

MATHEMATICAL RESULTS ON HARMONIC POLYNOMIALS

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ABSTRACT. Some years ago, the harmonic polynomial was introduced in order to understand better the harmonic topological index; for instance, it allows to obtain bounds of the harmonic index of the main products of graphs. Here, we obtain several properties of this polynomial, and we prove that several properties of graphs can be deduced from their harmonic polynomials. Also, we show that two graphs with the same harmonic polynomial have to be similar.

Keywords: Harmonic index; harmonic polynomial; degree-based topological indices

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1. INTRODUCTION

A topological descriptor is a single number that represents a chemical structure in graph-theoretical terms via the molecular graph, they play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations. A topological descriptor is called a topological index if it correlates with a molecular property. Topological indices are used to understand physicochemical properties of chemical compounds, since they capture some properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener [29].

Within all topological indices ones of the most investigated are the descriptors based on the valences of atoms in molecules (in graph-theoretical notions degrees of vertices of graph). Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best known such descriptor is the Randić connectivity index (R) [23]. There are more than thousand papers and a couple of books dealing with this molecular descriptor (see, e.g., [11], [19], [20], [25], [26] and the references therein).

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During many years, scientists were trying to improve the predictive power of the Randić index. This led to the introduction of a large number of new topological descriptors resembling the original Randić index. Two of the main successors of the Randić index are the first and second Zagreb indices, denoted by M_1 and M_2 , respectively, defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v) = \sum_{u \in V(G)} d_u^2, \quad M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

where uv denotes the edge of the graph G connecting the vertices u and v , and d_u is the degree of the vertex u . These indices have attracted growing interest, see e.g. [1], [2], [9], [21] (in particular, they are included in a number of programs used for the routine computation of topological indices).

Another remarkable topological descriptor is the *harmonic* index, defined in [7] as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

This index has attracted a great interest in the last years (see, e.g., [3], [8], [24], [30], and [32]).

With motivation from the first Zagreb and harmonic indices, *general sum-connectivity index* χ_α was defined by Zhou and Trinajstić in [33] as

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha,$$

with $\alpha \in \mathbb{R}$. Note that χ_1 is the first Zagreb index M_1 , $2\chi_{-1}$ is the harmonic index H , $\chi_{-1/2}$ is the sum-connectivity index, etc. Some mathematical properties of the general sum-connectivity index were given in [4], [24], [32], [33] and [34].

In [17] the *harmonic polynomial* of a graph G is defined as

$$H(G, x) := \sum_{uv \in E(G)} x^{d_u + d_v - 1},$$

and the harmonic polynomials of some graphs are computed. The harmonic polynomials of the line of some graphs are computed in [22]. In [15] this polynomial was used in order to obtain bounds of the harmonic index of the main products of graphs.

This polynomial gets its name from the fact that $2 \int_0^1 H(G, x) dx = H(G)$.

If G_1 and G_2 are disjoint graphs, then

$$H(G_1 \cup G_2, x) = H(G_1, x) + H(G_2, x).$$

Hence, considering connected graphs is not a restrictive condition.

The characterization of any graph by a polynomial is one of the open important problems in graph theory. In recent years there have been many works on graph polynomials (see, e.g., [27] and the references therein). The research in this area has been largely driven by the advantages offered by the use of computers: it is simpler to represent a graph by a polynomial (a vector with dimension $O(n)$) than by the adjacency matrix (an $n \times n$ matrix). Some parameters of a graph allow to define polynomials related to a graph. Although several polynomials are interesting since they compress information about the graph's structure, unfortunately, the well-known polynomials do not solve the problem of the characterization of any graph, since there are often non-isomorphic graphs with the same polynomial.

Throughout this paper, $G = (V, E) = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) graph without isolated vertices (every vertex has at least a neighbor). The main aim of this paper is to obtain several properties of the harmonic polynomial. We prove that several properties of graphs can be obtained from their harmonic polynomials: Corollary 2.8 characterizes regular and biregular graphs in terms of the zeros of their harmonic polynomials; Theorem 2.11 gives information about the connectedness, the diameter and the girth (the minimum length of the cycles) of a graph in terms of the degree of its harmonic polynomial; Proposition 2.20 shows that the cardinality of the set of pendant paths in a graph is precisely the coefficient of x^2 in its harmonic polynomial. Besides, Theorems 2.15, 2.16 and 2.17 relate the number of non-zero coefficients of the harmonic polynomial with the degree sequence of the polynomial. Theorem 2.24 shows that two graphs with the same harmonic polynomial have to be similar.

2. MAIN RESULTS

The following result appears in [17, Proposition 1].

Proposition 2.1. *If G is a k -regular graph with m edges, then $H(G, x) = mx^{2k-1}$.*

Propositions 2, 4, 5, 7 in [17] have the following consequences on the graphs: K_n (the complete graph with n vertices), C_n (the cycle with $n \geq 3$ vertices), Q_n (the n -dimensional hypercube), K_{n_1, n_2} (the complete bipartite graph with $n_1 + n_2$ vertices), P_n (the path graph with n vertices) and W_n (the wheel graph with $n \geq 4$ vertices).

Proposition 2.2. *We have*

$$\begin{aligned} H(K_n, x) &= \frac{1}{2}n(n-1)x^{2n-3}, & H(C_n, x) &= nx^3, \\ H(Q_n, x) &= n2^{n-1}x^{2n-1}, & H(K_{n_1, n_2}, x) &= n_1n_2x^{n_1+n_2-1}, \\ H(P_n, x) &= 2x^2 + (n-3)x^3, & H(W_n, x) &= (n-1)(x^{n+1} + x^5). \end{aligned}$$

Given a graph G , the *line graph* $\mathcal{L}(G)$ of G is a graph which has a vertex $w_e \in V(\mathcal{L}(G))$ for each edge $e \in E(G)$, and an edge joining w_{e_i} and w_{e_j} when e_i and e_j share a vertex (i.e., $\mathcal{L}(G)$ is the intersection graph of $E(G)$). It is easy to check that if $uv \in E(G)$, then the degree of $w_{uv} \in V(\mathcal{L}(G))$ is $d_u + d_v - 2$.

Line graphs were initially introduced in the papers [28] and [18], although the terminology of line graph was used in [14] for the first time. They are an active topic of research at this moment.

In the same paper, where Zagreb indices were introduced, the *forgotten topological index* (or *F-index*) is defined as

$$F(G) = \sum_{uv \in E(G)} (d_u^2 + d_v^2) = \sum_{u \in V(G)} d_u^3.$$

Both the forgotten topological index and the first Zagreb index were employed in the formulas for total π -electron energy in [13], as a measure of branching extent of the carbon-atom skeleton of the underlying molecule. However, this index never got attention except recently, when Furtula and Gutman in [10] established some basic properties of the F-index and showed that its predictive ability is almost similar to that of first Zagreb index and for the entropy and acetic factor, both of them yield correlation coefficients greater than 0.95.

Our first result shows that we can obtain information about the graph from the values of the harmonic polynomial (and its derivatives) at the point 1.

Proposition 2.3. *If G is a graph with n vertices, m edges, maximum degree Δ and minimum degree δ , then:*

- $H(G, 1) = m$,
- $H'(G, 1) + H(G, 1) = M_1(G)$,
- $H''(G, 1) - 2H(G, 1) = F(G) + 2M_2(G) - 3M_1(G)$,
- $H''(G, 1) + 2H(G, 1) = M_1(\mathcal{L}(G)) + M_1(G)$,
- $2H(G, 1)/\Delta \leq n \leq 2H(G, 1)/\delta$.

Proof. First of all, $H(G, 1) = \sum_{uv \in E(G)} 1 = m$. Also,

$$H'(G, 1) = \sum_{uv \in E(G)} (d_u + d_v) - \sum_{uv \in E(G)} 1 = M_1(G) - H(G, 1),$$

and

$$\begin{aligned}
 H''(G, 1) &= \sum_{uv \in E(G)} (d_u^2 + d_v^2) + 2 \sum_{uv \in E(G)} d_u d_v - 3 \sum_{uv \in E(G)} (d_u + d_v) + \sum_{uv \in E(G)} 2 \\
 &= F(G) + 2M_2(G) - 3M_1(G) + 2H(G, 1), \\
 H''(G, 1) &= \sum_{uv \in E(G)} (d_u + d_v - 2)(d_u + d_v - 2) + \sum_{uv \in E(G)} (d_u + d_v - 2) \\
 &= \sum_{uv \in E(G)} (d_u + d_v - 2)^2 + \sum_{uv \in E(G)} (d_u + d_v) - \sum_{uv \in E(G)} 2 \\
 &= M_1(\mathcal{L}(G)) + M_1(G) - 2H(G, 1).
 \end{aligned}$$

The inequalities $\delta n \leq 2m \leq \Delta n$ and the first item imply the fifth one. \square

Proposition 2.1 shows that any two k -regular graphs with the same cardinality of edges, have the same harmonic polynomial. It is natural to ask the following question: How many graphs can be characterized by their harmonic polynomials? This is a very difficult question, but there are partial answers: Proposition 2.3 gives that graphs with different cardinality of edges have different harmonic polynomials. This fact has the following interesting consequence.

Corollary 2.4. *If Γ is a proper subgraph of the graph G , then $H(\Gamma, x) \neq H(G, x)$.*

Also, Theorem 2.24 will show that two graphs with the same harmonic polynomial have to be similar, in some sense.

For each positive integer k , let us define the polynomial

$$Q_k(x) := (x-1)(x-2)\cdots(x-k) = x^k + \sum_{j=0}^{k-1} a_{k,j} x^j.$$

Note that Vieta's formulas allow to compute these coefficients $a_{k,j}$ in a very simple way:

$$a_{k,k-j} = (-1)^j \sum_{1 \leq i_1 < i_2 < \cdots < i_j \leq k} i_1 i_2 \cdots i_j.$$

In particular, we have $a_{k,k-1} = -\frac{1}{2}k(k+1)$ and $a_{k,0} = (-1)^k k!$.

Proposition 2.5. *If G is a graph and k is a positive integer, then*

$$H^{(k)}(G, 1) = \chi_k(G) + \sum_{j=0}^{k-1} a_{k,j} \chi_j(G).$$

Proof. We have

$$\begin{aligned}
 H^{(k)}(G, x) &= \sum_{uv \in E(G)} (d_u + d_v - 1)(d_u + d_v - 2) \cdots (d_u + d_v - k) x^{d_u + d_v - k - 1} \\
 &= \sum_{uv \in E(G)} Q_k(d_u + d_v) x^{d_u + d_v - k - 1}, \\
 H^{(k)}(G, 1) &= \sum_{uv \in E(G)} Q_k(d_u + d_v) = \sum_{uv \in E(G)} (d_u + d_v)^k + \sum_{j=0}^{k-1} \sum_{uv \in E(G)} a_{k,j} (d_u + d_v)^j \\
 &= \chi_k(G) + \sum_{j=0}^{k-1} a_{k,j} \chi_j(G).
 \end{aligned}$$

□

As usual, we denote by $\text{Deg } p(x)$ the degree of the polynomial $p(x)$, and by $\text{Deg}_{\min} p(x)$ the minimum degree of their monomials with non-zero coefficients.

Given a graph G , we have

$$\begin{aligned}
 \text{Deg } H(G, x) &= \max \{d_u + d_v - 1 \mid uv \in E(G)\}, \\
 \text{Deg}_{\min} H(G, x) &= \min \{d_u + d_v - 1 \mid uv \in E(G)\}.
 \end{aligned}$$

Recall that a *biregular* graph is a bipartite graph for which any vertex in one side of the given bipartition has degree Δ and any vertex in the other side of the bipartition has degree δ . We say that a graph is (Δ, δ) -*biregular* if we want to write explicitly the maximum and minimum degrees.

Proposition 2.6. *If G is a graph, then:*

- $H^{(k)}(G, x) \geq 0$ for every $k \geq 0$, $x \in [0, \infty)$ and $d_u + d_v - 1 \geq k$,
- $H(G, x) > 0$ on $(0, \infty)$ and $H(G, x)$ is strictly increasing on $[0, \infty)$,
- $H(G, x)$ is strictly convex on $[0, \infty)$ if and only if G is not isomorphic to a union of path graphs P_2 .

Proof. Since every coefficient of the polynomial $H(G, x)$ is non-negative, the first statement holds.

Since $\text{Deg}_{\min} H(G, x) \geq 2\delta - 1 \geq 1$, we have $H(G, x) > 0$ and $H'(G, x) > 0$ on $(0, \infty)$.

A graph G is not isomorphic to a union of path graphs P_2 if and only if $d_u + d_v \geq 3$ for some edge $uv \in E(G)$; this happens if and only if G satisfies $\text{Deg } H(G, x) \geq 2$; and this is equivalent to $H''(G, x) > 0$ on $(0, \infty)$. □

Let us denote by \mathfrak{G} the set of all regular and biregular connected graphs. We say that a set of graphs $\{G_i\}_{i=1}^k$, such that G_i has maximum degree Δ_i and minimum degree δ_i for each $1 \leq i \leq k$, is *coherent* if $G_i \subset \mathfrak{G}$ for

every $1 \leq i \leq k$, and $\Delta_i + \delta_i = \Delta_j + \delta_j$ for every $1 \leq i, j \leq k$. We say that a graph is *coherent* if the set of its connected components is coherent.

Given a graph G and a vertex $v \in V(G)$, we denote by $N(v)$ the set of neighbors of v .

Theorem 2.7. *Let G be a graph. $x = 0$ is the unique zero of $H(G, x)$ if and only if G is coherent.*

Proof. If G is coherent, let us consider the set of its connected components $\{G_i\}_{i=1}^k$. For each $1 \leq i \leq k$, G_i is either a regular or a biregular graph with m_i edges, maximum degree Δ_i and minimum degree δ_i ; hence, $H(G_i, x) = m_i x^{\Delta_i + \delta_i - 1}$. So, $m = m_1 + \dots + m_k$ is the cardinality of edges of G , $H(G, x) = mx^{\Delta_1 + \delta_1 - 1}$ and $x = 0$ is the unique zero of $H(G, x)$.

Assume now that $x = 0$ is the unique zero of $H(G, x)$; thus, $H(G, x) = ax^{b-1}$ for some positive integers a, b , and $d_u + d_v = b$ for every $uv \in E(G)$. Let us consider the set of connected components $\{G_i\}_{i=1}^k$ of G . Fix $1 \leq i \leq k$, and denote by Δ_i and δ_i the maximum and minimum degrees of G_i , respectively. Thus, for each fixed vertex $u \in V(G_i)$ we have $d_v = b - d_u$ for every $uv \in E(G_i)$, and every $v \in N(u)$ has the same degree $b - d_u$. In a similar way, if $w \in N(v)$, then $d_w = b - d_v = d_u$. Since G_i is a connected graph, G_i is either regular (if $\Delta_i = \delta_i$) or biregular (if $\Delta_i \neq \delta_i$), and $G_i \subset \mathfrak{G}$. Since $\Delta_i + \delta_i = b$ for every $1 \leq i \leq k$, we conclude that G is coherent. \square

The following consequence of Theorem 2.7 shows that it is possible to characterize regular and biregular connected graphs in terms of the zeros of their harmonic polynomials.

Corollary 2.8. *Let G be a connected graph. $x = 0$ is the unique zero of $H(G, x)$ if and only if G is either a regular or a biregular graph.*

The next result provides bounds of the harmonic index in terms of the values of the harmonic polynomial at the points 1 and $1/2$.

Proposition 2.9. *If G is a graph, then*

$$H(G) \geq 2H(G, 1/2),$$

and the equality in each inequality is attained if and only if G is isomorphic to a union of path graphs P_2 .

Proof. Hermite-Hadamard's inequality states that if $f : [0, 1] \rightarrow \mathbb{R}$ is a convex function, then

$$(2.1) \quad f(1/2) \leq \int_0^1 f(x) dx,$$

and if f is strictly convex, then the inequality is strict.

If G is not isomorphic to a union of path graphs P_2 , then Proposition 2.6 gives that $H(G, x)$ is a strictly convex function. Thus, (2.1) gives the result. If G is isomorphic to a union of m path graphs P_2 , then $H(G) = m$, $H(G, x) = mx$, $H(G, 1/2) = m/2$. Thus, $2H(G, 1/2) = H(G)$. \square

We say that a vertex $v \in V(G)$ in the graph G is *dominant* if $N(v) = V(G) \setminus \{v\}$.

Proposition 2.10. *Let G be a graph with n vertices, maximum degree Δ and minimum degree δ . Then:*

- $x = 0$ is a zero of $H(G, x)$ with multiplicity $\text{Deg}_{\min} H(G, x)$, where $2\delta - 1 \leq \text{Deg}_{\min} H(G, x) \leq \text{Deg} H(G, x) \leq 2\Delta - 1$,
- $\text{Deg} H(G, x) \leq 2n - 3$, and $\text{Deg} H(G, x) = 2n - 3$ if and only if there are at least two dominant neighbors in G ,
- if Γ is a subgraph of G , then $\text{Deg} H(\Gamma, x) \leq \text{Deg} H(G, x)$ and $\text{Deg}_{\min} H(\Gamma, x) \leq \text{Deg}_{\min} H(G, x)$.

Proof. Since

$$H(G, x) = \sum_{j=\text{Deg}_{\min} H(G, x)}^{\text{Deg} H(G, x)} c_j x^j,$$

for some constants c_j , $x = 0$ is a zero of $H(G, x)$ with multiplicity $\text{Deg}_{\min} H(G, x)$.

Since each j in the previous sum can be written as $d_u + d_v - 1$ for some $uv \in E(G)$, we have $2\delta - 1 \leq \text{Deg}_{\min} H(G, x) \leq \text{Deg} H(G, x) \leq 2\Delta - 1$.

Since $\Delta \leq n - 1$, we have $\text{Deg} H(G, x) \leq 2n - 3$. We have $\text{Deg} H(G, x) = 2n - 3$ if and only if there is an edge $uv \in E(G)$ with $d_u = d_v = n - 1$, and this holds is and only if u, v are dominant vertices in G .

Let Γ be a subgraph of G . The last statement holds, since the degree of a vertex in Γ is at most its degree in G . \square

The next result allows to obtain information about the connectedness, diameter and girth of a graph (the minimum length of its cycles) in terms of the degree of its harmonic polynomial.

Theorem 2.11. *Let G be a graph with n vertices. If $\text{Deg} H(G, x) \geq n$, then $g(G) = 3$. Furthermore, if G is a triangle-free graph and $\text{Deg} H(G, x) = n - 1$, then G is a connected graph and $\text{diam} G \leq 3$.*

Proof. Since $g(G) = 3$ if and only if G is not triangle-free, it suffices to prove that if G is a triangle-free graph, then $\text{Deg} H(G, x) \leq n - 1$. Since G is a triangle-free graph, then $N(u) \cap N(v) = \emptyset$ for every $uv \in E(G)$. Hence, $d_u + d_v \leq n$ for every $uv \in E(G)$, and $\text{Deg} H(G, x) \leq n - 1$.

Assume that G is a triangle-free graph and $\text{Deg} H(G, x) = n - 1$. Thus, there is an edge $uv \in E(G)$ with $d_u + d_v = n$. Since $N(u) \cap N(v) = \emptyset$, we have $N(u) \cup N(v) = V(G)$ and $d(w, \{u, v\}) \leq 1$ for every $w \in V(G)$. Consequently, $\text{diam} G \leq 3$ and G is a connected graph. \square

Denote by $K(p(x))$ the number of non-zero coefficients of the polynomial $p(x)$.

Theorem 2.12. *Let G be a graph with m edges. Then:*

- $1 \leq K(H(G, x)) \leq m$,
- $K(H(G, x)) = 1$ if and only if G is coherent,
- $K(H(G, x)) = m$ if and only if G is isomorphic to P_2 .

Proof. The first item is easy to see.

The proof of Theorem 2.7 gives that G is coherent if and only if $H(G, x) = ax^{b-1}$ for some positive integers a, b , and this is equivalent to $K(H(G, x)) = 1$.

If G is isomorphic to the path graph P_2 , then it is a regular graph with just an edge, and the previous item gives $K(H(G, x)) = 1 = m$.

Assume now that G is not isomorphic to P_2 . We consider several cases.

(1) G is connected. Thus, $3 \leq d_u + d_v \leq m + 1$ for every $uv \in E(G)$, i.e., $2 \leq d_u + d_v - 1 \leq m$. Since the m values of $d_u + d_v - 1$ belong to a set of $m - 1$ integers, there are two edges with the same value and we conclude that $K(H(G, x)) \leq m - 1$.

(2) G is not connected. So, G has connected components G_1, \dots, G_k , with $k \geq 2$. Denote by m_i the cardinality of the edges of G_i , thus $m = m_1 + \dots + m_k$.

(2.1) Assume that there exists some $1 \leq j \leq k$ such that G_j is not isomorphic to P_2 . So, (1) gives that $K(H(G_j, x)) \leq m_j - 1$, and this inequality and the first item give

$$K(H(G, x)) \leq \sum_{i=1}^k K(H(G_i, x)) \leq \sum_{i=1}^k m_i - 1 = m - 1.$$

(2.2) Assume that G_i is isomorphic to P_2 for every $1 \leq i \leq k$. So, $m = k \geq 2$,

$$H(G, x) = \sum_{i=1}^m H(G_i, x) = \sum_{i=1}^m x = mx,$$

and $K(H(G, x)) = 1 \leq k - 1 < m$. □

Theorem 2.12 has the following consequence.

Corollary 2.13. *If G is a graph with $m \geq 2$ edges, then $1 \leq K(H(G, x)) \leq m - 1$.*

Proposition 2.14. *Let G be a graph with n vertices, m edges, maximum degree Δ and minimum degree δ . Then:*

- $K(H(G, x)) \leq \text{Deg } H(G, x) - \text{Deg}_{\min} H(G, x) + 1$,
- $K(H(G, x)) \leq \min\{2\Delta - 2\delta + 1, m - 2\delta + 2\}$,
- if G is a triangle-free graph, then $K(H(G, x)) \leq n - 2\delta + 1$.

Proof. The first item holds since there are constants c_j with

$$H(G, x) = \sum_{j=\text{Deg}_{\min} H(G,x)}^{\text{Deg} H(G,x)} c_j x^j,$$

The first item and the bounds in Proposition 2.10 give

$$K(H(G, x)) \leq 2\Delta - 2\delta + 1.$$

Since $d_u + d_v \leq m + 1$ for every $uv \in E(G)$, we have $\text{Deg} H(G, x) \leq m$. This inequality, the first item and the first item in Proposition 2.10 give $K(H(G, x)) \leq m - 2\delta + 2$.

The third item is a consequence of the first one, the first item in Proposition 2.10 and Theorem 2.11. \square

Given a graph G , we say that $\{d_u\}_{u \in V(G)}$ is the *degree sequence* of G (if $d_{v_1} = d_{v_2}$ for some $v_1, v_2 \in V(G)$, then the value $d_{v_1} = d_{v_2}$ appears just once in $\{d_u\}_{u \in V(G)}$).

Let us denote by $\lceil t \rceil$ the upper integer part of $t \in \mathbb{R}$, i.e., the smallest integer greater or equal than t .

Theorem 2.15. *Let G be a graph. The following statements hold:*

- if the degree sequence of G has at most r terms, then

$$K(H(G, x)) \leq \frac{r(r+1)}{2},$$

- if $K(H(G, x)) \geq s$, then the degree sequence of G has at least

$$\left\lceil \frac{\sqrt{8s+1}-1}{2} \right\rceil$$

terms.

Proof. If the degree sequence of G has at most r terms, then the set of different values $d_u + d_v$ has cardinality at most $r(r+1)/2$ (2-combinations with repetition of a set of r elements). Thus, $K(H(G, x)) \leq r(r+1)/2$.

Assume that $K(H(G, x)) = S \geq s$, and denote by r the cardinality of the degree sequence of G . The first item gives

$$s \leq S \leq \frac{r(r+1)}{2}, \quad r^2 + r - 2s \geq 0, \quad r \geq \frac{\sqrt{8s+1}-1}{2},$$

and we obtain the desired inequality since r is an integer. \square

One can think that it might be possible to obtain a lower bound for $K(H(G, x))$ which is an increasing function of the cardinality of the degree sequence of G . However, this is not possible, as the following result shows.

Theorem 2.16. *Let G be a connected graph with a degree sequence of cardinality r .*

- If $r \leq 2$, then $K(H(G, x)) \geq 1$.
- If $r > 2$, then $K(H(G, x)) \geq 2$.

Furthermore, the bounds are sharp for each r .

Proof. The first statement is a consequence of Theorem 2.12.

Assume that $r > 2$. Since G is connected, there exist a path $\gamma = \{u_1, u_2, \dots, u_k\}$ in G and three vertices in $V(G) \cap \gamma$ with different degrees. Without loss of generality one can assume that

$$d_{u_1} \notin \{d_{u_2}, \dots, d_{u_k}\} \quad \text{and} \quad d_{u_k} \notin \{d_{u_1}, \dots, d_{u_{k-1}}\},$$

since otherwise u_1 and/or u_k can be removed from γ , and a shorter path with the same property is obtained. Also, we can assume that $d_{u_2} = d_{u_3} = \dots = d_{u_{k-2}} = d_{u_{k-1}}$. Thus, $d_{u_1} + d_{u_2} \neq d_{u_2} + d_{u_k} = d_{u_{k-1}} + d_{u_k}$ and, since $u_1 u_2, u_{k-1} u_k \in E(G)$, we conclude $K(H(G, x)) \geq 2$.

If G is a star graph with n vertices, then the degree sequence is $\{1, n-1\}$; thus $r = 1$ if $n = 2$, and $r = 2$ if $n > 2$. Since $H(G, x) = (n-1)x^{n-1}$, we have $K(H(G, x)) = 1$.

Consider the sequence $\{1, 2, \dots, r\}$ with $r > 2$. We are going to define a graph T_r (in fact, T_r is a tree) with degree sequence $\{1, 2, \dots, r\}$ and $K(H(T_r, x)) = 2$. Let us consider the (ordered) sequence $\{a_1, a_2, \dots, a_r\}$ obtained as a permutation of $\{1, 2, \dots, r\}$ in the following way. If r is even, then

$$\{a_1, a_2, \dots, a_r\} = \left\{ \frac{r}{2} + 1, \frac{r}{2}, \frac{r}{2} + 2, \frac{r}{2} - 1, \dots, r-1, 2, r, 1 \right\}.$$

If r is odd, then

$$\begin{aligned} & \{a_1, a_2, \dots, a_r\} = \\ & = \left\{ \frac{r+1}{2}, \frac{r+1}{2} + 1, \frac{r+1}{2} - 1, \frac{r+1}{2} + 2, \frac{r+1}{2} - 2, \dots, r-1, 2, r, 1 \right\}. \end{aligned}$$

In both cases we have that $a_j + a_{j+1}$ is either $r+1$ or $r+2$ for each $1 \leq j < r$. Consider a point v_1 , which will be the root of T_r . We define T_r inductively on the distance j from v_1 . We join v_1 with a_1 vertices (at distance 1 from v_1). If $u \in V(T_r)$ with $d_{T_r}(u, v_1) = j-1$ for some $1 < j < r$, then we join u with $a_j - 1$ vertices (at distance j from v_1). Note that if $u \in V(T_r)$, then $d_{T_r}(u, v_1) = j-1$ for some $1 \leq j < r$ and $d_u = a_j$. If $uv \in E(T_r)$, then without loss of generality we can assume that there exists $1 \leq j < r$ with $d_{T_r}(u, v_1) = j-1$ and $d_{T_r}(v, v_1) = j$. Therefore, $d_u + d_v = a_j + a_{j+1}$ is either $r+1$ or $r+2$, and so $K(H(T_r, x)) = 2$. \square

Theorem 2.17. *Let G be a graph.*

- If some connected component of G has a degree sequence of cardinality $r > 2$, then $K(H(G, x)) \geq 2$.
- For each $r \geq 1$, there exists a graph with a degree sequence of cardinality r and $K(H(G, x)) = 1$.

Proof. If there is a connected component G_i of G with degree sequence of cardinality $r > 2$, then Theorem 2.16 gives $K(H(G_i, x)) \geq 2$, and $K(H(G, x)) \geq K(H(G_i, x)) \geq 2$.

Fix any $r \geq 1$.

If r is even, then define G_r as the union of the complete bipartite graphs

$$K_{1,r}, K_{2,r-1}, \dots, K_{r/2-1, r/2+2}, K_{r/2, r/2+1}.$$

If r is odd, then define G_r as the union of the complete bipartite graphs

$$K_{1,r}, K_{2,r-1}, \dots, K_{(r+1)/2-1, (r+1)/2+1}, K_{(r+1)/2, (r+1)/2}.$$

In both cases, the degree sequence of G_r has cardinality r . If m denotes the cardinality of $E(G_r)$, then $H(G_r, x) = m x^r$ and $K(H(G_r, x)) = 1$. \square

Given a graph G , we say that the degree sequence of G is even (respectively, odd) if $\{d_u\}_{u \in V(G)}$ is a subset of the even (respectively, odd) integers.

Proposition 2.18. *Let G be a graph. Then $H(G, x)$ is an odd function if and only if the degree sequence of each connected component of G is either even or odd.*

Proof. If the degree sequence of each connected component of G is either even or odd, then $d_u + d_v - 1$ is odd for every $uv \in E(G)$. Since every exponent in $H(G, x)$ is odd, $H(G, x)$ is an odd function.

Assume now that $H(G, x)$ is an odd function. Thus, $d_u + d_v$ is even for every $uv \in E(G)$. Let us consider any fixed connected component G_i of G . If there is a vertex $u \in V(G_i)$ such that d_u is even, then d_v is even for every $v \in N(u)$. Since G_i is a connected graph, we conclude that the degree sequence of G_i is even. The same argument gives that if there is a vertex $u \in V(G_i)$ with d_u odd, the degree sequence of G_i is odd. \square

We say that the graph G has *alternated degree* if d_u and d_v have different oddity for every $u, v \in V(G)$ with $uv \in E(G)$.

From the above definition, the following result is obtained.

Proposition 2.19. *Let G be a graph. Then $H(G, x)$ is an even function if and only if G has alternated degree.*

An edge in a graph is said to be *pendant* if one of its vertices has degree 1. A path with length two in a graph is said to be a *pendant path* if it contains a pendant edge and a non-pendant edge.

Proposition 2.20. *Let G be a graph. Then, the cardinality of the pendant paths in G is the coefficient of x^2 in $H(G, x)$.*

Proof. There is a bijective correspondence between the pendant paths in G and the edges $uv \in E(G)$ with $d_u = 1$ and $d_v = 2$ (i.e., $d_u + d_v - 1 = 2$). This gives the result. \square

There are inequalities involving the harmonic and the first Zagreb indices ([16], [31, Theorem 2.5], [12, p.234]):

Theorem 2.21. *Let G be a graph with m edges, maximum degree Δ and minimum degree δ . Then*

$$\frac{2m^2}{M_1(G)} \leq H(G) \leq \frac{(\Delta + \delta)^2 m^2}{2\Delta\delta M_1(G)}.$$

The equality in the lower bound is attained if and only if $d_u + d_v$ is a constant for every $uv \in E(G)$. The equality in the upper bound is attained if G is regular.

We will use Theorem 2.21 in the proof of Proposition 2.22 below.

Considering the Zagreb indices, Fath-Tabar [6] defined the first Zagreb polynomial as

$$M_1(G, x) := \sum_{uv \in E(G)} x^{d_u + d_v}.$$

The harmonic and the first Zagreb indices are related by Theorem 2.21. Moreover, the harmonic and the first Zagreb polynomials are related by the equality $M_1(G, x) = x H(G, x)$.

The next result provides more bounds of $\text{Deg}_{\min} H(G, x)$ and $\text{Deg} H(G, x)$.

Proposition 2.22. *Let G be a graph with n vertices, m edges, maximum degree Δ and minimum degree δ . Then,*

$$2\delta - 1 \leq \text{Deg}_{\min} H(G, x) \leq \frac{H'(G, 1)}{m}, \quad \frac{4m}{n} - 1 \leq \text{Deg} H(G, x) \leq 2\Delta - 1.$$

Proof. The inequality $H(G) \leq n/2$ is a well-known upper bound for the harmonic index. Theorem 2.21 gives the lower bound $H(G) \geq 2m^2/M_1(G)$. Given $j \in \mathbb{N}$, let us define $c_j = c_j(G)$ as the cardinality of the set $\{uv \in E(G) \mid d_u + d_v - 1 = j\}$. We can write

$$H(G, x) = \sum_{j=\text{Deg}_{\min} H(G, x)}^{\text{Deg} H(G, x)} c_j x^j, \quad \text{with} \quad \sum_{j=\text{Deg}_{\min} H(G, x)}^{\text{Deg} H(G, x)} c_j = m.$$

Thus, we have

$$\begin{aligned}
 \frac{n}{2} &\geq H(G) = 2 \int_0^1 H(G, x) dx = \sum_{j=\text{Deg}_{\min} H(G, x)}^{\text{Deg} H(G, x)} \frac{2c_j}{j+1} \\
 &\geq \sum_{j=\text{Deg}_{\min} H(G, x)}^{\text{Deg} H(G, x)} \frac{2c_j}{\text{Deg} H(G, x) + 1} = \frac{2m}{\text{Deg} H(G, x) + 1}, \\
 \text{Deg} H(G, x) &\geq \frac{4m}{n} - 1, \\
 \frac{2m^2}{M_1(G)} &\leq H(G) = \sum_{j=\text{Deg}_{\min} H(G, x)}^{\text{Deg} H(G, x)} \frac{2c_j}{j+1} \leq \frac{2m}{\text{Deg}_{\min} H(G, x) + 1}, \\
 \text{Deg}_{\min} H(G, x) &\leq \frac{M_1(G)}{m} - 1 = \frac{M_1(G) - m}{m} = \frac{H'(G, 1)}{m}.
 \end{aligned}$$

Proposition 2.10 provides the other inequalities. \square

The next result allows to bound the harmonic index of a graph by using several parameters of its harmonic polynomial.

Given a graph G , let us denote by $c_{\min}(G)$ and $c_{\max}(G)$ the coefficients of $x^{\text{Deg}_{\min} H(G, x)}$ and $x^{\text{Deg} H(G, x)}$ in $H(G, x)$, respectively.

Proposition 2.23. *Let G be a graph with m edges. Then,*

$$\begin{aligned}
 &\frac{2c_{\min}(G)}{\text{Deg}_{\min} H(G, x) + 1} + \frac{2m - 2c_{\min}(G)}{\text{Deg} H(G, x) + 1} \leq H(G) \leq \\
 &\leq \frac{2c_{\max}(G)}{\text{Deg} H(G, x) + 1} + \frac{2m - 2c_{\max}(G)}{\text{Deg}_{\min} H(G, x) + 1}.
 \end{aligned}$$

Proof. As in the proof of Proposition 2.22, we obtain

$$H(G) = 2 \int_0^1 H(G, x) dx = \sum_{j=\text{Deg}_{\min} H(G, x)}^{\text{Deg} H(G, x)} \frac{2c_j}{j+1}.$$

Hence,

$$\begin{aligned}
 H(G) &= \frac{2c_{\min}(G)}{\text{Deg}_{\min} H(G, x) + 1} + \sum_{j=\text{Deg}_{\min} H(G, x)+1}^{\text{Deg} H(G, x)} \frac{2c_j}{j+1} \\
 &\geq \frac{2c_{\min}(G)}{\text{Deg}_{\min} H(G, x) + 1} + \sum_{j=\text{Deg}_{\min} H(G, x)+1}^{\text{Deg} H(G, x)} \frac{2c_j}{\text{Deg} H(G, x) + 1} \\
 &= \frac{2c_{\min}(G)}{\text{Deg}_{\min} H(G, x) + 1} + \frac{2m - 2c_{\min}(G)}{\text{Deg} H(G, x) + 1}, \\
 H(G) &= \frac{2c_{\max}(G)}{\text{Deg} H(G, x) + 1} + \sum_{j=\text{Deg}_{\min} H(G, x)}^{\text{Deg} H(G, x)-1} \frac{2c_j}{j+1} \\
 &\leq \frac{2c_{\max}(G)}{\text{Deg} H(G, x) + 1} + \sum_{j=\text{Deg}_{\min} H(G, x)}^{\text{Deg} H(G, x)-1} \frac{2c_j}{\text{Deg}_{\min} H(G, x) + 1} \\
 &= \frac{2c_{\max}(G)}{\text{Deg} H(G, x) + 1} + \frac{2m - 2c_{\max}(G)}{\text{Deg}_{\min} H(G, x) + 1}.
 \end{aligned}$$

□

Although two non-isomorphic graphs can have the same harmonic polynomial, Theorem 2.24 below shows that two graphs with the same harmonic polynomial have to be similar.

For each function $\mu : \mathbb{N} \rightarrow (0, \infty)$, let us define its associated topological indices

$$T_{\mu}(G) = \sum_{uv \in E(G)} \mu(d_u + d_v), \quad U_{\mu}(G) = \prod_{uv \in E(G)} \mu(d_u + d_v).$$

In particular, if $\mu(t) = t^{\alpha}$, then $T_{\mu} = \chi_{\alpha}$. The *modified first multiplicative Zagreb index* is defined in [5] by $\Pi_1^*(G) = \prod_{uv \in E(G)} (d_u + d_v)$. In particular, if $\mu(t) = t$, then $U_{\mu} = \Pi_1^*$.

Theorem 2.24. *If two graphs G_1 and G_2 have the same harmonic polynomial, then $T_{\mu}(G_1) = T_{\mu}(G_2)$ and $U_{\mu}(G_1) = U_{\mu}(G_2)$ for every function $\mu : \mathbb{N} \rightarrow (0, \infty)$. In particular, $\chi_{\alpha}(G_1) = \chi_{\alpha}(G_2)$ for every $\alpha \in \mathbb{R}$, and $\Pi_1^*(G_1) = \Pi_1^*(G_2)$.*

Proof. As in the proof of Proposition 2.22, given a graph G and $j \in \mathbb{N}$, we define $c_j(G)$ as the cardinality of the set $\{uv \in E(G) \mid d_u + d_v - 1 = j\}$. Thus, $H(G, x) = \sum_j c_j(G) x^j$. If $H(G_1, x) = H(G_2, x)$, then $c_j(G_1) = c_j(G_2)$ for every $j \in \mathbb{N}$. Since $T_{\mu}(G) = \sum_j c_j(G) \mu(j+1)$ and $U_{\mu}(G) = \prod_j \mu(j+1)^{c_j(G)}$ for every function $\mu : \mathbb{N} \rightarrow (0, \infty)$, we conclude that $T_{\mu}(G_1) = T_{\mu}(G_2)$ and $U_{\mu}(G_1) = U_{\mu}(G_2)$. □

We want to remark that if we consider a function $\mu : \mathbb{N} \rightarrow \mathbb{C}$ in the definition T_μ , then the argument in the proof of Theorem 2.24 also works. Thus, we can consider a family of functions $\{\mu_z\}$, where z is a complex variable, and we can define for each graph G the complex function $F_G(z) := T_{\mu_z}(G)$. So, if two graphs G_1 and G_2 have the same harmonic polynomial, then the complex functions $F_{G_1}(z)$ and $F_{G_2}(z)$ are the same. This holds, in particular, for the holomorphic function $F_G(z) := \sum_{uv \in E(G)} (d_u + d_v)^z$.

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