

Original Article

The Number of Perfect Matchings of $\{(3,4),4\}$ -fullerene

Huimin Jia¹, Rui Yang², Chuanjiao Yu³

^{1,2}School of Mathematics and Information Science, Henan Polytechnic University, Henan, China.

³Lushan No.1 Junior High School, Pingdingshan, Henan, China.

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Abstract - The problem of counting perfect matchings in graphs is an extremely difficult and important topic. In this paper, $\{(3,4),4\}$ -fullerene graphs are classified according to the cyclical edge-connectivity, and then we show that $\{(3,4),4\}$ -fullerene graph G with cyclical edge-connectivity 4 has exponentially many perfect matchings.

Keywords - $\{(3,4),4\}$ -fullerene, Perfect matching, Cyclic edge-connectivity.

1. Introduction

Counting perfect matchings is an important research subject in matching theory [1], which not only plays a significant role in understanding the structure of graphs. In early days, it was mainly to judge whether a graph has a perfect matching. In 1891, Petersen first proved that every 3-regular connected graph without more than two cut edges has a perfect matching [2]. In 1917, German mathematician Frobenius gave a sufficient and necessary condition for the existence of perfect matching in bipartite graphs [3].

In 1947, Tutte gave a sufficient and necessary condition for determining whether there is perfect matching in general graphs [4]. Gallai and Edmonds obtained Gallai Edmonds structure theorem through Gallai Edmonds standard decomposition. This theorem has a profound impact on the research of matching theory, and many important theorems can be derived from it, such as Tutte theorem and Berge formula. In addition, many results related to the number of perfect matchings of graphs can be derived from it [5-8]. With the deepening of research, it has not only developed into an important branch of graph theory, but also widely applied to other mathematical branches and disciplines, such as combinatorial optimization, mathematical modeling, and statistical physics.

As an important topological index, perfect matching number has been applied in many fields, such as estimating resonance energy and π -electron energy, calculating Pauling bond order, etc [9,10]. Due to the special structure and properties of fullerenes, they have great application prospects in biomedicine, energy, and daily life, which also encourages researchers to devote themselves to the synthesis of new and more complex fullerenes. Up to now, more than 30 fullerenes have been synthesized and characterized [11-15].

In recent years, the problem of counting perfect matchings of graphs has attracted many scholars' attention. In 1979, Valiant proved that the problem of calculating the number of perfect matchings of bipartite graph is NP-Hard [16]. Generally, it is very difficult to find a formula for the number of perfect matchings of a graph. Only for some graphs with special structures can we give its formula to calculate the number of perfect matchings.

In this paper, we study one of the $\{(a,b),k\}$ -fullerene, that is, the nature of $\{(3,4),4\}$ -fullerene. The concept of $\{(a,b),k\}$ -fullerene comes from Deza's (R,k) -fullerene [17], $\{(a,b),k\}$ -fullerene is defined as a k -regular graph ($k \geq 3$) embedded in sphere whose faces are of length a and b . Deza et al. proved that there are eight classes of $\{(a,b),k\}$ -fullerenes [18]. Since these eight classes of fullerenes contain most of the considered graphs, they have attracted much attention.

There is a classical class of fullerenes, namely $\{(5,6),3\}$ -fullerene. In 1998, Došlić gave a better lower bound of the number of perfect matchings of $\{(5,6),3\}$ -fullerene, that is, it contains at least $\frac{p}{2} + 1$ perfect matchings [19]. In 2001, Zhang et al. improved this result, that is, the $\{(5,6),3\}$ -fullerene with p vertices contain at least $\frac{3(p+2)}{4}$ perfect matchings [20]. In 2009, kardoš et al. proved that the $\{(5,6),3\}$ -fullerene with p vertices contain at least $2^{\frac{p-380}{61}}$ perfect matchings [21]. Up to now, some



scholars have given formulas for calculating the number of perfect matchings of some special graphs [22,23], but many open problems have not been solved.

In this paper, we discuss a special class of graphs, that is, $\{(3,4),4\}$ -fullerenes. The content of this paper is organized as follows. In the first part, we introduce the significance of calculating the number of perfect matchings of $\{(3,4),4\}$ -fullerenes and its development status.

In the second part, we introduce some basic concepts and symbols of graph theory used in this paper. In the third part, we classify $\{(3,4),4\}$ -fullerenes by using cyclical edge-connectivity. The cyclical edge-connectivity of $\{(3,4),4\}$ -fullerenes is 4 or 6. Then we divide the set of perfect matchings of $\{(3,4),4\}$ -fullerenes with cyclical edge-connectivity 4 into two independent sets and calculate the number of perfect matchings in the two sets. Finally, we collate all the results and obtain the formula for calculating the perfect matchings of $\{(3,4),4\}$ -fullerenes with cyclical edge-connectivity 4.

2. Definitions and Preliminary Results

Definition 2.1. A $\{(3,4),4\}$ -fullerene is defined as a 4-regular graph embedded in sphere whose faces are of length 3 and 4.

To simplify this paper, the $\{(3,4),4\}$ -fullerene in this paper also represents its planar embedded graph. By definition 2.1 and Euler formula, we get that there are 8 triangles in $\{(3,4),4\}$ -fullerene, and the smallest $\{(3,4),4\}$ -fullerene is an octahedron.

Definition 2.2. A matching M in graph G is a set of edges of G such that no two edges from M have a point in common.

Definition 2.3. Point $v \in V(G)$ incident with some edge from M is covered by matching M . Matching M is perfect if it covers every point of G .

Definition 2.4. A graph G is cyclically k -edge connected if at least k edges must be deleted from G in order to separate it into two components such that both contain a cycle. Obviously, if G is cyclically k -edge connected, it is cyclically m -edge connected, for all $1 \leq m \leq k$. Let us denote by $c\lambda(G)$ the greatest $k \in N$ such that G is cyclically k -edge connected, and call this number the cyclical edge-connectivity of G .

Definition 2.5. If the edge set $C \subset E(G)$ with $|C| = k$ satisfies $G - C$ is disconnected, then C is called k -edge cut set of a graph G . If at least two components of $G - C$ contain a cycle respectively, then C is called cyclical k -edge cut set of a graph G .

Since $\{(3,4),4\}$ -fullerene is 4-regular, each triangle emits six edges, these six edges form a cyclically 6-edge cut set, by the same taken, eight edges of each quadrilateral form a cyclically 8-edge cut set. We define the cyclically 6-edge cut set and cyclically 8-edge cut set as *trivial*, otherwise, *non-trivial*. The exact definition is as follows:

Definition 2.6. Let G be a graph and C a cyclical k -edge cut. If a component of $G - C$ contains only one single cycle, then C is *trivial*, otherwise, *non-trivial*.

For the cyclic edge-connectivity of $\{(3,4),4\}$ -fullerene graphs, we have the following conclusions.

Lemma 2.7. Every $\{(3,4),4\}$ -fullerene is cyclically 4-edge-connected [24].

Lemma 2.8. If the $\{(3,4),4\}$ -fullerene G has a cyclically 4-edge-cut $E = \{e_1, e_2, e_3, e_4\}$, then $G \cong Q_n$ (Q_n is the graph consisting of n concentric layers of quadrangles, capped on each end by a cap formed by four triangles which share a common vertex (see Fig.1)) [24].

Let G be $\{(3,4),4\}$ -fullerene, by Lemma 2.7, we can deduce that $c\lambda(G) \geq 4$, from the definition and degree sum formula of $\{(3,4),4\}$ -fullerene, we can know that $c\lambda(G)$ is an even number. We have the following lemma:

Lemma 2.9. Let G be a $\{(3,4),4\}$ -fullerene, then $c\lambda(G) \geq 4$ and $c\lambda(G) = 2m$.

Proof. It only needs to prove that $c\lambda(G)$ is even, let $c\lambda(G) = k$, the cyclically k edge-cut set $C = \{e_1, e_2, e_3, \dots, e_k\}$, G_1 is a component of $G - C$, then, we have

$$4|V(G_1)| - k = 2|E(G_1)| \tag{1}$$

Obviously, k is an even number.

Corollary 2.10. Let G be a $\{(3,4),4\}$ -fullerene, then $c\lambda(G) = 4$ or 6 .

Proof. By Lemma 2.9, the cyclical edge-connectivity of $\{(3,4),4\}$ -fullerene is 4, or 6, or 8, ..., and because each triangle emits six edges, these six edges form a trivial cyclically 6-edge cut set, so we can know that the cyclical edge-connectivity of G is 4 or 6.

For the definitions and symbols used in this paper but not shown in this paper, please refer to the literature [25]. For convenience, let N_n represents the number of perfect matchings of Q_n , by Corollary 2.10, $c\lambda(Q_n) = 4$.

With the above preparation, next, we can calculate the number of perfect matchings of $\{(3,4),4\}$ -fullerenes with cyclical edge-connectivity 4.

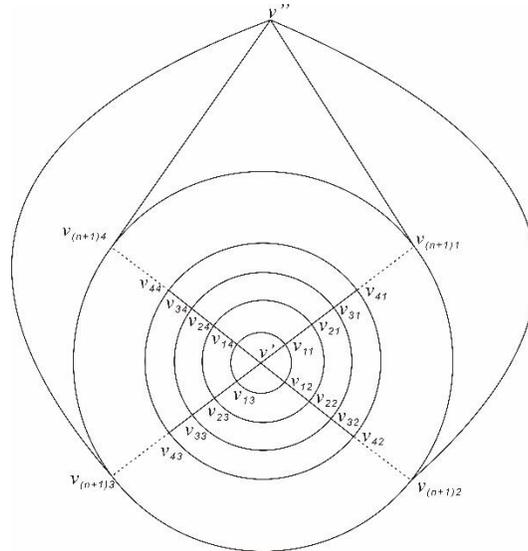


Fig. 1 The $\{(3,4),4\}$ -fullerene Q_n .

3. Main Results

Lemma 3.1. The number of perfect matchings of $\{(3,4),4\}$ -fullerenes Q_n equals $N_n = \sqrt{2} [(1 + \sqrt{2})^{n+2} - (1 - \sqrt{2})^{n+2}]$.

Proof. Obviously, Q_n have perfect matchings. For convenience, the plane embedding graph of Q_n is shown in Fig.1. Q_n consists of $n + 1$ concentric rings, each with four vertices and two vertices on two hats, these $n + 1$ concentric rings are respectively marked as $R_1, R_2, R_3, \dots, R_{n+1}$ from the inside to the outside.

Label the vertices of Q_n as follows: the vertices shared by four triangles on two hats are represented by v' and v'' respectively, the vertices on the i -th ring are recorded as $v_{i1}, v_{i2}, v_{i3}, v_{i4}$ ($i = 1, 2, \dots, n + 1$) in clockwise order, so that v_{i1}, v_{i3} and v_{i2}, v_{i4} are respectively on the same line (see Fig.1).

Let H be the set of perfect matchings of Q_n , then for any perfect matching $H \in H$, H must contain vertex v' . Let the set of perfect matchings containing $v'v_{11}, v'v_{12}, v'v_{13}, v'v_{14}$ be H_1, H_2, H_3, H_4 respectively, then $H_i \cap H_j = \emptyset$ ($i, j = 1, 2, 3, 4, i \neq j$)

and $\bigcup_{i=1}^4 H_i = H$, from the symmetry of graphs, $|H_i| = |H_j|$ ($i, j = 1, 2, 3, 4, i \neq j$), then

$$N_n = |H| = 4|H_1| \tag{2}$$

Next, we calculate the number of H_1 , for any perfect matching $H \in H_1$, $v'v_{11}$ must be covered by H , but there are two ways when v_{12} is covered, that is, $v_{12}v_{22} \in H$ or $v_{12}v_{13} \in H$. Let the set of perfect matchings covering $v'v_{11}, v_{12}v_{22}$ be H_1 and the set of perfect matchings covering $v'v_{11}, v_{12}v_{13}$ be H_2 , then $H_1 = H_1 \cup H_2$ and $H_1 \cap H_2 = \emptyset$, so

$$|H_1| = |H_1| + |H_2| \tag{3}$$

Next, we calculate the number of H_1 and H_2 , respectively.

Claim 1: $|H_1| = \frac{1}{4}N_{n-2} + \frac{1}{4}N_{n-1}$.

Proof. It is known that H_1 is a set of perfect matchings such that each M covers $v'_{11}, v_{12}v_{22}$ for $M \in H_1$. Next, we choose the vertex v_{13} , there are two ways when v_{13} is covered, that is, $v_{13}v_{23} \in H_1$ or $v_{13}v_{14} \in H_1$. Let the set of perfect matchings covering $v'_{11}, v_{12}v_{22}, v_{13}v_{23}$ be H_{11} and the set of perfect matches covering $v'_{11}, v_{12}v_{22}, v_{13}v_{14}$ be H_{12} , $H_1 = H_{11} \cup H_{12}$. We regard H_{11} and H_{12} as two cases to prove.

Case 1. Calculating the number of $n H_{11}$.

H_{11} has covered $v'_{11}, v_{12}v_{22}, v_{13}v_{23}$, so $v_{14}v_{24}$ must be covered by M for any $M \in H_{11}$. After selecting the edges, it is equivalent to removing vertices $v', v_{11}, v_{12}, v_{22}, v_{13}, v_{23}, v_{14}, v_{24}$, and it is known that M must cover $v_{21}v_{31}$ for any $M \in H_{11}$. We connect $v_{21}v_{32}, v_{21}v_{33}, v_{21}v_{34}$ respectively, then we get a $\{(3,4),4\}$ -fullerene Q_{n-2} (see Fig.2), and Q_{n-2} used v_{21} as the common adjacent vertex of a hat, let the number of Q_{n-2} be N_{n-2} , then

$$|H_{11}| = \frac{1}{4}N_{n-2} \tag{4}$$

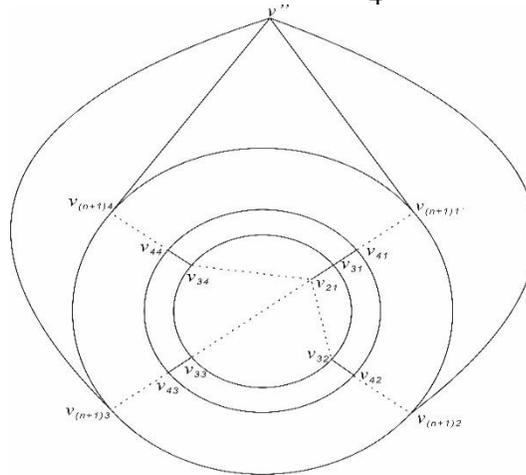


Fig. 2 The $\{(3,4),4\}$ -fullerene Q_{n-2} with v_{21} as the common vertex of a hat.

Case 2. Calculating the number of H_{12} .

H_{12} has covered $v'_{11}, v_{12}v_{22}, v_{13}v_{14}$, it is equivalent to removing vertices $v', v_{11}, v_{13}, v_{14}$ and we connect $v_{12}v_{21}, v_{12}v_{23}, v_{12}v_{24}$ (see Fig.3). Now, we get a $\{(3,4),4\}$ -fullerene Q_{n-1} and Q_{n-1} used v_{12} as the common adjacent vertex of a hat, also as the number of Q_{n-1} is N_{n-1} , then

$$|H_{12}| = \frac{1}{4}N_{n-1} \tag{5}$$

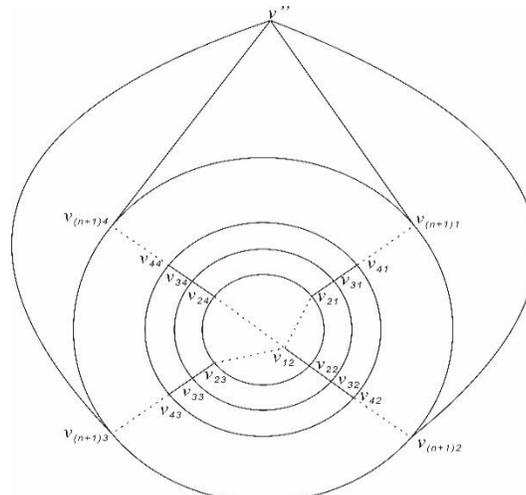


Fig. 3 The $\{(3,4),4\}$ -fullerene Q_{n-1} with v_{12} as the common vertex of a hat.

Since $|H_1| = |H_{11}| + |H_{12}|$, then

$$|H_1| = \frac{1}{4}N_{n-2} + \frac{1}{4}N_{n-1} \tag{6}$$

Claim 2: $|H_2| = \frac{1}{4}N_{n-1}$.

Proof. It is known that H_2 is a set of perfect matchings such that each M covers $v'v_{11}, v_{12}v_{13}$ for $M \in H_2$. After selecting these edges, it is equivalent to removing vertices $v', v_{11}, v_{12}, v_{13}$, and it is known that H_2 must cover $v_{14}v_{24}$. Now, we respectively connect $v_{14}v_{21}, v_{14}v_{22}, v_{14}v_{23}$, then we get a $\{(3,4),4\}$ -fullerene Q_{n-1} (see Fig.4) and Q_{n-1} used v_{14} as the common adjacent vertex of a hat.

As the above, we have

$$|H_2| = \frac{1}{4}N_{n-1} \tag{7}$$

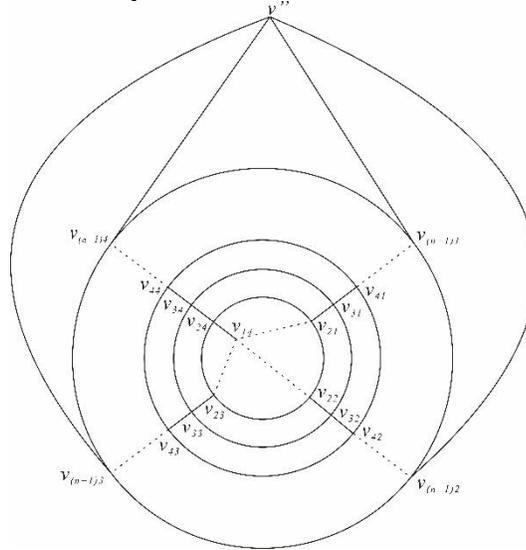


Fig 4. The $\{(3,4),4\}$ -fullerene Q_{n-1} with v_{14} as the common vertex of a hat.

From (3),(6),(7), then

$$|H_1| = |H_1| + |H_2| = \frac{1}{4}N_{n-2} + \frac{1}{4}N_{n-1} + \frac{1}{4}N_{n-1} = \frac{1}{4}N_{n-2} + \frac{1}{2}N_{n-1} \tag{8}$$

By equation (2), $|H| = N_n = 4|H_1| = 2N_{n-1} + N_{n-2}$, then

$$N_n = 2N_{n-1} + N_{n-2} \tag{9}$$

We can use the method like solve differential equations in ordinary differential equations for calculating N_n , its characteristic equation is as follows:

$$q^2 - 2q - 1 = 0 \tag{10}$$

We get two characteristic roots:

$$q_1 = 1 + \sqrt{2}, q_2 = 1 - \sqrt{2} \tag{11}$$

Therefore, its general solution is as follows:

$$N_n = c_1(1 + \sqrt{2})^n + c_2(1 - \sqrt{2})^n \tag{12}$$

To calculate N_n , take the two initial values $N_0 = 8$ and $N_1 = 20$ into the equation (12). We get a set of equations as follows:

$$\begin{cases} c_1 + c_2 = 8(n = 0) \\ c_1(1 + \sqrt{2}) + c_2(1 - \sqrt{2}) = 20(n = 1) \end{cases} \tag{13}$$

Then

$$c_1 = 4 + 3\sqrt{2}, c_2 = 4 - 3\sqrt{2} \tag{14}$$

Take c_1, c_2 into the equation (12), then we get N_n , Lemma 3.1 has been completed. From the above lemmas and corollaries, we have the following theorem.

Theorem 3.2. If $c\lambda(G) = 4$, the number of perfect matchings of $\{(3,4),4\}$ -fullerene G with p vertices equals

$$N(p) = \sqrt{2} \left[(1 + \sqrt{2})^{\frac{p-6}{4}+2} - (1 - \sqrt{2})^{\frac{p-6}{4}+2} \right].$$

Proof. By Lemma 2.8, Lemma 3.1 and Corollary 2.10, $c\lambda(G) = 4$, $G \cong Q_n$, the number of perfect matchings of Q_n equals $N_n = \sqrt{2} \left[(1 + \sqrt{2})^{n+2} - (1 - \sqrt{2})^{n+2} \right]$.

According to the structure of Q_n , so $|V(G)| = |V(Q_n)| = 4(n+1) + 2 = p$ ($6 \leq p \leq 4n+6$) then $n = \frac{p-6}{4}$. So the number of perfect matchings of $\{(3,4),4\}$ -fullerene G with p vertices equals $N(p) = \sqrt{2} \left[(1 + \sqrt{2})^{\frac{p-6}{4}+2} - (1 - \sqrt{2})^{\frac{p-6}{4}+2} \right]$.

4. Conclusion

So far, we have obtained a formula for calculating the number of perfect matchings of $\{(3,4),4\}$ -fullerene with cyclical edge-connectivity 4. Similarly, we find that this formula has exponential order.

Secondly, it is worth noting that in Theorem 3.2, the formula for calculating the number of perfect matchings of $\{(3,4),4\}$ -fullerenes includes the irrational number " $\sqrt{2}$ " and the variable " p ". But what is more interesting is that it is just like the general formula of Fibonacci series, when p is equal to the number of vertices of the $\{(3,4),4\}$ -fullerene, this irrational number " $\sqrt{2}$ " can always be eliminated, so we can always get integer results. For example, when $p = 10$, $N(10) = 20$.

References

- [1] L. Lovász, M. D. Plummer, "Matching Theory," *American Mathematical Society*, 2009.
- [2] J. Petersen, "The Theory of Regular Graphs," *Acta Mathematica*, vol. 15, pp. 193-220, 1891.
- [3] G. Frobenius, "About Decomposable Determinants," *Reimer*, 1917.
- [4] W. T. Tutte, "The Factorization of Linear Graphs," *Journal of the London Mathematical Society*, vol. 1, no. 2, pp. 107-111, 1947.
- [5] Y. Liu, J. Hao, "The Enumeration of Near-Perfect Matchings of Factor-Critical Graphs," *Discrete Mathematics*, vol. 243, no. 1-3, pp. 259-266, 2002.
- [6] M. Jünger, G. Reinelt, W. R. Pulleyblank, "On Partitioning the Edges of Graphs Into Connected Subgraphs," *Journal of Graph Theory*, vol. 9, no. 4, pp. 539-549, 1985.
- [7] H. Lin, "On the Structure of Graphs with Exactly Two Near-Perfect Matchings," *Ars Combinatoria*, vol. 99, pp. 353-358, 2011.
- [8] B. Spille, L. Szegő, "A Gallai-Edmonds-Type Structure Theorem for Path-Matchings," *Journal of Graph Theory*, vol. 46, no. 2, pp. 93-102, 2011.
- [9] G. G. Hall, "A Graphical Model of a Class of Molecules," *International Journal of Mathematical Education in Science and Technology*, vol. 4, no. 3, pp. 233-240, 1973.
- [10] R. Swinborne-Sheldrake, W. C. Herndon, I. Gutman, "Kekulé Structures and Resonance Energies of Benzenoid Hydrocarbons," *Tetrahedron Letters*, vol. 16, no. 10, pp. 755-758, 1975.
- [11] F. Diederich, R. Ettl, Y. Rubin, et al., "The Higher Fullerenes: Isolation and Characterization of C_{76} , C_{84} , C_{90} , C_{94} , and $C_{70}O$, an Oxide of $D_{5h}-C_{70}$," *Science*, vol. 252, no. 5005, pp. 548-551, 1991.
- [12] K. Kikuchi, N. Nakahara, T. Wakabayashi, et al., "NMR Characterization of Isomers of C_{78} , C_{82} and C_{84} Fullerenes," *Nature*, vol. 357, no. 6374, pp. 142-145, 1992.
- [13] T. J. S. Dennis, T. Kai, K. Asato, et al., "Isolation and Characterization by C-13 NMR Spectroscopy of C_{84} Fullerene Minor Isomers," *The Journal of Physical Chemistry A*, vol. 103, no. 44, pp. 8747-8752, 1999.
- [14] J. Crassous, J. Rivera, N. S. Fender, et al., "Chemistry of C_{84} : Separation of Three Constitutional Isomers and Optical Resolution of D_2-C_{84} by Using the "Bingel-Retro-Bingel" Strategy," *Angewandte Chemie International Edition*, vol. 38, no. 11, pp. 1613-1617, 1999.
- [15] G. W. Wang, M. Saunders, A. Khong, et al., "A New Method for Separating the Isomeric C_{84} Fullerenes," *Journal of the American Chemical Society*, vol. 122, no. 13, pp. 3216-3217, 2000.
- [16] L. G. Valiant, "The Complexity of Computing the Permanent," *Theoretical Computer Science*, vol. 8, no. 2, pp. 189-201, 1979.
- [17] M. Deza, M. Sikirić, "Spheric Analogs of Fullerenes," *Ecole Normale Supérieure, Paris, and Rudjer Boskovic Institute, Zagreb*, 2012.
- [18] M. Deza, M. Sikirić, M. Shtogrin, "Fullerene-Like Spheres with Faces of Negative Curvature," *Diamond and Related Nanostructures*, Springer, Dordrecht, pp. 251-274, 2013.
- [19] T. Došlić, "On Lower Bounds of Number of Perfect Matchings in Fullerene Graphs," *Journal of Mathematical Chemistry*, vol. 24, no. 4, pp. 359-364, 1998.
- [20] H. Zhang, F. Zhang, "New Lower Bound on the Number of Perfect Matchings in Fullerene Graphs," *Journal of Mathematical Chemistry*, vol. 30, no. 3, pp. 343-347, 2001.

- [21] F. Kardoš, D. Král, J. Miskuf, et al., “Fullerene Graphs have Exponentially Many Perfect Matchings,” arXiv preprint arXiv:0801.1438, 2008.
- [22] Tang Baoxiang, Ren Han, “*Perfect Matching Numbers in Two Types of 3-Regular Graphs*,” Journal of Sun Yat-Sen University, Natural Science Edition, vol. 53, no. 5, pp. 54-58, 2014.
- [23] Tang Baoxiang, Ren Han, “*Perfect Matching Numbers in 3-Class 3-Regular Graph*,” Journal of Central China Normal University, Natural Science Edition, vol. 48, no. 5, 2014.
- [24] R. Yang, C. Liu, S. Wu, “The Facial Resonance of $\{(3, 4), 4\}$ -Fullerene,” *Journal of Com-Binatorial Mathematics and Combinatorial Computing*.
- [25] J. A. Bondy, U. S. R. Murty, “Graph Theory,” *Graduate Texts in Mathematics*, Springer, New York, 2008.