Computing counting polynomials of leapfrog fullerenes $F_{26\times3^n}$

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Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. The omega polynomial was defined as $\Omega(G,x)=\sum_c m\cdot x^c$, in which *m*(*G*, *c*) is the number of strips of length *c*. 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. In this paper, the Omega and Sadhana polynomials of a new infinite class of fullerenes constructed by leapfrog principle is computed.

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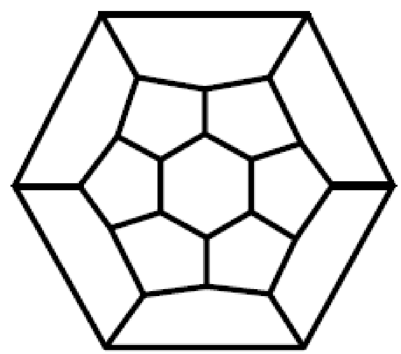
1. Introduction

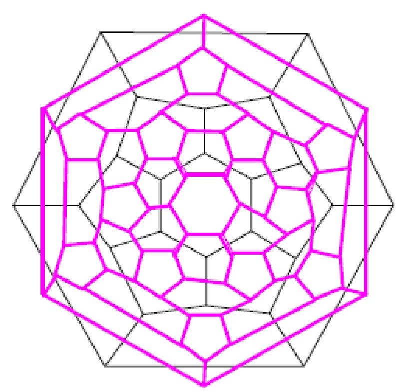
The discovery of C_{60} bucky-ball, which has a nanometer-scale hollow spherical structure in 1985 by Kroto [1, 2] and Smalley revealed a new form of existence of carbon element other than graphite, diamond and amorphous carbon [3, 4]. A fullerene graph is a cubic 3-connected plane graph. Let *p*, *h*, *n* and m be the number of pentagons, 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 = (5*p*+6*h*)/3, the number of edges is *m* = (5*p*+6*h*)/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 (5p+6h)/3 – (5p+6h)/2 + *p* + *h* = 2, and therefore *p* = 12, *n* = 2*h* + 20 and *m* = 3*h* + 30. This implies that such molecules, made entirely of *n* carbon atoms, have 12 pentagonal and (*n*/2 − 10) hexagonal faces, while $n \neq 22$ is a natural number equal or greater than 20.

Let *G* = (*V, E*) be a connected graph with the vertices set *V* = *V*(*G*) and the edges set *E* = *E*(*G*), without loops and multiple edges. The distance *d*(*x,y*) between *x* and *y* is defined as the length of a minimum path between x and y.

Let *G* be a fullerene graph on n vertices. A leapfrog transform G^l of *G* is a graph on 3*n* vertices obtained by truncating the dual of *G*. Hence, $G^l = Tr(G^*)$, where G^* denotes the dual of *G*. It is easy to check that G^l itself is a fullerene graph. We say that G^l is a leapfrog fullerene obtained from *G* and write $G^l = Le(G)$. In the other word, for a given fullerene F_n put an extra vertex into the centre of each face of F_n. Then connect these new vertices with all the vertices surrounding the corresponding face. Then the dual polyhedron is again a fullerene having 3*n* vertices 12 pentagonal and (3*n*/2)-10 hexagonal faces. From Fig. 1, one can see that $Le(C_{20}) = C_{60}$. For a more thorough introduction and treatment of leapfrog fullerenes we refer the reader to [5, 6]. Through this paper all notations are standard and mainly taken from [7, 8, 14-23].



F_{24}



$Le(F_{24})$

Fig. 1. The leapfrog of graph F_{24}.

Two edges $e = ab$ and $f = xy$ of G are called codistant, "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. 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 $E(G)$ a union of disjoint orthogonal cuts. If any two consecutive edges of an edge-cut sequence are topologically parallel within the same face of the covering, such a sequence is called a quasi-orthogonal cut *qoc* strip. Let G be an arbitrary connected graph and s_1, s_2, ..., s_k be the *ops* strips of a plane graph G. Then the *ops* strips form a partition of $E(G)$ and the Ω-polynomial15 of G is defined as

$$\Omega(x) = \sum_{i=1}^{k} x^{|S_i|} \quad (1)$$

Let now consider the set of edges *co*-distant to edge e in G, $c(e)$. A θ - polynomial counting the edges equidistant to all the reference edges e, is written as

$$\theta(x) = \sum_{e \in E(G)} x^{|C(e)|} \quad (2)$$

A third polynomial also related to the ops in G, but counting the non-opposite edges is the *Sadhana Sd* polynomial defined as

$$Sd(x) = \sum_{i=1}^{k} x^{|E|-|S_i|} \quad (3)$$

The Sadhana index $Sd(G)$ for counting *qoc* strips in G was defined by Khadikar et al [12, 13] as $Sd(x) = \sum_{i=1}^{k} |E(G)| - |S_i|$. By definition of Omega polynomial, one can obtain the Sadhana polynomial by replacing $x^{|S_i|}$ with $x^{|E|-|S_i|}$ in omega polynomial. Then the Sadhana index will be the first derivative of $Sd(x)$ evaluated at $x = 1$.

2. Main results and discussion

The aim of this paper is computing Omega and Sadhana polynomials of leapfrog fullerenes of F_{26}. In the other word by using the leapfrog principle we can construct an infinite class of fullerenes denoted by $F_{26\times3^n}$. We compute Omega and Sadhana polynomials of $F_{26\times3^n}$. To do it at first we should consider the following examples.

Example 1. Let F_{20} be a fullerene with 20 vertices depicted in Fig. 2. It is easy to see that $|E(F_{20})| = 30$. By computing the quasi-orthogonal cut *qoc* strips of F_{20} one can see that the Omega and Sadhana polynomials are as $\Omega(F_{20}, x) = 30x$ and $Sd(F_{20}, x) = 30x^{29}$.

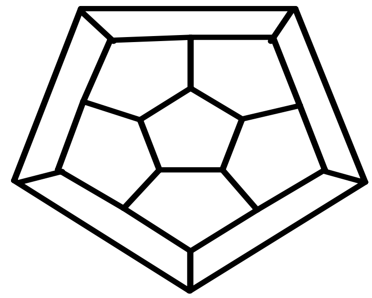
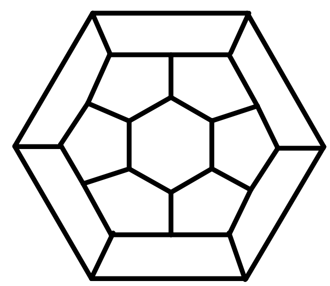
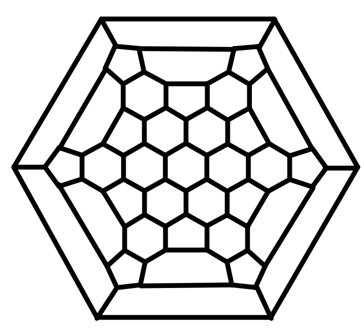


Fig. 2. The graph of fullerene F_{20}.

Example 2. Consider the fullerene graph F_{24}. This fullerene graph has 36 edges. Similar to example 1 one can see that $\Omega(F_{24}, x) = 24x + 6x^2$ and so, $Sd(F_{24}, x)= 24x^{35} + 6x^{34}$. In Fig. 3 one can see the planer graphs F_{24} and $Le(F_{24})$.



F_{24}



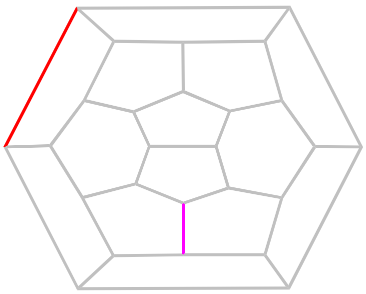
$Le(F_{24})$

Fig. 3. The leapfrog of graph F_{24}.

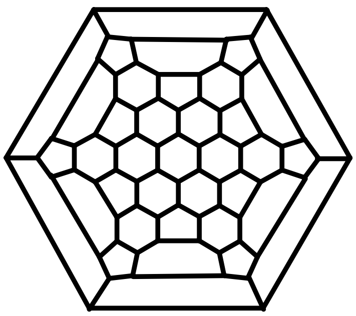
Example 3. Consider the fullerene graph F_{26}. This fullerene graph has 39 edges. Similar to example 1,2 one can see that $\Omega(F_{26}, x) = 21x + 9x^2$ and so, $Sd(F_{24}, x)= 21x^{38} + 9x^{37}$. By computing these polynomials for the leapfrog fullerene we have:

$$\Omega(\mathrm{Le}\ (\mathrm{C26}), \mathrm{x}) = 24\mathrm{x}^3 + 6\mathrm{x}^6 + \mathrm{x}^9.$$

In Fig. 4 one can see fullerenes F_{26} and $Le(F_{26})$.



F_{26}



$Le(F_{26})$

Fig. 4. The leapfrog of graph F_{26}.

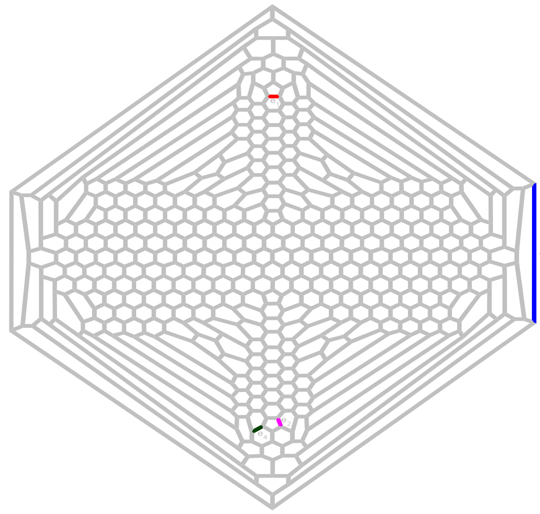
By continuing of this method we can consult the graph of fullerene $\mathrm{F}_{26\times 3^{n}}$. It is necessary to consider two cases. At first suppose n be even. By Fig. 5(i), one can prove there are four types of edges for *qoc* strips. We denote them by e_1, e_2, e_3 and e_4. By the table 1, $|C(e_1)| = 3^{n/2}$, $|C(e_2)| = 2 \times 3^{n/2}$, $|C(e_3)| = 2 \times 3^{n/2+1}$ and $|C(e_4)| = 7 \times 3^{n/2+1}$. In the other word there are 21, 9, $3(3^{n/2}-1)$ and $3^{n/2}-1$ edges of type e_1, e_2, e_3 and e_4, respectively. Now let n be odd. By the same way we can see there are four types of edges for *qoc* strips. We name them by e_1, e_2, e_3 and e_4. On the other hand $|C(e_1)| = 3^{(n+1)/2}$, $|C(e_2)| = 2 \times 3^{(n+1)/2}$, $|C(e_3)| = 3^{(n+3)/2}$ and $|C(e_4)| = 11 \times 3^{(n+3)/2}$ and one can see that there are 24, 6, $3^{n/2} - 1$, $2 \times 3^{(n-1)/2}-1$ and $3^{(n-1)/2}-1$ edges of type e_1, e_2, e_3 and e_4, respectively. Hence, we proved the following theorem:

Theorem 4. Consider the fullerene graph $\mathrm{F}_{26\times 3^{n}}$ $(n \geq 2)$ depicted in Fig. 5. Then the Omega polynomial is as follows:

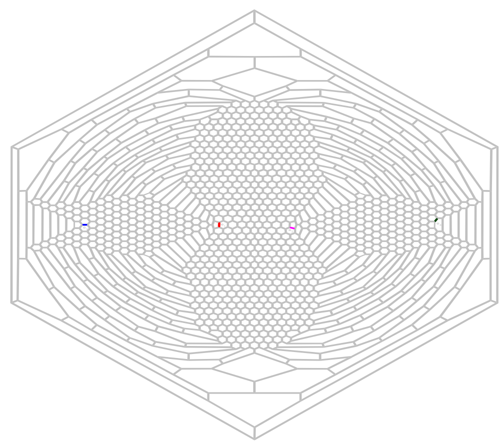
$$\Omega(x) = \begin{cases} 24x^{3^{(n+1)/2}} + 6x^{2\times 3^{(n+1)/2}} + (2\times 3^{(n-1)/2}-1)x^{3^{(n+3)/2}} + (3^{(n-1)/2}-1)x^{11\times 3^{(n+3)/2}} & 2 \nmid n \\ 21x^{3^{n/2}} + 9x^{2\times 3^{n/2}} + (3^{n/2}-1)(3x^{2\times 3^{n/2+1}} + x^{7\times 3^{n/2+1}}) & 2 \mid n \end{cases}$$

Corollary 5. For the fullerene graph $\mathrm{F}_{26\times 3^{n}}$ $(n \geq 2)$ the Sadhana polynomial is as follows:

$$Sd(x) = \begin{cases} 24x^{|E|-3^{(n+1)/2}} + 6x^{|E|-2\times 3^{(n+1)/2}} + (2\times 3^{(n-1)/2}-1)x^{|E|-3^{(n+3)/2}} + (3^{(n-1)/2}-1)x^{|E|-11\times 3^{(n+3)/2}} & 2 \nmid n \\ 21x^{|E|-3^{n/2}} + 9x^{|E|-2\times 3^{n/2}} + (3^{n/2}-1)(3x^{|E|-2\times 3^{n/2+1}} + x^{|E|-7\times 3^{n/2+1}}) & 2 \mid n \end{cases}.$$



(a)



(b)

Fig. 5. (a). The graph of $F_{26\times 3^{n}}$ for $n = 3$; (b). The graph of $F_{26\times 3^{n}}$ for $n = 4$.

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