On the harmonic index and harmonic polynomial of Caterpillars with diameter four

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Received 16 February 2015; Accepted 5 March 2015

ACADEMIC EDITOR: ALI REZA ASHRAFI

ABSTRACT The harmonic index $H(G)$, of a graph G is defined as the sum of weights $2(\deg(u)+\deg(v))^{-1}$ of all edges in $E(G)$, where *deg (u)* denotes the degree of a vertex *u* in *V(G).* In this paper we define the harmonic polynomial of G as $H(G,x)=\sum_{uv\in E(G)} 2x^{\deg(u)+\deg(v)-1}$, where $\int_0^1 H(G,x)\,dx = H(G)$. We present explicit formula for the values of harmonic polynomial for several families of specific graphs and we find the lower and upper bound for harmonic index in Caterpillars of diameter 4.

KEYWORDS Harmonic index · harmonic polynomial · Randić index.

1. INTRODUCTION

All graphs in this paper are finite, simple and connected. For terms and concepts not defined here we refer the reader to any of several standard monographs such as, e.g., [1, 2]. Let G be a graph on n vertices. We denote the vertex set and the edge set of G by $V(G)$ and $E(G)$, respectively. Also we denote $n=|V(G)|$ and $m=|E(G)|$. For two vertices u and v of $V(G)$ the distance between u and v denoted by $d(u,v)$ and defined as the length of any shortest path connecting u and v in G. For a given vertex u of $V(G)$ its eccentricity $\varepsilon(u)$ is the largest distance between u and any other vertices of G. The maximum eccentricity over all vertices of G is called the diameter of G and is denoted by $D(G)$.

The structure property relationship quantity makes a connection between the structure and properties of molecules. In 1975, Randić proposed a new structural descriptor

[3], which is defined as the sum of the weights $(\deg(u)\deg(v))^{-1/2}$ of all edges uv of G. It is defined as $R(G)=\sum_{uv\in E(G)}(\deg(u)\deg(v))^{-1/2}$. Later, the Randić index had been extended as the general Randić index by replacing *–1/2* with any real number α and denoted by $R_\alpha(G)=\sum_{uv\in E(G)}(\deg(u)\deg(v))^{\alpha}$.

The harmonic index is one of the most important indices in chemical and mathematical fields. It is a variant of the Randić index which is the most successful molecular descriptor in structure-property and structure activity relationships studies. The harmonic index gives somewhat better correlations with physical and chemical properties comparing with the well known Randić index.

The harmonic index $H(G)$ of a graph G is defined as $H(G)=2\sum_{uv\in E(G)}(\deg(u)\deg(v))^{-1}$. This index was first appeared in [4]. Estimating bounds for $H(G)$ is of great interest, and many results have been obtained. For example, Favaron et al. [5] considered the relationship between the harmonic index and the eigenvalues of graphs; Zhong [6–8] determined the minimum and maximum values of the harmonic index for simple connected graphs, trees, unicyclic graphs and bicyclic graphs, and characterized the corresponding extremal graphs, respectively. It turns out that trees with maximum and minimum harmonic index are the path P_n and the star S_n, respectively. And the star S_n also reaches the minimum harmonic index in simple connected graphs. Li and Shiu [9] studied how the harmonic index behaves when the graph is under perturbations and provided a simpler method for determining unicyclic graphs with maximum and minimum harmonic index among all unicyclic graphs, respectively. Moreover, lower bounds for harmonic index are also obtained in [9] and [10], respectively. Recently, Deng et al. [11] studied the relationship between the harmonic index and the chromatic number of a graph G, and obtained the lower bound for $H(G)$ in terms of its chromatic number. Lv and Li [12] studied the relationship between the harmonic index and the matching number for trees, and determined the trees with minimum harmonic index among trees with a perfect matching and among trees with a given matching number, respectively. The relationship between the harmonic index and the matching number for unicyclic graphs, The graph with minimum harmonic index among all unicyclic graphs with a perfect matching and the graph with minimum harmonic index among all unicyclic graphs with a given matching number are determined in [13].

In this paper, **for the first time** the harmonic polynomial of a graph G is defined as $H(G,x)=2\sum_{uv\in E(G)}x^{\deg(u)+\deg(v)-1}$, where $\int_0^1 H(G,x)\,dx=H(G)$. We obtain explicit formulas for the harmonic polynomial of several familiar classes of graphs.

Proposition 1. [4] $H(G) \le R(G)$ with equality if and only if G is a regular graph.

Proposition 2. If G is a k-regular graph, then $H(G,x) = 2m\, x^{2k-1}$ and $H(G) = n/2$.

Proof. Since G is k–regular, so for every edge in G we have $x^{\deg(u)+\deg(v)-1} = x^{2k-1}$ and hence, $H(G,x) = 2m\, x^{2k-1}$. Computation of $H(G)$ with using this fact that in k–regular graphs $m = nk/2$ is straightforward.

Proposition 3. We have

(1) $H(K_n, x) = n(n-1)x^{2n-3}$;

(2) $H(C_n, x) = 2nx^3$;

(3) $H(\Pi_n, x) = 6nx^5$;

(4) $H(A_n, x) = 8nx^7$;

(5) $H(Q_n, x) = n2^n x^{2n-1}$.

Here by K_n, C_n, Π_n, A_n and Q_n we denote the complete graph on n vertices, the cycle on n vertices, the n−sided prism, the n−sided antiprism, and the n−dimensional hypercube, respectively, as shown in Figure 1.

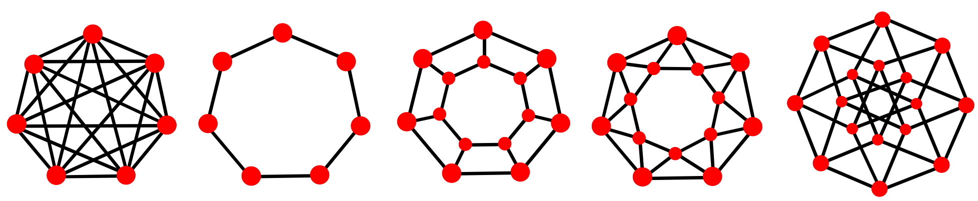

Figure 1. The graphs K_7, C_7, Π_7, A_7 and Q_7 from left to right.

Proof. The proof can obtain by using of Proposition 2.

The following results can be easily obtained by a straightforward computation.

Proposition 4. Let $K_{m,n}$, be a complete bipartite graph on $m+n$ vertices. For $m,n \ge 2$, we have $H(K_{m,n}, x) = 2mnx^{m+n-1}$. In particular $H(K_{n,n}, x) = 2n^2x^{2n-1}$ for $n \ge 2$.

For the case of complete bipartite graphs $K_{m,n}$, when one of the classes of bipartition is of size 1 is treated separately. In order to facilitate the comparison with other trees on n vertices, we find it more convenient to state the result as follows.

Proposition 5. Let $S_n = K_{1,n-1}$ be a star on $n \geq 3$ vertices. Then $H(S_n, x) = 2(n-1)x^{n-1}$.

Proposition 6. Let W_n and B_n denote the graphs of the pyramid and the bipyramid with $n-$gonal base. Then $H(W_n, x) = 2n(x^5 + x^{n+2})$ and $H(B_n, x) = 2n(x^7 + 2x^{n+3})$, (Figure 2). (The pyramid graph W_n is also known as the wheel graph on *n* spokes.)

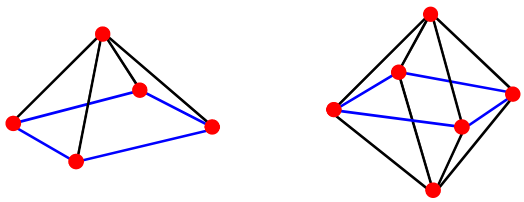

Figure 2. Pyramid and bipyramid graphs.

It is remained to compute the harmonic polynomial for the graph path P_n, in which harmonic index reach to maximum value in trees.

Proposition 7. Let P_n be a path with n vertices. Then $H(P_n, x) = 4x^2 + 2(n-3)x^3$.

2. HARMONIC POLYNOMIAL AND HARMONIC INDEX IN CATERPILLARS

In this section we try to compute the harmonic polynomial and harmonic index in Caterpillars. Recall first that a Caterpillar is a tree in which the removal of all terminal vertices (i.e. those of degree 1) gives a path.

Let $\mathrm{T}(m_0, m_1, \ldots, m_{d-1}, m_d)$ be a Caterpillar obtained from a path of length *d* say P by attaching to its i^{th} vertex $m_i(\geq 0)$ hanging edges $(i = 0,1,\ldots,d-1,d)$, (Figure 3). Clearly, $\mathrm{T} = T(m_0, m_1, \ldots, m_{d-1}, m_d)$ is of diameter *d* only if $m_0 = m_d = 0$; note also that T has $n = d + 1 + \sum_{i=0}^{d} m_i$ vertices and $m = d + \sum_{i=0}^{d} m_i$ edges.

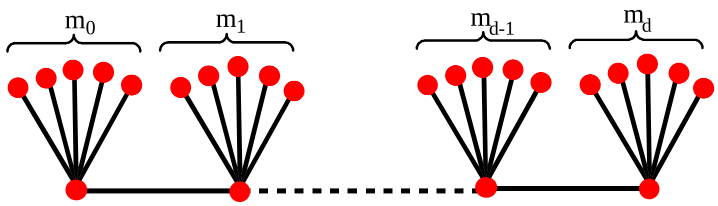

Figure 3. Caterpillar $\mathrm{T}(m_0, m_1, \ldots, m_{d-1}, m_d)$.

Theorem 8.

a) The harmonic polynomial of Caterpillar $\mathrm{T}(m_0, m_1, \ldots, m_{d-1}, m_d)$ is equal to

$$H(\mathrm{T}(m_0, m_1, \ldots, m_{d-1}, m_d), x) = \sum_{i=1}^{d-1} 2m_i x^{m_i+2} + \sum_{i=1}^{d-2} 2x^{m_i+m_{i+1}+3} + 2m_0 x^{m_0+1} + 2m_d x^{m_d+1} + 2x^{m_0+m_1+2} + 2x^{m_{d-1}+m_d+2}$$

b) The harmonic index of $\mathrm{T}(m_0, m_1, \ldots, m_{d-1}, m_d)$ is equal to

$$H(\mathrm{T}(m_0, m_1, \ldots, m_{d-1}, m_d)) = \sum_{i=1}^{d-1} \frac{2m_i}{m_i+3} + \sum_{i=1}^{d-2} \frac{2}{m_i+m_{i+1}+4} + \frac{2m_0}{m_0+2} + \frac{2m_d}{m_d+2} + \frac{2}{m_0+m_1+3} + \frac{2}{m_{d-1}+m_d+3}$$

Proof. We partition the set of edges into two subsets. First the edges on path P, and second the terminal edges. For the first kind of edges we have:

$$\sum_{uv\in E(G)} 2x^{d_u+d_v-1} = 2x^{m_0+m_1+2} + \sum_{i=1}^{d-2} 2x^{m_i+m_{i+1}+3} + 2x^{m_{d-1}+m_d+2}$$

and for the second partition we have:

$$\sum_{uv\in E(G)} 2x^{d_u+d_v-1} = 2m_0 x^{m_0+1} + \sum_{i=1}^{d-1} 2m_i x^{m_i+2} + 2m_d x^{m_d+1}.$$

The proof of part (b) is obvious from the definition. □

We restrict our computation to the Caterpillars with diameter four. These Caterpillars in terms of length of path P are divided to three kind; length 3, 4 and 5. We show these three kind briefly by $\mathrm{T}(a,b,c)$, $\mathrm{T}(0,b,c,d)$ and $\mathrm{T}(0,b,c,d,0)$. It is easy to see that $\mathrm{T}(0,b,c,d) \cong T(b+1,c,d)$ and $\mathrm{T}(0,b,c,d,0) \cong T(b+1,c,d+1)$, (Figure 4). Therefore for finding extremal graphs in this family, it is enough to work with first kind of Caterpillars. By using Theorem 8 we have:

$$H(\mathrm{T}(a,b,c), x) = 2ax^{a+1} + 2bx^{b+2} + 2cx^{c+1} + 2x^{a+b+2} + 2x^{b+c+2}$$

and

$$H(\mathrm{T}(a,b,c)) = \frac{2a}{a+2} + \frac{2b}{b+3} + \frac{2c}{c+2} + \frac{2}{a+b+3} + \frac{2}{b+c+3}.$$

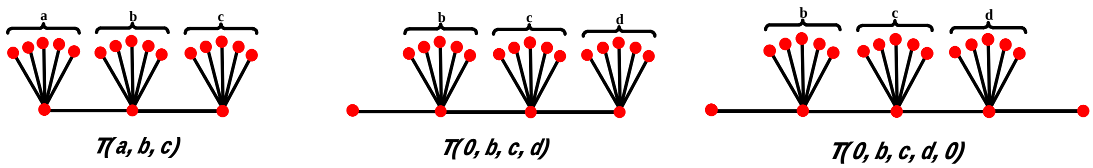

Figure 4. Caterpillars of diameter 4.

Theorem 9. Let $T(a,b,c)$ be a Caterpillar with diameter 4 , also $a \geq 1$ and $c \geq 2$. Then $H(T(a,b,c)) \leq H(T(a+1,b,c-1))$ and equation is hold if and only if $a = \left\lfloor \frac{n-3-b}{2} \right\rfloor$ and $c = \left\lceil \frac{n-3-b}{2} \right\rceil$.

Proof. Without loss of generality, assume that $a < c$. If $a \geq c$, with using the fact that $T(a,b,c) \cong T(c,b,a)$, we can replace a with c. Let the vertices on path P are denoted by α, β, γ with the degree sequence $a+1, b+2, c+1$, respectively. Since $a \geq 1$ after transformation, the degree of α increases and degree of β decreases by one. We will consider the difference $\Delta = H(T(a,b,c)) - H(T(a+1,b,c-1))$ in two cases.

- **Case 1:** $b = 0$. In this case we have:

$$\Delta = \frac{-4}{(a+2)(a+3)} + \frac{4}{(c+2)(c+1)} + \frac{2}{(a+3)(a+4)} + \frac{-2}{(c+3)(c+2)}$$
$$= \frac{-4}{a+2} + \frac{4}{a+3} + \frac{-4}{c+2} + \frac{4}{c+1} + \frac{2}{a+3} + \frac{-2}{a+4} + \frac{2}{c+3} + \frac{-2}{c+2}$$
$$= \left(\frac{6}{a+3} - \frac{6}{c+2}\right) + \left(\frac{4}{c+1} - \frac{4}{a+2}\right) + \left(\frac{2}{c+3} - \frac{2}{a+4}\right).$$

Since $a < c$, we have $c = a + k$ for some positive integer k. So

$$\Delta = \left(\frac{6}{a+3} - \frac{6}{a+k+2}\right) + \left(\frac{4}{a+k+1} - \frac{4}{a+2}\right) + \left(\frac{2}{a+k+3} - \frac{2}{a+4}\right)$$
$$= -\frac{2\begin{pmatrix}10a^4 + 22a^3k + 13a^2k^2 + ak^3 + 106a^3 + 192a^2k + 88ak^2 \\ + 6k^3 + 398a^2 + 533ak + 132k^2 + 626a + 474k + 348\end{pmatrix}}{(a+2)(a+3)(a+4)(a+k+1)(a+k+2)(a+k+3)} \leq 0$$

- **Case2:** $b > 0$. Since for every $a,b,c \geq 1$ we have:

$$\frac{2}{a+b+3} - \frac{2}{a+b+4} + \frac{2}{a+b+k+3} - \frac{2}{a+b+k+2} \leq \frac{2}{a+3} - \frac{2}{a+4} + \frac{2}{a+k+3} - \frac{2}{a+k+2},$$

so in this case we have also: $\Delta \le 0$. It is obvious that the equality is hold for $a = \left\lfloor \frac{n-3-b}{2} \right\rfloor$ and $c = \left\lceil \frac{n-3-b}{2} \right\rceil$. □

Collorally 10. When b is fixed, the maximum and minimum values of harmonic index occur in $\mathrm{T}\left(\left\lfloor \frac{n-3-b}{2} \right\rfloor, b, \left\lceil \frac{n-3-b}{2} \right\rceil\right)$ and $\mathrm{T}(1, b, n-b-4)$, respectively.

Proof. The proof is straightforward. □

Theorem 9 and Collarally 10 are useful when b is a fixed number. While for fixed a (similarly for c) we have the following theorem.

Theorem 11. Let $\mathrm{T}(a,b,c)$ are Caterpillars with diameter 4, where $a \ge 1$ and $c \ge 2$. Then

$$H(\mathrm{T}(a,b,c)) \le H(T(a,b+1,c-1))$$

and

$$H(\mathrm{T}(a+1,b,c-1)) \ge H(T(a,b+1,c-1)).$$

Proof. The proof is similar to the proof of Theorem 9. □

The following corollary is immediate consequence of Theorem 11.

Corollary 12. When a is fixed, the maximum and minimum values of harmonic index occur in $\mathrm{T}\left(a, \left\lfloor \frac{n-3-a}{2} \right\rfloor, \left\lceil \frac{n-3-a}{2} \right\rceil\right)$ and $\mathrm{T}(a, 0, n-a-3)$, respectively.

Our main theorem is the following theorem.

Theorem 13. For every Caterpillar,

$$H(T(1,0,n-4)) \le H(\mathrm{T}(a,b,c)) \le$$

$$\begin{cases} H\left(T\left(\left\lceil \frac{n-3}{3} \right\rceil, \left\lfloor \frac{n-3}{3} \right\rfloor, n - \left\lceil \frac{n-3}{3} \right\rceil - \left\lfloor \frac{n-3}{3} \right\rfloor - 3\right)\right) & n < 19, \\ H\left(T\left(\left\lfloor \frac{n-3}{3} \right\rfloor, \left\lceil \frac{n-3}{3} \right\rceil, n - \left\lceil \frac{n-3}{3} \right\rceil - \left\lfloor \frac{n-3}{3} \right\rfloor - 3\right)\right) & n \ge 19. \end{cases}$$

Proof. By easy calculation we can prove theorem for $n<19$ and $n=19$. Suppose that $n>19$. Then we have:

$$H\left(T(\left\lfloor\frac{n-3}{3}\right\rfloor,\left\lceil\frac{n-3}{3}\right\rceil,n-\left\lceil\frac{n-3}{3}\right\rceil-\left\lfloor\frac{n-3}{3}\right\rfloor-3)\right)\leq H\left(T(\left\lceil\frac{n-3}{3}\right\rceil,\left\lfloor\frac{n-3}{3}\right\rfloor,n-\left\lceil\frac{n-3}{3}\right\rceil-\left\lfloor\frac{n-3}{3}\right\rfloor-3)\right).$$

Now by using a similar method to the proof of Theorem 9 the proof is complete.

Example. The harmonic index for n=16 are presented in the following table. We know that in this kind of Caterpillars $a+b+c=n-3$. So the lower and upper bounds occur in T(1,0,12) and T(4,4,5) as have been shown in Table 1.

Table 1. Harmonic index for n = 16.

	$a=1$	$a=2$	$a=3$	$a=4$	$a=5$	$a=6$
$b=0$	**3.0142**	3.2352	3.3538	3.4220	3.4604	3.4778
$b=1$	3.3924	3.6428	3.7760	3.8500	3.8882	3.9000
$b=2$	3.6000	3.8650	4.0038	4.0778	4.1104	
$b=3$	3.7220	3.9928	4.1316	4.2000	4.2208	
$b=4$	3.7928	4.0634	4.1968	**4.2532**		
$b=5$	3.8278	4.0928	4.2142	4.2500		
$b=6$	3.8334	4.0866	4.1872			
$b=7$	3.8104	4.0428	4.1076			
$b=8$	3.7546	3.9512				
$b=9$	3.6538	3.7858				
$b=10$	3.4814					
$b=11$	3.1714					

3. CONCLUSION

In this paper the lower and upper bound for harmonic index of Caterpillars with diameter four is computed. To the best of our knowledge it is the first paper considering the harmonic polynomial of a graph. We think it is possible to extend these calculations for other important families of graphs.

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