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On the Number of Paths, Independent Sets, and Matchings of Low Order in (4,6)−Fullerenes

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Abstract

A (4,6)−fullerene graph is a 3-regular planar graph which faces are squares or hexagons. In this paper, we first compute the number of paths of low order in a fullerene. Then apply these numbers to obtain the number of independent sets and k-matchings in fullerenes, when k = 1, 2, 3, 4.

1. Introduction

The graphs considered here are finite, loopless and contains no multiple edges. Fullerenes are allotropes of carbon with a spherical nanostructure was discovered for the first time in 1985 by Kroto et al. [13,14]. An (r,s)−fullerene is a cage polyhedral carbon molecule such that all faces are r− or s−gons. Throughout this paper (r , s) = (4 , 6) and fullerene means (4,6)-fullerene.

Let F be a fullerene and s, h, n and m be the number of quadrangles, hexagons, carbon atoms and bonds between them, respectively. Since each atom lies in exactly 3 faces and each

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edge lies in 2 faces, the number of atoms is $n = (4s+6h)/3$, the number of edges is $m = (4s+6h)/2 = 3/2n$ and the number of faces is $f = s + h$. From the Euler's formula one can deduce that $(4s + 6h)/3 – (4s + 6h)/2 + s + h = 2$, and therefore $s = 6$, $n = 2h + 8$ and $m = 3h + 12$. This implies that such molecules made up entirely of n carbon atoms and having 6 quadrangles and $(n/2 - 4)$ hexagonal faces [1]. In Figure 1, a (4,6)–fullerene with 40 carbon atoms is depicted.

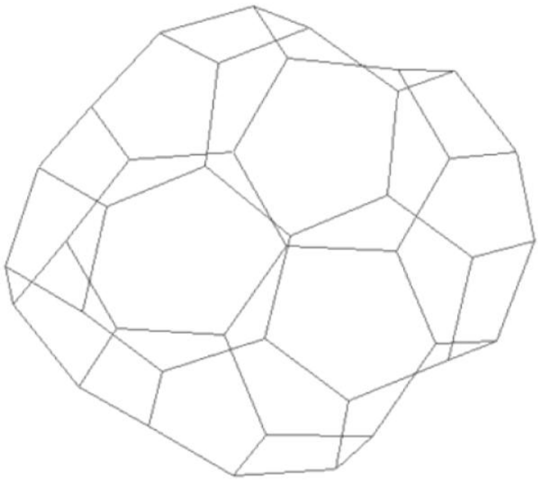

Figure 1. A (4,6)–Fullerene Molecule Containing 40 Carbon Atoms.

Suppose G is a graph. A matching M in G is a set of pairwise non-adjacent edges. A vertex $x \in V(G)$ is called M−saturated if it is incident to an edge in M. Otherwise x is called unsaturated. A k-matching is a matching with k edges. By M(G,k) we denote the number of k–matchings in G. It is easy to see that M(G,1) is equal to the number of edges in G. A maximum matching is a matching with the largest possible number of edges. A perfect matching L is a maximal matching such that all vertices of the graph are covered by L, see [2−5] for details.

Throughout this paper our notation is standard and taken mainly from the standard book on graph theory. We encourage the reader to consult [6−11] for background material as well as basic computational techniques for matchings and independent sets in a graph. The path and cycle with n vertices are called n–path and n–cycle, respectively. Suppose G is a graph. An independent set for G is a subset of V(G), no two of which are adjacent. The size of an independent set is the number of vertices it contains. The number of independent sets with size k in G is denoted by $Ind_k(G)$.

2. Main Results

Suppose G is a graph. Define $P_k(G)$ and $M_k(G)$ to be the number of k–paths and matchings of G, respectively. In this section, exact formulas for the number of k–path, $k \leq 8$, k–independent set and k–matchings, k = 2, 3, 4, in a fullerene graph are computed. The following theorem is crucial throughout this section:

Theorem 1. If F is a fullerene graph with m edges then

i) $P_k(F) = 2^{k-2}m$, k = 2, 3, 4;

ii) $P_5(F) = 8m - 24$;

iii) $P_6(F) = 16m - 48$;

iv) $P_7(F) = 30m - 24$;

v) $P_8(F) = 60m$.

Proof. (i) Since every edge is a path with 2 vertices, $P_2(F) = m$ and since a (4,6)–fullerene is a cubic graph, the number of paths containing three vertices is 3n = 2m. Thus $P_3(F) = 2m$. To count the number of paths with four vertices, we choose an edges e = uv in F. To construct a 4–path in F, we have to choose two edges of F such that each of them is incident to exactly one endpoint of e. Therefore, we have $P_4(F) = m \times 2 \times 2 = 4m$.

(ii) Consider a vertex u of F. For constructing 5–paths with u as its midpoint, we have eight choices. On the other hand, we must remove the cases that a quadrangle is constructed. Notice that each quadrangle will be counted four times in this way. So, $P_5(F) = 8m - 24$.

(iii) For calculation of $P_6(F)$, we first choose an edge e = uv and construct a 6-path where e is its centre. To do this, we have four choices for 3–paths start at u and the same number for 3–paths start at v. But there are $4 \times 2 \times 6 = 48$ cases that we find a quadrangle with a hanging edge. Thus $P_6(F) = 4 \times 4 \times |E(F)| - 48 = 16m - 48$.

(iv) To calculate $P_7(F)$, we choose a vertex v and then paste two 4–paths to v. There are 32 ways to choice these two paths. Two edges incident to v have three ways and another edge have exactly two ways to choice. By subtracting the cases that six edges give a hexagon or a subgraph constructed from a quadrangle and a 3–path with unifying a pendant of 3–path with a vertex of quadrangle, we have $P_7(F) = 32m – 6h – 48 = 30m – 24$.

(v) In this case we apply a similar method as iii. We choose an edge e = uv and count the number of 4–paths start at u and in v. Then we have to omit the cases that we find one of the following subgraphs:

- A subgraph H_1 isomorphic to hexagon T with a pendant.
- A subgraph H_2 constructed from a quadrangle and a 4–path by unifying a pendant of 4–path and a vertex of quadrangle. □

By a similar argument as iv, $P_8(F) = 64m – 12h – 48 = 60m$. □

We now apply Theorem 1 to count the number of k–matchings and k–independent sets in a (4,6) fullerene graph.

Theorem 2. Suppose F is a (4,6)–fullerene graph. Then,

i. $M(F,2) = \frac{9}{2}h^2 + \frac{57}{2}h + 42,$

ii. $M(F,3) = \frac{9}{2}h^3 + \frac{189}{6}h^2 - 65h + 44,$

iii. $M(F,4) = \frac{27}{8}h^4 + \frac{81}{4}h^3 - \frac{375}{8}h^2 - \frac{1827}{4}h - 621.$

where h is the number of hexagons in F.

Proof. (i) Since for every vertex e, f $\in$ E(G), either e and f have a common vertex or they constitute a matching, $M(F,2) + P_3(F) = \binom{3h+12}{2}$. By Theorem 1(i), $P_3(F) = 2m = 6h + 24$, as desired.

(ii) To prove, we use a similar argument as those are given in [12, Theorem 3.1]. We will use the formula $M(F,3)=\binom{m}{3}-(m-2)P_3(F)+P_4(F)+2n$. This is obtained from the number of all 3–subsets minus the numbers of 3–subsets which are not 3–matchings. We add an edge to each 3–path that is outside of this path and notice that these are the only subsets which do not represent 3–matchings. This yields the second term. However, every 4–path *ijkl* has been counted twice and so we have to add the third term. Finally, any subset {ij, ik, il}, where i is a vertex of degree 3, has been counted thrice and so we must add the last term. We now apply Theorem 1(i) to complete our argument.

(iii) In this case, we can see that P(F,4) is the number of 4–subsets of edges in F minus the number of those 4–subsets that do not represent 4–matchings. The possible subgraphs which do not represent 4–matchings are shown in Figure 2. □

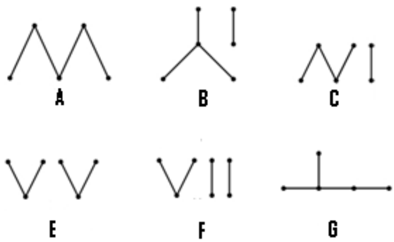

Figure 2. The Possible 4–Subsets of Edges which are not 4–Matching.

Let N(A), N(B), N(C), N(E), N(F) and N(G) are the number of subgraphs isomorphic to those are depicted in Figure 2. Then we have:

- N(A): This a 5–path that are counted in Theorem 1(i). By this theorem N(A) = 24h + 72.
- N(B): Choose a vertex v, three edges incident to v and an edge e which do not have common neighbor. Then we have N(B) = n(m–9) = 6(h+4)(h+1) = $6h^2$ + 30h + 24.
- N(C): For computing N(C), we choose a 4-path and an edge disjoint from the 4–path. Then N(C) = 36(h + 4)(h + 1) = $36h^2$ + 180h + 144.

- N(E): To compute N(E), we have to choose two vertices a and b without common neighbors and then four edges f_1, f_2, f_3 and f_4 such that a is the common vertex of f_1, f_2 and b is the common vertex of f_3, f_4. Then we have:

$$N(E) = 9n(n-3)/2 = 27(h+4)(h+3) = 27h^2 + 189h + 324.$$

- N(F): We have to count the number of disjoint 2–matching and a 3–path in F. We have $N(F) = 3M(F,2)(n-4) = 6M(F,2)(h+2) = (6\binom{3h+12}{2} - 36h - 144)(h+2) = 27h^3 + 225h^2 + 594h + 504$.
- N(G): In this case, we must count the number of subgraphs of F constructed from a 4–path T and a vertex adjacent to a vertex of degree 2 in T. By Theorem 1, the number of 4–path is $P_4(F)$ and there are two choices for the vertex. Therefore, $N(G) = 2P_4(F) = 12h + 48$.

Therefore,

$$\begin{aligned}
M(F,4) &= \binom{3h+30}{4} - 60h^2 - 273h - 3270 - 6(h-8)M(F,2) \\
&= \binom{3h+12}{4} - [27h^3 + 225h^2 + 594h + 504 + 27h^2 + 189h + 324 + 36h^2 \\
&\quad + 180h + 72 + 6h^2 + 30h + 24 + 24h + 144 + 12h + 48] \\
&= \frac{27}{8}h^4 + \frac{81}{4}h^3 - \frac{375}{8}h^2 - \frac{1827}{4}h - 621,
\end{aligned}$$

which completes the proof. ■

Theorem 3. Suppose F is a (4,6)–fullerene graph.

i. $Ind_2(F) = 2h^2 + 12h + 16$,

ii. $Ind_3(F) = \frac{1}{3}(4h^3 + 24h^2 + 2h - 120)$,

iii. $Ind_4(F) = \binom{2h+8}{4} - (3h+12)\binom{2h+6}{2} + \binom{3h+12}{2} + 12h^2 + 80h + 140$,

where h is the number of hexagons in F.

Proof. Clearly, $Ind_2(F) + P_2(F) = \binom{n}{2}$. This proves (i).

(ii) This is obtained from the number of all triples of vertices by subtracting the number of those triples that do not represent 3−independent sets. We consider two types of vertices that are not independent which are named vertices of type 1 and type 2, respectively. We also consider two types of subgraphs in F. The type 1 subgraphs are those constructed from an edge f and a vertex non-incident to f, and the type 2 are subgraphs isomorphic to a 3−path. Clearly, the number of subgraphs of type 1 is m(n – 2) and the number of type 2 subgraphs is $P_3(F)$. However, every 3−path *ijkl* has been counted twice. Therefore,

$$\mathrm{Ind}_3(F) = \binom{2h+20}{3} - 6(h+10)^2 + 12h + 120 = \frac{1}{3}\left(4h^3 + 24h^2 + 2h - 120\right).$$

(iii) Since g(F) = 4, there are exactly four different types of sets of four vertices that are not independent. To count the number of 4−independent set, we have to count the number of all 4−subsets of vertices and then subtract the number of those 4−subsets that do not represent 4−independent set. The 4−subsets that do not represent 4−independent set are isomorphic to a subgraph constructed from an edge and two components each of them is a vertex, a 2−matching, a 3−path with a vertex outside the path, a 4−path and a 3−star. Notice that the 4−paths and 3−stars are counted twice. By substituting the number of mentioned subgraphs the result is proved. □

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