Modified eccentric connectivity index of fullerenes

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ABSTRACT. The eccentric connectivity index of a graph is defined as $\xi(\Gamma) = \sum_{u \in V(\Gamma)} \deg_{\Gamma}(u) e(u)$, where $\deg_{\Gamma}(u)$ denotes the degree of the vertex $u$ in $\Gamma$ 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 $\Gamma$ 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 $\Gamma$, was proposed by Sharma et al. [12] as

$$\zeta(\Gamma) = \sum_{u \in V(\Gamma)} \deg_{\Gamma}(u) e(u),$$  \hspace{1cm} (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 $\Gamma$ defined by Ghorbani et.al [8] as

$$ECP(\Gamma,x) = \sum_{u \in V(\Gamma)} \deg_{\Gamma}(u) x^{e(u)}.$$  \hspace{1cm} (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 \( \Gamma \) as follows:

\[
\Theta(\Gamma) = \sum_{u \in V(\Gamma)} e(u).
\] (3)

An automorphism of graph \( \Gamma \) is a bijection \( \alpha \) 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 \( \Gamma \) is a graph with automorphism group \( Aut(\Gamma) \), then the modified eccentric connectivity index of \( \Gamma \) is defined as:

\[
\hat{\xi}(\Gamma) = \sum_{u \in V(\Gamma)} \deg_r(u)\hat{e}(u),
\] (4)

where \( \hat{e}(u)=\max\{d(u,a(u))\mid a \in Aut(\Gamma)\} \). 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 \( \Gamma \) those two quantities are related as \( \hat{\xi}(\Gamma) = k\hat{\Theta}(\Gamma) \).

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

\[
\hat{\xi}(\Gamma) = \sum_{i=1}^{k} |V_i(\Gamma)|\deg_r(v_i)\hat{e}(v_i),
\] (5)

where \( v_i \) is an arbitrary vertex of \( V_i \).

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

For given graph \( \Gamma \), the difference between eccentric connectivity and modified eccentric connectivity indices can be defined as follows:

\[
\varepsilon(\Gamma) = \xi(\Gamma) - \hat{\xi}(\Gamma).
\] (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 necessarily 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

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

If $n \geq 2$ is even, then

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

and if $n \geq 3$ is odd, then

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

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,

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

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

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

2) If \(n\) is odd, then

\[
\xi(P_n \times C_n) = |V(C_n)| \times \left(2 \times 3 \times \left|E(P_n)\right| + \left\lceil \frac{|E(C_n)|}{2} \right\rceil\right) + 4 \times \sum_{i=1}^{\lfloor |E(C_n)|/2 \rfloor - 1} \left(\left|E(P_n)\right| + i\right) + 4 \times |E(P_n)| \\
= 2n \left(3(n-1+\lfloor n/2 \rfloor) + 4 \sum_{i=1}^{\lfloor n/2 \rfloor - 1} (n-1+i) + 2(n-1)\right) \\
= 2n(2\lfloor n/2 \rfloor^2 + 4n\lfloor n/2 \rfloor - 3\lfloor n/2 \rfloor + n - 1),
\]

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

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

\[
e(P_n \times C_n) = \begin{cases} 
    n^2(n-2n^2) & n \mid 2 \\
    4n(4n[n/2] - n - 3[n/2]^2 + 1) & n \not\mid 2
\end{cases}
\]

Example 5. Let \(S_n\) is a star graph on \(n\) vertices, then the vertices of \(S_n\) can be divided into 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 \( \xi(W_n) = 7(n-1) \) and \( \varepsilon(W_n) = 6(n-1) \). 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 \( n = 5i - 1 \) (\( i \geq 1 \)) and otherwise it is isomorphic with cyclic group \( \mathbb{Z}_2 \).

![Figure 1. 2-D and 3-D graph \( F_{20n+4} \) for \( n = 3 \).](image-url)
In Table 1, the eccentric connectivity of fullerenes $\zeta(F_{2n+4})$ are computed, $3 \leq n \leq 16$. For $n \geq 17$ we have the following theorem for the eccentric connectivity of this class of fullerenes.

**Theorem 3.** The eccentric connectivity of the fullerene $F_{20n+6}$ ($n \geq 17$) is

$$\zeta(F_{2n+4}) = 90n^2 + 84n + 45.$$  \hspace{1cm} (7)

**Proof.** By means of group action of automorphism group of $F_{2n+4}$ 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.

<table>
<thead>
<tr>
<th>Types of vertices</th>
<th>$e(u)$</th>
<th>No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type 1</td>
<td>$2n+2$</td>
<td>7</td>
</tr>
<tr>
<td>Type 2</td>
<td>$2n+1$</td>
<td>11</td>
</tr>
<tr>
<td>Type 3</td>
<td>$2n$</td>
<td>16</td>
</tr>
<tr>
<td>Type 4</td>
<td>$n+1$</td>
<td>10</td>
</tr>
<tr>
<td>Type 5</td>
<td>$2n-i$ ($1 \leq i \leq n-2$)</td>
<td>20</td>
</tr>
</tbody>
</table>

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

![Graph Image]
Fig. 3. Five different types of vertices in fullerene $F_{20n+4}$, where $n \geq 17$.

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

By continuing this method, the eccentric connectivity polynomial of the fullerene $F_{20n+4}$ ($n \geq 17$), 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

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

**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.

<table>
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</tr>
<tr>
<td>Type 2</td>
<td>( 2n+1 )</td>
<td>12</td>
</tr>
<tr>
<td>Type 3</td>
<td>( 2n )</td>
<td>16</td>
</tr>
<tr>
<td>Type 4</td>
<td>( n+1 )</td>
<td>10</td>
</tr>
<tr>
<td>Type 5</td>
<td>( 2n-i ) (1( \leq i \leq n-2 ))</td>
<td>20</td>
</tr>
</tbody>
</table>

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, \( \zeta(F_{20n+6})=90n^2 + 96n + 54 \) 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 $n \geq 17$.

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

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\xi(F_{20n+6})$</th>
<th>$n$</th>
<th>$\xi(F_{20n+6})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>2838</td>
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<td>5</td>
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<td></td>
</tr>
</tbody>
</table>

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.
REFERENCES


