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Computing omega and Sadhana polynomials of an infinite class of fullerenes $F_{4\times 3^n}$

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The Omega polynomial was defined by M. V. Diudea as $\Omega(x)=\sum_{e=uv} x^{n(e)}$, where the number of edges co -distant with e is denoted by n(e). One can obtain the Sadhana polynomial by replacing $x^{n(e)}$ with $x^{|E|-n(e)}$ in Omega polynomial. Then the Sadhana index will be the first derivative of Sd(x) evaluated at x = 1. In the present study, compute the Omega and Sadhana polynomials of a new infinite class of fullerenes is computed for the first time.

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1. Introduction

Although graph theory is one of the younger branches of mathematics, it is fundamental to a number of applied fields, including operations research, computer science, and nanostructures. In this paper we discuss the basic concepts of graph theory from the point of view of nanostructures.

Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. The discovery of C_{60} bucky-ball, which has a nanometer-scale hollow spherical structure in 1985 by Kroto and Smalley revealed a new form of existence of carbon element other than graphite, diamond and amorphous carbon [1, 2]. In many of mathematical papers fullerenes with pentagonal and hexagonal faces were studied but other structures of fullerenes are very important too. In this paper we consider a class of fullerenes $F_{4\times 3^n}$ with trigonal and hexagonal faces. 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. Suppose p, h, n and m be the number of trigonal, hexagons, carbon atoms and bonds between them, in a given fullerene F. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is n = (3p+6h)/3, the number of edges is m = (3p+6h)/2 = 3/2n and the number of faces is f = p + h. By the Euler's formula n − m + f = 2, one can deduce that (3p+6h)/3 – (3p+6h)/2 + p + h = 2, and therefore p = 4. This implies that such molecules, made entirely of n carbon atoms, have 4 trigonal and (n/2 – 2) hexagonal faces.

The distance d(x, y) between x and y is defined as the length of a minimum path between x and y. Two edges e = ab and f = xy of G are called co -distant, "e co f", if and only if d(a, x) = d(b, y) = k and d(a, y) = d(b, x) = k+1 or vice versa, for a non-negative integer k. It is easy to see that the relation "co" is reflexive and symmetric but it is not necessary to be transitive. The Omega polynomial has been defined by M. V. Diudea as follows [3-7]:

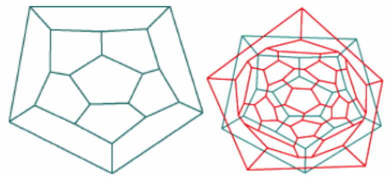
$$\Omega(x)=\sum_e x^{n(e)}$$

where, n(e) denotes the number of edges co –distant with the edge e. It is easy to see that the Omega polynomial $\Omega(x)$ counts equidistant edges in graph G.

A topological index of a graph G is a numeric quantity related to G. The oldest topological index is the Wiener index which introduced by Harold Wiener [7]. The Sadhana index Sd(G) for counting qoc strips in G was defined by Khadikar et al.[8,9] as $Sd(G)=\sum_e(|E(G)|-n(e))$. Also, the Sadhana polynomial of a graph G as defined by Ashrafi et al. [10] as $Sd(x)=\sum_e x^{|E|-n(e)}$ By definition of Omega polynomial, one can obtain the Sadhana polynomial by replacing $x^{n(e)}$ with $x^{|E|-n(e)}$ in omega polynomial. Then the Sadhana index will be the first derivative of Sd(x) evaluated at x = 1.

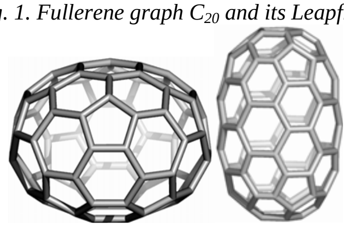
A method [11,12] has been described on how to construct a fullerene C_{3n} from a fullerene C_n having the same or even a bigger symmetry group as C_n. This method is called the Leapfrog principle. If one starts with a C_n cluster with icosahedral symmetry, all the new clusters will be of the same symmetry, since this is the biggest symmetry group in 3-dimensional space. In the first step, an extra vertex has to be put into the centre of each face of C_n. Then, these new vertices have to be connected with all the vertices surrounding the corresponding face. Then, the dual polyhedron is again a fullerene having 3n vertices, 12 pentagonal and (3n/2) – 10 hexagonal faces.

Throughout this paper, our notation is standard and taken from the standard book of graph theory [13]. In Fig. 1, one can see that the fullerene graph C_{20} and its Leapfrog, namely C_{60}. Also, in Figs. 2 the 3 dimentional Leapfrog graph of C_{24} and C_{30} are depicted. We denote the Leapfrog of graph G by Le(F).



$Le(C_{20}) = C_{60}$.

Fig. 1. Fullerene graph C_{20} and its Leapfrog.



$L(C_{20}) = C_{60}$.

Fig. 2. $Le(C_{24})$ and $Le(C_{30})$.

We encourage the reader to consult papers by Ashrafi et al. and Ghorbani et al. [14-28].

2. Results and discussion

In this section by using definition of Omega and Sadhana polynomials, we compute these counting polynomials for a special class of fullerenes, namely $F_{4\times 3^n}$. In other word, $F_{4\times 3^n}$ is an infinite family of fullerenes with 4×3^n carbon atoms and $2\times 3^{n+1}$ bonds (the graph G, Figure 1 is n=1) constructed by Leapfrog principle. At first we should to compute some computational examples.

Example 1. Suppose F_{12} denotes the fullerene graph on 12 vertices (Figure 3). The co – distant edges are shown by the same colours. Then $\Omega(x) = 6x^3$ and $Sd(x) = 6x^9$.

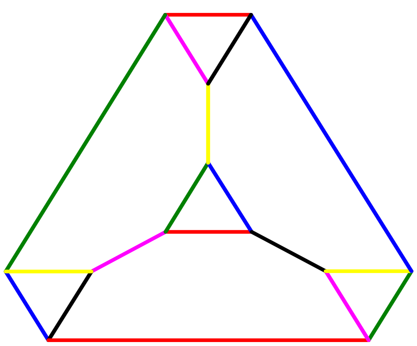


Fig. 3. The fullerene graph F_{12}.

Example 2. Consider the fullerene graph F_{36} with 36 vertices, Fig. 4. Then one can see that $\Omega(x) = 6x^6 + 6x^3$ and $Sd(x) = 6x^{30} + 6x^{33}$.

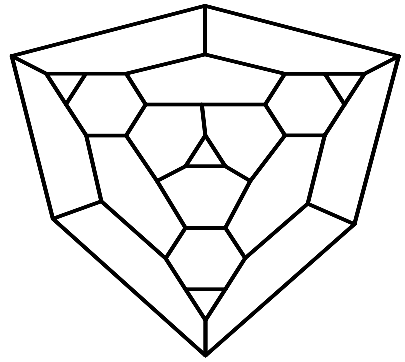


Fig. 4. The fullerene fraph F_{36}.

Example 3. The Omega and Sadhana polynomials of fullerene graph F_{108} (Figure 5) are as follows:

$$\Omega(x) = 6x^9 + 6x^{18} \text{ and } Sd(x) = 6x^{90} + 6x^{99}.$$

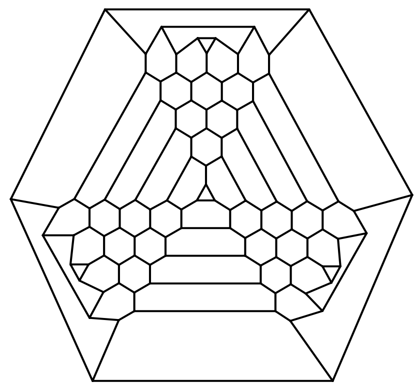


Fig. 5. The fullerene graph F_{108}.

Theorem. Consider the fullerene graph $F_{4\times 3^n}$, see Fig. 6. Then

$$\Omega(x) = \begin{cases} 6x^{3^{\frac{n+1}{2}}} + \left(\sum_{k=0}^{\frac{n-1}{2}} 6\times 3^k\right) x^{6\times 3^{\frac{n-1}{2}}} & 2 \nmid n \\ 6x^{3^{\frac{n}{2}+1}} + \left(\sum_{k=0}^{\frac{n}{2}-1} 6\times 3^k\right) x^{6\times 3^{\frac{n}{2}}} & 2 \mid n \end{cases}.$$

Proof. By Fig. 6, there are two distinct cases of qoc strips. We denote the corresponding edges by e_1 and e_2. By using Table 1 and Fig. 6 the proof is completed.

Table 1. The number of co-distant edges of e_i, $i = 1, 2$.

No.	Number of co-distant edges	Type of Edges
$\Omega(x) = \begin{cases} \sum_{k=0}^{\frac{n-1}{2}} 6\times 3^k & 2 \nmid n \\ \sum_{k=0}^{\frac{n}{2}-1} 6\times 3^k & 2 \mid n \end{cases}.$	18	e_1
6	9	e_2

Corollary 1.

$$Sd(x)=\begin{cases} 6x^{|E|-3^{\frac{n+1}{2}}}+\left(\sum_{k=0}^{\frac{n-1}{2}} 6\times 3^k\right)x^{|E|-6\times 3^{\frac{n-1}{2}}} & 2\nmid n \\ 6x^{|E|-3^{\frac{n}{2}+1}}+\left(\sum_{k=0}^{\frac{n}{2}-1} 6\times 3^k\right)x^{|E|-6\times 3^{\frac{n}{2}}} & 2\mid n \end{cases}.$$

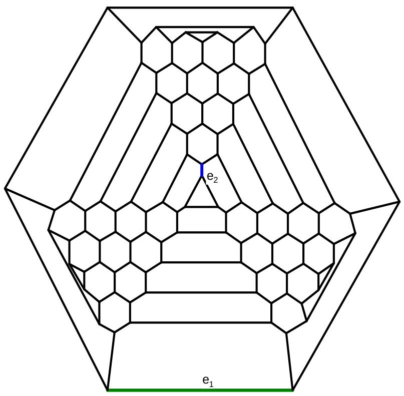


Fig. 6.The graph of fullerene $F_{4\times 3^n}$ *for n = 3.*

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