Number of Matchings of Low Order in (4,6)-Fullerene Graphs*

Zhi–Feng Wei a,b , Heping Zhang a†

^a School of Mathematics and Statistics, Lanzhou University, Lanzhou, Gansu 730000, P. R. China

^bCuiying Honors College, Lanzhou University, Lanzhou, Gansu 730000, P. R. China

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Abstract

We obtain the formulae for the numbers of 4-matchings and 5-matchings in terms of the number of hexagonal faces in (4, 6)-fullerene graphs by studying structural classification of 6-cycles and some local structural properties, which correct the corresponding wrong results published. Furthermore, we obtain a formula for the number of 6-matchings in tubular (4, 6)-fullerenes in terms of the number of hexagonal faces, and a formula for the number of 6-matchings in the other (4,6)-fullerenes in terms of the numbers of hexagonal faces and dual-squares.

1 Introduction

Let G be a graph with vertex set V(G) and edge set E(G). We use n(G) and m(G) to denote the numbers of vertices and edges of G respectively. If G is understood, then we use such notations without reference to G. A k-matching (or a matching of order k) of G is a set of k pairwise nonadjacent edges. A (4,6)-fullerene graph, a mathematical model of a boron-nitrogen fullerene, is a plane cubic graph with exactly six square faces and $\frac{n}{2}-4$ hexagonal faces. It is known that every (4,6)-fullerene graph is bipartite and 3-connected [15].

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[†]Corresponding author.

The number of matchings in a graph is of significance in theory and applications. The matching polynomial of a graph G was defined as $\sum_{k=0}^{\nu} (-1)^k M(G,k) x^{n-2k}$ in [5,6], where ν denotes the size of a maximum matching and M(G,k) the number of k-matchings. All roots of the matching polynomial are real, and the sequence $M(G,0), M(G,1), \ldots, M(G,\nu)$ is log-concave (cf. [12]). In 1971, Hosoya found a correlation between boiling point of some hydrocarbons and the total number of matchings in their molecular graphs [8].

There has already been some research into the enumeration of low order matchings. Klabjan and Mohar [10] counted the matchings of order at most 5 in hexagonal systems. Behmaram [2] established a formula for the number of 4-matchings in triangle-free graphs with respect to the number of vertices, edges, degrees and 4-cycles. Vesalian and Asgari [13], and Vesalian et al. [14] counted the 5-matchings and 6-matchings in graphs with girth at least 5 and 6, respectively. However, their methods and results are not applicable to (4,6)-fullerene graphs. Behmaram et al. [3] recently studied the number of matchings of order no more than 4 in (4,6)-fullerene graphs. But, all 6-cycles of (4,6)-fullerene graphs were mistakenly identified with hexagonal faces. We can give many (4,6)-fullerene graphs with 6-cycles which do not bound faces. This together with an error in counting the 5-length paths of (4,6)-fullerene graphs leads to wrong formulae for the numbers of 4-matchings [3] and 5-matchings [11]. So, we first give a classification of 6-cycles of (4,6)-fullerene graphs in Theorem 2.7. Then we correct the above errors and derive the enumeration result for 6-matchings of (4,6)-fullerene graphs. It turns out that there is not a unified formula for the number of 6-matchings in (4,6)-fullerenes, so we give two formulae for 6-matchings in (4, 6)-fullerenes according to different graph structures.

This paper is organized as follows. In section 2, we study the structure of 6-cycles and obtain a structural classification of (4,6)-fullerene graphs and some local properties. In section 3, by establishing a series of recurrence relations, we deduce the enumeration of higher order matchings to lower order ones. We obtain not only the correct formulae for the numbers of 4-matchings and 5-matchings but also the formulae for the numbers of 6-matchings. Meanwhile, we enumerate some other subgraphs of (4,6)-fullerene graphs.

2 A classification of (4,6)-fullerene graphs

Let G be a graph. We say G is cyclically k-edge-connected if G cannot be separated into two components, each containing a cycle, by deletion of fewer than k edges. We call the greatest integer k such that G is cyclically k-edge-connected the cyclical edge-connectivity of G, denoted by $\zeta(G)$. If G is a (4,6)-fullerene graph, then $\zeta(G)=3$ or 4 (cf. [4]). A tubular (4,6)-fullerene graph consists of $t \geq 0$ concentric layers of three hexagons, capped on each end by a cap formed by three squares. We denote such a tubular (4,6)-fullerene graph with t layers of hexagonal faces by T_t . Figure 1 presents T_3 (Notice that the three dangling edges in the outside area actually connect to the same vertex). In the degenerate case t=0, we get the ordinary cube. The family of all such tubes $T_t, t \geq 1$, is denoted by \mathcal{T} [4].



Figure 1. A tubular (4,6)-fullerene graph T_3 with 3 hexagon-layers.

In a (4, 6)-fullerene graph G, h(G) denotes the number of hexagonal faces.

Lemma 2.1. Let G be a (4,6)-fullerene graph. Then we have

- (i) [3] n = 2h + 8, m = 3h + 12;
- (ii) $h \neq 1$;
- (iii) Any two faces of G cannot have more than one common edge; and
- (iv) [4] $G \in \mathcal{T}$ if and only if $\zeta(G) = 3$.

Lemma 2.2. [9] Let G be a (4,6)-fullerene graph and C a 4-cycle in G. Then C must be a facial cycle of G.

2.1 Structure of 6-cycles

For a (4,6)-fullerene graph G, Lemma 2.2 claims that a 4-cycle must be a facial cycle. But a 6-cycle is not necessarily a facial cycle. So we will study the structure of 6-cycles in (4,6)-fullerene graphs.

We call the two subgraphs in Figure 2 dual-square and square-cap, respectively. For convenience, a boundary 6-cycle of a plane graph is often represented by the name of this graph if this will not lead to confusion.

By Lemma 2.1(iv) and the fact that $\zeta(G) = 3$ or 4, we only need to study the following two cases: $\zeta(G) = 4$ (equivalently, $G \notin \mathcal{T}$) and $\zeta(G) = 3$ (equivalently, $G \in \mathcal{T}$).

Lemma 2.3. [9] Given a (4,6)-fullerene graph $G \notin \mathcal{T}$, if C is a 6-cycle of G, then C is either

- (i) a hexagonal facial cycle, or
- (ii) a dual-square, or
- (iii) a square-cap.

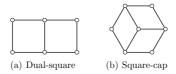


Figure 2. Two types of 6-cycle in (4,6)-fullerene graphs.

Lemma 2.4. For a (4,6)-fullerene graph G with $h \ge 2$, if G has a square-cap subgraph, then $\zeta(G) = 3$ and G is thus tubular.

Proof. This is a direct inference from Lemma 2.1(iv).

By Lemma 2.4, we can strengthen Lemma 2.3 as follows.

Lemma 2.5. For a (4,6)-fullerene graph $G \notin \mathcal{T}$ other than the cube, if C is a 6-cycle of G, then C is either a hexagonal facial cycle or a dual-square.

We call the graph in Figure 3 "a square-cap with 2 hexagon-layers". Generally, we have "a square cap with k hexagon-layers", where $k \ge 1$.

Lemma 2.6. Given a tubular (4,6)-fullerene graph T_t with $t \ge 1$, if C is a 6-cycle of T_t , then C is either

- (i) a hexagonal facial cycle, or
- (ii) a dual-square, or
- (iii) a square-cap, or
- (iv) the boundary of a square-cap with hexagon-layers.



Figure 3. A square-cap with 2 hexagon-layers.

Proof. We first give partitions of $E(T_t)$ and $V(T_t)$ according to the concentric layers of T_t . We first fix one of the two square-caps, and the 0-layer is the set of edges of the fixed square-cap. The 1-layer is the boundary edges of the square-cap with 1 hexagon-layer. In general, we define the i-layer as the boundary edges of the square-cap with i hexagon-layers for $1 \leq i \leq t-1$. The t-layer of T_t is defined as the set of edges of the other square-cap in T_t . Thus, the i-layer is an edge set L_i , $0 \leq i \leq t$. We define \widetilde{L}_i as the set of vertices incident with edges in L_i . Then $V(T_t) = \bigcup_{i=0}^t \widetilde{L}_i$. We call the set of edges linking \widetilde{L}_i and \widetilde{L}_{i+1} the i-bridge B_i , $0 \leq i \leq t-1$. Thus $E(T_t) = (\bigcup_{i=0}^t L_i) \cup (\bigcup_{j=0}^{t-1} B_j)$.

If $E(C) \subseteq L_i$ for some $0 \leqslant i \leqslant t$, one can easily check this result. Otherwise, $E(C) \cap B_i \neq \emptyset$ for some $i, 0 \leqslant i \leqslant t-1$. We claim that C is a hexagonal facial cycle.

Let $C=u_1u_2u_3u_4u_5u_6u_1$. Without loss of generality, we suppose that $u_1u_2\in E(C)\cap B_i$. Since B_i is an edge-cut, C has another edge in B_i , say vw, where $v,w\in V(C)\setminus\{u_1,u_2\}$. Further we assume that $u_1,v\in \widetilde{L}_i$ and $u_2,w\in \widetilde{L}_{i+1}$. We now consider the distance d(u,v) between vertices u and v of T_t (the length of a shortest path between u and v). It is obvious that $d(u_1,v)=d(u_2,w)=2$. Since the common neighbour of u_1 and v (respectively, u_2 and w) is unique, the 2-path linking u_1 and v (respectively, u_2 and w) is also unique and thus located in L_i (L_{i+1} , respectively). This implies $|E(C)\cap L_i|=|E(C)\cap L_{i+1}|=2$. Hence we have $w=u_4, v=u_5$ and C is a hexagonal facial cycle.

Combining Lemmas 2.5 and 2.6, we have

Theorem 2.7 (Structure of 6-cycles). Let G be a (4,6)-fullerene graph and C a 6-cycle in G. Then C is a hexagonal facial cycle, a dual-square, a square-cap or a square-cap with hexagon-layers.

2.2 Local structural properties

Lemma 2.4 is interesting since we can determine the global structure of the graph from its local behavior. Analogous situations can be found in the following two propositions.

Proposition 2.8. Let G be a (4,6)-fullerene graph that has at least 4 square faces arranged in a line. Then G is either a cube or a hexagonal prism.

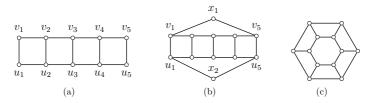


Figure 4. Graphs for proof of Proposition 2.8.

Proof. Suppose that G is not a cube and has a subgraph as depicted in Figure 4(a). Next we show that G is a hexagonal prism.

Since G is a bipartite graph, $v_1v_5 \notin E(G)$, and the path $v_1v_2v_3v_4v_5$ lies on the boundary of a hexagonal face of G. That means that G has a vertex x_1 adjacent to both v_1 and v_5 such that the 6-cycle $x_1v_1v_2v_3v_4v_5x_1$ is a hexagonal face. Similarly, there is another vertex x_2 adjacent to both u_1 and u_5 such that $x_2u_1u_2u_3u_4u_5x_2$ is a hexagonal face (see Figure 4(b)). Now, we get a subgraph of G as shown in Figure 4(b) whose boundary is 6-cycle $x_1v_1u_1x_2u_5v_5x_1$. There are exactly two vertices of degree 2 on this 6-cycle. By Theorem 2.7 this 6-cycle must be a dual-square and $x_1x_2 \in E(G)$. Now G is a hexagonal prism (Figure 4(c)).

Proposition 2.9. For a (4,6)-fullerene graph G, if there are some three square faces arranged in a line, then the other three square faces are also arranged in a line.

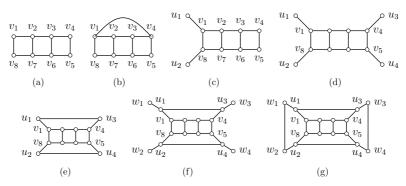


Figure 5. Graphs for proof of Proposition 2.9.

Proof. If there are more than 3 square faces arranged in a line, Proposition 2.8 implies that G is either a cube or a hexagonal prism and the conclusion holds. So suppose that G has some exactly three square faces arranged in a line. That is, the referred 3 square faces form a subgraph as shown in Figure 5(a) whose vertices are labelled so that each of edges v_1v_8 and v_4v_5 belongs to a hexagonal face. Let $C = v_1v_2v_3v_4v_5v_6v_7v_8v_1$.

Because G is bipartite, $v_1v_5, v_4v_8 \notin E(G)$. If $v_1v_4 \in E(G)$ (Figure 5(b)), then Theorem 2.7 implies that 6-cycle $v_1v_4v_5v_6v_7v_8v_1$ is a dual-square, so $v_5v_8 \in E(G)$. That is, v_1v_8 belongs to two squares, a contradiction. Hence $v_1v_4 \notin E(G)$, similarly, $v_5v_8 \notin E(G)$.

Therefore, there are vertices u_1 and u_2 which are adjacent to v_1 and v_8 respectively (Figure 5(c)). If $u_2v_4 \in E(G)$, 6-cycle $v_4v_5v_6v_7v_8u_2v_4$ is a dual-square by Lemma 2.5, but this is impossible. Hence $u_2v_4 \notin E(G)$, and similarly $u_1v_5 \notin E(G)$. So G has a vertex u_3 adjacent to v_4 , and a vertex u_4 adjacent to v_5 (Figure 5(d)). Since G is a (4,6)fullerene, $u_1u_3, u_2u_4 \in E(G)$, and G has a subgraph as in Figure 5(e). Since v_1v_8 and v_4v_5 belong to a hexagonal face, $u_1u_2, u_3u_4 \notin E(G)$. As above, G has vertices w_1, w_2, w_3, w_4 satisfying $w_iu_i \in E(G)$, i = 1, 2, 3, 4 (Figure 5(f)). Further, we have $w_1w_2, w_3w_4 \in E(G)$ (Figure 5(g)). Since 8-cycle $w_1u_1u_3w_3w_4u_4u_2w_2w_1$ has a similar structure with G. If $w_1w_3 \in E(G)$, then $w_2w_4 \in E(G)$. In this case graph G has already been determined (Figure 6(a)), and the theorem holds. If $w_1w_3 \notin E(G)$, then $w_2w_4 \notin E(G)$. The theorem also follows from analogous arguments as above.

Remark 2.10. In the above proof, we have actually ascertained the whole graph structure. To be precise, we have exactly two groups of squares. In each group there are 3 squares arranged in a line. If such two groups of squares have some common edges, the corresponding (4,6)-fullerene graphs must be cube and hexagonal prism. Otherwise, hexagonal faces are distributed around the two square groups of squares (See Figure 6 for two examples). For ease of terminology, we say the latter kind of (4,6)-fullerene graphs are of "lantern structure", which is important in the following enumeration.

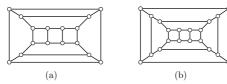


Figure 6. Two examples of (4,6)-fullerene of lantern structure.

2.3 Classification theorem

A (4,6)-fullerene graph is said to be of *dispersive structure* if has neither three squares arranged in a line nor a square-cap. In the case of dispersive structure, every square face is adjacent to at most one square face.

Theorem 2.11. Let G be a (4,6)-fullerene graph. Then G can be of one of the following 4 types:

- (i) a cube,
- (ii) a hexagonal prism,
- (iii) a tubular graph with at least one hexagon-layer,
- (iv) a (4,6)-fullerene graph of lantern structure, and
- (v) a (4,6)-fullerene graph of dispersive structure.

Proof. If h=0, then G is a cube. So we suppose $h\geqslant 2$. If $\zeta(G)=3$, then G has a square-cap and is of tubular structure with at least one hexagon-layer. Further, we suppose $\zeta(G)=4$. If there are at least 4 squares arranged in a line, G is a hexagonal prism by Proposition 2.8. If some exactly 3 squares are arranged in a line, then G is of lantern structure by Proposition 2.9. For the remaining (4,6)-fullerene graph, it has neither three squares arranged in a line nor a square-cap. Hence it is of dispersive structure.

As an application of Theorem 2.11, we count 6-cycles.

Corollary 2.12. Let G be a (4,6)-fullerene graph. Then

- (i) if G is a cube, then the number of 6-cycles is 16,
- (ii) if $G = T_t$ ($t \ge 1$), then the number of 6-cycles is 4t + 7,
- (iii) if $G \notin \mathcal{T}$ other than the cube, then the number of 6-cycles is h + y, where y is the number of dual-squares.
- *Proof.* (i) In a cube, there are in total 12 dual-squares. Also there are exactly four 6-cycles that are boundaries of square-caps.
- (ii) T_t ($t \ge 1$) has 3t hexagonal faces, 6 dual-squares and (t+1) 6-cycles that are boundaries of square-caps with or without hexagonal-layers. Lemma 2.6 demonstrates our result.
- (iii) If $G \notin \mathcal{T}$ other than the cube and has y dual-squares, by Lemma 2.5 the number of 6-cycles is h + y.

3 Number of low-order matchings

Let G be a (4,6)-fullerene graph. We will consider several small subgraphs of (4,6)fullerene graphs. Those of interest to us are shown in Figure 7 and will be denoted by C, D, E, H, \ldots, W as shown in the figure. For a subgraph S of G, let N(S) be the number of subgraphs of G that are isomorphic to S.

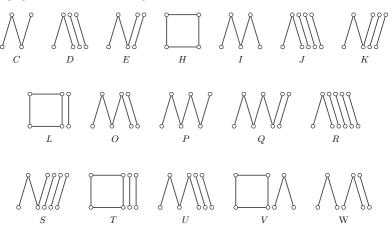


Figure 7. Some possible subgraphs of a (4,6)-fullerene graph.

Lemma 3.1. Let G be a (4,6)-fullerene graph. Then

(i) [3]
$$N(C) = 4m$$
, $N(I) = 8m - 24$;

(ii) [11]
$$N(O) = 72h^2 + 240h + 120$$
, $N(L) = 18h + 24$.

Lemma 3.2. Let G be a (4,6)-fullerene graph. Then N(P)=48h+120, $N(T)=27h^2+27h+12$ and N(V)=36h+24.

Proof. To count N(P), we choose one path of length 3 first and then choose an edge from the two endpoints of the path independently. Noting that the chosen 3-length path may lie on a square, we have

$$N(P) = (N(C) - 6 \times 4) \times 2 \times 2 + 6 \times 4 = 48h + 120.$$

We now consider N(T). We choose a square and then two edges not incident to the chosen square. Then we can get a subgraph T or V. N(V) can be calculated through the following formula

$$N(V) = 6 \times (n-8) \times 3 + 6 \times 4 = 36h + 24.$$

Thus, we have

$$N(T) = 6 \times {m-8 \choose 2} - N(V) = 27h^2 + 27h + 12.$$

Remark 3.3. The number N(P) is not consistent with that in [3]. Behmaram et al. obtained N(P) by choosing an edge at first and then extending the path to both directions. With this in mind [3] gives a formula $N(P) = m \times 4 \times 4 - 48$, where 48 deals with some cases in which the original edge is located in a square and the resulted graph after extension is a square with a hanging edge. However, they did not notice whether the original edge is in a square and the extension process would be restricted. Thus the formula is not correct. Since Li et al. [11] obtain the enumeration of 5-matching by applying the N(P) from [3], their formula is also wrong. Moreover, a similar extension restriction leads to a mistake in the calculation of N(W) in [11].

Lemma 3.4. [3, 11] Let G be a (4,6)-fullerene graph. Then we have

$$\begin{split} &M(G,1) = 3h + 12, \\ &M(G,2) = \frac{9}{2}h^2 + \frac{57}{2}h + 42, \\ &M(G,3) = \frac{9}{2}h^3 + \frac{63}{2}h^2 + 65h + 44. \end{split}$$

3.1 Recurrence relations

Lemma 3.5. Let G be a (4,6)-fullerene graph. We have

(*i*)

$$M(G,5) \times (m-5) = 6 \times M(G,6) + 2 \times N(R) + N(S),$$
 (3.1a)

$$M(G,5) \times 10 \times 2 = 2 \times N(R) + 2 \times N(S),$$
 (3.1b)

$$M(G,4) \times 4 \times 4 = N(S) + 4 \times N(T) + 2 \times N(U) + N(Q),$$
 (3.1c)

$$N(K) \times 2 \times 2 = 2 \times N(U) + 2 \times N(Q) + 8 \times N(T); \tag{3.1d}$$

(ii)

$$M(G,4) \times (m-4) = 5 \times M(G,5) + 2 \times N(J) + N(K),$$
 (3.2a)

$$M(G, 4) \times 8 \times 2 = 2 \times N(J) + 2 \times N(K),$$
 (3.2b)

$$M(G,3) \times 3 \times 4 = N(K) + 4 \times N(L) + 2 \times N(O) + N(P);$$
 (3.2c)

(iii)

$$M(G,3) \times (m-3) = 4 \times M(G,4) + 2 \times N(D) + N(E),$$
 (3.3a)

$$M(G,3) \times 6 \times 2 = 2 \times N(D) + 2 \times N(E), \tag{3.3b}$$

$$M(G, 2) \times 2 \times 4 = N(E) + 4 \times N(H) + 2 \times N(I).$$
 (3.3c)

Proof. We only give the proof of equation system (3.1). The proofs of systems (3.2) and (3.3) are essentially the same and omitted here.

To prove (3.1a), we choose a 5-matching first and then add an arbitrary edge. We use an ordered pair to represent such a choice: the first coordinate indicates the chosen 5-matching and the second one stands for the chosen edge. By the elementary counting principle, the number of such ordered pairs (which equals the number of ways to do the above process) is

$$M(G,5) \times (m-5).$$

Hereinafter, we say a subgraph of G and an ordered pair described above are correlated if the process represented by the pair leads to the subgraph. It is obvious that after the above process, the resulted subgraph of G could only be a 6-matching, a subgraph R or a subgraph S. Each 6-matching correlates 6 ordered pairs. Similarly, for each subgraph R (respectively, S), there are two (respectively, one) correlated pairs. Thus, the number of representation pairs is

$$6 \times M(G,6) + 2 \times N(R) + N(S).$$

Hence (3.1a) is proved and we take in consideration a second process for the proof of (3.1b). First, we choose a 5-matching and fix one of its vertices, then we choose one edge incident with the chosen vertex that is not in the 5-matching. Similarly, we define ordered triples to represent the above process: the first coordinate indicates the 5-matching chosen, while the second one is for the fixed vertex and the last one for the chosen edge. The number of such ordered triples is

$$M(G,5) \times 10 \times 2.$$

The resulted subgraph of G after such a process could only be a subgraph R, or a subgraph S. Each subgraph R correlates to two representation triples since we have 2 ways to determine the initially chosen 5-matching for a given a subgraph R. As for each

subgraph S we have two ways to determine the fixed vertex, each subgraph S correlates to two triples. Thus, the number of representation triples equals

$$2 \times N(R) + 2 \times N(S)$$
.

We have proved (3.1b).

To prove (3.1c), we choose a 4-matching first and fix one edge of this 4-matching, then we add one edge for each end vertex of the fixed edge. Again, the number of representation ordered triples is

$$M(G,4) \times 4 \times 4$$
.

Once we execute the above process, the resulted subgraph of G should be S, T, U, or Q. Each subgraph T correlates to 4 triples, since for a given T, we have 2 ways to determine the initial 4-matching and further if the 4-matching is determined we have 2 ways to determine the fixed edge. Similarly, each subgraph U (respectively, S and Q) correlates to two (respectively, one and one) ordered triples. Thus, the number of representation triples equals

$$4 \times N(T) + 2 \times N(U) + N(Q) + N(S).$$

Therefore (3.1c) is proved and we turn to (3.1d). To this end, we choose a subgraph K first and fix one end-vertex of the 3-length path in K, then we add one edge incident with the fixed vertex. And we use ordered triples to represent the process as above: the first coordinate indicates the subgraph K chosen, the second coordinate stands for the fixed vertex and the third one means the added edge. Then the number of representation triples is $N(K) \times 2 \times 2$. The resulted graph of such a process is either a subgraph U, Q or T. For each U or Q, there are two triples correlated since we have two ways to determine the initial K. For each T, it is easy to check that there are 8 correlated triples. Hence (3.1d) holds.

By (3.2c), we have

Corollary 3.6. $N(K) = 54h^3 + 234h^2 + 180h + 72$.

Theorem 3.7. For a (4,6)-fullerene graph G, we have

$$M(G,4) = \frac{27}{8}h^4 + \frac{81}{4}h^3 + \frac{273}{8}h^2 + \frac{117}{4}h + 9,$$
(3.4a)

$$M(G,5) = \frac{81}{40}h^5 + \frac{27}{4}h^4 - \frac{9}{8}h^3 + \frac{39}{4}h^2 - \frac{27}{5}h,$$
(3.4b)

$$M(G,6) = \frac{81}{80}h^6 - \frac{81}{80}h^5 - \frac{99}{16}h^4 + \frac{405}{16}h^3 - \frac{2833}{40}h^2 - \frac{123}{10}h - 16 + \frac{N(Q)}{6}.$$
 (3.4c)

Proof. Calculating (3.3a) - (3.3b) + (3.3c), (3.2a) - (3.2b) + (3.2c) and (3.1a) - (3.1b) + (3.1c) - (3.1d), respectively, we get

$$4M(G,4) + 4N(H) + 2N(I) = (m-15)M(G,3) + 8M(G,2);$$

$$5M(G,5) + 4N(L) + 2N(O) + N(P) = (m-20)M(G,4) + 12M(G,3);$$

$$6M(G,6) + 4N(K) - 4N(T) = (m-25)M(G,5) + 16M(G,4) + N(Q).$$

Equivalently,

$$\begin{split} M(G,4) &= \frac{m-15}{4} M(G,3) + 2M(G,2) - N(H) - \frac{1}{2} N(I); \\ M(G,5) &= \frac{m-20}{5} M(G,4) + \frac{12}{5} M(G,3) - \frac{4}{5} N(L) - \frac{2}{5} N(O) - \frac{1}{5} N(P); \\ M(G,6) &= \frac{m-25}{6} M(G,5) + \frac{8}{3} M(G,4) - \frac{2}{3} N(K) + \frac{2}{3} N(T) + \frac{1}{6} N(Q). \end{split}$$

That is a series of recurrence relations. Our theorem follows immediately.

Theorem 3.7 has already given the expressions of M(G,4) and M(G,5), and the enumeration of 6-matchings is now reduced to the calculation of N(Q). In addition, we have the following corollary from Lemma 3.5.

Corollary 3.8. Let G be a (4,6)-fullerene graph. We have

$$N(E) = 36h^2 + 180h + 168; (3.5)$$

$$N(D) = 27h^3 + 153h^2 + 210h + 96; (3.6)$$

$$N(J) = 27h^4 + 108h^3 + 39h^2 + 54h; (3.7)$$

$$N(U) = 108h^{3} + 360h^{2} + 252h + 96 - N(Q);$$
(3.8)

$$N(S) = 54h^4 + 108h^3 - 282h^2 - 144h - 96 + N(Q);$$
(3.9)

$$N(R) = \frac{81}{4}h^5 + \frac{27}{2}h^4 - \frac{477}{4}h^3 + \frac{759}{2}h^2 + 90h + 96 - N(Q).$$
 (3.10)

Proof. (3.3c) gives N(E) = 8M(G, 2) - 4N(H) - 2N(I), so we have (3.5). (3.3b) gives N(D) = 6M(G, 3) - N(E), so (3.6) follows. By (3.2b), N(J) = 8M(G, 4) - N(K), which leads to (3.7). By (3.1d), N(U) = 2N(K) - 4N(T) - N(Q), which leads to (3.8).

Substracting (3.1c) with (3.1d), we get N(S) = 16M(G, 4) - 4N(K) + 4N(T) + N(Q), so (3.9) holds. It follows from (3.1b) that N(R) = 10M(G, 5) - N(S), and (3.10) is proved.

3.2 Number of 6-matchings

In the following, we calculate N(Q) for (4,6)-fullerene graphs according to their different structures.

Lemma 3.9. Let $G = T_t$ $(t \ge 1)$ be a tubular (4,6)-fullerene graph. Then

$$N(Q) = 144h^2 + 320h + 42.$$

Proof. To calculate N(Q), we choose a path of length 5 (a subgraph P) first and then choose an edge disjoint with the path. We should notice that a 5-length path may be in a 6-cycle and some 3 consecutive edges of the path may be located in a 4-cycle.

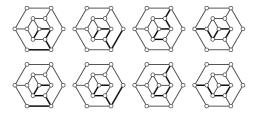


Figure 8. Examples of 5-length path having its head 3 edges in a square.



Figure 9. 5-length path "embedded" in a dual-square.

First we consider the case that the 5-length path chosen is in a 6-cycle. For different types of 6-cycle, hexagonal faces, boundary of square-cap with or without hexagon-layers and dual-square, we have m-12, m-12 and m-11 ways to add one edge, respectively. Hence, the number of subgraph Q in this case is

$$h\times 6\times (m-12)+(t+1)\times 6\times (m-12)+6\times 6\times (m-11).$$

Then we consider the case that some 3 consecutive edges of the 5-length path chosen are in a 4-cycle. If the inner 3 edges of the path is in a square (not including the circumstance

where the whole path is in a dual-square), we have 6×2 such paths and m-12 ways to select the nomadic edge. If the 5-length path has its "head" 3 edges in a square as shown in Figure 8, then the number of related subgraph Q is $6 \times 8 \times (m-12)$. If the path is embedded in a dual-square as shown in Figure 9, the number of Q is $6 \times 2 \times (m-11)$.

In the remaining cases, the number of Q is

$$[N(P) - h \times 6 - (t+1) \times 6 - 6 \times 6 - 6 \times 2 - 6 \times 8 - 6 \times 2] \times (m-13).$$

Thus, we have

$$\begin{split} N(Q) &= 6h \times (m-12) + (t+1) \times 6 \times (m-12) + 36 \times (m-11) \\ &+ 12 \times (m-12) + 48 \times (m-12) + 12 \times (m-11) \\ &+ [N(P) - 6h - (t+1) \times 6 - 36 - 12 - 48 - 12] \times (m-13). \end{split}$$

Note that h = 3t, and the proof is complete.

Lemma 3.10. For a (4,6)-fullerene graph $G \notin \mathcal{T}$ other than the cube, we have $N(Q) = 144h^2 + 318h + 6y$, where y is the number of dual-squares of G.

Proof. We assume that there are x_k squares that have precisely k neighbouring square faces, where $0 \le k \le 2$. As in the proof of Lemma 3.9, we consider different types of 5-length paths (subgraph P).

First, if the 5-length path chosen is in a 6-cycle, then by Theorem 2.11 the number of resulted Q is

$$h \times 6 \times (m-12) + y \times 6 \times (m-11).$$

Second, we consider whether some 3 consecutive edges of the chosen path are in a square. Also we should notice that the three edges in one square might be the "head" three edges or the "inner" three edges. We deal with a special case in the first place where the 5-length path chosen is embedded in a dual-square as shown in Figure 9, the number of such resulted Q is $2y \times (m-11)$. For the other cases,

(a) if the square has no neighbouring squares, then the number of resulted Q is

$$x_0 \times 4 \times 2 \times 2 \times (m-12) + x_0 \times 4 \times (m-12);$$

(b) if the square has one neighbouring square, then the number of resulted Q is

$$x_1 \times 12 \times (m-12) + x_1 \times 3 \times (m-12);$$

(c) if the square has two neighbouring squares, then the number of resulted Q is

$$x_2 \times 8 \times (m-12) + x_2 \times 2 \times (m-12).$$

Third, in the remaining cases, the number of resulted Q is

$$[N(P) - 6h - 6y - 2y - 20x_0 - 15x_1 - 10x_2] \times (m - 13).$$

Thus, we have

$$N(Q) = 6h \times (m - 12) + 6y \times (m - 11)$$

$$+ 2y \times (m - 11) + (20x_0 + 15x_1 + 10x_2) \times (m - 12)$$

$$+ [N(P) - 6h - 6y - 2y - (20x_0 + 15x_1 + 10x_2)] \times (m - 13).$$

Observe that in a (4,6)-fullerene of lantern structure $x_0 = 0$, $x_1 = 4$, $x_2 = 2$, y = 4, in a (4,6)-fullerene of dispersive structure $x_0 = 6 - 2y$, $x_1 = 2y$, $x_2 = 0$, and in a hexagonal prism, $x_0 = x_1 = 0$, $x_2 = 6$, y = 6. An elementary calculation completes our proof.

Lemma 3.11. If G is a cube, then M(G, 6) = 0 and N(Q) = 96.

Proof. Theorem 3.7 claims that M(G,5) = 0, which implies M(G,6) = 0. Further, N(Q) = 96 by (3.4c).

Now, we are in position to declare our enumeration result for 6-matchings.

Theorem 3.12. Let G be a (4,6)-fullerene graph.

- (i) If G is a cube, then M(G,6) = 0.
- (ii) If $G \in \mathcal{T}$, then

$$M(G,6) = \frac{81}{80}h^6 - \frac{81}{80}h^5 - \frac{99}{16}h^4 + \frac{405}{16}h^3 - \frac{1873}{40}h^2 + \frac{1231}{30}h - 9.$$

(iii) If $G \notin \mathcal{T}$ is different from the cube and has y dual-squares, then

$$M(G,6) = \frac{81}{80}h^6 - \frac{81}{80}h^5 - \frac{99}{16}h^4 + \frac{405}{16}h^3 - \frac{1873}{40}h^2 + \frac{407}{10}h - 16 + y.$$

Proof. M(G,6) in a cube has already been calculated in Lemma 3.11. (3.4c) together with Lemmas 3.9 and 3.10 imply our results for the other two cases.

Corollary 3.13. Let G be a (4,6)-fullerene graph.

(i) If G is a cube, then
$$N(U) = N(S) = N(R) = 0$$
.

(ii) If $G \in \mathcal{T}$, then

$$\begin{split} N(U) &= 108h^3 + 216h^2 - 68h + 54; \\ N(S) &= 54h^4 + 108h^3 - 138h^2 + 176h - 54; \\ N(R) &= \frac{81}{4}h^5 + \frac{27}{2}h^4 - \frac{477}{4}h^3 + \frac{471}{2}h^2 - 230h + 54. \end{split}$$

(iii) If $G \notin \mathcal{T}$ is different from the cube and has y dual-squares, then

$$\begin{split} N(U) &= 108h^3 + 216h^2 - 66h - 6y + 96; \\ N(S) &= 54h^4 + 108h^3 - 138h^2 + 174h + 6y - 96; \\ N(R) &= \frac{81}{4}h^5 + \frac{27}{2}h^4 - \frac{477}{4}h^3 + \frac{471}{2}h^2 - 228h - 6y + 96. \end{split}$$

Proof. This corollary follows from Corollary 3.8, and Lemmas 3.9, 3.10 and 3.11 immediately.

References

- R. Balakrishnan, K. Ranganathan, A Textbook of Graph Theory, Springer, New York, 2012.
- [2] A. Behmaram, On the number of 4-matchings in graphs, MATCH Commun. Math. Comput. Chem. 62 (2009) 381–388.
- [3] A. Behmaram, H. Yousefi-Azari, A. R. Ashrafi, On the number of paths, independent set, and matchings of low order in (4,6)-fullerenes, MATCH Commun. Math. Comput. Chem. 69 (2013) 25–32.
- [4] T. Došlić, Cyclical edge-connectivity of fullerene graphs and (k, 6)-cages, J. Math. Chem. 33 (2003) 103–111.
- [5] E. J. Farrel, An introduction to matching polynomials, J. Comb. Theory B 27 (1979) 75–86.
- [6] I. Gutman, The matching polynomial, MATCH Commun. Math. Comput. Chem. 6 (1979) 75–91.
- [7] F. Harary, Graph Theory, Addison-Wesley, Boston, 1969.
- [8] H. Hosoya, Topological index. a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, Bull. Chem. Soc. Jpn. 44 (1971) 2332–2339.
- [9] X. Jiang, H. Zhang, On forcing matching number of boron-nitrogen fullerene graphs, Discr. Appl. Math. 159 (2011) 1581-1593.

- [10] D. Klabjan, B. Mohar, The number of matchings of low order in hexagonal systems, Discr. Math. 186 (1999) 167–175.
- [11] Y. Li, J. Du, J. Tu, On the number of 5-matchings in boron-nitrogen fullerene graphs, Ars Comb. 123 (2015) 207–214.
- [12] L. Lovász, M. D. Plummer, Matching Theory, North-Holland, Amsterdam, 1986.
- [13] R. Vesalian , F. Asgari, Number of 5-matchings in graphs, MATCH Commun. Math. Comput. Chem. 69 (2013) 33–46.
- [14] R. Vesalian, R. Namazi, F. Asgari, Number of 6-matchings in graphs, MATCH Commun. Math. Comput. Chem. 73 (2015) 239–265.
- [15] H. Zhang, S. Liu, 2-resonance of plane bipartite graphs and its applications to boronnitrogen fullerenes, *Discr. Appl. Math.* 158 (2010) 1559–1569.