b,c})^{\varepsilon} / g(m) h(n) , \tag{4}$$

where ε and k_{bc} are constants. The quantities $g(m)$ and $h(n)$ are functions of m and n, respectively:

$$\begin{aligned} g(m) &\equiv \prod_{g=1}^{m} (u^2 x^2 + v^2 y^2 + w^2 z^2 \cos^2[g\pi/(m+1)])^{\beta} \\ &\equiv \prod_{g=1}^{m} f(g, m+1) , \end{aligned} \tag{5}$$

$$\begin{aligned} h(n) &\equiv \prod_{h=1}^{n} (u'^2 x^2 + v'^2 y^2 + w'^2 z^2 \cos^2[h\pi/(n+1)])^{\gamma} \\ &\equiv \prod_{h=1}^{n} f(h, n+1) , \end{aligned} \tag{6}$$

where $\beta, \gamma, u, v, w, u', v'$ and w' are constants.

The matrix $\tilde{D}_{2,m,n,b,c}$ is obtained by diagonalizing the anti-symmetrical matrix $D_{2,m,n,b,c}$. The latter matrix shows the bonding relation among the lattice points defined as follows.

Each lattice point p in an $l \times m \times n$ rectangular lattice is generally expressed by use of the coordinates of a lattice point (i, j, k) as follows:

$$(i, j, k) \leftrightarrow p = i + (j-1)l + (k-1)lm . \tag{7}$$

Examples of numbering in the $2 \times 2 \times n$, $\overline{m \times n}$ and $2 \times 3 \times n$ lattices are shown in refs. [8–10].

The $lmn/2$ dimers occupy the pairs of sites p_1 and p_2, p_3 and p_4, p_5 and p_6, etc., for the configuration

$$C = |p_1; p_2|p_3; p_4|p_5; p_6| \dots |p_{lmn-1}; p_{lmn}| . \tag{8}$$

The lattice points of a given configuration are assigned in the canonical order:

$$\begin{aligned} &p_1 < p_2 ; p_3 < p_4 ; \dots ; p_{lmn-1} < p_{lmn} ; \\ &p_1 < p_3 < \dots , p_{lmn-1} . \end{aligned} \tag{9}$$

In the case of $2 \times l \times m$ lattices the anti-symmetrical matrix mentioned above is

$$\begin{aligned} D_{2,m,n,b,c} = {} & x Q_2 \otimes E_m \otimes E_n + y_b F_2 \otimes Q_m \otimes E_n \\ & + z'_c E_2 \otimes E_m \otimes Q_n . \end{aligned} \tag{10}$$

The set of variables, real x, y_b and pure-imaginary z'_c, stand for the variables related to the two lattice points [8] which correspond to x, y and z directions of the lattice, respectively.

The determinantal element expressing the relation between the lattice points is as follows:

$$\begin{aligned} &D(i,j,k;i+1,j,k) = x\,, \\ &D(i,j,k;i,j+1,k) = (-1)^i y\,, \\ &D(i,j,k;i,j,k+1) = z\,, \\ &\quad i=1,2\,; \quad j=1,2,\ldots,m\,; \quad k=1,2,\ldots,n\,. \end{aligned} \tag{11}$$

By use of the Kasteleyn's method [1,8,9] the matrix $D_{2,m,n,b,c}$ can be diagonalized as

$$\begin{aligned} \tilde{D}_{2,m,n,b,c} &= U_2^{-1} \otimes U_m^{-1} \otimes U_n^{-1} D_{2,m,n,b,c} U_2 \otimes U_m \otimes U_n \\ &= x U_2^{-1} Q_2 U_2 \otimes U_m^{-1} E_m U_m \otimes U_n^{-1} E_n U_n \\ &\quad + y_b U_2^{-1} F_2 U_2 \otimes U_m^{-1} Q_m U_m \otimes U_n^{-1} E_n U_n \\ &\quad + z'_c U_2^{-1} E_2 U_2 \otimes U_m^{-1} E_m U_m \otimes U_n^{-1} Q_n U_n\,. \end{aligned} \tag{12}$$

When Λ_f, M_g and N_h are defined by the eigenvalues λ_f, μ_g and ν_h,

$$\begin{aligned} &\Lambda_f \equiv x\lambda_f (f=1,2)\,; \quad \lambda_f = 2i\cos[f\pi/(l+1)]\,, \\ &M_g \equiv y\mu_g (g=1,2,\ldots,m)\,; \quad \mu_g = 2i\cos[g\pi/(m+1)]\,, \\ &N_h \equiv z'\nu_h (h=1,2,\ldots,n)\,; \quad \nu_h = 2i\cos[h\pi/(n+1)]\,, \end{aligned} \tag{13}$$

the determinant of $\tilde{D}_{2,m,n,b,c}$ can be expressed as

$$\det \tilde{D}_{2,m,n,b,c} = \prod_{g=1}^{m} \prod_{h=1}^{n} (N_h^2 + x^2 - M_g^2)\,. \tag{14}$$

The relations $\Lambda_1 + \Lambda_2 = 0$ and $\Lambda_1 \Lambda_2 = x^2$ are used for deriving eq. (14).

Using the above determinant, the perfect matching number of the $2 \times m \times n$ lattice is obtained as

$$K_{2,m,n} = \sum_{b=1}^{b'} \sum_{c=1}^{c'} k_{b,c} \prod_{g=1}^{[m/2]} \prod_{h=1}^{n} (x^2 - y_b^2 \mu_g^2 + z_c'^2 \nu_h^2)^{2\varepsilon} / g(m) h(n)\,. \tag{15}$$

Substituting each eigenvalue in eq. (13) into eq. (15), $K_{2,m,n}$ is expressed as

$$\begin{aligned} K_{2,m,n}(y_b, z_c) = &\sum_{b=1}^{b'} \sum_{c=1}^{c'} k_{b,c} \prod_{g=1}^{m'} \prod_{h=1}^{n} \left(x^2 + 4y_b^2 \cos^2 \frac{g\pi}{m+1} + 4z_c^2 \cos^2 \frac{h\pi}{n+1} \right)^{2\varepsilon} \\ &/ g(m') h(n)\,, \end{aligned} \tag{16}$$

where

$$\begin{aligned} &m' = [m/2]\,, \\ &z_c^2 \equiv -z_c'^2 > 0\,. \end{aligned} \tag{17}$$

The numbers b' and c' are supposed to be finite in eq. (16). An example of the $2 \times 3 \times 4$ lattice is shown as follows:

$$K_{2,3,4}(y_b, z_c)$$
$$= \sum_{b=1}^{b'=5} \sum_{c=1}^{c'=1} k_{b,c} \prod_{g=1}^{[3/2]} \prod_{h=1}^{4} \left(x^2 + 4y_b^2 - \cos^2 \frac{g\pi}{3+1} + 4zc^2 \cos^2 \frac{h\pi}{4+1} \right)^{2\varepsilon} / g\left(\left[\frac{3}{2}\right]\right) h(4)$$
$$= \sum_{b=1}^{5} \sqrt{-\bar{A}_b A_b} (\bar{Q}_b - Q_b) (\det \tilde{D}_{4,b})^{1/4} / \prod_{h=1}^{4} \left[x^2 - 4z^2 \cos^2 \left(\frac{h\pi}{4+1} \right) \right]^{1/4},$$

where

$$(\det \tilde{D}_{4,b})^{1/4} = \prod_{h=1}^{4} \left[x^2 + 2y_b^2 - 4z^2 \cos^2 \left(\frac{h\pi}{4+1} \right) \right]^{1/2} \left[x^2 - 4z^2 \cos^2 \left(\frac{h\pi}{4+1} \right) \right]^{1/4}$$

and

$$g([3/2]) = 1 .$$

(See ref. [10, eq. (40)]).

When y_q^2 and z_r^2 form a couple of variables giving the maximum value for the quantity expressed by the parentheses ( ) in eq. (16), the number K is expressed as

$$K_{2,m,n}(y_b, z_c) = \bar{K}_{2,m,n}$$
$$\times \frac{\left\{ k_{q,r} + \sum_{b,c} k_{b,c} \prod_{g=1}^{m'} \prod_{h=1}^{n} \left(x^2 + 4y_b^2 \cos^2 \frac{g\pi}{m+1} + 4z_c^2 \cos^2 \frac{h\pi}{n+1} \right)^{2\varepsilon} / \bar{K}_{2,m,n} \right\}}{g(m')h(n)}, \tag{18}$$

where

$$\bar{K}_{2,m,n} \equiv \bar{K}_{2,m,n}(y_q, z_r) \equiv \prod_{g=1}^{m'} \prod_{h=1}^{n} \left(x^2 + 4y_q^2 \cos^2 \frac{g\pi}{m+1} + 4z_r^2 \cos^2 \frac{h\pi}{n+1} \right)^{2\varepsilon} . \tag{19}$$

3. Perfect matching numbers of infinite lattices

The limits of $g(m)$ and $h(n)$ are respectively given by

$$\lim_{m \to \infty} g(m)^{1/m} = \frac{2\beta}{\pi} \int_0^{\pi/2} (u^2 x^2 + v^2 y^2 \cos^2 \phi + w^2 z^2) \, d\phi , \tag{20}$$

$$\lim_{n \to \infty} h(n)^{1/n} = \frac{2\gamma}{\pi} \int_0^{\pi/2} (u'^2 x^2 + v'^2 y^2 + w'^2 z^2 \cos^2 \theta) \, d\theta . \tag{21}$$

If the following equations are supposed to be connected with eqs. (20) and (21),

$$\lim_{m\to\infty} g(m)^{1/m} = 1\,,$$
$$\lim_{n\to\infty} h(n)^{1/n} = 1\,, \tag{22}$$

then

$$\lim_{m,n\to\infty} \ln K_{2,m,n}(y_q, z_r)^{1/mn} = \lim_{m,n\to\infty} \ln \bar{K}_{2,m,n}(y_q, z_r)^{1/mn}\,, \tag{23}$$

because the term following $\sum$ in eq. (18) becomes zero when m and n approach infinity. Namely, it is supposed that the value $K(y_q, z_r)$ for an infinitely large system becomes $\bar{K}(y_q, z_r)$ in the same system.

The quantity $\bar{K}_{2,m,n}(y_q, z_r)$ can be changed into

$$\bar{K}_{2,m,n}(y_q, z_r) = (y_q^{\varepsilon})^{2mn} \times \prod_{g=1}^{m'} \prod_{h=1}^{n'} \{4(\xi^2 + \eta^2 \cos^2[h\pi/(n+1)] + \cos^2[g\pi/(m+1)])\}^{4\varepsilon}\,, \quad n' = [n/2]\,, \tag{24}$$

where

$$\xi^2 \equiv x^2/4y_q^2 \tag{25}$$

and

$$\eta^2 \equiv z_r^2/y_q^2\,. \tag{26}$$

Using the definition

$$u^2 \equiv \xi^2 + \eta^2 \cos^2[h\pi/(n+1)]\,, \tag{27}$$

$\bar{K}_{2,m,n}$ becomes

$$\bar{K}_{2,m,n} = y_q^{2\varepsilon mn} \left\{ \prod_{h=1}^{n'} \prod_{g=1}^{m'} 4(u^2 + \cos^2[g\pi/(m+1)]) \right\}. \tag{28}$$

We know the following identity:

$$\prod_{g=1}^{m'} 4(u^2 + \cos^2[g\pi/(m+1)]) \equiv \{[u + (1+u^2)^{1/2}]^{m+1} - [u - (1+u^2)^{1/2}]^{m+1}\}/2(1+u^2)^{1/2} \tag{29}$$

(see ref. [1, eq. (14)]). When m approaches infinity, i.e., in an infinitely long rectangle with a finite cross section $2 \times n$ (see fig. 1), the quantity (rhs of eq. (29)) $^{1/m}$ becomes $u + (1+u^2)^{1/2}$. Then we have

$$K_n \equiv \lim_{m\to\infty} \bar{K}_{2,m,n}^{1/m} = y_q^{2\varepsilon n} \left(\prod_{h=1}^{n'} [u + (1+u^2)^{1/2}] \right)^{4\varepsilon}. \tag{30}$$

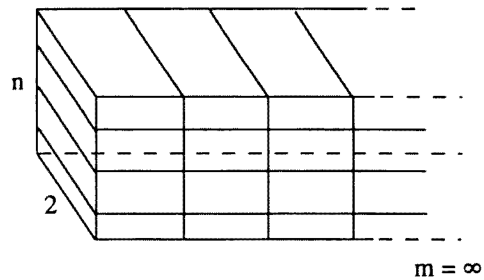

Fig. 1. Infinitely long rectangular prism with a finite cross section of the 2 × n square lattice.

In an infinitely wide lattice like a rectangular board with width 2 (see fig. 2) we get

$$K \equiv \lim_{n\to\infty} K_n^{1/n} = \lim_{n\to\infty} y_q^{2\varepsilon} \left(\prod_{h=1}^{n'} [u + (1+u^2)^{1/2}] \right)^{4\varepsilon/n} , \tag{31}$$

and then we have

$$\ln K = 2\varepsilon \ln y_q + \lim_{n\to\infty} \frac{2\varepsilon}{n} \sum_{h=1}^{n} \ln[u + (1+u^2)^{1/2}] . \tag{32}$$

Equation (16) can be transformed into an integral form as

$$\ln K = 2\varepsilon \ln y_q + \frac{4\varepsilon}{\pi} \int_0^{\pi/2} \ln([\xi^2 + \eta^2 \cos^2\phi]^{1/2} + [1 + \xi^2 + \eta^2 \cos^2\phi]^{1/2})\, d\phi . \tag{33}$$

Kasteleyn treated $m \times n$ planar lattices with width zero [1] and he could calculate the integral more easily. However, it is difficult to calculate analytically the integral in eq. (33). Substituting $\varepsilon = 1/4$ and $x = 0$, i.e. $\xi = 0$, eq. (33) becomes

$$\ln K = \tfrac{1}{2} \ln y_q + \frac{1}{\pi} \int_0^{\pi/2} \ln\{\eta \cos\phi + (1 + \eta^2 \cos^2\phi)^{1/2}\} . \tag{34}$$

Equation (34) is the same as eq. (17) of ref. [1]. Namely, our solution (33) contains the one by Kasteleyn as a special case. In the case of $y_q = 1 = z_r$, the value K^2 becomes as follows:

$$K^2(y_q = 1, \eta = 1) = 1.79162 .$$

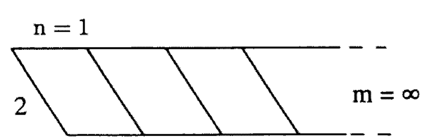

Fig. 2. Infinitely long square lattice with width 2.

The above value is of course the same as the one obtained by Kasteleyn.

Equation (33) can be written as

$$\ln K = \frac{1}{\pi}\int_0^{\pi/2} \ln\left(\left[\frac{x^2}{4} + z_r^2\cos^2\phi\right]^{1/2} + \left[y_q^2 + \frac{x^2}{4} + z_r^2\cos^2\phi\right]^{1/2}\right) d\phi . \qquad (35)$$

It is to be noted that there is a factor 1/4 in front of x^2 because the width of the x-direction is not zero in the lattice $2 \times m \times n$.

The generalization of eq. (35) to $l \times m \times n$ lattices will be the next problem to be solved.

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