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Harmonic Index and Harmonic Polynomial on Graph Operations

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Abstract: Some years ago, the harmonic polynomial was introduced to study the harmonic topological index. Here, using this polynomial, we obtain several properties of the harmonic index of many classical symmetric operations of graphs: Cartesian product, corona product, join, Cartesian sum and lexicographic product. Some upper and lower bounds for the harmonic indices of these operations of graphs, in terms of related indices, are derived from known bounds on the integral of a product on nonnegative convex functions. Besides, we provide an algorithm that computes the harmonic polynomial with complexity $O(n^2)$.

Keywords: harmonic index; harmonic polynomial; inverse degree index; products of graphs; algorithm

1. Introduction

A single number representing a chemical structure, by means of the corresponding molecular graph, is known as topological descriptor. Topological descriptors play a prominent role in mathematical chemistry, particularly in studies of quantitative structure–property and quantitative structure–activity relationships. Moreover, a topological descriptor is called a topological index if it has a mutual relationship with a molecular property. Thus, since topological indices encode some characteristics of a molecule in a single number, they can be used to study physicochemical properties of chemical compounds.

After the seminal work of Wiener [1], many topological indices have been defined and analysed. Among all topological indices, probably the most studied is the Randić connectivity index (R) [2]. Several hundred papers and, at least, two books report studies of R (see, for example, [3–7] and references therein). Moreover, with the aim of improving the predictive power of R, many additional topological descriptors (similar to R) have been proposed. In fact, the first and second Zagreb indices, M_1 and M_2, respectively, can be considered as the main successors of R. They are defined as

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

where uv is the edge of G between vertices u and v, and d_u is the degree of vertex u. Both M_1 and M_2 have recently attracted much interest (see, e.g., [8–11]) (in particular, they are included in algorithms used to compute topological indices).

Another remarkable topological descriptor is the *harmonic* index, defined in [12] as

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

This index has attracted a great interest in the lasts years (see, e.g., [13–18]). In particular, in [16] appear relations for the harmonic index of some operations of graphs.

In [19], 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. For more information on the study of polynomials associated with topological indices and their practical applications, see, e.g., [20–23].

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

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., [21,24] 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 graphs 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.

Polynomials have proved to be useful in the study of several topological indices. There are many papers studying topological indices on graph operations (see, e.g., [25–27]).

Along this work, $G = (V, E) = (V(G), E(G))$ indicates a finite, undirected and simple (i.e., without multiple edges and loops) graph with $E \neq \emptyset$. The main aim of this paper is to obtain several computational properties of the harmonic polynomial. In Section 2, we obtain closed formulas to compute the harmonic polynomial of many classical symmetric operations of graphs: Cartesian product, corona product, join, Cartesian sum and lexicographic product. These formulas are interesting by themselves and, furthermore, allow to obtain new inequalities for the harmonic index of these operations of graphs. Besides, we provide in the last section an algorithm that computes this polynomial with complexity $O(n^2)$.

We would like to stress that the symmetry property present in the operations on graphs studied here (Cartesian product, corona product, join, Cartesian sum and lexicographic product) was an essential tool in the study of the topological indexes, because it allowed us to obtain closed formulas for the harmonic polynomial and to deduce the optimal bounds for that index.

2. Definitions and Background

The following result appears in Proposition 1 of [19].

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

Propositions 2, 4, 5, 7 in [19] 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. *We have*

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

In Propositions 2.3 and 2.6 in [28] appear the following result.

Proposition 3. *If G is a graph with m edges, then:*

- $H^{(k)}(G,x)\geq 0$ *for every* $k\geq 0$ *and* $x\in[0,\infty)$;
- $H(G,x)>0$ *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; *and*
- $0=H(G,0)\leq H(G,x)\leq H(G,1)=m$ *for every* $x\in[0,1]$.

Considering the Zagreb indices, Fath-Tabar [29] 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 several inequalities (see [30], Theorem 2.5 [31] and [32], p. 234). Moreover, the harmonic and the first Zagreb polynomials are related by the equality $M_1(G,x)=x\,H(G,x)$,

In [33], Shuxian defined the following polynomial related to the first Zagreb index as

$$M_1^*(G,x):=\sum_{u\in V(G)}d_ux^{d_u}.$$

Given a graph G, let us denote by $S(G)$ its *subdivision graph*. $S(G)$ is constructed from G by inserting an additional vertex into each of its edges. Concerning $S(G)$, in Theorem 2.1 of [25], the following result appears.

Theorem 1. *For the subdivision graph $S(G)$ of G, the first Zagreb polynomial is*

$$M_1(S(G),x)=x^2M_1^*(G,x).$$

Since the harmonic and the first Zagreb polynomials are related by the equality $M_1(G,x)=x\,H(G,x)$, we have the following result for the harmonic polynomial of the subdivision graph.

Proposition 4. *Given a graph G, the harmonic polynomial of its subdivision graph $S(G)$ is*

$$H(S(G),x)=x\,M_1^*(G,x).$$

Similarly, we can obtain the harmonic polynomial for the other operations on graphs appearing in [25].

Next, we obtain the harmonic polynomial for other classical operations: Cartesian product, corona product, join, Cartesian sum and lexicographic product. It is important to stress that, since large graphs are composed by smaller ones by the use of products of graphs (and, as a consequence, their properties are strongly related), the study of products of graphs is a relevant and timely research subject.

Let us recall the definitions of these classical products in graph theory.

The *Cartesian product* $G_1 \times G_2$ of the graphs G_1 and G_2 has the vertex set $V(G_1 \times G_2) = V(G_1) \times V(G_2)$ and $(u_i, v_j)(u_k, v_l)$ is an edge of $G_1 \times G_2$ if $u_i = u_k$ and $v_j v_l \in E(G_2)$, or $u_i u_k \in E(G_1)$ and $v_j = v_l$.

Given two graphs G_1 and G_2, we define the *corona product* $G_1 \circ G_2$ as the graph obtained by adding to G_1, $|V(G_1)|$ copies of G_2 and joining each vertex of the i-th copy with the vertex $v_i \in V(G_1)$.

The *join* $G_1 + G_2$ is defined as the graph obtained by taking one copy of G_1 and one copy of G_2, and joining by an edge each vertex of G_1 with each vertex of G_2.

The *Cartesian sum* $G_1 \oplus G_2$ of the graphs G_1 and G_2 has the vertex set $V(G_1 \oplus G_2) = V(G_1) \times V(G_2)$ and $(u_i, v_j)(u_k, v_l)$ is an edge of $G_1 \oplus G_2$ if $u_i u_k \in E(G_1)$ or $v_j v_l \in E(G_2)$.

The *lexicographic product* $G_1 \odot G_2$ of the graphs G_1 and G_2 has $V(G_1) \times V(G_2)$ as vertex set, so that two distinct vertices $(u_i, v_j), (u_k, v_l)$ of $V(G_1 \odot G_2)$ are adjacent if either $u_i u_k \in E(G_1)$, or $u_i = u_k$ and $v_j v_l \in E(G_2)$.

Let us introduce another topological index that will be very useful in this work.

The *inverse degree* $ID(G)$ of a graph G is defined by

$$ID(G) := \sum_{u \in V(G)} \frac{1}{d_u} = \sum_{uv \in E(G)} \Big(\frac{1}{d_u^2} + \frac{1}{d_v^2} \Big).$$

It is relevant to mention that the surmises inferred through the computer program Graffiti [12] attracted the attention of researchers. Thus, since then, several studies (see, e.g., [34–38]) focusing on relationships between $ID(G)$ and other graph invariants (such as diameter, edge-connectivity, matching number and Wiener index) have appeared in the literature.

Let us define the *inverse degree polynomial* of a graph G as

$$ID(G, x) = \sum_{u \in V(G)} x^{d_u - 1}.$$

Thus, we have $\int_0^1 ID(G, x)\, dx = ID(G)$. Note that $x(xID(G, x))' = M_1^*(G, x)$.

The following result summarizes some interesting properties of the inverse degree polynomial. Recall that a vertex of a graph is said to be *pendant* if it has degree 1.

Proposition 5. *If G is a graph with n vertices and k pendant vertices, then:*

- $ID^{(j)}(G, x) \geq 0$ *for every* $j \geq 0$ *and* $x \in [0, \infty)$;
- $ID(G, x) > 0$ *on* $(0, \infty)$;
- $ID(G, x)$ *is strictly increasing on* $[0, \infty)$ *if and only if G is not isomorphic to a union of path graphs* P_2;
- $ID(G, x)$ *is strictly convex on* $[0, \infty)$ *if and only if G is not isomorphic to a union of path graphs; and*
- $k = ID(G, 0) \leq ID(G, x) \leq ID(G, 1) = n$ *for every* $x \in [0, 1]$.

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

Since every coefficient of the polynomial $ID(G, x)$ is non-negative and $ID(G, x)$ is not identically zero, we have $ID(G, x) > 0$ on $(0, \infty)$.

Since every coefficient of the polynomial $ID(G, x)$ is non-negative, we have $ID'(G, x) > 0$ on $(0, \infty)$ if and only if there exists a vertex $u \in V(G)$ with $d_u \geq 2$, and this holds if and only if G is not isomorphic to a union of path graphs P_2.

Similarly, $ID(G, x)$ is strictly convex on $[0, \infty)$ if and only if there exists a vertex $u \in V(G)$ with $d_u \geq 3$, and this holds if and only if G is not isomorphic to a union of path graphs.

Finally, if $x \in [0, 1]$, then

$$k = ID(G,0) \le \sum_{u \in V(G)} x^{d_u - 1} \le \sum_{u \in V(G)} 1 = ID(G,1) = n.$$

□

Proposition 4 has the following consequence, which illustrates how these polynomials associated to topological indices provide information about the topological indices themselves.

Corollary 1. *Given a graph G with maximum degree Δ, the harmonic index of the subdivision graph $S(G)$ satisfies*

$$H(S(G)) \le 2\Delta\, ID(G).$$

Proof. Proposition 4 gives

$$H(S(G)) = 2\int_0^1 H(S(G),x)\,dx = 2\int_0^1 x\,M_1^*(G,x)\,dx = 2\int_0^1 x \sum_{u \in V(G)} d_u x^{d_u} dx$$
$$\le 2\Delta \int_0^1 \sum_{u \in V(G)} x^{d_u - 1} dx = 2\Delta \int_0^1 ID(G,x)\,dx = 2\Delta\, ID(G).$$

□

3. Computation of the Harmonic Index of Graph Operations

Let us start with the formula of the harmonic polynomial of the Cartesian product.

Theorem 2. *Given two graphs G_1 and G_2, the harmonic polynomial of the Cartesian product $G_1 \times G_2$ is*

$$H(G_1 \times G_2, x) = x^2 H(G_1,x)\, ID(G_2,x^2) + x^2 H(G_2,x)\, ID(G_1,x^2).$$

Proof. Denote by n_1 and n_2 the cardinality of the vertices of G_1 and G_2, respectively.

Note that if $(u_i, v_j) \in V(G_1 \times G_2)$, then $d_{(u_i,v_j)} = d_{u_i} + d_{v_j}$.

If $(u_i, v_k)(u_j, v_k) \in E(G_1 \times G_2)$, then the corresponding monomial of the harmonic polynomial is

$$x^{d_{u_i} + d_{v_k} + d_{u_j} + d_{v_k} - 1} = x^{2d_{v_k}} x^{d_{u_i} + d_{u_j} - 1}.$$

Hence,

$$\sum_{k=1}^{n_2} \sum_{u_i u_j \in E(G_1)} x^{2d_{v_k}} x^{d_{u_i} + d_{u_j} - 1} = x^2 \sum_{k=1}^{n_2} (x^2)^{d_{v_k} - 1} \sum_{u_i u_j \in E(G_1)} x^{d_{u_i} + d_{u_j} - 1} = x^2 ID(G_2, x^2)\, H(G_1, x).$$

The same argument gives that the sum of the monomials corresponding to $(u_k, v_i)(u_k, v_j) \in E(G_1 \times G_2)$ is $x^2 H(G_2,x)\, ID(G_1,x^2)$, and the equality holds. □

Next, we present two useful improvements (for convex functions) of the well-known Chebyshev's inequalities.

Lemma 1 ([39]). *Let $f_1, \ldots, f_k$ be non-negative convex functions defined on the interval $[0,1]$. Then,*

$$\int_0^1 \prod_{i=1}^k f_i(x)\,dx \ge \frac{2^k}{k+1} \prod_{i=1}^k \int_0^1 f_i(x)\,dx\,.$$

Lemma 2 (Corollary 5.2 [40])**.** *Let $f_1, \ldots, f_k$ be non-negative convex functions defined on the interval $[0,1]$. Then*

$$\int_0^1 \prod_{i=1}^k f_i(x)\,dx \le \frac{2}{k+1}\left(\prod_{i=1}^k \int_0^1 f_i(x)\,dx\right)^{1/k}\left(\prod_{i=1}^k (f_i(0)+f_i(1))\right)^{1-1/k}.$$

Theorem 3. *Given two graphs G_1 and G_2 with n_1 and n_2 vertices, and m_1 and m_2 edges, respectively, the harmonic index of the Cartesian product $G_1 \times G_2$ satisfies*

$$\begin{aligned}
H(G_1\times G_2) &\ge \frac{1}{2}H(G_1)\,ID(G_2) + \frac{1}{2}H(G_2)\,ID(G_1),\\
H(G_1\times G_2) &\le \min\left\{\frac{2}{3}\Big(m_1n_2H(G_1)\,ID(G_2)\Big)^{1/2}, \frac{1}{2}\Big(m_1^2n_2^2H(G_1)\,ID(G_2)\Big)^{1/3}\right\}\\
&\quad+\min\left\{\frac{2}{3}\Big(m_2n_1H(G_2)\,ID(G_1)\Big)^{1/2}, \frac{1}{2}\Big(m_2^2n_1^2H(G_2)\,ID(G_1)\Big)^{1/3}\right\}.
\end{aligned}$$

Proof. Propositions 3 and 5 give that $H(G_1,x), ID(G_2,x^2), H(G_2,x), ID(G_1,x^2)$ are non-negative convex functions. Thus, Lemma 1 gives

$$\begin{aligned}
\int_0^1 2x^2H(G_1,x)\,ID(G_2,x^2)\,dx &\ge \frac{2^3}{3+1}\int_0^1 x\,dx\int_0^1 H(G_1,x)\,dx\int_0^1 2xID(G_2,x^2)\,dx\\
&= 2\,\frac{1}{2}\int_0^1 H(G_1,x)\,dx\int_0^1 ID(G_2,x)\,dx = \frac{1}{2}H(G_1)\,ID(G_2).
\end{aligned}$$

Similarly,

$$\int_0^1 2x^2H(G_2,x)\,ID(G_1,x^2)\,dx \ge \frac{1}{2}H(G_2)\,ID(G_1).$$

These inequalities, Theorem 2 and $H(G_1\times G_2) = 2\int_0^1 H(G_1\times G_2,x)\,dx$ give the lower bound.

Lemma 2 and Propositions 3 and 5 give

$$\begin{aligned}
\int_0^1 2x^2H(G_1,x)\,ID(G_2,x^2)\,dx &\le \int_0^1 2x\,H(G_1,x)\,ID(G_2,x^2)\,dx\\
&\le \frac{2}{3}\left(\int_0^1 H(G_1,x)\,dx\int_0^1 2xID(G_2,x^2)\,dx\right)^{1/2}\big(2H(G_1,1)\,ID(G_2,1)\big)^{1/2}\\
&= \frac{2}{3}\Big(m_1n_2H(G_1)\,ID(G_2)\Big)^{1/2}.
\end{aligned}$$

In addition, Lemma 2 and Propositions 3 and 5 give

$$\begin{aligned}
\int_0^1 2x^2H(G_1,x)\,ID(G_2,x^2)\,dx &\le \frac{1}{2}\left(\int_0^1 x\,dx\int_0^1 H(G_1,x)\,dx\int_0^1 2xID(G_2,x^2)\,dx\right)^{1/3}\big(2H(G_1,1)\,ID(G_2,1)\big)^{2/3}\\
&= \frac{1}{2}\Big(m_1^2n_2^2H(G_1)\,ID(G_2)\Big)^{1/3}.
\end{aligned}$$

These inequalities give

$$\int_0^1 2x^2H(G_1,x)\,ID(G_2,x^2)\,dx \le \min\left\{\frac{2}{3}\Big(m_1n_2H(G_1)\,ID(G_2)\Big)^{1/2}, \frac{1}{2}\Big(m_1^2n_2^2H(G_1)\,ID(G_2)\Big)^{1/3}\right\}.$$

Similarly,

$$\int_0^1 2x^2H(G_2,x)\,ID(G_1,x^2)\,dx \le \min\left\{\frac{2}{3}\Big(m_2n_1H(G_2)\,ID(G_1)\Big)^{1/2}, \frac{1}{2}\Big(m_2^2n_1^2H(G_2)\,ID(G_1)\Big)^{1/3}\right\}.$$

These inequalities, Theorem 2 and $H(G_1 \times G_2) = 2\int_0^1 H(G_1 \times G_2, x)\,dx$ give the upper bound. □

Theorem 4. *Given two graphs G_1 and G_2, with n_1 and n_2 vertices, respectively, the harmonic polynomial of the corona product $G_1 \circ G_2$ is*

$$H(G_1 \circ G_2, x) = x^{2n_2} H(G_1, x) + n_1 x^2 H(G_2, x) + x^{n_2+2} ID(G_1, x)\, ID(G_2, x).$$

Proof. The degree of $u \in V(G_1)$, considered as a vertex of $G_1 \circ G_2$, is $d_u + n_2$. The degree of any copy v' of $v \in V(G_2)$, considered as a vertex of $G_1 \circ G_2$, is $d_v + 1$.

If $u_i u_j \in E(G_1)$, then the corresponding monomial of the harmonic polynomial of $G_1 \circ G_2$ is

$$x^{d_{u_i}+n_2+d_{u_j}+n_2-1} = x^{2n_2} x^{d_{u_i}+d_{u_j}-1}.$$

Hence,

$$\sum_{u_i u_j \in E(G_1)} x^{2n_2} x^{d_{u_i}+d_{u_j}-1} = x^{2n_2} \sum_{u_i u_j \in E(G_1)} x^{d_{u_i}+d_{u_j}-1} = x^{2n_2} H(G_1, x).$$

If $v_i v_j \in E(G_2)$, then each corresponding monomial of the harmonic polynomial of $G_1 \circ G_2$ is

$$x^{d_{v_i}+1+d_{v_j}+1-1} = x^2 x^{d_{v_i}+d_{v_j}-1}.$$

Therefore,

$$\sum_{v_i v_j \in E(G_2)} x^2 x^{d_{v_i}+d_{v_j}-1} = x^2 \sum_{v_i v_j \in E(G_2)} x^{d_{v_i}+d_{v_j}-1} = x^2 H(G_2, x).$$

If we add the corresponding polynomials of the n_1 copies of G_2, then we obtain $n_1 x^2 H(G_2, x)$.

If $u_i v_j' \in E(G_1 \circ G_2)$ with $u_i \in V(G_1)$ and $v_j \in V(G_2)$, then the corresponding monomial of the harmonic polynomial is

$$x^{d_{u_i}+n_2+d_{v_j}+1-1} = x^{n_2+2} x^{d_{u_i}-1} x^{d_{v_j}-1}.$$

Hence,

$$\sum_{i=1}^{n_1} \sum_{j=1}^{n_2} x^{n_2+2} x^{d_{u_i}-1} x^{d_{v_j}-1} = x^{n_2+2} \sum_{i=1}^{n_1} x^{d_{u_i}-1} \sum_{j=1}^{n_2} x^{d_{v_j}-1} = x^{n_2+2} ID(G_1, x)\, ID(G_2, x).$$

Thus, the equality holds. □

Theorem 5. *Given two graphs G_1 and G_2 with n_1 and n_2 vertices, m_1 and m_2 edges, and k_1 and k_2 pendant vertices, respectively, the harmonic index of the corona product $G_1 \circ G_2$ satisfies*

$$\begin{aligned}
H(G_1 \circ G_2) &\geq \frac{4}{3(2n_2+1)}\, H(G_1) + \frac{4n_1}{9}\, H(G_1) + \frac{4}{n_2+3}\, ID(G_1)\, ID(G_2),\\
H(G_1 \circ G_2) &\leq \frac{2}{3}\Big(\frac{2m_1}{2n_2+1} H(G_1)\Big)^{1/2} + \frac{2n_1}{3}\Big(\frac{2m_2}{3} H(G_2)\Big)^{1/2}\\
&\quad + \Big(\frac{1}{n_2+3}\, ID(G_1)\, ID(G_2) (n_1+k_1)^2 (n_2+k_2)^2\Big)^{1/3}.
\end{aligned}$$

Proof. Lemma 1 gives

$$\begin{aligned}
\int_0^1 2x^{2n_2} H(G_1, x)\,dx &\geq \frac{4}{3}\int_0^1 x^{2n_2} dx \int_0^1 2\,H(G_1, x)\,dx = \frac{4}{3(2n_2+1)}\, H(G_1),\\
\int_0^1 2n_1 x^2 H(G_2, x)\,dx &\geq \frac{4n_1}{3}\int_0^1 x^2 dx \int_0^1 2\,H(G_1, x)\,dx = \frac{4n_1}{9}\, H(G_1),
\end{aligned}$$

$$\int_0^1 2x^{n_2+2} ID(G_1,x)\, ID(G_2,x)\, dx \geq \frac{8}{4}\int_0^1 2x^{n_2+2}dx \int_0^1 ID(G_1,x)\, dx \int_0^1 ID(G_2,x)\, dx$$
$$= \frac{4}{n_2+3}\, ID(G_1)\, ID(G_2).$$

These inequalities, Theorem 4 and $H(G_1 \circ G_2) = 2\int_0^1 H(G_1 \circ G_2, x)\, dx$ give the lower bound. Lemma 2 and Proposition 3 give

$$\int_0^1 2x^{2n_2} H(G_1,x)\, dx \leq \frac{2}{3}\left(\int_0^1 x^{2n_2}dx \int_0^1 2\,H(G_1,x)\, dx\right)^{1/2} \left(2H(G_1,1)\right)^{1/2}$$
$$= \frac{2}{3}\Big(\frac{2m_1}{2n_2+1} H(G_1)\Big)^{1/2}.$$

In addition, Lemma 2 and Proposition 3 give

$$\int_0^1 2n_1 x^2 H(G_2,x)\, dx \leq \frac{2n_1}{3}\left(\int_0^1 x^2 dx \int_0^1 2\,H(G_2,x)\, dx\right)^{1/2} \left(2H(G_2,1)\right)^{1/2}$$
$$= \frac{2n_1}{3}\Big(\frac{2m_2}{3} H(G_2)\Big)^{1/2}.$$

Lemma 2 and Proposition 5 give

$$\int_0^1 2x^{n_2+2} ID(G_1,x)\, ID(G_2,x)\, dx \leq \frac{2}{4}\, 2\left(\int_0^1 x^{n_2+2}dx \int_0^1 ID(G_1,x)\, dx \int_0^1 ID(G_2,x)\, dx\right)^{1/3}$$
$$\cdot \left((ID(G_1,1)+ID(G_1,0))(ID(G_2,1)+ID(G_2,0))\right)^{2/3}$$
$$= \left(\frac{1}{n_2+3}\, ID(G_1)\, ID(G_2)(n_1+k_1)^2(n_2+k_2)^2\right)^{1/3}.$$

These inequalities, Theorem 4 and $H(G_1 \circ G_2) = 2\int_0^1 H(G_1 \circ G_2, x)\, dx$ give the upper bound. □

Theorem 6. *Given two graphs G_1 and G_2, with n_1 and n_2 vertices, respectively, the harmonic polynomial of the join $G_1 + G_2$ is*

$$H(G_1+G_2,x) = x^{2n_2} H(G_1,x) + x^{2n_1} H(G_2,x) + x^{n_1+n_2+1} ID(G_1,x)\, ID(G_2,x).$$

Proof. The degree of $u \in V(G_1)$, considered as a vertex of $G_1 + G_2$, is $d_u + n_2$. The degree of $v \in V(G_2)$, considered as a vertex of $G_1 + G_2$, is $d_v + n_1$.

If $u_i u_j \in E(G_1)$, then the corresponding monomial of the harmonic polynomial of $G_1 + G_2$ is

$$x^{d_{u_i}+n_2+d_{u_j}+n_2-1} = x^{2n_2} x^{d_{u_i}+d_{u_j}-1}.$$

Hence,

$$\sum_{u_i u_j \in E(G_1)} x^{2n_2} x^{d_{u_i}+d_{u_j}-1} = x^{2n_2} \sum_{u_i u_j \in E(G_1)} x^{d_{u_i}+d_{u_j}-1} = x^{2n_2} H(G_1,x).$$

If $v_i v_j \in E(G_2)$, then the corresponding monomial of the harmonic polynomial of $G_1 + G_2$ is

$$x^{d_{v_i}+n_1+d_{v_j}+n_1-1} = x^{2n_1} x^{d_{v_i}+d_{v_j}-1}.$$

Therefore,

$$\sum_{v_i v_j \in E(G_2)} x^{2n_1} x^{d_{v_i}+d_{v_j}-1} = x^{2n_1} \sum_{v_i v_j \in E(G_2)} x^{d_{v_i}+d_{v_j}-1} = x^{2n_1} H(G_2,x).$$

If $u_i v_j \in E(G_1 + G_2)$ with $u_i \in V(G_1)$ and $v_j \in V(G_2)$, then the corresponding monomial of the harmonic polynomial is

$$x^{d_{u_i}+n_2+d_{v_j}+n_1-1} = x^{n_1+n_2+1} x^{d_{u_i}-1} x^{d_{v_j}-1}.$$

Hence,

$$\sum_{i=1}^{n_1} \sum_{j=1}^{n_2} x^{n_1+n_2+1} x^{d_{u_i}-1} x^{d_{v_j}-1} = x^{n_1+n_2+1} \sum_{i=1}^{n_1} x^{d_{u_i}-1} \sum_{j=1}^{n_2} x^{d_{v_j}-1} = x^{n_1+n_2+1} ID(G_1, x)\, ID(G_2, x),$$

Thus, the equality holds. □

Theorem 7. *Given two graphs G_1 and G_2 with n_1 and n_2 vertices, m_1 and m_2 edges, and k_1 and k_2 pendant vertices, respectively, the harmonic index of the join $G_1 + G_2$ satisfies*

$$\begin{aligned} H(G_1 + G_2) &\geq \frac{4}{3(2n_2+1)} H(G_1) + \frac{4}{3(2n_1+1)} H(G_2) + \frac{4}{n_1+n_2+2} ID(G_1)\, ID(G_2), \\ H(G_1 + G_2) &\leq \frac{2}{3}\Big(\frac{2m_1}{2n_2+1} H(G_1)\Big)^{1/2} + \frac{2}{3}\Big(\frac{2m_2}{2n_1+1} H(G_2)\Big)^{1/2} \\ &\quad + \Big(\frac{1}{n_1+n_2+2} ID(G_1)\, ID(G_2)(n_1+k_1)^2(n_2+k_2)^2\Big)^{1/3}. \end{aligned}$$

Proof. We have seen in the proof of Theorem 5 that

$$\frac{4}{3(2n_2+1)} H(G_1) \leq \int_0^1 2x^{2n_2} H(G_1, x)\, dx \leq \frac{2}{3}\Big(\frac{2m_1}{2n_2+1} H(G_1)\Big)^{1/2}.$$

Similarly, we obtain

$$\frac{4}{3(2n_1+1)} H(G_2) \leq \int_0^1 2x^{2n_1} H(G_2, x)\, dx \leq \frac{2}{3}\Big(\frac{2m_2}{2n_1+1} H(G_2)\Big)^{1/2}.$$

Lemma 1 gives

$$\begin{aligned} \int_0^1 2x^{n_1+n_2+1} ID(G_1, x)\, ID(G_2, x)\, dx &\geq \frac{8}{4} \int_0^1 2x^{n_1+n_2+1} dx \int_0^1 ID(G_1, x)\, dx \int_0^1 ID(G_2, x)\, dx \\ &= \frac{4}{n_1+n_2+2} ID(G_1)\, ID(G_2). \end{aligned}$$

Lemma 2 and Proposition 5 give

$$\begin{aligned} \int_0^1 2x^{n_1+n_2+1} ID(G_1, x)\, ID(G_2, x)\, dx &\leq \frac{2}{4}\, 2 \Big(\int_0^1 x^{n_1+n_2+1} dx \int_0^1 ID(G_1, x)\, dx \int_0^1 ID(G_2, x)\, dx\Big)^{1/3} \\ &\quad \cdot \big((ID(G_1,1) + ID(G_1,0))(ID(G_2,1) + ID(G_2,0))\big)^{2/3} \\ &= \Big(\frac{1}{n_1+n_2+2} ID(G_1)\, ID(G_2)(n_1+k_1)^2(n_2+k_2)^2\Big)^{1/3}. \end{aligned}$$

These inequalities, Theorem 6 and $H(G_1 + G_2) = 2\int_0^1 H(G_1 + G_2, x)\, dx$ give the bounds. □

Theorem 8. *Given two graphs G_1 and G_2, with n_1 and n_2 vertices, respectively, the harmonic polynomial of the Cartesian sum $G_1 \oplus G_2$ is*

$$\begin{aligned} H(G_1 \oplus G_2, x) &= x^{2n_1+n_2-1} H(G_1, x^{n_2})\, ID^2(G_2, x^{n_1}) + x^{n_1+2n_2-1} H(G_2, x^{n_1})\, ID^2(G_1, x^{n_2}) \\ &\quad - x^{n_1+n_2-1} H(G_1, x^{n_2})\, H(G_2, x^{n_1}). \end{aligned}$$

Proof. Note that if $(u_i, v_j) \in V(G_1 \oplus G_2)$, then $d_{(u_i,v_j)} = n_2 d_{u_i} + n_1 d_{v_j}$.

If $(u_i, v_j)(u_k, v_l) \in E(G_1 \oplus G_2)$, then the corresponding monomial of the harmonic polynomial is

$$\begin{aligned} x^{n_2 d_{u_i} + n_1 d_{v_j} + n_2 d_{u_k} + n_1 d_{v_l} - 1} &= x^{2n_1+n_2-1} (x^{n_2})^{d_{u_i}+d_{u_k}-1} (x^{n_1})^{d_{v_j}-1} (x^{n_1})^{d_{v_l}-1} \\ &= x^{n_1+n_2-1} (x^{n_2})^{d_{u_i}+d_{u_k}-1} (x^{n_1})^{d_{v_j}+d_{v_l}-1}. \end{aligned}$$

Hence, the sum of the corresponding monomials with $u_i u_k \in E(G_1)$ is

$$\begin{aligned} &\sum_{j,l=1}^{n_2} \sum_{u_i u_k \in E(G_1)} x^{2n_1+n_2-1} (x^{n_2})^{d_{u_i}+d_{u_k}-1} (x^{n_1})^{d_{v_j}-1} (x^{n_1})^{d_{v_l}-1} \\ &= x^{2n_1+n_2-1} \sum_{j=1}^{n_2} (x^{n_1})^{d_{v_j}-1} \sum_{l=1}^{n_2} (x^{n_1})^{d_{v_l}-1} \sum_{u_i u_k \in E(G_1)} (x^{n_2})^{d_{u_i}+d_{u_k}-1} \\ &= x^{2n_1+n_2-1} H(G_1, x^{n_2})\, ID^2(G_2, x^{n_1}). \end{aligned}$$

Similarly, the sum of the corresponding monomials with $v_j v_l \in E(G_2)$ is

$$x^{n_1+2n_2-1} H(G_2, x^{n_1})\, ID^2(G_1, x^{n_2}).$$

If we add these two terms, then we take into account twice the corresponding monomials with $u_i u_k \in E(G_1)$ and $v_j v_l \in E(G_2)$:

$$\begin{aligned} &\sum_{u_i u_k \in E(G_1)} \sum_{v_j v_l \in E(G_2)} x^{n_1+n_2-1} (x^{n_2})^{d_{u_i}+d_{u_k}-1} (x^{n_1})^{d_{v_j}+d_{v_l}-1} \\ &= x^{n_1+n_2-1} \sum_{u_i u_k \in E(G_1)} (x^{n_2})^{d_{u_i}+d_{u_k}-1} \sum_{v_j v_l \in E(G_2)} (x^{n_1})^{d_{v_j}+d_{v_l}-1} \\ &= x^{n_1+n_2-1} H(G_1, x^{n_2})\, H(G_2, x^{n_1}). \end{aligned}$$

Hence, the equality holds. □

Theorem 9. *Given two graphs G_1 and G_2 with n_1 and n_2 vertices, and m_1 and m_2 edges, respectively, the harmonic index of the Cartesian sum $G_1 \oplus G_2$ satisfies*

$$\begin{aligned} H(G_1 \oplus G_2) &\geq \frac{16}{15 n_1^2 n_2} H(G_1)\, ID^2(G_2) + \frac{16}{15 n_1 n_2^2} H(G_2)\, ID^2(G_1) \\ &\quad - \frac{2}{3} \Big(\frac{m_1 m_2}{n_1 n_2} H(G_1)\, H(G_2) \Big)^{1/2}, \\ H(G_1 \oplus G_2) &\leq \frac{n_2}{2} \Big(\frac{4 m_1^2}{n_1^2} H(G_1)\, ID^2(G_2) \Big)^{1/3} + \frac{n_1}{2} \Big(\frac{4 m_2^2}{n_2^2} H(G_2)\, ID^2(G_1) \Big)^{1/3} \\ &\quad - \frac{1}{2 n_1 n_2} H(G_1)\, H(G_2). \end{aligned}$$

Proof. Lemma 1 gives

$$\begin{aligned} \int_0^1 2x^{2n_1+n_2-1} H(G_1, x^{n_2})\, ID^2(G_2, x^{n_1})\, dx &\geq \frac{16}{5} \int_0^1 x^2 dx \int_0^1 2x^{n_2-1} H(G_1, x^{n_2})\, dx \\ &\quad \cdot \int_0^1 x^{n_1-1} ID(G_2, x^{n_1})\, dx \int_0^1 x^{n_1-1} ID(G_2, x^{n_1})\, dx \\ &= \frac{16}{15 n_1^2 n_2} H(G_1)\, ID^2(G_2), \end{aligned}$$

$$\int_0^1 2x^{n_1+n_2-1} H(G_1, x^{n_2})\, H(G_2, x^{n_1})\, dx \geq \frac{8}{4} \int_0^1 x\, dx \int_0^1 2x^{n_2-1} H(G_1, x^{n_2})\, dx \int_0^1 x^{n_1-1} H(G_2, x^{n_1})\, dx$$
$$= \frac{1}{2n_1 n_2}\, H(G_1)\, H(G_2).$$

The same argument gives

$$\int_0^1 2x^{n_1+2n_2-1} H(G_2, x^{n_1})\, ID^2(G_1, x^{n_2})\, dx \geq \frac{16}{15 n_1 n_2^2}\, H(G_2)\, ID^2(G_1).$$

Lemma 2 and Propositions 3 and 5 give

$$\int_0^1 2x^{2n_1+n_2-1} H(G_1, x^{n_2})\, ID^2(G_2, x^{n_1})\, dx \leq \int_0^1 2x^{n_2-1} H(G_1, x^{n_2})\, x^{2n_1-2} ID^2(G_2, x^{n_1})\, dx$$
$$\leq \frac{2}{4} \left(\int_0^1 2x^{n_2-1} H(G_1, x^{n_2})\, dx \int_0^1 x^{n_1-1} ID(G_2, x^{n_1})\, dx \int_0^1 x^{n_1-1} ID(G_2, x^{n_1})\, dx \right)^{1/3}$$
$$\cdot \left(2H(G_1, 1)\, ID(G_2, 1)\, ID(G_2, 1)\right)^{2/3} = \frac{1}{2} \left(\frac{1}{n_2 n_1^2}\, H(G_1)\, ID^2(G_2) \right)^{1/3} \left(2m_1 n_2^2\right)^{2/3}$$
$$= \frac{n_2}{2} \left(\frac{4m_1^2}{n_1^2}\, H(G_1)\, ID^2(G_2) \right)^{1/3}.$$

The same argument gives

$$\int_0^1 2x^{n_1+2n_2-1} H(G_2, x^{n_1})\, ID^2(G_1, x^{n_2})\, dx \leq \frac{n_1}{2} \left(\frac{4m_2^2}{n_2^2}\, H(G_2)\, ID^2(G_1) \right)^{1/3}.$$

In addition, Lemma 2 and Proposition 3 give

$$\int_0^1 2x^{n_1+n_2-1} H(G_1, x^{n_2})\, H(G_2, x^{n_1})\, dx \leq \frac{1}{2} \int_0^1 2x^{n_2-1} H(G_1, x^{n_2})\, 2x^{n_1-1} H(G_2, x^{n_1})\, dx$$
$$\leq \frac{1}{2}\, \frac{2}{3} \left(\int_0^1 2x^{n_2-1} H(G_1, x^{n_2})\, dx \int_0^1 2x^{n_1-1} H(G_2, x^{n_1})\, dx \right)^{1/2} \left(2H(G_1, 1)\, 2H(G_2, 1)\right)^{1/2}$$
$$= \frac{2}{3} \left(\frac{m_1 m_2}{n_1 n_2}\, H(G_1)\, H(G_2) \right)^{1/2}.$$

These inequalities, Theorem 8 and $H(G_1 \oplus G_2) = 2\int_0^1 H(G_1 \oplus G_2, x)\, dx$ give the desired bounds. □

Theorem 10. *Given two graphs G_1 and G_2, with n_1 and n_2 vertices, respectively, the harmonic polynomial of the lexicographic product $G_1 \odot G_2$ is*

$$H(G_1 \odot G_2, x) = x^{2n_2} ID(G_1, x^{2n_2})\, H(G_2, x) + x^{n_2+1} H(G_1, x^{n_2})\, ID^2(G_2, x).$$

Proof. Note that if $(u_i, v_j) \in V(G_1 \odot G_2)$, then $d_{(u_i,v_j)} = n_2 d_{u_i} + d_{v_j}$.

If $(u_i, v_j)(u_i, v_k) \in E(G_1 \odot G_2)$, then the corresponding monomial of the harmonic polynomial is

$$x^{n_2 d_{u_i} + d_{v_j} + n_2 d_{u_i} + d_{v_k} - 1} = x^{2n_2} (x^{2n_2})^{d_{u_i}-1} x^{d_{v_j} + d_{v_k} - 1}.$$

Hence,

$$\sum_{i=1}^{n_1} \sum_{v_j v_k \in E(G_2)} x^{2n_2} (x^{2n_2})^{d_{u_i}-1} x^{d_{v_j}+d_{v_k}-1} = x^{2n_2} \sum_{i=1}^{n_1} (x^{2n_2})^{d_{u_i}-1} \sum_{v_j v_k \in E(G_2)} x^{d_{v_j}+d_{v_k}-1}$$
$$= x^{2n_2} ID(G_1, x^{2n_2})\, H(G_2, x).$$

If $(u_i, v_j)(u_k, v_l) \in E(G_1 \odot G_2)$ with $u_i u_k \in E(G_1)$, then the corresponding monomial of the harmonic polynomial is

$$x^{n_2 d_{u_i} + d_{v_j} + n_2 d_{u_k} + d_{v_l} - 1} = x^{n_2+1} (x^{n_2})^{d_{u_i} + d_{u_k} - 1} x^{d_{v_j} - 1} x^{d_{v_l} - 1}.$$

Hence, the sum of their corresponding monomials is

$$\begin{aligned}
&\sum_{u_i u_k \in E(G_1)} \sum_{j,l=1}^{n_2} x^{n_2+1} (x^{n_2})^{d_{u_i} + d_{u_k} - 1} x^{d_{v_j} - 1} x^{d_{v_l} - 1} \\
&= x^{n_2+1} \sum_{u_i u_k \in E(G_1)} (x^{n_2})^{d_{u_i} + d_{u_k} - 1} \sum_{j=1}^{n_2} x^{d_{v_j} - 1} \sum_{l=1}^{n_2} x^{d_{v_l} - 1} \\
&= x^{n_2+1} H(G_1, x^{n_2})\, ID^2(G_2, x).
\end{aligned}$$

We obtain the desired equality by adding these two terms. □

Theorem 11. *Given two graphs G_1 and G_2 with n_1 and n_2 vertices, m_1 and m_2 edges, and k_1 and k_2 pendant vertices, respectively, the harmonic index of the lexicographic product $G_1 \odot G_2$ satisfies*

$$\begin{aligned}
H(G_1 \odot G_2) &\geq \frac{1}{2n_2}\, ID(G_1)\, H(G_2) + \frac{16}{15 n_2}\, H(G_1)\, ID^2(G_2) \\
H(G_1 \odot G_2) &\leq \frac{2}{3} \Big(\frac{n_1 m_2}{n_2}\, ID(G_1)\, H(G_2) \Big)^{1/2} + \frac{1}{2} \Big(\frac{4 m_1^2}{n_2}\, H(G_1)\, ID^2(G_2) (n_2 + k_2)^4 \Big)^{1/3}.
\end{aligned}$$

Proof. Lemma 1 gives

$$\begin{aligned}
\int_0^1 2x^{2n_2} ID(G_1, x^{2n_2})\, H(G_2, x)\, dx &\geq \frac{8}{4} \int_0^1 x\, dx \int_0^1 x^{2n_2 - 1} ID(G_1, x^{2n_2})\, dx \int_0^1 2H(G_2, x)\, dx \\
&= \frac{1}{2n_2}\, ID(G_1)\, H(G_2), \\
\int_0^1 2x^{n_2+1} H(G_1, x^{n_2})\, ID^2(G_2, x)\, dx &\geq \frac{16}{5} \int_0^1 x^2\, dx \int_0^1 2x^{n_2 - 1} H(G_1, x^{n_2})\, dx \int_0^1 ID(G_2, x)\, dx \int_0^1 ID(G_2, x)\, dx \\
&= \frac{16}{15 n_2}\, H(G_1)\, ID^2(G_2).
\end{aligned}$$

Lemma 2 and Propositions 3 and 5 give

$$\begin{aligned}
\int_0^1 2x^{2n_2} ID(G_1, x^{2n_2})\, H(G_2, x)\, dx &\leq \int_0^1 x^{2n_2 - 1} ID(G_1, x^{2n_2})\, 2H(G_2, x)\, dx \\
&\leq \frac{2}{3} \left(\int_0^1 x^{2n_2 - 1} ID(G_1, x^{2n_2})\, dx \int_0^1 2H(G_2, x)\, dx \right)^{1/2} \big(ID(G_1, 1)\, 2H(G_2, 1) \big)^{1/2} \\
&= \frac{2}{3} \Big(\frac{n_1 m_2}{n_2}\, ID(G_1)\, H(G_2) \Big)^{1/2}, \\
\int_0^1 2x^{n_2+1} H(G_1, x^{n_2})\, ID^2(G_2, x)\, dx &\leq \int_0^1 2x^{n_2 - 1} H(G_1, x^{n_2})\, ID^2(G_2, x)\, dx \\
&\leq \frac{2}{4} \left(\int_0^1 2x^{n_2 - 1} H(G_1, x^{n_2})\, dx \int_0^1 ID(G_2, x)\, dx \int_0^1 ID(G_2, x)\, dx \right)^{1/3} \\
&\quad \cdot \big(2H(G_1, 1)\, (ID(G_2, 1) + ID(G_2, 0))^2 \big)^{2/3} \\
&= \frac{1}{2} \Big(\frac{4 m_1^2}{n_2}\, H(G_1)\, ID^2(G_2) (n_2 + k_2)^4 \Big)^{1/3}.
\end{aligned}$$

These inequalities, Theorem 10 and $H(G_1 \odot G_2) = 2 \int_0^1 H(G_1 \odot G_2, x)\, dx$ give the bounds. □

4. Algorithm for the Computation of the Harmonic Polynomial

The procedure shown in Algorithm 1 allows to compute the harmonic polynomial of a graph G with n vertices. This algorithm for computing the harmonic polynomial of a graph shows a complexity $O(n^2)$.

Algorithm 1 procedure Harmonic-Polynomial

Require: AM(G)—Adjacency matrix of G.
n = order(AM(G))
HPolynomial = [0] $*(2*(n-1))$
let D be a list with the degree of each vertex
for all i with $i \in \{1, 2, ...n-1\}$ **do**
  for all j with $j \in \{i+1, i+2, ...n\}$ **do**
    if AM[i][j] == 1 **then**
      $v = D[i]$
      $u = D[j]$
      HPolynomial[$v+u-1$] = HPolynomial [$v+u-1$] + 1
    end if
  end for
end for
return HPolynomial

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