On F-Polynomial, Multiple and Hyper F-Index of Some Molecular Graphs

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Abstract. A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix which represent the whole graph, and these representations are aimed to be uniquely defined for that graph. Topological index is a numeric quantity with a graph which characterizes the topology of the graph and is invariant under graph automorphism. In this paper, we compute *F-polynomial*, *Multiple F-index* and *Hyper F-index* for some special graphs.

Introduction

A graph $G = (V, E)$ with vertex set V and edge set E is connected, if there exists a connection between any pair of vertices in G . For a graph G , the degree of a vertex v is the number of edges incident with v and denoted by $d_G(v)$.

Topological indices are numbers associated with molecular graphs for the purpose of allowing quantitative structure-activity/property relationships [6]. Topological indices correlate certain physico-chemical properties like boiling point, stability, strain energy etc of chemical compounds.

The idea of topological index appears from work done by Harold Wiener (see [9]) in 1947 although he was working on boiling point of Paraffin. He called this index as Wiener index and then theory of topological index started. A pair of molecular descriptors known as the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$, first appeared in the topological formula for the total π - *electron* energy of conjugated molecules that has been derived in 1972 by I. Gutman and N. Trinajstić (see [5]). The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a molecular graph G are respectively defined as

$$M_1(G) = \sum_{u \in V(G)} d_G^2(u) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v).$$

In the same paper, another topological index, defined as the sum of cubed degrees of the vertices of a graph, was also shown to relate π - *electron* energy. However, this index was never studied in detail then. In 2015, Furtula and Gutman [2] have restudied this index to establish some basic properties and have also demonstrated that the predictive ability of this index is similar to that of the first Zagreb index with respect to entropy and acetic factors of the molecules and both first Zagreb index and this index yield correlation coefficients greater than 0.95. They named this index the "*Forgotten topological index*" or "*F-index*". In symbolic notation, the *F-index* is given as follows:

$$F(G) = \sum_{u \in V(G)} d_G^3(u) = \sum_{uv \in E(G)} [d_G^2(u) + d_G^2(v)].$$

Similar to the *first Zagreb polynomial* [4], *first multiple Zagreb index* [3] and *hyper Zagreb index* [8], the *F-polynomial*, *multiple F-index* and *hyper F-index* of a graph G respectively are defined as

$$F(G, x) = \sum_{uv \in E(G)} x^{[d_G^2(u) + d_G^2(v)]} \quad (1)$$

$$PF(G) = \prod_{uv \in E(G)} [d_G^2(u) + d_G^2(v)] \quad (2)$$

$$HF(G) = \sum_{uv \in E(G)} [d_G^2(u) + d_G^2(v)]^2. \quad (3)$$

Siddiqui et al. in [7] presented the Zagreb indices and Zagreb polynomials of different nanostar dendrimers. In [1], N.De et al. computed F-index and F-polynomial of six infinite classes of dendrimer nanostars, namely: $NS_1[n]$, $NS_2[n]$, $NS_3[n]$, $NS_4[n]$, $NS_5[n]$ and D_n . In this paper, we obtain, F-polynomial, multiple and hyper F-index for some molecular graphs namely *Dandelion graph*, *Friendship graph*, *Comet graph*, *t-fold bristled graph* of P_n and C_n , *Fence* and *Closed fence graph*, *Tadpole graph*, *Ladder graph* and *Wheel*.

Fig. 1: Dandelion graph $D(17, 8)$

Main Results

Let $D(n, l)$ be a Dandelion graph with n vertices, consisted of a copy of the star S_{n-l} and a copy of a path P_l with vertices $p_0, p_1, \dots, p_{l-1}$, where p_0 is identified with a star center. (See Fig. 1)

Theorem 1. Let $D(n, l)$ be a Dandelion graph. Then

$$\begin{aligned} F(D(n, l), x) &= x^5 + (n-l)x^{(n-l+1)^2+1} + x^{(n-l+1)^2+4} + (l-3)x^8 \\ PF(D(n, l)) &= 5 \times [1 + (n-l+1)^2]^{(n-l)} \times [4 + (n-l+1)^2] \times 8^{(l-3)} \\ HF(D(n, l)) &= 25 + (n-l)[1 + (n-l+1)^2]^2 + [4 + (n-l+1)^2]^2 + 64(l-3). \end{aligned}$$

Proof. Let G be a Dandelion graph $D(n, l)$. The edge set of G is divided into four edge partition based on the degrees of end vertices. We have

$$E(G) = \bigcup_{i=1}^4 E_i(G)$$

where

$$\begin{aligned} E_1(G) &= \{e = uv \in E(G) : d_G(u) = 1 \text{ and } d_G(v) = 2\} \\ E_2(G) &= \{e = uv \in E(G) : d_G(u) = 1 \text{ and } d_G(v) = n-l+1\} \\ E_3(G) &= \{e = uv \in E(G) : d_G(u) = n-l+1 \text{ and } d_G(v) = 2\} \\ E_4(G) &= \{e = uv \in E(G) : d_G(u) = 2 \text{ and } d_G(v) = 2\}. \end{aligned}$$

Hence, $|E_1(G)| = 1$, $|E_2(G)| = n - l$, $|E_3(G)| = 1$ and $|E_4(G)| = l - 3$. Now using Eqs.(1)-(3), we have

$$\begin{aligned}
 F(G, x) &= \sum_{uv \in E(G)} x^{[d_G^2(u) + d_G^2(v)]} \\
 &= \sum_{uv \in E_1(G)} x^{[d_G^2(u) + d_G^2(v)]} + \sum_{uv \in E_2(G)} x^{[d_G^2(u) + d_G^2(v)]} \\
 &+ \sum_{uv \in E_3(G)} x^{[d_G^2(u) + d_G^2(v)]} + \sum_{uv \in E_4(G)} x^{[d_G^2(u) + d_G^2(v)]} \\
 &= \sum_{uv \in E_1(G)} x^5 + \sum_{uv \in E_2(G)} x^{(n-l+1)^2+1} + \sum_{uv \in E_3(G)} x^{(n-l+1)^2+4} + \sum_{uv \in E_4(G)} x^8 \\
 &= |E_1(G)|x^5 + |E_2(G)|x^{(n-l+1)^2+1} + |E_3(G)|x^{(n-l+1)^2+4} + |E_4(G)|x^8 \\
 &= x^5 + (n-l)x^{(n-l+1)^2+1} + x^{(n-l+1)^2+4} + (l-3)x^8
 \end{aligned}$$

$$\begin{aligned}
 PF(G) &= \prod_{uv \in E(G)} [d_G^2(u) + d_G^2(v)] \\
 &= \prod_{uv \in E_1(G)} [d_G^2(u) + d_G^2(v)] \times \prod_{uv \in E_2(G)} [d_G^2(u) + d_G^2(v)] \\
 &\times \prod_{uv \in E_3(G)} [d_G^2(u) + d_G^2(v)] \times \prod_{uv \in E_4(G)} [d_G^2(u) + d_G^2(v)] \\
 &= 5^{|E_1(G)|} \times [(n-l+1)^2 + 1]^{|E_2(G)|} \times [(n-l+1)^2 + 4]^{|E_3(G)|} \times 8^{|E_4(G)|} \\
 &= 5 \times [(n-l+1)^2 + 1]^{(n-l)} \times [(n-l+1)^2 + 4] \times 8^{(l-3)}
 \end{aligned}$$

$$\begin{aligned}
 HF(G) &= \sum_{uv \in E(G)} [d_G^2(u) + d_G^2(v)]^2 \\
 &= \sum_{uv \in E_1(G)} [d_G^2(u) + d_G^2(v)]^2 + \sum_{uv \in E_2(G)} [d_G^2(u) + d_G^2(v)]^2 \\
 &+ \sum_{uv \in E_3(G)} [d_G^2(u) + d_G^2(v)]^2 + \sum_{uv \in E_4(G)} [d_G^2(u) + d_G^2(v)]^2 \\
 &= 25|E_1(G)| + [(n-l+1)^2 + 1]^2|E_2(G)| + [(n-l+1)^2 + 4]^2|E_3(G)| + 64|E_4(G)| \\
 &= 25 + (n-l)[(n-l+1)^2 + 1]^2 + [(n-l+1)^2 + 4]^2 + 64(l-3).
 \end{aligned}$$

□

A friendship graph (or Dutch windmill graph) F_m is a graph with $2m + 1$ vertices and $3m$ edges constructed by joining m copies of the cycle graph C_3 with a common vertex. (See Fig. 2)

Theorem 2. Let F_m be a friendship graph. Then

$$\begin{aligned}
 F(F_m, x) &= 2mx^{4m^2+4} + mx^8 \\
 PF(F_m) &= (4 + 4m^2)^{2m} \times 8^m \\
 HF(F_m) &= 2m(4 + 4m^2)^2 + 64m.
 \end{aligned}$$

 Fig. 2: Friendship graph F_m

Proof. Let G be a friendship graph F_m . The edge set of G is divided into two edge partition based on degrees of end vertices as follow:

$$E_1(G) = \{e = uv \in E(G) : d_G(u) = 2m \text{ and } d_G(v) = 2\}$$

$$E_2(G) = \{e = uv \in E(G) : d_G(u) = 2 \text{ and } d_G(v) = 2\}.$$

Hence, $|E_1(G)| = 2m$ and $|E_2(G)| = m$. Now using Eqs.(1)-(3) we have

$$\begin{aligned} F(G, x) &= \sum_{uv \in E(G)} x^{[d_G^2(u) + d_G^2(v)]} \\ &= \sum_{uv \in E_1(G)} x^{[d_G^2(u) + d_G^2(v)]} + \sum_{uv \in E_2(G)} x^{[d_G^2(u) + d_G^2(v)]} \\ &= \sum_{uv \in E_1(G)} x^{4m^2 + 4} + \sum_{uv \in E_2(G)} x^8 \\ &= |E_1(G)|x^{4m^2 + 4} + |E_2(G)|x^8 \\ &= 2mx^{4m^2 + 4} + mx^8 \end{aligned}$$

$$\begin{aligned} PF(G) &= \prod_{uv \in E(G)} [d_G^2(u) + d_G^2(v)] \\ &= \prod_{uv \in E_1(G)} [d_G^2(u) + d_G^2(v)] \times \prod_{uv \in E_2(G)} [d_G^2(u) + d_G^2(v)] \\ &= (4 + 4m^2)^{|E_1(G)|} \times 8^{|E_2(G)|} \\ &= (4 + 4m^2)^{2m} \times 8^m \end{aligned}$$

$$\begin{aligned} HF(G) &= \sum_{uv \in E(G)} [d_G^2(u) + d_G^2(v)]^2 \\ &= \sum_{uv \in E_1(G)} [d_G^2(u) + d_G^2(v)]^2 + \sum_{uv \in E_2(G)} [d_G^2(u) + d_G^2(v)]^2 \\ &= (4 + 4m^2)^2 |E_1(G)| + 64 |E_2(G)| \\ &= 2m(4 + 4m^2)^2 + 64m. \end{aligned}$$

□

For a positive integer $l \leq n$ let $C(n, l)$ be the comet graph with n vertices, consisted of a copy of the complete graph K_{n-l+1} and a copy of the path P_l , with vertices $p_0, p_1, \dots, p_{l-1}$, where p_0 is identified with a vertex from K_{n-l+1} . (See Fig. 3)

Fig. 3: Comet graph $C(7, 3)$

Theorem 3. Let $C(n, l)$ be a comet graph. Then

$$F(C(n, l), x) = x^5 + (l - 3)x^8 + (n - l)x^{(n-l+1)^2+(n-l)^2} + \frac{(n-l)(n-l-1)}{2}x^{2(n-l)^2} + x^{(n-l+1)^2+4}$$

$$PF(C(n, l)) = 5 \times 8^{(l-3)} \times [(n-l+1)^2 + (n-l)^2]^{(n-l)} \times [2(n-l)^2]^{\frac{(n-l)(n-l-1)}{2}} \times [(n-l+1)^2 + 4]$$

$$HF(C(n, l)) = 25 + 64(l-3) + (n-l)[(n-l+1)^2 + (n-l)^2]^2 + 2(n-l)^4[(n-l)(n-l-1)] + [4 + (n-l+1)^2]^2.$$

Proof. Let G be a Comet graph $C(n, l)$. The edge set of G is divided into five partition based on degrees of end vertices. We have

$$E_1(G) = \{e = uv \in E(G) : d_G(u) = 1 \text{ and } d_G(v) = 2\}$$

$$E_2(G) = \{e = uv \in E(G) : d_G(u) = 2 \text{ and } d_G(v) = 2\}$$

$$E_3(G) = \{e = uv \in E(G) : d_G(u) = n-l+1 \text{ and } d_G(v) = n-l\}$$

$$E_4(G) = \{e = uv \in E(G) : d_G(u) = n-l \text{ and } d_G(v) = n-l\}$$

$$E_5(G) = \{e = uv \in E(G) : d_G(u) = 2 \text{ and } d_G(v) = n-l+1\}.$$

Hence, $|E_1(G)| = 1$, $|E_2(G)| = l - 3$, $|E_3(G)| = n - l$, $|E_4(G)| = \frac{(n-l)(n-l-1)}{2}$ and $|E_5(G)| = 1$. Similar to the above theorems and using Eqs.(1)-(3) we have

$$\begin{aligned} F(G, x) &= \sum_{uv \in E_1(G)} x^{[d_G^2(u) + d_G^2(v)]} + \dots + \sum_{uv \in E_5(G)} x^{[d_G^2(u) + d_G^2(v)]} \\ &= x^5 + (l - 3)x^8 + (n - l)x^{(n-l+1)^2+(n-l)^2} + \frac{(n-l)(n-l-1)}{2}x^{2(n-l)^2} + x^{(n-l+1)^2+4} \end{aligned}$$

$$\begin{aligned} PF(G) &= \prod_{uv \in E_1(G)} [d_G^2(u) + d_G^2(v)] \times \dots \times \prod_{uv \in E_5(G)} [d_G^2(u) + d_G^2(v)] \\ &= 5 \times 8^{(l-3)} \times [(n-l+1)^2 + (n-l)^2]^{(n-l)} \times [2(n-l)^2]^{\frac{(n-l)(n-l-1)}{2}} \times [(n-l+1)^2 + 4] \end{aligned}$$

$$\begin{aligned} HF(G) &= \sum_{uv \in E_1(G)} [d_G^2(u) + d_G^2(v)]^2 + \dots + \sum_{uv \in E_5(G)} [d_G^2(u) + d_G^2(v)]^2 \\ &= 25 + 64(l - 3) + (n - l)[(n-l+1)^2 + (n-l)^2]^2 + 2(n-l)^5(n-l-1) \\ &\quad + [4 + (n-l+1)^2]^2. \end{aligned}$$

 Fig. 4: t -fold bristled graph of P_n and C_n

□

For a given graph G , its t -fold bristled graph $Brs_t(G)$ is obtained by attaching t vertices of degree one to each vertex of G .

Theorem 4. Let $Brs_t(P_n)$ be a t -fold bristled graph of P_n (See Fig. 4). Then

$$F(Brs_t(P_n)) = 2tx^{(t+1)^2+1} + t(n-2)x^{(t+2)^2+1} + 2x^{(t+1)^2+(t+2)^2} + (n-3)x^{2(t+2)^2}$$

$$PF(Brs_t(P_n)) = [(t+1)^2 + 1]^{2t} \times [(t+2)^2 + 1]^{t(n-2)} \times [(t+1)^2 + (t+2)^2]^2 \times [2(t+2)^2]^{n-3}$$

$$HF(Brs_t(P_n)) = 2t[(t+1)^2 + 1]^2 + t(n-2)[(t+2)^2 + 1]^2 + 2[(t+1)^2 + (t+2)^2]^2 + 4(n-3)(t+2)^4.$$

Proof. Let G be a t -fold Bristled graph of P_n . The edge set of G is divided into four partition based on degrees of end vertices. we have

$$E_1(G) = \{e = uv \in E(G) : d_G(u) = 1 \text{ and } d_G(v) = t+1\}$$

$$E_2(G) = \{e = uv \in E(G) : d_G(u) = 1 \text{ and } d_G(v) = t+2\}$$

$$E_3(G) = \{e = uv \in E(G) : d_G(u) = t+1 \text{ and } d_G(v) = t+2\}$$

$$E_4(G) = \{e = uv \in E(G) : d_G(u) = t+2 \text{ and } d_G(v) = t+2\}.$$

Hence, $|E_1(G)| = 2t$, $|E_2(G)| = t(n-2)$, $|E_3(G)| = 2$ and $|E_4(G)| = n-3$. Similar to the above theorems and using Eqs.(1)-(3) the proof is easy. □

Fig. 5: Fence and Closed fence graphs

For the Fence graph $P_n[P_2]$ (See Fig. 5), we can divided the edge set into three edge partition based on degrees of end vertices. we have

$$E_1(P_n[P_2]) = \{e = uv \in E(P_n[P_2]) : d_G(u) = 3 \text{ and } d_G(v) = 3\}$$

$$E_2(P_n[P_2]) = \{e = uv \in E(P_n[P_2]) : d_G(u) = 3 \text{ and } d_G(v) = 5\}$$

$$E_3(P_n[P_2]) = \{e = uv \in E(P_n[P_2]) : d_G(u) = 5 \text{ and } d_G(v) = 5\}.$$

Hence, $|E_1(P_n[P_2])| = 2$, $|E_2(P_n[P_2])| = 8$ and $|E_3(P_n[P_2])| = 5n - 14$. Using Eqs.(1)-(3), we have,

Theorem 5. *Let $P_n[P_2]$ be a Fence graph with $2n$ vertices. Then*

$$F(P_n[P_2], x) = 2x^{18} + 8x^{34} + (5n - 14)x^{50}$$

$$PF(P_n[P_2]) = 18^2 \times 34^8 \times 50^{5n-14}$$

$$HF(P_n[P_2]) = 9896 + 2500(5n - 14).$$

Fig. 6: Tadpole graph $T_{4,3}$

A Tadpole graph $T_{n,k}$ is a special type of graph consisting of a cycle graph on n (at least 3) vertices and a path graph with k vertices, connected with a bridge. (See Fig. 6) For the Tadpole graph $T_{n,k}$ we can divide the edge set into three partition based on degrees of end vertices as follows:

$$E_1(T_{n,k}) = \{e = uv \in E(P_n[P_2]) : d_G(u) = 2 \text{ and } d_G(v) = 2\}$$

$$E_2(T_{n,k}) = \{e = uv \in E(P_n[P_2]) : d_G(u) = 3 \text{ and } d_G(v) = 2\}$$

$$E_3(T_{n,k}) = \{e = uv \in E(P_n[P_2]) : d_G(u) = 1 \text{ and } d_G(v) = 2\}.$$

Hence, $|E_1(T_{n,k})| = n + k - 4$, $|E_2(T_{n,k})| = 3$ and $|E_3(T_{n,k})| = 1$. Using Eqs.(1)-(3) we have,

Theorem 6. *Let $T_{n,k}$ be a Tadpole graph. Then*

$$F(T_{n,k}, x) = (n + k - 4)x^8 + 3x^{13} + x^5$$

$$PF(T_{n,k}) = 8^{n+k-4} \times 13^3 \times 5$$

$$HF(T_{n,k}) = 64(n + k - 4) + 532.$$

Fig. 7: Ladder graphs L_1, L_2, L_3, L_4, L_5

With reference to the above theorems the proofs of the next four results are easy. So we omit the proofs.

Theorem 7. Let L_n be a Ladder graph obtained as the Cartesian product of two path graphs, one of which has only one edge(See Fig. 7). Then

$$F(L_n, x) = 2x^8 + 4x^{13} + (n - 2)x^{18}$$

$$PF(L_n) = 8^2 \times 13^4 \times 18^{n-2}$$

$$HF(L_n) = 804 + 324(n - 2).$$

Theorem 8. Let $Brst_t[C_n]$ be a t -fold bristled graph of C_n (See Fig. 4). Then

$$F(Brst_t[C_n], x) = tnx^{(t+2)^2+1} + nx^{2(t+2)^2}$$

$$PF(Brst_t[C_n]) = [(t + 2)^2 + 1]^{tn} \times [2(t + 2)^2]^n$$

$$HF(Brst_t[C_n]) = tn[(t + 2)^2 + 1]^2 + 4n(t + 2)^4.$$

Theorem 9. Let $C_n[P_2]$ be a Closed fence graph with $2n$ vertices(See Fig. 5). Then

$$F(C_n[P_2], x) = (5n - 2)x^{50}$$

$$PF(C_n[P_2]) = 50^{5n-2}$$

$$HF(C_n[P_2]) = 2500(5n - 2).$$

Theorem 10. Let W_{n+1} be a Wheel graph. Then

$$F(W_{n+1}, x) = nx^{18} + nx^{n^2+9}$$

$$PF(W_{n+1}) = 18^n \times [9 + n^2]^n$$

$$HF(W_{n+1}) = 324n + n[9 + n^2]^2.$$

Having computed above indices, it is not difficult for computing other degree-based indices such as Randic index, Multiplicative Zagreb indices etc., for the graphs applied in this article. For instance, in the following two theorems we compute Randic polynomial, Multiple Randic index, and Hyper Randic index for the Fence graph and Tadpole graph. The proofs are easy, so we omit the proofs.

The Randic polynomial, Multiple Randic index, and Hyper Randic index of a graph G respectively are defined as

$$\chi(G, x) = \sum_{uv \in E(G)} x^{\frac{1}{\sqrt{d(u)d(v)}}}$$

$$P\chi(G(x)) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$$

$$H\chi(G(x)) = \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{d(u)d(v)}} \right)^2.$$

Theorem 11. Let $P_n[P_2]$ be a Fence graph with $2n$ vertices. Then

$$\chi(P_n[P_2], x) = 2x^{\frac{1}{3}} + 8x^{\frac{1}{\sqrt{15}}} + (5n - 14)x^{\frac{1}{5}}$$

$$P\chi(P_n[P_2]) = \frac{1}{9} \left(\frac{1}{\sqrt{15}} \right)^8 \left(\frac{1}{5} \right)^{5n-14}$$

$$H\chi(P_n[P_2]) = \frac{2}{9} + \frac{8}{15} + \frac{5n - 14}{25}.$$

Theorem 12. Let $T_{n,k}$ be a Tadpole graph. Then

$$\chi(T_{n,k}, x) = (n + k - 4)x^{\frac{1}{2}} + 3x^{\frac{1}{\sqrt{6}}} + x^{\frac{1}{\sqrt{2}}}$$

$$P\chi(T_{n,k}) = \left(\frac{1}{2} \right)^{n+k-4} \left(\frac{1}{\sqrt{6}} \right)^3 \left(\frac{1}{\sqrt{2}} \right)$$

$$H\chi(T_{n,k}) = \frac{n + k - 4}{4} + 1.$$

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