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On the Number of Matchings and Independent Sets in (3,6)−Fullerenes

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Abstract

A (3,6)−Fullerene is a 3−regular planar graph whose faces are triangles and hexagons. In this paper we compute the number of paths, independent sets and k−matchings of small size in an arbitrary (3,6)−fullerene. Then we compute the Wiener polarity of these graphs. We also present a lower bound for the number of perfect matching in these cubic graphs.

1. Introduction

We consider only finite graphs without loops and multiple edges. Let G be such a graph and let n and m be the number of its vertices and edges, respectively. A (k;6)−fullerene is a cubic planar graph whose faces have sizes k and 6. The only values of k for which a (k,6)−fullerene exists are 3, 4 and 5. The (3,6)−fullerenes have received recent attention from chemists due to their similarity to ordinary fullerenes. The Euler's formula implies that an n−vertex (3,6)−fullerene has exactly four faces of size 3 and n/2 − 2 hexagons. A (3,6)−fullerene is called ITR if its triangles have no common edge. In this paper we study this class of chemically interested fullerenes, see [1–4] for details.

A matching of graph G is a subgraph of G such that every edge shares no vertex with any other edge. That is, each vertex in matching M has degree one. A k-matching is a matching of size k and $M_k(G)$ denotes the number of k–matching in G. It is easily seen that $M_1(G)$ is equal to the number of edges in G. A perfect matching is a matching such that exactly one edge of the matching is incident on each vertex of the graph. In other word perfect matching is a matching of size n/2.

In Chemistry, perfect matching called Kekulé structure and have some application in stability of molecular graphs. for example, fullerene is a molecule consisting entirely of carbon atoms. Each carbon is three connected to other carbon atoms by one double bound and two single bound. The set of doubled bonds in a fullerene is precisely a perfect matching in corresponding its molecular graph. It turns out that the number of perfect matching is highly related to the stability of the molecule. We encourage to the interested readers to consult papers [5–10] for some useful algorithms for calculation of Kekulé structures.

The matching polynomial of graph is defined as $\mu(G,x) = \sum_{k=0}^{\frac{n}{2}}(-1)^k M_k\,(G)x^{n-2k}$. A graph G is called matching unique if it is uniquely determined by its matching polynomial, It is easy to see that the house graph and the complete bipartite graph $K_{2,3}$ have the same matching polynomial and so non-isomorphic graphs do not necessarily have distinct matching polynomials, See [6] for more details. In this paper, we computed exact formula for the small coefficient of matching polynomial.

Throughout this paper, our notation is standard and taken mainly from [11] and other standard books on graph theory. The path and cycle with n vertices are called n–path and n–cycle, respectively. Suppose that G and H are two graphs. A splice of G and H by vertices a $\in$ V(G) and b $\in$ V(H) is the graph obtained by identifying the vertices a and b. 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, [12,13]. The set of all independent sets of G is denoted by Ind(G). Finally, d(G,k) denotes the number of ordered vertices with distance k, where the distance between two vertices is defined as the number of edges in a shortest path connecting them. We encourage the interested readers to consult [14–18] for more information on the results of this paper.

In this paper, we continue our earlier works on computing the number of independent sets of size k and k–matchings in fullerene graphs. Here, we consider (3,6)-fullerenes and compute these factors for small values of k.

2. Main results

For a graph G, $P_k(G)$, $M_k(G)$ and $Ind_k(G)$ denote the number of k-paths, k-matchings and k independent set of G, respectively. In this section, exact formulas for the number of k-path, $k \leq 7$, k–independent set and k-matchings, k = 2, 3 in a (3,6)–fullerene are presented.

Theorem 1. If F is a (3,6)–fullerene graph with m edges then

i) $P_2(F) = m$, $P_3(F) = 2m$, $P_4(F) = 4m - 12$ and $P_7(F) = 30m$;

ii) If F is ITR then $P_5(F) = 8m - 24$ and $P_6(F) = 16m - 24$;

iii) If F have exactly two induced subgraphs A and B such that $A \cong B \cong K_4 - e$ then $P_5(F) = 8m - 32$ and $P_6(F) = 16m - 32$.

Proof. (i) Clearly, $P_2(F) = m$ and $P_3(F) = \sum_{i=1}^{n}\binom{d_i}{2} = 3n = 2m$. To count the number of paths with four vertices, choose an edge e = uv of F. To construct a 4–path in F, we have to choose two edges of F, each of them incident to exactly one endpoint of e. But there are 12 undesirable cases and so $P_4(F) = m \times 2 \times 2 - 12 = 4m - 12$. To complete this part, we choose a vertex u. Then we paste two 3-paths to u. There are 32m ways to choice these two paths. By subtracting the cases that six edges give a hexagon or a the splice of a triangle and a path of length 3, we have 12 choices and so $P_7(F) = 32m - 6h - 12 = 30m$, where h denotes the number of hexagons.

(ii) To calculate $P_5(F)$, we first choose one vertex u and construct a 5–path with u as its centre. There are n choices for the vertex u and $3 \times 2 \times 2$ cases for edges attach to u. By subtraction of the cases that we have the splice of a triangle and K_2, we have $P_5(F) = 12n - 24 = 8m - 24$. To compute $P_6(F)$, we choose an edge e = uv. Then we paste a 3-path to u and another to v. There are m choice for e and $4 \times 4 = 16$ ways to choice these two paths. We now subtract the cases that we find the splice of a triangle and a path of length 3. Thus, $P_6(F) = 16m - 24$, as desired.

(iii) To compute $P_5(F)$, we notice that there is a new undesirable case that we obtain an induced subgraph isomorphic to $K_4 - e$. There are $4 \times 2 = 8$ choices for such induced subgraphs. So, by our calculation in the case (ii), $P_5(F) = 8m - 24 - 8 = 8m - 32$. To end the proof, we compute $P_6(F)$. A similar argument shows that $P_6(F) = 16m - 32$.

▼

The Wiener polarity index of the molecular graph G is defined as $W_p(G) = d(G,3)$ [19,20]. In the best of our knowledge, the Wiener polarity index had some information about the applicability of this topological index. We now apply the previous theorem to compute the Wiener polarity index, the number of k–matchings and the number of k–independent sets in a fullerene graph.

Corollary 2. Suppose F is a n-vertex (3,6)–fullerene. Then $W_p(F) = 9/2n - 6$.

Proof. By Theorem 2, the number of 3–paths is $P_4(F) = 4m - 12$. We have to subtract the cases that a hexagon is constructed. If h is the number of hexagons and m is the number of edges then $W_p(F) = 4m - 12 - 3h = 3m - 6 = 9/2n - 6$.

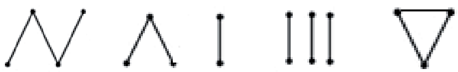
▼

Theorem 3. If F is a (3,6)–fullerene with exactly n vertices and m edges. Then

1) $M_2(F) = \dfrac{m^2 - 5m}{2}$,

2) $M_3(F) = \dbinom{m}{3} - 2m^2 + 8m - 16$,

Proof. Suppose that e and f are two arbitrary edges of F. Then either e and f have a common vertex or {e,f} is 2-matching of F. Thus, $P_3(F) + M_2(F) = m(m-1)/2$ and by Theorem 1(i), $M_2(F) = m(m - 5)/2$. To prove the second part, we have to count the number of 3–matchings. We choose three different edges e_1, e_2 and e_3. Then we have four different types for these edges which are depicted in Figure 1.



A B C D

Figure 1. Four Different Types for the Edges e_1, e_2 and e_3.

If N(T) denotes the number of triangles then we have:

$$M_3(F) + (m-2)P_3(F) - P_4(F) + N(T) = \binom{m}{3}.$$

We now again apply Theorem 1 to deduce that

$$M_3(F) = \binom{m}{3}. - 2m^2 + 8m - 16.$$

▼

Theorem 4. Every n–vertex (3,6)–fullerene has at least $2^{(n-76)/61}$ perfect matching.

Proof. Suppose W is a maximal set of hexagons without common edge in F. Since each member of W has exactly two perfect matching, there are at least $2^{|W|}$ perfect matchings in F. So, it is enough to prove that there exists a maximal set W of independent hexagons such that $|W| \geq (n-76)/122$. Consider an embedding of F into plane and construct its dual, F*, as follows: The vertices F* are in correspondence with plane regions of F and two vertices are adjacent if the corresponding regions have a common edge. Notice that F has exactly four triangles. So, we have a four element set $U = \{u_1, u_2, u_3, u_4\}$ in F* corresponding to triangles of F. Choose vertices $w_1, w_2, \ldots, w_t$ of F* in the following way:

i) The distance between each of w_i and u_j, $1 \leq i \leq t$ and $1 \leq j \leq 4$, are at least three,

ii) The distance between w_i and w_j, $1 \leq i \neq j \leq t$, are at least five.

Set $W = \{w_1, w_2, ..., w_t\}$. If the members of W satisfy these conditions then we can construct a perfect matching for F [21, Theorem 2.1]. Choose a fixed vertex u_i. Then u_i has exactly three neighbours and at most six second neighbours in F*. Therefore, there are at most 4(1 + 3 + 6) = 40 vertices in F* with distance smaller than 3 from u_i. On the other hand, since each w_i has degree six, there are 6d vertices in F* with distance d from w_i. So, for each w_i, there are at most 1 + 6 + 12 + 18 + 24 = 61 vertices with distance smaller than five from w_i. Therefore, $|W| \geq (n/2 + 2 - 40)/61 = (n - 76)/122$.

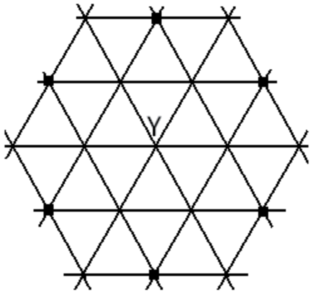


Figure 2. The Configuration of the Hexagon Y and the Six Vertices in F*.

We now extend W to a perfect matching of F. The Tait's theorem states that the edge set of every planar cubic bridgeless graph is the union of three perfect matchings. We colour these three perfect matching by different colours. By four colour theorem, we can colour F* in a way that each hexagon Y has the same colour as six hexagons depicted in Figure 2. Therefore, we have 6|W| disjoint hexagons and so 2|W| of these hexagons having the same colour the corresponding edges of these hexagons give us the desired perfect matchings of F. This completes the proof.

▼

Theorem 5. Suppose F is a (3,6)–fullerene with exactly h hexagons. Then,

i) $Ind_2(F) = 2h^2 + 4h$,

ii) $Ind_3(F) = 1/3(4h^3-10h+36)$.

Proof. For each 2–element set $\{u,v\} \subseteq V(F)$, u an v are adjacent or is an independent set, as desired. The second part is obtained from the nu mber of all triples of vertices by subtracting the number of those triples that do not represent 3–independent sets. There are three different types of vertices, type 1, type 2 and type 3, that are not independent. The type 1 subgraphs are those constructed from an edge f and a vertex non-incident to f, the type 2 are subgraphs isomorphic to a 3–path, and type 3 are triangles. Notice that every 3–path has been counted twice and each triangle has been counted thrice. Therefore, the number of subgraphs of type 1 is m(n–2), the number of type 2 is $P_3(F)$ and the number of type 3 is four. Therefore, $Ind_3(F) = 1/3(4h^3-10h+36)$, proving the theorem.

▼

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