Computing Vertex PI, Omega and Sadhana Polynomials of $F_{12(2n+1)}$ Fullerenes

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ABSTRACT

The topological index of a graph G is a numeric quantity related to G which is invariant under automorphisms of G. The vertex PI polynomial is defined as $\text{PI}_v(G) = \sum_{e \in G} n_u(e) + n_v(e)$. Then Omega polynomial $\Omega(G,x)$ for counting qoc strips in G is defined as $\Omega(G,x) = \sum m(G,c)x^c$ with $m(G,c)$ being the number of strips of length c. In this paper, a new infinite class of fullerenes is constructed. The vertex PI, omega and Sadhana polynomials of this class of fullerenes are computed for the first time.

Keywords: Fullerene, vertex PI polynomial, Omega polynomial, Sadhana polynomial.

1. INTRODUCTION

Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. Fullerenes $F_n$ can be drawn for $n = 20$ and for all even $n \geq 24$. They have $n$ carbon atoms, $3n/2$ bonds, 12 pentagonal and $n/2-10$ hexagonal faces. The most important member of the family of fullerenes is $C_{60}$ [1,2].

Let $\Sigma$ be the class of finite graphs. A topological index is a function $\text{Top}$ from $\Sigma$ into real numbers with this property that $\text{Top}(G) = \text{Top}(H)$, if G and H are isomorphic.

Let $G = (V,E)$ be a connected bipartite graph with the vertex set $V = V(G)$ and the edge set $E = E(G)$, without loops and multiple edges. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of G whose distance to the vertex v is smaller than u. The vertex PI index is a topological index which is introduced in [3]. It is defined as the sum of $[n_u(e) + n_v(e)]$, over all edges of a graph G. Let G be an arbitrary graph. Two edges $e = uv$ and $f = xy$ of G are called codistant (briefly: e co f ) if they obey the
topologically parallel edges relation. For some edges of a connected graph $G$ there are the following relations satisfied [4,5]:

$$e \co e \iff f \co e$$

$$e \co f, f \co h \Rightarrow e \co h$$

though the last relation is not always valid.

Set $C(e) := \{f \in E(G) \mid f \co e\}$. If the relation “co” is transitive on $C(e)$ then $C(e)$ is called an orthogonal cut “oc” of the graph $G$. The graph $G$ is called co-graph if and only if the edge set $E(G)$ is the union of disjoint orthogonal cuts.

Let $m(G,c)$ be the number of qoc strips of length $c$ (i.e., the number of cut-off edges) in the graph $G$, for the sake of simplicity, $m(G,c)$ will hereafter be written as $m$. Three counting polynomials have been defined [6-8] on the ground of qoc strips:

$$\Omega(G, x) = \sum_{c} m \cdot x^{c}, \quad \Theta(G, x) = \sum_{c} m \cdot c \cdot x^{c} \quad \text{and} \quad \Pi(G, x) = \sum_{c} m \cdot c \cdot x^{c-c}. \quad \Omega(G, x)$$

and $\Theta(G, x)$ polynomials count equidistant edges in $G$ while $\Pi(G, x)$, non-equidistant edges. In a counting polynomial, the first derivative (in $x=1$) defines the type of property which is counted; for the three polynomials they are:

$$\Omega'(G,1) = \sum_{c} m \cdot c \cdot |E(G)|, \quad \Theta'(G,1) = \sum_{c} m \cdot c \cdot 2 \quad \text{and} \quad \Pi'(G,1) = \sum_{c} m \cdot c \cdot (e - c).$$

If $G$ is bipartite, then a qoc starts and ends out of $G$ and so $\Omega(G, 1) = r / 2$, in which $r$ is the number of edges in out of $G$.

The Sadhana index $Sd(G)$ for counting qoc strips in $G$ was defined by Khadikar et. al. [9,10] as $Sd(G)=\sum_{c} m(G,c)(|E(G)|-c)$, where $m(G,c)$ is the number of strips of length $c$.

We now define the Sadhana polynomial of a graph $G$ as $Sd(G,x) = \sum_{c} m(G,c) \cdot x^{|E| - c}$. By definition of Omega polynomial, one can obtain the Sadhana polynomial by replacing $x^{c}$ with $x^{|E| - c}$ in omega polynomial. Then the Sadhana index will be the first derivative of $Sd(G, x)$ evaluated at $x = 1$. Herein, our notation is standard and taken from the standard book of graph theory [11-17].

Example 1. Let $C_n$ denotes the cycle of length $n$.

$$\Omega(C_n, x) = \begin{cases} \frac{n}{2} x^{2} & 2 \mid n \\ nx & 2 \nmid n \end{cases} \quad \text{and} \quad Sd(C_n, x) = \begin{cases} \frac{n}{2} x^{n-2} & 2 \mid n \\ nx^{n-1} & 2 \nmid n \end{cases}. $$

Example 2. Suppose $K_n$ denotes the complete graph on $n$ vertices. Then we have:
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$$\Omega(K_n, x) = \begin{cases} \frac{n}{2} \left( x^{\frac{n}{2}} + x^{\frac{n-1}{2}} \right) & 2 \mid n \\ \frac{n}{n} x^{\frac{n}{2}} & 2 \nmid n \end{cases}$$ and $Sd(K_n, x) = \begin{cases} \frac{n}{2} \left( x^{\frac{n}{2}}(n-2) + x^{\frac{n-2}{2}} \right) & 2 \mid n \\ \frac{n}{n} x^{\frac{n}{2}} & 2 \nmid n \end{cases}$

Example 3. Let $T_n$ be a tree on $n$ vertices. We know that $|E(T_n)| = n - 1$. So,
$$\Omega(T_n, x) = \Theta(T_n, x) = (n - 1)x, \quad Sd(T_n, x) = \Pi(T_n, x) = (n - 1)x^{n-2}.$$

2. **Main Results and Discussion**

The aim of this section is to compute the counting polynomials of equidistant (Omega, Sadhana and Theta polynomials) of an infinite family $F_{12(2n+1)}$ of fullerenes with $12(2n+1)$ carbon atoms and $36n+18$ bonds (the graph $F_{12(2n+1)}$, Figure 1 is $n = 4$).

**Theorem 4.** The omega polynomial of fullerene graph $F_{12(2n+1)}$ for $n \geq 2$ is as follows:
$$\Omega(F_{12(2n+1)}, x) = 12x^3 + 12x^{2n-2} + 6x^{n-1} + 3x^{2n+4}.$$  

**Proof.** By figure 1, there are four distinct cases of qoc strips. We denote the corresponding edges by $f_1$, $f_2$, $f_3$ and $f_4$. By the table 1 proof is completed.

<table>
<thead>
<tr>
<th>Edge</th>
<th>Co distance</th>
<th>Number of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f_1$</td>
<td>3</td>
<td>12</td>
</tr>
<tr>
<td>$f_2$</td>
<td>2n-2</td>
<td>12</td>
</tr>
<tr>
<td>$f_3$</td>
<td>2n+4</td>
<td>3</td>
</tr>
<tr>
<td>$f_4$</td>
<td>n-1</td>
<td>6</td>
</tr>
</tbody>
</table>

Table 1. The Number of Equidistant Edges.

**Corollary 5.** The Sadhana polynomial of fullerene graph $F_{12(2n+1)}$ is as follows:
$$Sd(F_{12(2n+1)}, x) = 12x^{36n+15} + 12x^{34n+20} + 6x^{35n+19} + 3x^{34n+14}.$$  

Now, we are ready to compute the vertex PI polynomial of fullerene graph $F_{12(2n+1)}$. It is well-known fact that an acyclic graph $T$ does not have cycles and so $n_u(e|G) + n_v(e|G) = |V(T)|$. Thus $P_i(T) = |V(T)|, |E(T)|$. Since a fullerene graph $F$ has 12 pentagonal faces, $P_i(F) < |V(F)|, |E(F)|$. Let $G$ be a connected graph. The $P_i$ polynomials of $G$ are defined as $P_i(G; x) = \sum_{e=uv \in E(G)} x^{n_u(e|G) + n_v(e|G)}$. Obviously $P_i(G, 1) = P_i(G)$ and $P_i(G, 1) =$...
\[ |E(G)|. \text{ Define } N(e) = |V| - (n_u(e) + n_v(e)). \text{ Then } PI_v(G) = \sum_{e \in E(G)} [V| - N(e)] = |V| \cdot |E| - \sum_{e \in E(G)} N(e) \text{ and we have:} \]

\[
PI_v(G, x) = \sum_{e \in \mathcal{E}(G)} x^{n_u(e) + n_v(e)} = \sum_{e \in \mathcal{E}(G)} x^{V(G) - N(e)} = x^{V(G)} \cdot \sum_{e \in \mathcal{E}(G)} x^{-N(e)}.
\]

**Figure 1.** The graph of fullerene $F_{12(2n+1)}$ for $n = 4$.

**Example 6.** Suppose $F_{30}$ denotes the fullerene graph on 30 vertices, see Figure 2. Then $PI_v(F_{30}, x) = 10x^{20} + 10x^{22} + 20x^{26} + 5x^{30}$ and so $PI_v(F_{30}) = 1090$.

**Figure 2.** The Fullerene Graph $F_{30}$. 
Theorem 7. The vertex PI polynomial of fullerene graph $F_{12(2n+1)}$ for $n \geq 2$ is as follows:

$$
\text{PI}_v(F_{12(2n+1)}, x) = 24x^{24n-64} + 12x^{24n-44} + 12x^{24n-12} + 6(n-3)x^{24n-4} + 24x^{24n-2} + 24x^{24n} + 24x^{24n+6} + 24x^{24n+8} + 24x^{24n+10} + 6(5n-22)x^{24n+12}.
$$

Proof. From Figures 3, one can see that there are ten types of edges of fullerene graph $F_{12(2n+1)}$. We denote the corresponding edges by $e_1, e_2, \ldots, e_{10}$. By table 2 the proof is completed.

<table>
<thead>
<tr>
<th>Edge</th>
<th>Number of vertex which are codistance from two ends of edges</th>
<th>Num</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_1$</td>
<td>0</td>
<td>6(5n-22)</td>
</tr>
<tr>
<td>$e_2$</td>
<td>2</td>
<td>12</td>
</tr>
<tr>
<td>$e_3$</td>
<td>4</td>
<td>12</td>
</tr>
<tr>
<td>$e_4$</td>
<td>6</td>
<td>24</td>
</tr>
<tr>
<td>$e_5$</td>
<td>12</td>
<td>24</td>
</tr>
<tr>
<td>$e_6$</td>
<td>14</td>
<td>24</td>
</tr>
<tr>
<td>$e_7$</td>
<td>16</td>
<td>6(n-3)</td>
</tr>
<tr>
<td>$e_8$</td>
<td>24</td>
<td>12</td>
</tr>
<tr>
<td>$e_9$</td>
<td>56</td>
<td>12</td>
</tr>
<tr>
<td>$e_{10}$</td>
<td>76</td>
<td>24</td>
</tr>
</tbody>
</table>

Table 2. Computing $N(e)$ for Different Edges.

![Figure 3](https://example.com/figure3.png)

Figure 3. Types of Edges of Fullerene Graph $F_{12(2n+1)}$. 
REFERENCES