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On the number of Kekule structures of a type of oblate rectangles*

Weigen Yan[1,2]** Fuji Zhang[2]
1. Department of Mathematics, Teacher's College, Jimei University, Xiamen 361021, P.R.China.
2. Department of Mathematics, Xiamen University, Xiamen 361005, P.R.China

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Abstract Let $\#\mathbf{R}^j(m,n)$ be the number of Kekule structures of the oblate rectangle $\mathbf{R}^j(m,n)$. Chen et al obtained some formulas for $\#\mathbf{R}^j(m,n)$ and expected to obtain an explicit formula for $\#\mathbf{R}^j(m,n)$ in which there are not trigonometric functions. In this paper, by using a theorem discovered by M.Ciucu, we obtain a formula for $\#\mathbf{R}^j(m,2^{n+1}-2)(n \geq 0)$) in addition to the previously known formulas. Particularly, this makes possible to obtain the limit value of the quantities of $\frac{\log \#\mathbf{R}^j(m,2^{n+1}-2)}{mn}$ when $m \to \infty$ and $n \to \infty$.

1. Introduction

A hexagonal system is a finite connected graph without cut vertices in which every interior face is bounded by a regular hexagon of side length 1. Hexagonal systems are the natural graph representations of benzenoid hydrocarbons. A perfect matching of a graph G is a set of independent edges of G covering all vertices of G, which is called Kekule structure in chemistry. Since a hexagonal system with at least one Kekule structure is the carbon atoms skeleton of a benezenoid hydrocarbon molecule, various topological properties of hexagonal systems were extensively treated by chemists. See for example the prestigious books [7, 18-20] of S.J.Cyvin and I.Gutman. The number of Kekule structures is an important topological index which had been applied for estimation of the resonant energy and $\pi-$electron energy and calculation of Pauling bond order ([22, 25, 30]). So far, enumerative problems on Kekule structures of hexagonal systems are still considerable for mathematicians, physicists and chemists([6, 26, 32]).

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**Corresponding author, E-mail address: weigenyan@263.net

The hexagonal system whose structure is indicated in Figure 1 is called the oblate rectangle and is denoted by $\mathbf{R}^j(m,n)$. This is a hexagonal systems with Kekule structures (see chapter 9 in [7]).

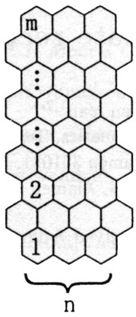


Fig. 1 $\mathbf{R}^j(m,n)$.

Throughout this paper, let $\#G$ denote the number of perfect matchings of a graph G.

For $\#\mathbf{R}^j(m,n)$ with fixed $m \leq 8$ or $n \leq 5$, explicit formulas were obtained in [1-4, 8-14, 16, 21, 24, 29] (or see S.J.Cyvin and I.Gutman's book [7]). In [4], by using the John-Sachs theorem from [23], a determinant formula for $\#\mathbf{R}^j(m,n)$ was obtained as follows.

Proposition 1[4, 7]

$$\#\mathbf{R}^j(m,n) = \begin{vmatrix} C_{n+2}^2 & C_{n+3}^4 & C_{n+4}^6 & \cdots & C_{n+m}^{2m-2} & C_{n+m}^{2m-1} \\ (n+2) & C_{n+3}^3 & C_{n+4}^5 & \cdots & C_{n+m}^{2m-3} & C_{n+m}^{2m-2} \\ 0 & (n+2) & C_{n+3}^3 & \cdots & C_{n+m-1}^{2m-5} & C_{n+m-1}^{2m-4} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & (n+2) & C_{n+2}^2 \end{vmatrix} . \tag{1}$$

This is an $m \times m$ determinant. The first row and last column are special.

In [5], by using the transfer-matrix method (see P.R.Stanley [28]), a formula for $\#\mathbf{R}^j(m,n)$ was obtained as follows:

Proposition 2[5] For fixed n, we have

$$\#\mathbf{R}^j(m,n) = \frac{2}{n+2} \sum_{k=1}^{n+1} \left[\cot \frac{k\pi}{2(n+2)} \right]^2 \lambda_k^{m-1}, \tag{2}$$

where only odd values of k give nonvanishing terms, and $\lambda_k = \frac{n+2}{4} \left[\sin \frac{k\pi}{2(n+2)} \right]^{-2}$.

Chen et al in [5] claimed the above formulas (1) and (2) could not be called being "explicit", since formula (2) contained trigonometric functions and formula (1) was expressed by a determinant whose entries are expressed by combinatorial numbers, particularly, we could not obtain an asymptotic estimation in terms of formula (1), which is physicists and chemists concern (see section 3.4 in [5]). Furthermore, it was claimed in [5] that an "explicit" formula for $\#\mathrm{R}^j(m,n)$, where both m and n were arbitrary, was not known, and seemed not likely ever to be found. In this paper, we use some results from [31] and a theorem from M.Ciucu [6] to obtain the following formula (3) for $\#\mathrm{R}^j(m,2^{n+1}-2)$ in addition to the previously known formulas (1) and (2). Particularly, this makes possible to obtain the limit value of the quantities of $\frac{\log \#\mathrm{R}^j(m,2^{n+1}-2)}{mn}$ when $m\to\infty$ and $n\to\infty$.

In order to give formula (3) for $\#\mathrm{R}^j(m,2^{n+1}-2)$, we introduce some notations as follows. Denote by $\{S_n\}_{n\geq 0}^{\infty}$ the following sequence of the sets.

$$S_n=\left\{2\pm\sqrt{2\pm\sqrt{2\pm\sqrt{\cdots\pm\sqrt{2\pm\sqrt{2}}}}}\right\},$$

where all 2^n combinations of signs have to be considered. It is obvious that there are 2^n different real numbers in S_n.

In this paper, we prove the following results:

1. For fixed $n\geq 0$, we have

$$\#\mathrm{R}^j(m,2^{n+1}-2)=2^{m(n+1)-2n-1}\sum_{\theta\in S_n}\frac{4-\theta}{\theta^m}, \tag{3}$$

where the summation ranges over every number in S_n.

2. We have

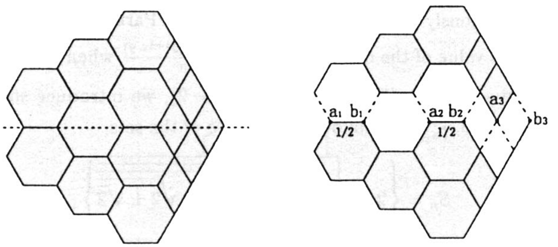
$$\lim_{(m,n)\to(\infty,\infty)}\frac{\log \#\mathrm{R}^j(m,2^{n+1}-2)}{mn}=\log 2. \tag{4}$$

2. Breaking the oblate rectangle into two parts

Now we use a theorem from M.Ciucu [6] to factorize the number of Kekule structures of $\mathrm{R}^j(m,n)$. Roughly speaking, break the oblate rectangle $\mathrm{R}^j(m,n)$ into two subgraphs $\mathrm{R}^j_+(m,n)$ and $\mathrm{R}^j_-(m,n)$. Before we state it we need a few definitions. First, let G be a graph and assign to each of its edges a number, the weight of the edge. Then the weight of a perfect matching of G is the product of all weights of edges contained in the perfect matching. The weighted enumeration $M(G)$ is just the sum of the weights of all possible perfect matchings. If every edge has weight 1 then $M(G)$ reduces to $\#G$ (the number of perfect matchings of G).

Let G be a plane graph. We say G is symmetric if it is invariant under the reflection across some straight line. Figure 2(a) shows an example of a symmetric graph. A weighted symmetric graph is a symmetric graph equipped with weight on every edge of

G that is constant on the orbits of the reflection. The width of a symmetric graph G, denoted by $\omega(G)$, is defined to be half the number of vertices of G lying on the symmetric axis. Clearly, if $\omega(G)$ is not an integer then $M(G) = 0$. Hence we suppose that there are even number of vertices of G lying on the symmetric axis.



(a) (b)

Fig2. (a). A symmetric graph G. (b). The cutting operations of symmetric graph G.

Let G be a weighted symmetric bipartite graph with symmetric axis l, which we consider to be horizontal. Let $a_1, b_1, a_2, b_2, \cdots, a_{\omega(G)}, b_{\omega(G)}$ be the vertices lying on l as they occur from left to right. Let us color the vertices of G in two bipartition classes black and white. For definiteness, choose the leftmost vertex lying on the symmetric axis l to be white. We define two subgraphs G_+ and G_- as follows. Perform cutting operations above all white $a_i's$ and black $b_i's$ and below all black $a_i's$ and white $b_i's$. Note that this procedure yields cuts of the same kind at the endpoints of each edge lying on l. Reduce the weight of each such edge by half, leave all other weights unchanged. Since l separates G, the graph produced by above precess is disconnected into one component lying above l, which we denote by G_+, and one below l, denoted by G_-. Figure 2(b) illustrates this procedure for the graph pictured in Figure 2(a) (the edges whose weights have been reduced by half are marked by $\frac{1}{2}$).

Now we can state the matchings factorization theorem from [6] as follows:

Lemma 2.1[6] Let G be a planar bipartite weighted, symmetric graph, which splits into two parts G_+ and G_- after removal of the vertices of the symmetric axis. Then

$$M(G) = 2^{\omega(G)} M(G_+) M(G_-),$$

where $M(G)$ denotes the weighted count of perfect matchings of graph G, and G_+ and G_- denote the upper and lower half obtained by the procedure of separating G as described above. $\omega(G)$ is the width of G, which is half the number of vertices of G lying on the symmetric axis.

We apply lemma 2.1 to the oblate rectangle $\mathbf{R}^j(m,2n)$, showed in Figure 3(a). In our cases, $\mathbf{R}^j_{\pm}(m,2n)$ are shown in Fig. 3(b) and 3(c), respectively.

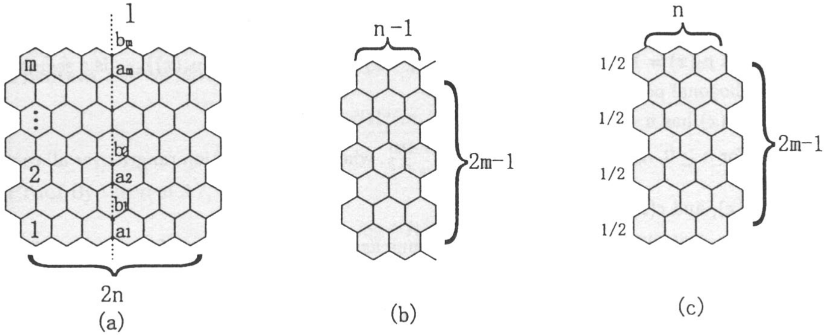


Fig 3. (a). $R^j(m,2n)$. (b). $R^j_+(m,2n)$. (c). $R^j_-(m,2n)$.

By lemma 2.1, we have:

Lemma 2.2

$$\#\mathbf{R}^j(m,2n) = 2^m M(\mathbf{R}^j_+(m,2n))M(\mathbf{R}^j_-(m,2n)).$$

where $\mathbf{R}^j_{\pm}(m,2n)$ are shown in Fig. 3(b) and 3(c), respectively.

By lemma 2.2, we need to count $M(\mathbf{R}^j_+(m,2n))$ and $M(\mathbf{R}^j_-(m,2n))$.

Lemma 2.3[15] Let G be a simple graph, and $e=(u,v)$ be an edge in G, then $\#G = \#G\backslash e + \#G\backslash uv$, where $G\backslash e$ is the graph obtained from G by deleting edge e, and $G\backslash uv$ denotes the induced subgraph of G obtained by deleting vertices u and v from G.

The following result is immediate from lemma 2.3.

Lemma 2.4(see chapter 9 in [7]) Let $\mathbf{R}^j_+(m,2n)$ be the same as in lemma 2.2. Then

$$M(\mathbf{R}^j_+(m,2n)) = (n+1)^{m-1}.$$

3. Main results

Let $\mathbf{R}^j_-(m,2n))$ be the same as in lemma 2.2, and let $A_{n,m} = M(\mathbf{R}^j_-(m,2n))$, and $h_n(x) = \sum_{m\geq 0} A_{n,m}x^m$ for fixed $n \geq 0$, where $A_{0,m} = (\frac{1}{2})^m$, and $f_0(x) = \frac{2}{2-x}$. By using lemma 2.3 and the theory of orthogonal polynomials, we obtained the following results in [31].

Lemma 3.1[31] Let $P_{-1}(x) = 2$, $P_0(x) = 2-x$, and $P_n(x) = (2-x)^{n+1} + \sum_{j=1}^{\lceil \frac{n}{2} \rceil} (-1)^j [C_{n+1-j}^{j} + C_{n-j}^{j-1}](2-x)^{n+1-2j}$ for $n \geq 1$, where $\lceil \frac{n}{2} \rceil$ denotes the least integer no less than $\frac{n}{2}$. Then $h_n(x) = \frac{P_{n-1}(x)}{P_n(x)}$ for $n \geq 0$.

Lemma 3.2[31] Let $\{P_n(x)\}_{n \geq -1}$ be the same as in lemma 3.1. Then we have
(1). $P_n(x) = (2-x)P_{n-1}(x) - P_{n-2}(x)$ for $n \geq 1$, where $P_{-1}(x) = 2$, and $P_0(x) = 2-x$.
(2). Let $p_0(x) = 1$, and $p_n(x) = (-1)^{n-1} P_{n-1}(x)$ for $n \geq 1$. Then $\{p_n(x)\}_{n \geq 0}$ is a sequence of orthogonal polynomials.
(3). $P_n(x)$ has $n+1$ different real roots.
(4). For $n \geq 0$, $h_n(x) = \frac{P_{n-1}(x)}{P_n(x)} = \sum_{\theta : P_n(\theta)=0} \frac{c(\theta)}{x-\theta}$; where the summation ranges over all roots of $P_n(x)$, and $c(\theta) = \frac{P_{n-1}(\theta)}{P_n'(\theta)}$.

Lemma 3.3[31] Let $\{P_n(x)\}_{n \geq 0}$ be the same as in lemma 3.1. Then, for $n \geq 0$, we have

$$P_n(x) = \left(\frac{2 - x + \sqrt{x^2 - 4x}}{2} \right)^{n+1} + \left(\frac{2 - x - \sqrt{x^2 - 4x}}{2} \right)^{n+1}. \tag{5}$$

Lemma 3.4[31] Let $\mathbf{R}_{-}^{j}(m, 2n)$ be the same as in lemma 2.2. Then

$$M(\mathbf{R}_{-}^{j}(m, 2n)) = A_{n,m} = \frac{1}{2n+2} \sum_{\theta : P_n(\theta)=0} \frac{4-\theta}{\theta^m}.$$

Where the summation ranges over all zeros θ of $P_n(x)$.

Lemma 3.5 Let $\{P_i(x)\}_{i \geq -1}$ be the same as in lemma 3.1. Then the set of roots of $P_{2^n-1}(x)$ is S_n for any $n \geq 0$.

Proof By lemma 3.2, $P_{2^0-1}(x) = 2 - x, P_{2^1-1}(x) = (2-x)(2-x) - 2 = 2 - 4x + x^2$. Hence when $n = 0$ or 1 the lemma holds. We assume inductively the lemma holds for $n = k$. Then the set of roots of $P_{2^k-1}(x)$ is S_k. Noting equation (5), we have

$$P_{2^k-1}[(2-x)^2] = \left(\frac{2-(2-x)^2 + \sqrt{(2-x)^2 - 4(2-x)^2}}{2} \right)^{2^k} + \left(\frac{2-(2-x)^2 - \sqrt{(2-x)^2 - 4(2-x)^2}}{2} \right)^{2^k}$$

$$= \left(\frac{-x^2+4x-2+\sqrt{(2-x)^2[x^2-4x]}}{2} \right)^{2^k} + \left(\frac{-x^2+4x-2-\sqrt{(2-x)^2[x^2-4x]}}{2} \right)^{2^k} = P_{2^{k+1}-1}(x).$$

Hence every root of $P_{2^{k+1}-1}(x)$ has the form $2 \pm \sqrt{c}$, where $c \in S_k$. This shows that the set of $P_{2^{k+1}-1}(x)$ is S_{k+1}. Hence, by the induction, the lemma is thus proved.

The following result is immediate from lemmas 3.4 and 3.5.

Corollary 3.6 Let $\mathbf{R}_{-}^{j}(m, 2n)$ be the same as in lemma 2.2. Then

$$M(\mathbf{R}_{-}^{j}(m, 2^{n+1} - 2)) = A_{2^n-1,m} = \frac{1}{2^{n+1}} \sum_{\theta \in S_n} \frac{4-\theta}{\theta^m}.$$

where the summation ranges over every number θ in S_n.
Theorem 3.7 For $n \geq 0$, we have

$$\#\mathrm{R}^j(m, 2^{n+1} - 2) = 2^{m(n+1)-2n-1} \sum_{\theta \in S_n} \frac{4-\theta}{\theta^m}.$$

Theorem 3.7 follows from lemmas 2.2 and 2.4 and corollary 3.6. Furthermore, we can easily prove the following theorem.
Theorem 3.8 We have

$$\lim_{(m,n)\to(\infty,\infty)} \frac{\log \#\mathrm{R}^j(m, 2^{n+1} - 2)}{mn} = \log 2.$$

Proof By theorem 3.7, we have

$$\lim_{(m,n)\to(\infty,\infty)} \frac{\log \#\mathrm{R}^j(m, 2^{n+1} - 2)}{mn}$$

$$= \lim_{(m,n)\to(\infty,\infty)} \frac{[m(n+1) - 2n - 1]\log 2 + \log[\sum_{\theta \in S_n} \frac{4-\theta}{\theta^m}]}{mn}$$

$$= \log 2 + \lim_{(m,n)\to(\infty,\infty)} \frac{\log[\sum_{\theta \in S_n} \frac{4-\theta}{\theta^m}]}{mn}.$$

Let $\theta_{\min} = \inf\{S_n\}$, and $\theta_{\max} = \sup\{S_n\}$. Noting that we have

$$\frac{\log\left\{2^n[\frac{4-\theta_{\max}}{\theta^m_{\max}}]\right\}}{mn} \leq \frac{\log[\sum_{\theta \in S_n} \frac{4-\theta}{\theta^m}]}{mn} \leq \frac{\log\left\{2^n[\frac{4-\theta_{\min}}{\theta^m_{\min}}]\right\}}{mn},$$

by routine calculation, we can prove that

$$\lim_{(m,n)\to(\infty,\infty)} \frac{\log\left\{2^n[\frac{4-\theta_{\max}}{\theta^m_{\max}}]\right\}}{mn} = \lim_{(m,n)\to(\infty,\infty)} \frac{\log\left\{2^n[\frac{4-\theta_{\min}}{\theta^m_{\min}}]\right\}}{mn} = 0.$$

Hence we have

$$\lim_{(m,n)\to(\infty,\infty)} \frac{\log \#\mathrm{R}^j(m, 2^{n+1} - 2)}{mn} = \log 2.$$

The theorem thus follows.

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