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Modified eccentric connectivity index of fullerenes

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ABSTRACT. The eccentric connectivity index of a graph is defined as $\xi(\Gamma)=\Sigma_{u\in V(\Gamma)}\deg_\Gamma(u)e(u)$, where $\deg_\Gamma(u)$ denotes the degree of the vertex u in Γ and $e(u)$ is the eccentricity of vertex u. In this paper, the modified eccentric connectivity index of two infinite classes of fullerenes is computed.

Keywords: automorphism group, eccentric connectivity index, fullerene graph.

1. INTRODUCTION

Throughout this paper, all graphs are simple and connected. The vertex and edge sets of graph Γ are denoted by $V(\Gamma)$ and $E(\Gamma)$, respectively.

For two vertices $x,y\in V(\Gamma)$ the distance $d(x,y)$ is defined as the length of a shortest path between them. The eccentric connectivity index of the molecular graph Γ, was proposed by Sharma et al. [12] as

$$\xi(\Gamma)=\sum_{u\in V(\Gamma)}\deg_\Gamma(u)e(u), \quad (1)$$

where $\deg_\Gamma(u)$ denotes the degree of vertex u and $e(u)=\max\{d(u,x)\,|\,x\in V(\Gamma)\}$, see [1,2,3,7,10] for details. The eccentric connectivity polynomial of a graph Γ defined by Ghorbani et.al [8] as

$$ECP(\Gamma,x)=\sum_{u\in V(\Gamma)}\deg_\Gamma(u)x^{e(u)}. \quad (2)$$

Then the eccentric connectivity index is the first derivative of $ECP(\Gamma,x)$ evaluated at $x = 1$.

Došlić et al. [4] defined the total eccentricity of the graph Γ as follows:

$$\Theta(\Gamma)=\sum_{u\in V(\Gamma)} e(u). \quad (3)$$

An automorphism of graph Γ is a bijection α on $V(\Gamma)$ with this property that $e=xy$ is an edge if and only if $\alpha(e)=\alpha(x)\alpha(y)$ is an edge. The set of all automorphisms under the composition of mappings as an operation forms a group and we denote it by $Aut(\Gamma)$.

2. Results and Discussions

Graovać and Pisanski in [6] defined an algebraic version of Wiener index and they called it as modified Wiener index. Here, by following their work , we can define an algebraic approach for generalizing the eccentric connectivity index by automorphism group of the graph under consideration. We call this new version of eccentric connectivity index as symmetric eccentric connectivity index or modified eccentric connectivity index. Assume that Γ is a graph with automorphism group $Aut(\Gamma)$, then the modified eccentric connectivity index of Γ is defined as:

$$\hat{\xi}(\Gamma)=\sum_{u\in V(\Gamma)} \deg_{\Gamma}(u)\hat{e}(u), \quad (4)$$

where $\hat{e}(u)=\max\{d(u,\alpha(u))\mid \alpha\in Aut(\Gamma)\}$. The modified-total eccentricity then can be defined as $\hat{\Theta}(\Gamma)=\sum_{u\in V(\Gamma)}\hat{e}(u)$. For the k-regular graph Γ those two quantities are related as $\hat{\xi}(\Gamma)=k\hat{\Theta}(\Gamma)$.

Theorem 1. [9] Let Γ is a graph with automorphism group $Aut(\Gamma)$ and vertex set $V(\Gamma)$. Let $V_1, V_2, \ldots, V_k$ be all orbits of action $Aut(\Gamma)$ on $V(\Gamma)$. Then

$$\hat{\xi}(\Gamma)=\sum_{i=1}^{k}|V_i(\Gamma)|\deg_{\Gamma}(v_i)\hat{e}(v_i), \quad (5)$$

where v_i is an arbitrary vertex of V_i.

Corollary 2. [9] Let Γ is a vertex-transitive graph, then $\hat{\xi}(\Gamma)=\xi(\Gamma)$.

For given graph Γ, the difference between eccentric connectivity and modified eccentric connectivity indices can be defined as follows:

$$\varepsilon(\Gamma)=\xi(\Gamma)-\hat{\xi}(\Gamma). \quad (6)$$

By Corollary 2, it is clear that for a vertex-transitive graph, we have $\varepsilon(\Gamma)=0$. In general, the difference number determines the number of orbits of a graph under the group automorphism action. In other words, if the action of automorphism group of graph on the set of vertices has one orbit, then clearly the difference number is zero and the maximum possible of orbits which is equal with the number of vertices yields the maximum value of difference number. It should be noted that this value is not necessary a positive integer and it may be a negative. However, it seems that this value is zero if the considered graph is vertex-transitive and we left it as an open problem.

Example 1. It is easy to see that the symmetry group of complete graph K_n is isomorphic to the symmetric group S_n and so K_n is vertex-transitive with $\hat{\xi}(K_n) = n(n-1)$. Thus Corollary 2 implies that $\varepsilon(K_n) = 0$.

Example 2. Let K_{n_1,n_2} is a complete bipartite graph on $n = n_1 + n_2$ vertices, if $n_1 = n_2 = n/2$, then $K_{n/2,n/2}$ is vertex-transitive and Corollary 2 yields that $\varepsilon(K_{n/2,n/2}) = 0$. In addition, if $n_1 \neq n_2$, K_{n_1,n_2} is not vertex-transitive and clearly $\hat{\xi}(K_{n_1,n_2}) = \xi(K_{n_1,n_2}) = 4n_1n_2$. This means that $\varepsilon(K_{n_1,n_2}) = 0$.

Example 3. Let P_n is a path on n vertices, it is not difficult to see that the symmetry group of P_n is isomorphic with cyclic group $\mathbb{Z}_2 = \langle \alpha \rangle$ where

$$\alpha = \begin{cases} (1\ n)(2\ n-1)\ldots((n-1)/2\ \ (n+3)/2) & n \text{ is odd} \\ (1\ n)(2\ n-1)\ldots(n/2\ \ (n+3)/2) & n \text{ is even} \end{cases}.$$

If $n \geq 2$ is even, then

$$\hat{\xi}(P_n) = 2(n-1) + 4\sum_{i=1}^{(n/2)-1}(2i-1) = 2(n-1) + 4\left((n^2/4) - n + 1\right) = n^2 - 2n + 2,$$

and if $n \geq 3$ is odd, then $\hat{\xi}(P_n) = 2(n-1) + 4\sum_{i=1}^{\lfloor n/2 \rfloor - 1}(2i) = 2(n-1) + 4\left(\lfloor n/2 \rfloor^2 - \lfloor n/2 \rfloor\right)$. On the other hand, by a direct computation, one can see that for $n \geq 2$ and even, $\xi(P_n) = (3n^2/2) - 3n + 2$ and for $n \geq 3$ and odd, $\xi(P_n) = 3(n^2 - 1)/2$. Hence,

$$\varepsilon(\Gamma) = \begin{cases} n\left((n/2) - 1\right) & n \text{ is even} \\ (3n^2 - 1)/2 + 4\left(\lfloor n/2 \rfloor^2 - \lfloor n/2 \rfloor\right) - 5n & n \text{ is odd} \end{cases}.$$

Example 4. For the Cartesian product of a path and a cycle on n vertices, the eccentric connectivity and modified eccentric connectivity indices, can be computed as follows:

1) If n is even, then

$$\xi(P_n \times C_n) = 2\times|V(C_n)|\times\left(3\times\left(|E(P_n)|+\frac{|E(C_n)|}{2}\right)+4\times\sum_{i=1}^{(|E(C_n)|/2)-1}(|E(P_n)|+i)\right)$$
$$= 2n\left(3(n-1+(n/2))+4((5n^2/8)-(7n/4)+1)\right)$$
$$= n(5n^2-5n+2),$$

$$\hat{\xi}(P_n \times C_n) = 2\times|V(C_n)|\times\left(3\times\left(|E(P_n)|+\frac{|E(C_n)|}{2}\right)+4\times\sum_{i=1}^{(|E(C_n)|/2)-1}\left(\frac{|E(C_n)|}{2}+|E(P_n)|-2i\right)\right)$$
$$= 2n\left(3(n-1+(n/2))+4((n^2/2)-(3n/2)+1)\right)$$
$$= n(4n^2-3n+2).$$

2) If n is odd, then

$$\xi(P_n \times C_n) = |V(C_n)|\times\left(2\times\left(3\times\left(|E(P_n)|+\left[\frac{|E(C_n)|}{2}\right]\right)+4\times\sum_{i=1}^{[|E(C_n)|/2]-1}(|E(P_n)|+i)\right)+4\times|E(P_n)|\right)$$
$$= 2n\left(3(n-1+[n/2])+4\sum_{i=1}^{[n/2]-1}(n-1+i)+2(n-1)\right)$$
$$= 2n(2[n/2]^2+4n[n/2]-3[n/2]+n-1),$$
$$\hat{\xi}(P_n \times C_n) = |V(C_n)|\times\left(2\times\left(3\times\left(|E(P_n)|+\left[\frac{E(C_n)}{2}\right]\right)+4\sum_{i=1}^{[E(C_n)/2]-1}\left(\left[\frac{E(C_n)}{2}\right]+2i\right)\right)+4\left[\frac{E(C_n)}{2}\right]\right)$$
$$= 2n\left(3(n-1+[n/2])+4\sum_{i=1}^{[n/2]-1}([n/2]+2i)+2[n/2]\right)$$
$$= 6n\left(\frac{8}{3}[n/2]^2+n-[n/2]-1\right).$$

Thus, by using the definition of difference number, we have

$$\varepsilon(P_n \times C_n) = \begin{cases} n^2(n-2n^2) & n|2 \\ 4n\left(4n[n/2]-n-3[n/2]^2+1\right) & n\nmid 2 \end{cases}.$$

Example 5. Let S_n is a star graph on n vertices, then the vertices of S_n can be divided in to sets. The vertex of degree $n-1$ composes a singleton orbit and the other vertices compose the second orbit. This means that the automorphism group of S_n is isomorphic with symmetric group $Sym(n-1)$. Hence, $\hat{\xi}(S_n) = 2(n-1)$. On the other hand $\xi(S_n)=3(n-1)$. Thus, $\varepsilon(S_n)=n-1$. Similarly, for Wheel graph W_n on *n* vertices $\hat{\xi}(W_n)=7(n-1)$ and $\xi(W_n)=6(n-1)$. Then we conclude that $\varepsilon(W_n)=n-1$.

3. Application in fullerene graphs

A graph is called three regular or cubic, if the degree of each vertex is three. It is said to be 3-connected, if there does not exist a set of two vertices whose removal disconnects the graph. A planar, cubic and 3-connected graph is called a fullerene graph if all faces are pentagons and hexagons. The importance of fullerene graphs is for their applications in fullerene chemistry. This new topic has been developed after pioneering work of Kroto et al. [11]. The mathematical properties of fullerene graphs are a new branch of nanoscience started by pioneering work of Fowler et al. in [5].

The aim of this section is to compute the modified eccentric connectivity index for two classes of fullerenes, namely fullerene series F_{20n+4} ($n\geq 3$) and F_{20n+6} ($n\geq 4$), see Figures 1,3 respectively. The symmetry group of the fullerene F_{20n+4} is $\mathbb{Z}_2$. The symmetry group of fullerene graph F_{20n+6} is isomorphic to non-cyclic abelian group $\mathbb{Z}_2\times\mathbb{Z}_2$, when *n*=5*i*-1 (*i*≥1) and otherwise it is isomorphic with cyclic group $\mathbb{Z}_2$.

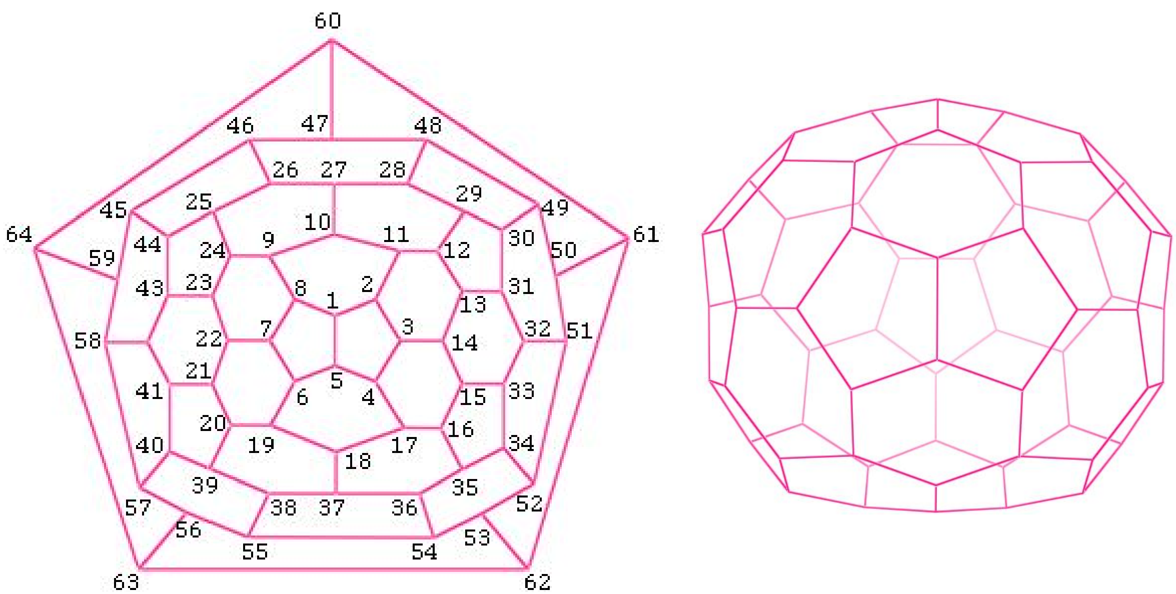

Figure 1. 2-*D* and 3-*D* graph F_{20n+4} for n = 3.

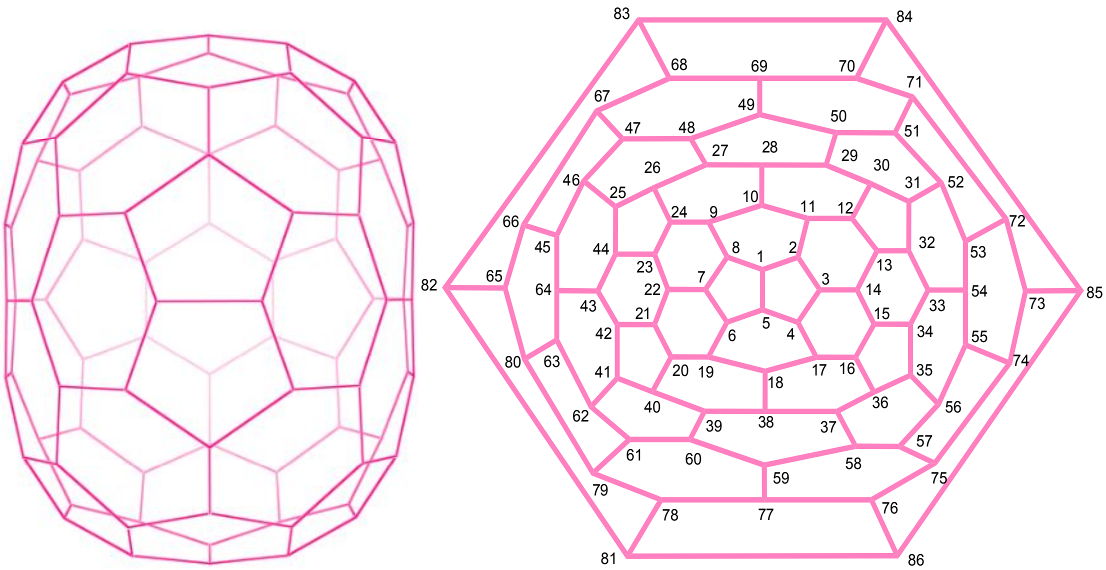

Figure 2. *2-D* and *3-D* graph F_{20n+6} for n = 4.

In Table 1, the eccentric connectivity of fullerenes $\xi(F_{20n+4})$ are computed, 3≤n≤16. For n≥17 we have the following theorem for the eccentric connectivity of this class of fullerenes.

Theorem 3. The eccentric connectivity of the fullerene F_{20n+4} (n≥17) is

$$\xi(F_{20n+4}) = 90n^2 + 84n + 45. \quad (7)$$

Proof. By means of group action of automorphism group of F_{20n+4} on the set of vertices, one can see that there are five types of vertices of fullerene graph as reported in the following table, see also Figure 3.

Types of vertices	$e(u)$	No.
Type 1	2n+2	7
Type 2	2n+1	11
Type 3	2n	16
Type 4	n+1	10
Type 5	2n-i (1≤i≤n-2)	20

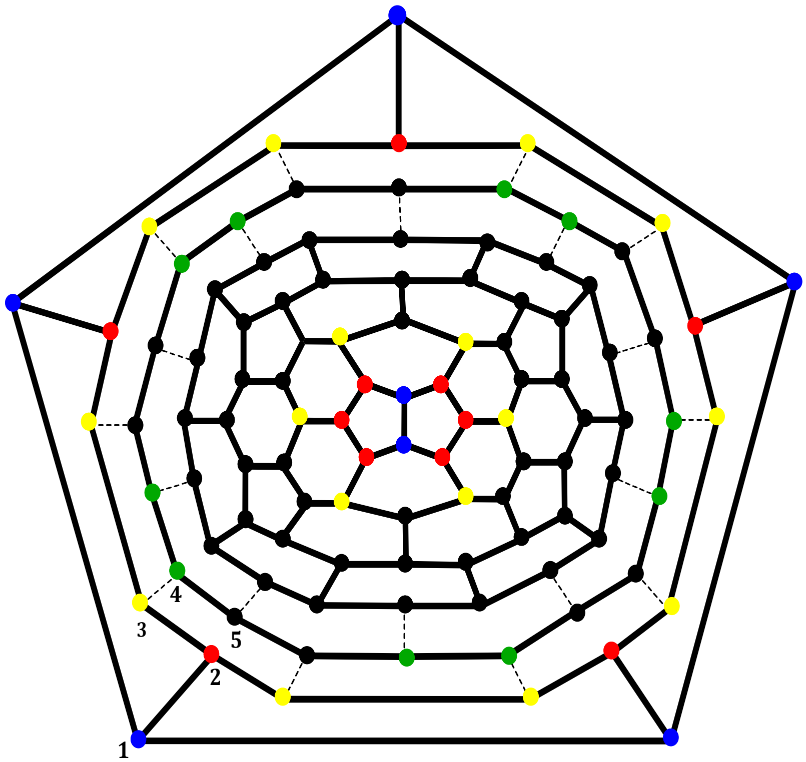

Fig. 3. Five different types of vertices in fullerene F_{20n+4}, where n≥17.

n	$\xi(F_{20n+4})$	n	$\xi(F_{20n+4})$
3	1740	10	10317
4	2724	11	12141
5	3699	12	14205
6	4773	13	16449
7	5949	14	18927
8	7257	15	21588
9	8673	16	24444

Table 1. The eccentric connectivity index of $\xi(F_{20n+4})$ for 3≤n≤16.

By continuing this method, the eccentric connectivity polynomial of the fullerene F_{20n+4} (n ≥17), can be computed as follows (see Fig. 3):

$$ECP(F_{20n+4},x) = 60x^{2n+1}\frac{x^{2n-1}-1}{x-1} + 21x^{2n+2} + 33x^{2n+1} + 48x^{2n} + 30x^{n+1}.$$

Thus, $\xi(F_{20n+4}) = 90n^2 + 84n + 45$ and the proof is completed.

Theorem 4. For the fullerene graph F_{20n+4} for $n \geq 17$, we have

$$\varepsilon(F_{20n+4}) = \begin{cases} 90n^2 - 216n + 315 & n \text{ is even} \\ 90n^2 - 216n + 261 & n \text{ is odd} \end{cases}.$$

Proof. By applying the methods of [1,4] for $n \geq 3$ we have:

$$\hat{\xi}(F_{20n+4}) = \begin{cases} 300n - 270 & n \text{ is even} \\ 300n - 216 & n \text{ is odd} \end{cases}. \quad (8)$$

The proof can be resulted from *Eq*.(7) and *Eq*.(8).

Theorem 5. The eccentric connectivity of the fullerene F_{20n+6} ($n \geq 17$) is

$$\xi(F_{20n+6}) = 90n^2 + 96n + 54. \quad (9)$$

Proof. By means of group action of automorphism group of F_{20n+6} on the set of vertices, one can see that there are five types of vertices of fullerene graph as reported in the following table, see also Fig. 4.

Types of vertices	$e(u)$	No.
Type 1	$2n+2$	8
Type 2	$2n+1$	12
Type 3	$2n$	16
Type 4	$n+1$	10
Type 5	$2n$-i ($1 \leq i \leq n$-2)	20

By continuing this method, the eccentric connectivity polynomial of the fullerene F_{20n+6} ($n \geq 17$), can be computed as follows (see Fig. 4):

$$ECP(F_{20n+6}, x) = 60x^{2n+1}\frac{x^{2n-1} - 1}{x - 1} + 24x^{2n+2} + 36x^{2n+1} + 48x^{2n} + 30x^{n+1}.$$

Thus, $\xi(F_{20n+6}) = 90n^2 + 96n + 54$ and the proof is completed.

Theorem 6. For the fullerene graph F_{20n+6} for $n \geq 17$, we have

$$\varepsilon(F_{20n+6}) = 90n^2 - 504n + 588.$$

Proof. By applying the methods of [1,4] for $n \geq 4$ we have:

$$\hat{\xi}(F_{20n+6}) = 600n - 534. \quad (10)$$

The proof can be resulted from *Eq*.(9) and *Eq*.(10).

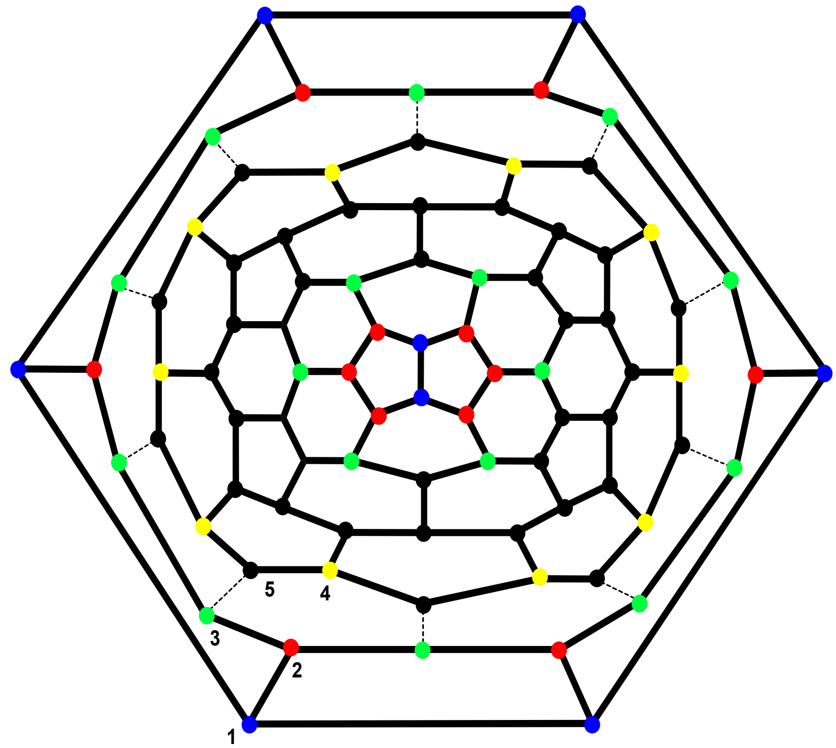

Fig. 4. five different types of vertices in fullerene F_{20n+6}, where n≥17.

n	$\xi(F_{20n+6})$	n	$\xi(F_{20n+6})$
4	2838	11	12288
5	3774	12	14364
6	4854	13	16620
7	6030	14	19110
8	7368	15	21780
9	8796	16	24648
10	10452		

Table 2. The eccentric connectivity index of $\xi(F_{20n+6})$ for 4≤n≤16.

4. CONCLUSION

In this paper, we computed the modified eccentric connectivity index of two infinite families of fullerene graphs and then we obtained the difference between eccentric connectivity and modified eccentric connectivity indices.

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