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On the Entire Harmonic Index and Entire Harmonic Polynomial of Graphs

Anwar Saleh *,† and Samirah H. Alsulami †

Department of Mathematics and Statistics, Faculty of Science, University of Jeddah, Jeddah 21589, Saudi Arabia; shalsulami@uj.edu.sa

* Correspondence: asaleh1@uj.edu.sa

† These authors contributed equally to this work.

Abstract: A topological descriptor is a numerical parameter that describes a chemical structure using the related molecular graph. Topological descriptors have significance in mathematical chemistry, particularly for studying QSPR and QSAR. In addition, if a topological descriptor has a reciprocal link with a molecular attribute, it is referred to as a topological index. The use of topological indices can help to examine the physicochemical features of chemical compounds because they encode certain attributes of a molecule. The Randić index is a molecular structure descriptor that has several applications in chemistry and medicine. In this paper, we introduce a new version of the Randić index to the inclusion of the intermolecular forces between bonds with atoms, referred to as an entire Harmonic index (EHI), and we present the entire Harmonic polynomial (EHP) of a graph. Specific formulas have been obtained for certain graph classes, and graph operations have been obtained. Bounds and some important results have been found. Furthermore, we demonstrate that the correlation coefficients for the new index lie between 0.909 and 1. In the context of enthalpy of formation and π-electronic energy, the acquired values are significantly higher than those observed for the Harmonic index and the Randić index.

Keywords: entire indices; Harmonic index; entire Harmonic index; entire Harmonic polynomial

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1. Introduction

We restrict our attention to finite, undirected, and simple graphs, and we refer to such a graph as $G = (V, E)$, where V is the vertex set, and E is the edge set. The symbols P_n, C_n, S_n, and K_n denote a path, cycle, star, and complete graph of order n, respectively. For any element on the graph, either vertex or edge, the degree $deg(x)$ of the element x is the number of edges joining to x; in particular, the degree of the edge uv is the sum of the degrees of the vertices u and v minus two. Readers seeking in-depth explanations of the terms or notations not elaborated upon here are directed to [1].

A topological descriptor is a numerical representation of a chemical structure using the molecular graph. When this descriptor also correlates with a molecular property, it is referred to as a topological index. These indices are used to gain insights into the physicochemical properties of chemical compounds. The significance of these indices lies in their ability to capture multiple properties of a molecule in a single numerical value. As a result, numerous topological indices have been developed and analyzed. There is a rich history of topological indices. The relationship between graph properties and chemical characteristics has been explored for decades through the development of diverse topological indices. The pioneering work by Wiener (1947) [2] established the Wiener index, which quantifies the total distance between all pairs of vertices in a graph, and showed its correlation with the boiling point of paraffins. This marked the foundation for distance-based indices. Building on this, Gutman and Trinajstić (1972) [3] introduced the first and second Zagreb indices, based on vertex degrees, to relate to the π-electron energy of molecules. These pioneering works inspired a surge in the development of topological indices for diverse chemical applications. Within distance-based indices, degree-based indices have gained notable relevance (cf. [4,5]). For a comprehensive overview of degree and distance-based indices, readers can refer to [6–8]. More recently, Ali and Trinajstić (2018) [9] revisited the first, second, and modified first Zagreb connection indices. Subsequently, the connection distance and degree connection indices were investigated in [10]. The value of connection number-based indices was further solidified by Javaid et al. (2014) [11], who demonstrated their strong correlation with various thermodynamic properties. In order to examine the many chemical characteristics of molecular networks (structures), these findings encouraged other mathematicians and chemists to create new topological indices. Extensive research has delved into numerous aspects of the Zagreb indices, including their bounds, extremal graphs, and connections to other graph invariants. For in-depth studies, refer to [12–24]. Alwardi et al. introduced and studied some versions of entire Zagreb indices of graphs, see [25–27]. Some bounds for the first and second entire Zagreb indices were introduced in [28]. The generalization of entire topological indices was introduced very recently in [29]. The Randić index, a versatile topological descriptor [30], developed by Randić in 1975, captures the branching structure of carbon skeletons and exhibits correlations with numerous chemical properties. Initially termed the "branching index" and later the "molecular connectivity index", it remains a prominent tool in diverse chemical assessments and was defined as:

$$\chi(G) = \sum_{uv \in E(G)} (deg(u)deg(v))^{-1/2}.$$

The Harmonic index, an alternative to the Randić index [31], is defined for a graph G as:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{deg(u) + deg(v)}.$$

The sum-connectivity index of a graph G [32], denoted by ${}^{s}\chi(G)$, is defined as

$${}^{s}\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg(u) + deg(v)}}.$$

In the same way, in [33], the Harmonic polynomial is defined as

$$H(G, x) = \sum_{uv \in E(G)} x^{deg(u)+deg(v)-1}.$$

Motivated by the works [25–27,29–32] and the large applications of these topological indices, here, we introduce the entire Harmonic index of the graph along with the entire Harmonic polynomial.

Definition 1. *Consider a simple graph G with vertices V and edges E. We define a set $B(G)$ containing pairs of elements $\{x, y\}$ such that x and y are adjacent or incident. Then, the entire Harmonic index is defined as,*

$$H^{\mathcal{E}}(G) = 2 \sum_{\{x,y\} \in B(G)} (deg(x) + deg(y))^{-1}.$$

Additionally, the entire Harmonic polynomial can be defined as

$$H^{\mathcal{E}}(G, z) = 2 \sum_{\{x,y\} \in B(G)} z^{deg(x)+deg(y)-1}.$$

Precise formulae of this index along with the associated polynomial for significant graph families are derived, and some important properties and relations are established.

The motivation for developing this new index is that the existing Harmonic index is limited in its ability to capture the interactions (forces) between edges and vertices, in addition to the interactions between vertices alone.

2. The Informative Power for Chemical Modeling

The field of mathematical chemistry utilizes math and chemistry to analyze chemical reactions and properties. In their work ([34]), Randić and Trinajstić highlight the potential of relating theoretical indices to experimental properties of benchmark datasets to assess the chemical significance of graph invariants. Following this approach, this section explores the applicability of the entire Harmonic index to elucidating structural features of molecules through the quantitative structure–property relationship (QSPR) methodology. Specifically, we focus on evaluating the effectiveness of the entire Harmonic index as a descriptor for QSPR modeling of various physicochemical properties across diverse molecules. The choice of benzenoid hydrocarbons, with their well-defined structures, allows us to represent both cyclic and acyclic chemical systems for this investigation. So, we examine the significance of the entire Harmonic index for predicting for key properties like the total π-electronic energy (E_π), enthalpy of formation (Δ_f^o), and boiling points (Bp) of 16 lower benzenoid hydrocarbons, see Figure 1.

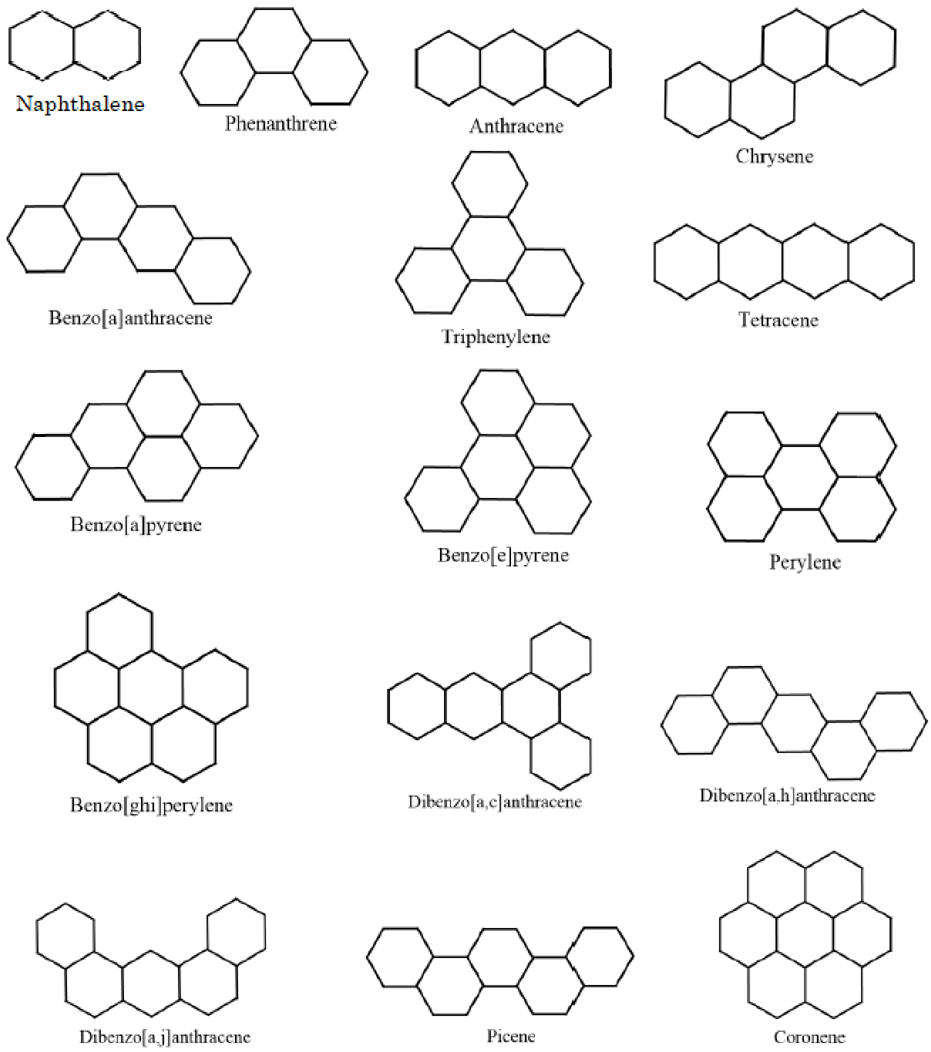

Figure 1. The 16 lower benzenoid hydrocarbons.

The experimental data of the total π-electronic energy (E_π), enthalpy of formation (Δ_f^o), and boiling points (Bp) are taken from NIST databases [35] and retrieved from [36].

Analysis of the data in Table 1 highlights the emergence of the entire Harmonic index as a promising descriptor for diverse physicochemical properties. Constructed linear models in SPSS demonstrate statistically significant correlations with the boiling point $(r = 0.996)$, enthalpy of formation $(r = 0.909)$, and, notably, a perfect correlation with total π-electronic energy $(r = 1)$, suggesting exceptional predictive potential for this property. Furthermore, Table 2 reveals the consistent advantage of the entire Harmonic index over the traditional Harmonic index, underlining its significance as a novel topological index for modeling chemical and physical properties.

Table 1. Experimental total π-electronic energy ($\mathbf{E_\pi}$), enthalpy of formation (**EF**), boiling points (**BP**) and theoretical indices for benzenoid hydrocarbons.

SN	The Compounds	E_π	EF	BP	EH	H	R	SC
1	naphthalene	13.6832	141	218	19.8475	4.9333	4.9663	5.1971
2	phenanthrene	19.4483	202.7	338	27.8665	6.8999	6.9495	7.408
3	anthracene	19.3137	222.6	340	27.7618	6.8666	6.9327	7.3942
4	chrysene	25.1922	271.1	431	35.8856	8.8666	8.9327	9.619
5	tetraphene or Benz(a)anthracene	25.1012	277.1	425	35.78	8.8333	8.9158	9.6051
6	triphenylene	25.2745	275.1	429	36.057	8.8999	8.9495	9.6328
7	naphthacene or TETRACENE	24.9308	310.5	440	35.6761	9.7999	8.899	9.5913
8	benzo[a]pyrene	28.222	296	496	39.9618	9.8333	9.9158	10.8299
9	benzo[e]pyrene	28.3361	289.9	493	40.1998	9.8666	9.9327	10.8437
10	perylene	28.2453	319.2	497	40.0998	9.8666	9.9327	10.8437
11	benzo[ghi]perylene	31.4251	301.2	542	44.1428	10.8333	10.9158	12.0546
12	dibenzo[a,c]anthracene	30.9418	348	535	43.9713	10.8333	10.9158	11.8299
13	dibenz[a,h]anthracene	30.8805	335	536	43.7999	10.7999	10.899	11.8161
14	dibenz[a,j]anthracene	30.8795	336.3	531	44.0618	10.7999	10.899	11.8161
15	picene	30.9432	336.9	519	43.9046	10.8333	10.9158	11.8299
16	coronene	34.5718	296.7	590	48.5189	11.8	11.899	13.2655

Table 2. Correlations of the entire Harmonic index and key descriptors with diverse properties of benzenoid hydrocarbons.

	Boiling Point	Enthalpy of Formation	Pi Electronic Energy
Entire Harmonic index	0.996	0.909	1
Harmonic index	0.990	0.933	0.984
Randić index	0.996	0.915	0.999
The sum-connectivity index	0.997	0.901	1

Figure 2 visually portrays the linear relationships between the entire Harmonic index and three critical properties of benzenoid hydrocarbons: the boiling point (BP), enthalpy of formation (EF), and π-electronic energy.

The linear QSPR model yielded the following predictive regression equations, linking the entire Harmonic index (EH) to critical physicochemical properties:

Boiling point (Bp): $Bp = -20.7621 + EH(12.6613)$.

Enthalpy of formation (EF): $EF = 32.5122 + EH(6.6483)$.

π-electronic energy (Eπ): $E_\pi = -0.75589 + +EH(0.7233)$.

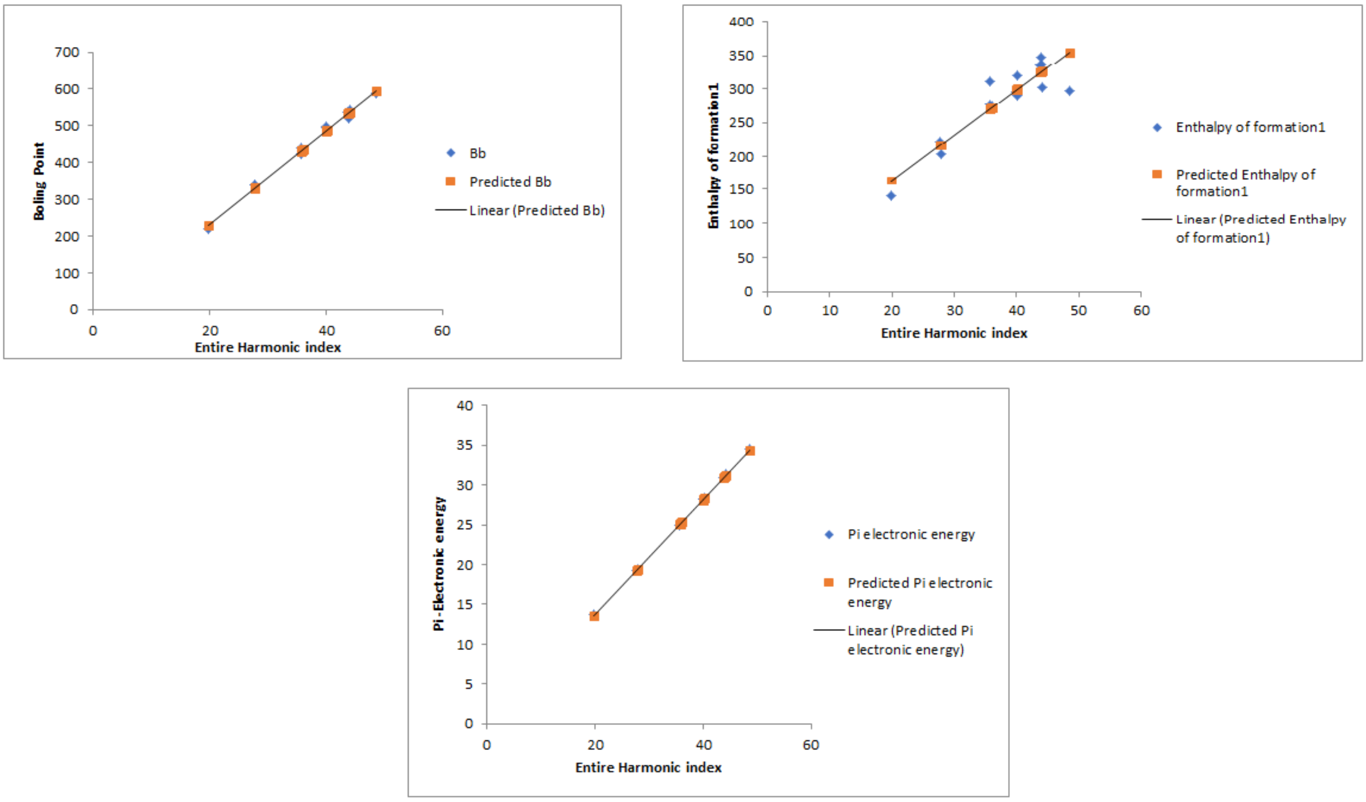

Figure 2. Linear fitting of the BP, EF, and π electronic energy predicted by the entire Harmonic index.

3. Mathematical Results on Some Significant Families of Graphs

In this section, we obtain precise formulae for the entire Harmonic index along with the associated polynomial for significant graph families of standard graphs.

Observation 1. *Let G be a graph with q edges and a first Zagreb index M_1. Then,*

1. $H^{\mathcal{E}}(G) = \int_0^1 H^{\mathcal{E}}(G,z)\,dz.$
2. $|B(G)| = 2m + \dfrac{M_1}{2}.$
3. $H^{\mathcal{E}}(G) = H(G) + H_e(G) + 2\sum_{v \text{ incident to } e}(deg(v) + deg(e))^{-1}.$

The line graph $L(G)$ captures the relationships between the edges of the original graph. Each vertex in $L(G)$ represents an edge in the original graph, and two edges in L(G) are connected if the corresponding edges in the original graph are "neighbors" (meaning they share a common vertex) [1].

Proposition 1. *For a regular graph G of n vertices with degree k greater than* 2*,*

i. $H^{\mathcal{E}}(G) = \frac{12nk - 4n + 3nk^2}{4(3k-2)}.$
ii. $H^{\mathcal{E}}(G,z) = nkz^{2k-1} + nk(k-1)z^{4k-5} + 2nkz^{3k-3}.$

Proof. G. a regular graph, contains n vertices and each vertex has a degree equal to or more than 2. Hence, it contains $nk/2$ edges, and the number of edges on $L(G)$ is

$$\frac{1}{2}\sum_{v \in V(G)} (deg(v))^2 - q = \frac{nk^2}{2} - \frac{nk}{2} = \frac{kn(k-1)}{2}.$$

Hence,

$$H^{\mathcal{E}}(G) = \frac{kn}{2}\frac{2}{2k} + \frac{kn(k-1)}{2}\frac{2}{(4k-4)} + kn\frac{2}{3k-2}$$
$$= \frac{12nk - 4n + 3nk^2}{4(3k-2)}.$$

In the same procedure, we obtain

$$H^{\mathcal{E}}(G, z) = nkz^{2k-1} + nk(k-1)z^{4k-5} + 2nkz^{3k-3}.$$

□

Corollary 1. *For the complete graph K_n and the cycle C_n, where $n \geq 3$,*

1. $H^{\mathcal{E}}(K_n) = \frac{3n^3+6n^2-13n}{4(3n-5)}$.
2. $H^{\mathcal{E}}(K_n, z) = n^2z^{2n-3} - nz^{2n-3} + n^3z^{4n-9} - 3n^2z^{4n-9} + 2nz^{4n-9} + 2n^2z^{3n^2-3n-6} -2nz^{3n^2-3n-6}$.
3. $H^{\mathcal{E}}(C_n) = 2\,n$.
4. $H^{\mathcal{E}}(C_n, z) = 8nz^3$.

Proposition 2. *For any path P_n, with $n \geq 4$ vertices,*

1. $H^{\mathcal{E}}(P_n) = \frac{4n-1}{2}$.
2. $H^{\mathcal{E}}(P_n, z) = 2z + 6z^2 + (4n-13)z^3$.

Proof. In a path P_n with $n \geq 4$ vertices and $n-1$ edges, the degree of each vertex and edge is 2, except for the endpoints. Both the first and last vertices, v_1 and v_n, have degree 1, as they only connect to one other vertex. Similarly, the edges connecting them to other vertices, e_1 and e_n, also have degree 1. Therefore,

$$\begin{aligned} H^{\mathcal{E}}(P_n) =& (n-3)/2 + 4/3 + (n-4)/2 \\ &+ \frac{4}{3} + n + \frac{4}{3} - 3 + 2 \\ =& \frac{4n-1}{2}. \end{aligned}$$

By using the same data about the degrees of the vertices and edges, we have achieved part (ii).

$$H^{\mathcal{E}}(P_n, z) = 2z + 6z^2 + (4n-13)z^3.$$

□

Proposition 3. *For any complete bipartite graph $K_{a,b}$, $H^{\mathcal{E}}(K_{a,b}) = \frac{2ab}{a+b} + \frac{ab}{2} + 2ab \left(\frac{1}{2a+b-2} + \frac{1}{2b+a-2}\right)$.*

Proof. Let the vertices of $K_{a,b}$ be labeled as $v_1, v_2, \ldots, v_a, v_{a+1}, v_{a+2}, \ldots, v_b$. Then,

$$\begin{aligned} H^{\mathcal{E}}(K_{a,b}) =& \frac{2ab}{a+b} + \left(\frac{1}{2}(a^2b + b^2a) - ab\right)\frac{2}{2(a+b-2)} \\ &+ 2ab\frac{1}{a+(a+b-2)} + 2ab\frac{1}{b+(a+b-2)} \\ =& \frac{2ab}{a+b} + \frac{ab}{2} + 2ab\left(\frac{1}{2a+b-2} + \frac{1}{2b+a-2}\right). \end{aligned}$$

A graph that has r distinct paths connecting two specific vertices is called an r-bridge graph. We denote it as $Q(k_1, ..., k_r)$, where $k_1, ..., k_r$ represent the lengths of each of the r paths. The r-bridge is a generalization of theta graphs, see Figure 3. □

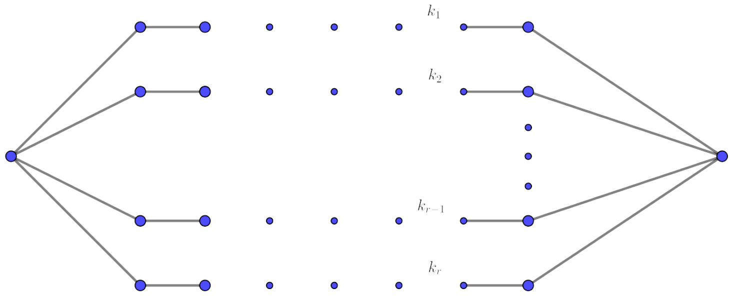

Figure 3. r-bridge graph.

Lemma 1. *For any multi-bridge graph $G \cong Q(k_1, k_2, ..., k_r)$,*

$$H(G) = \frac{4r}{r+2} - r + \frac{1}{2}\sum_{i=1}^{r} k_i.$$

Proof. For a multi-bridge graph $G \cong Q(k_1, k_2, ..., k_r)$, we have

$$\begin{aligned} H(G) =& (k_1 - 2)\frac{2}{4} + (k_2 - 2)\frac{2}{4} + ... + (k_r - 2)\frac{2}{4} + 4\frac{r}{r+2} \\ =& \frac{4r}{r+2} - r + \frac{1}{2}\sum_{i=1}^{r} k_i. \end{aligned}$$

□

Lemma 2. *For the multi-bridge graph $G = Q(k_1, k_2, ..., k_r)$, we have*

$$H_e(G) = \frac{4r}{r+2} - \frac{r+2}{2} + \frac{1}{2}\sum_{i=1}^{r} k_i.$$

Proof. By the definition of the edge version of the Harmonic index, we obtain

$$\begin{aligned} H_e(G) =& (k_1 - 3)\frac{1}{2} + (k_2 - 3)\frac{1}{2} + ... + (k_r - 3)\frac{1}{2} + \frac{4r}{r+2} + \frac{-2-r}{2} \\ =& \frac{4r}{r+2} - \frac{r+2}{2} + \frac{1}{2}\sum_{i=1}^{r} k_i \end{aligned}$$

□

Theorem 1. *Let $G \cong Q(k_1, ..., k_r)$ be the multi-bridge graph. Then,*

$$H^{\mathcal{E}}(G) = \frac{12r}{r+1} - \frac{7r-2}{2} + 2\sum_{i=1}^{r} k_i.$$

Proof. Since $G \cong Q(k_1, ..., k_r)$, applying Observation 1, we obtain

$$H^{\mathcal{E}}(G) = H(G) + H_e(G) + 2\sum_{v \text{ incident to } e} (deg(v) + deg(e))^{-1}.$$

□

It is easy to see that

$$2\sum_{v\text{ incident to }e}(deg(v)+deg(e))^{-1} = 2(k_1-2)\frac{2}{4}+2(k_2-2)\frac{2}{4}+\ldots+2(k_r-2)\frac{2}{4}+2+\frac{4r}{r+2}$$
$$=\frac{4r}{r+2}-2(r-1)+\sum_{i=1}^{r}k_i.$$

So using Lemmas 1 and 2, we obtain

$$H^{\mathcal{E}}(G)=\frac{12r}{r+1}-\frac{7r-2}{2}+2\sum_{i=1}^{r}k_i.$$

To prove some results, we need some specific sets defined for a graph $G=(V,E)$, as follows:

- $V_{a,b}(G)=\{\{u,v\}\}$, if there is an edge between u and v.
- $E_{a,b}(G)=\{\{e,f\}\}$, if edges e and f share both endpoints and have degrees a and b, respectively.
- $A_{a,b}(G)=\{\{v,f\}\}$, if vertex v and edge f are incident and have degrees a and b, respectively.

In the realm of hydrocarbons, pentacene stands out for its unique structure. Comprised of five fused benzene rings, this vibrant purple powder exhibits semiconducting properties. However, its beauty is fleeting, as exposure to light and air causes pentacene to gradually degrade. The linear form, known as $[n]$-pentacene, is pictured in Figure 4.

Figure 4. Linear $[n]$-Pentacene.

Lemma 3. *For any linear $[n]$-Pentacene graph G,*

$$H(G)=\frac{160n+1}{15}.$$

Proof. Let G be the $[n]$-Pentacene graph, from the definition of the $[n]$-Pentacene graph G; clearly, it has $22n$ vertices and $28n-2$ edges, and the degrees of the vertices are either two or four. We can see that $|V_{2,2}|=6$, $|V_{2,3}|=20n-4$, and $|V_{3,3}|=8n-4$; so,

$$H(G)=\frac{2}{4}|V_{2,2}|+\frac{2}{5}|V_{2,3}|+\frac{2}{6}|V_{3,3}|=\frac{160n+1}{15}.$$

□

Lemma 4. *For any linear $[n]$-Pentacene graph G,*

$$H_e(G)=\frac{1455n-107}{105}.$$

Proof. Let G be the $[n]$-Pentacene graph, from the definition of the $[n]$-Pentacene graph G; clearly, it has $28n-2$ edges, and the degrees of the edges are either two, three, or four. By simple counting, we obtain $|E_{2,2}|=4$, $|E_{2,3}|=4$, $|E_{3,3}|=18n-4$, $|E_{4,3}|=24n-8$, and $|E_{4,4}|=4n-4$; so,

$$H(G)=\frac{2}{4}|E_{2,2}|+\frac{2}{5}|E_{2,3}|+\frac{2}{6}|E_{3,3}|+\frac{2}{7}|E_{4,3}|+\frac{2}{8}|E_{4,4}|.$$

Therefore,

$$H(G) = \frac{8}{4} + \frac{8}{5} + \frac{2}{6}(18n-4) + \frac{2}{7}(24n-8) + \frac{2}{8}(4n-4) = \frac{1455n-107}{105}.$$

□

Theorem 2. *For any linear $[n]$-Pentacene graph G,*

$$H^{\mathcal{E}}(G) = \frac{4595n+42}{105}.$$

Proof. Let G be any $[n]$-Pentacene graph, by using Observation 1, we obtain

$$H^{\mathcal{E}}(G) = H(G) + H_e(G) + 2\sum_{v \text{ incident to } e} (deg(v) + deg(e))^{-1}.$$

To obtain $2\sum_{v \text{ incident to } e}(deg(v)+deg(e))^{-1}$, we have $|A_{2,3}| = 20n-4$, $|A_{2,2}| = 12$, $|A_{3,3}| = 20n-4$, and $|A_{3,4}| = 16n-6$. Then,

$$2\sum_{v \text{ incident to } e} (deg(v)+deg(e))^{-1} = \frac{24}{4} + \frac{2}{5}(20n-4) + \frac{2}{6}(20n-4) + \frac{2}{7}(16n-6)$$
$$= \frac{2020n+142}{105}. \quad (1)$$

Then by Lemmas 3 and 4, and Equation (1), we obtain

$$H^{\mathcal{E}}(G) = \frac{160n+1}{15} + \frac{1455n-107}{105} + \frac{2020n+142}{105} = \frac{4595n+42}{105}.$$

□

Proposition 4. *Let $G \cong W_n$ be a wheel graph that contains $n+1$ vertices. Then,*

$$H^{\mathcal{E}}(G) = \frac{278n^6 + 5097n^5 + 30725n^4 + 75075n^3 + 70445n^2 + 23292n}{84(n+1)(n+3)(n+4)(n+5)(2n+1)}.$$

Proof. For the graph $G \cong W_n$, we can see that $|V_{3,3}| = n$, $|V_{3,n}| = n$, $|E_{4,4}| = n$, $|E_{4,n+1}| = 2n$, $|E_{(n+1),(1+n)}| = n(n-1)/2$, $|A_{3,4}| = 2n$, $|A_{3,(n+1)}| = n$, and $|A_{n,n+1}| = n$. Then, by Observation 1,

$$H^{\mathcal{E}}(G) = \tfrac{n}{3} + \tfrac{2n}{n+3} + \tfrac{n}{4} + \tfrac{4n}{n+5} + \tfrac{n(n-1)}{2(n+1)} + \tfrac{4n}{7} + \tfrac{2n}{n+4} + \tfrac{2n}{2n+1},$$
$$= \tfrac{278n^6+5097n^5+30725n^4+75075n^3+70445n^2+23292n}{84(n+3)(n+5)(n+1)(n+4)(2n+1)}.$$

□

4. Entire Harmonic Index under Some Common Graph Operations

In this section, we focus on determining the Harmonic index for a variety of graph operations applied to common graph types.

We present the Cartesian product of two graphs $G_1 \square G_2$, where $V(G_1)$, $V(G_2)$, $E(G_1)$, and $E(G_2)$ are the vertex sets and edge set of G_1 and G_2, respectively. The resulting graph has the vertex set $V(G_1) \times V(G_2)$, and two vertices (a,b) and (c,d) are adjacent, if and only if either ($a = c$ and $bd \in E(G_2)$) or ($b = d$ and $ac \in E(G_1)$) [1].

Lemma 5. *For any positive integers s and t with $s, t \geq 4$, if G is the Cartesian product between the paths P_t and P_s, then*

$$H(G) = \frac{210st - 5s - 5t - 36}{420}.$$

Proof. Let s, t be any positive integers such that $s, t \geq 4$ and $G \cong P_t \Box P_s$. Let $V_{a,b} = \{\{u.v\} : uv \in E(G)\, such\ that\, deg(u) = a\ and\ deg(v) = b\}$; so, we have $|V_{2,3}| = 8, |V_{3,3}| = (2s + 2t - 12), |V_{3,4}| = 2s + 2t - 8$, and $|V_{4,4}| = 2st - 5s - 5t + 12$. Then,

$$H(G) \quad = \quad \frac{16}{5} + (2s + 2t - 12)\frac{2}{6} + (2s + 2t - 8)\frac{2}{7} + (2st - 5s - 5t + 12)\frac{2}{8}.$$

Hence, $H(G) = \frac{210st-5s-5t-36}{420}$. □

Lemma 6. *If $s, t \geq 4$, and $G \cong P_t \Box P_s$, then*

$$H_e(G) = \frac{6930st - 3605s - 3605t - 456}{6930}.$$

Proof. Let $s, t \geq 4$, and $G \cong P_t \Box P_s$. Then, we can see that $|E_{3,3}| = 4$, $|E_{3,4}| = 8$, $|E_{4,4}| = 2(s - 4) + 2(t - 4)$, $|E_{3,5}| = 8$, $|E_{4,5}| = 4(s - 3) + 4(t - 3)$, $|E_{5,5}| = 4$, $|E_{6,5}| = 4(s - 3) + 4(t - 3) + 2(t - 2) + 2(s - 2) = 6s + 6t - 32$, and $|E_{6,6}| = (s - 4)(t - 2) + 4(s - 4)(t - 3) + 4(t - 3) + (s - 2)(t - 4) = 6st - 18s - 18t + 52$, and then,

$$H_e(G) = \frac{8}{6} + \frac{16}{7} + (2s + 2t - 16)\frac{2}{8} + \frac{16}{8} + (4s + 4t - 24)\frac{2}{9} + \frac{8}{10} + (6s + 6t - 32)\frac{2}{11} + (6st - 18s - 18t + 52)\frac{2}{12}.$$

Hence,

$$H_e(G) = \frac{6930st - 3605s - 3605t - 456}{6930}.$$

□

Theorem 3. *For any positive integers s and t with $s, t \geq 4$, if G is the Cartesian product between the paths P_t and P_s, then*

$$H^{\mathcal{E}}(G) = \frac{10626st - 2055s - 2055t - 4660}{4620}.$$

Proof. By applying Observation 1, we obtain

$$H^{\mathcal{E}}(G) = H(G) + H_e(G) + 2 \sum_{v \text{ incident to } e} (deg(v) + deg(e))^{-1}.$$

To obtain $2\sum_{v \text{ incident to } e}(deg(v) + deg(e))^{-1}$, we have $|A_{2,3}| = 8$, $|A_{3,3}| = 8$, $|A_{3,4}| = 4(s - 3) + 4(t - 3) = 4s + 4t - 24$, $|A_{3,5}| = 2(s - 2) + 2(t - 2) = 2s + 2t - 8$, $|A_{4,5}| = 2s + 2t - 8$, and $|A_{4,6}| = 2(s - 3)(t - 2) + 2(t - 3)(s - 2) = 4st - 10s - 10t + 24$. Then,

$$\begin{aligned} 2 \sum_{v \text{ incident to } e} (deg(v) + deg(e))^{-1} &= \frac{16}{5} + \frac{16}{9} + (4s + 4t - 24)\frac{2}{7} \\ &+ (2s + 2t - 8)\frac{2}{8} + (2s + 2t - 8)\frac{2}{9} + (4st - 10s - 10t + 24)\frac{2}{10} \\ &= \frac{504st + 55s + 55t - 540}{630}. \end{aligned} \tag{2}$$

Building upon Lemmas 5 and 6, and applying Equation (2), we obtain

$$H^{\mathcal{E}}(G) = \frac{210st - 5s - 5t - 36}{420} + \frac{6930st - 3605s - 3605t - 456}{6930} + \frac{504st + 55s + 55t - 540}{630} = -\frac{2055s - 10626st + 2055t + 4660}{4620}.$$

□

Lemma 7. *Let S and t be positive integers such that $s \geq 4$ and $t \geq 3$; if G is the Cartesian product between the path P_s and the cycle C_t, then*

$$H(G) = \frac{42ts - t}{84}.$$

Proof. Suppose that S and t are positive integers such that $s \geq 4$ and $t \geq 3$, and G is the Cartesian product between the path P_s and the cycle C_t; then, it is easy to see that $|V_{3,3}| = 2t$, $|V_{3,4}| = 2t$, and $|V_{4,4}| = t(s-2) + t(s-3)$, and then, $H(G) = 2t\frac{2}{6} + 2t\frac{2}{7} + (t(s-2) + t(s-3))\frac{2}{8}$. Therefore,

$$H(G) = \frac{42ts - t}{84}.$$

□

Lemma 8. *Let S and t be positive integers such that $s \geq 4$ and $t \geq 3$; if G is the Cartesian product between the path P_s and the cycle C_t, then*

$$H_e(G) = \frac{198ts - 103t}{198}.$$

Proof. Let $s \geq 4$ and $t \geq 3$; if $G \cong P_s \Box C_t$, it is easy to see that $|E_{4,4}| = 2t$, $|E_{4,5}| = 4t$, $|E_{5,6}| = 6t$, and $|E_{6,6}| = 6ts - 18t$. Therefore,

$$H_e(G) = 2t\frac{2}{8} + 4t\frac{2}{9} + 6t\frac{2}{11} + (6ts - 18t)\frac{2}{12}.$$

Hence,

$$H_e(G) = \frac{198ts - 103t}{198}.$$

□

Theorem 4. *Let S and t be positive integers such that $s \geq 4$ and $t \geq 3$; if G is the Cartesian product between the path P_s and the cycle C_t, then*

$$H^{\mathcal{E}}(G) = \frac{t(3542s - 685)}{1540}.$$

Proof. Let s, t be any positive integers such that $s \geq 4$ and $t \geq 3$, if $G \cong P_s \Box C_t$; then, using Observation 1, we have

$$H^{\mathcal{E}}(G) = H(G) + H_e(G) + 2\sum_{v \text{ incident to } e} (deg(v) + deg(e))^{-1}.$$

To obtain $2\sum_{v \text{ incident to } e}(deg(v) + deg(e))^{-1}$, let $A_{a,b}$ be the set of all subsets $\{v, e\}$ where v is a vertex in G, e is an edge in G, and v is incident with e, such that $deg(v) = a$ and $deg(e) = b$; then, we have, $|A_{3,4}| = 4t$, $|A_{3,5}| = 2t$, $|A_{4,5}| = 2t$, and $|A_{4,6}| = 4t(s-4) + 6t = 4ts - 10t$, and then,

$$2\sum_{v \text{ incident to } e} (deg(v) + deg(e))^{-1} = 4t\frac{2}{7} + 2t\frac{2}{8} + 2t\frac{2}{9} + (4ts - 10t)\frac{2}{10} = \frac{504ts + 55t}{630}. \quad (3)$$

By virtue of Lemmas 7 and 8 and invoking Equation (3), we obtain

$$H^{\mathcal{E}}(G) = \frac{42ts - t}{84} + \frac{198ts - 103t}{198} + \frac{504ts + 55t}{630} = \frac{t(3542s - 685)}{1540}.$$

□

Lemma 9. *Let G be the Stacked Book Graph $S_m \Box P_n$, where $n \geq 5$ and $m \geq 1$. Then,*

$$H(G) = \frac{(5n-3)(m-1)}{15} + \frac{4(m-1)}{m+2} + \frac{2(m-1)(n-2)}{m+4} + \frac{4}{2m+1} + \frac{2(n-3)}{2m+2}.$$

Proof. Let $G \cong S_m \Box P_n$; then, it is easy to see that $|V_{2,3}| = 2(m-1)$, $|V_{2,m}| = 2(m-1)$, $|V_{3,3}| = (m-1)(n-2)$, $|V_{m+1,3}| = (m-1)(n-2)$, $|V_{m+1,m}| = 2$, and $|V_{m+1,m+1}| = n-3$, and then,

$$\begin{aligned} H(G) &= \frac{4(m-1)}{5} + \frac{4(m-1)}{m+2} + \frac{2(m-1)(n-3)}{6} + \frac{2(m-1)(n-2)}{m+4} \\ &\quad + \frac{4}{2m+1} + \frac{2(n-3)}{2m+2} \\ &= \frac{(5n-3)(m-1)}{15} + \frac{4(m-1)}{m+2} + \frac{2(m-1)(n-2)}{m+4} + \frac{4}{2m+1} + \frac{2(n-3)}{2m+2}. \end{aligned}$$

□

Lemma 10. *Let G be the Stacked Book Graph $S_m \Box P_n$, where $n \geq 5$ and $m \geq 1$. Then,*

$$\begin{aligned} H_e(G) = \frac{(m-1)(m-2)}{m} &+ \frac{4(m-1)}{m+3} + \frac{4(m-1)}{3m-1} + \frac{(7n-12)(m-1)}{28} + \frac{(m-4)}{2m} + \frac{4(m-1)}{3m+1} \\ &+ \frac{4(n-3)(m-1)}{3m+2} + \frac{4(n-3)(m-1)}{m+6} \\ &+ \frac{4(m-1)}{m+5} + \frac{4}{4m-1} + \frac{(n-2)(m-1)(m-2)}{2m+4}. \end{aligned}$$

Proof. Let $G \cong S_m \Box P_n$; then, we can obtain $|E_{m,m}| = (m-1)(m-2)$, $|E_{m,3}| = 2(m-1)$, $|E_{m,2m-1}| = 2(m-1)$, $|E_{4,4}| = (m-1)(n-4)$, $|E_{3,4}| = 2(m-1)$, $|E_{2m,2m}| = n-4$, $|E_{m+2,2m-1}| = 2(m-1)$, $|E_{m+2,2m}| = 2(n-3)(m-1)$, $|E_{m+2,4}| = 2(n-3)(m-1)$, $|E_{m+2,3}| = 2(m-1)$, $|E_{2m-1,2m}| = 2$, and $|E_{m+2,m+2}| = 1/2(n-2)(m-1)(m-2)$, and then

$$\begin{aligned} H_e(G) &= \frac{(m-1)(m-2)}{m} + \frac{4(m-1)}{m+3} + \frac{4(m-1)}{3m-1} + \frac{(m-1)(n-4)}{4} + \frac{4(m-1)}{7} + \frac{(m-4)}{2m} \\ &\quad + \frac{4(m-1)}{3m+1} + \frac{4(n-3)(m-1)}{3m+2} + \frac{4(n-3)(m-1)}{m+6} + \frac{4(m-1)}{m+5} \\ &\quad + \frac{4}{4m-1} + \frac{(n-2)(m-1)(m-2)}{2m+4} \\ &= \frac{(m-1)(m-2)}{m} + \frac{4(m-1)}{m+3} + \frac{4(m-1)}{3m-1} + \frac{(7n-12)(m-1)}{28} + \frac{(m-4)}{2m} \\ &\quad + \frac{4(m-1)}{3m+1} + \frac{4(n-3)(m-1)}{3m+2} + \frac{4(n-3)(m-1)}{m+6} + \frac{4(m-1)}{m+5} + \frac{4}{4m-1} \\ &\quad + \frac{(n-2)(m-1)(m-2)}{2m+4}. \end{aligned}$$

□

Theorem 5. *Let G be the Stacked Book Graph $S_m \Box P_n$, where $n \geq 5$ and $m \geq 1$. Then,*

$$H^{\mathcal{E}}(G) = \frac{8(m-1)}{m+2} + \frac{2n(m-1)}{m+5} + \frac{6m^2-9m+2}{6m} + \frac{(m-1)(485n-368)}{420} + \frac{4}{3m-1} + \frac{4(n-3)}{3m+1} + \frac{2(m-1)(n-2)}{2m+3} + \frac{4(m-1)}{m+3} + \frac{4(m-1)}{3m-1} + \frac{4(m-1)}{3m+1} + \frac{4(n-3)(m-1)}{3m+2} + \frac{4(n-3)(m-1)}{m+6} + \frac{4}{4m-1} + \frac{(n-2)(m-1)(m-2)}{2m+4} + \frac{2(m-1)(n-2)}{m+4} + \frac{4}{2m+1} + \frac{2(n-3)}{2m+2}.$$

Proof. Let G be any Stacked Book Graph $S_m \square P_n$, where $n \geq 5$ and $m \geq 1$, as in Figure 5; using Observation 1, we have

$$H^{\mathcal{E}}(G) = H(G) + H_e(G) + 2 \sum_{v \text{ incident to } e} (deg(v) + deg(e))^{-1}.$$

We have $|A_{2,3}| = |A_{2,m}| = |A_{3,3}| = 2(m-1)$, $|A_{3,4}| = 2(n-3)(m-1)$, $|A_{3,m+2}| = (n-2)(m-1)$, $|A_{m,m}| = 2(m-1)$, $|A_{m,2m-1}| = |A_{m+1,2m-1}| = 2$, $|A_{m+1,2m}| = 2(n-3)$, and $|A_{m+1,m+2}| = (m-1)(n-2)$. Therefore,

$$\begin{aligned} 2 \sum_{v \text{ incident to } e} (deg(v) + deg(e))^{-1} &= \frac{4(m-1)}{5} + \frac{4(m-1)}{m+2} + \frac{4(m-1)}{6} + \frac{4(m-1)(n-3)}{7} \\ &+ \frac{2(m-1)(n-2)}{m+5} + \frac{(m-1)}{m} + \frac{4}{3m-1} + \frac{4}{3m} + \frac{4(n-3)}{3m+1} + \frac{2(m-1)(n-2)}{2m+3} \\ &= \frac{2(30n-13)(m-1)}{105} + \frac{4(m-1)}{m+2} + \frac{2(m-1)(n-2)}{m+5} + \frac{(m-1)}{m} \\ &+ \frac{4}{3m-1} + \frac{4}{3m} + \frac{4(n-3)}{3m+1} + \frac{2(m-1)(n-2)}{2m+3}. \end{aligned} \quad (4)$$

By virtue of Lemmas 9 and 10 and invoking Equation (4), we obtain

$$\begin{aligned} H^{\mathcal{E}}(G) &= \frac{(m-1)(485n-368)}{420} + \frac{4(m-1)}{m+2} + \frac{2(m-1)(n-2)}{m+5} + \frac{(m-1)}{m} \\ &+ \frac{4}{3m-1} + \frac{4}{3m} + \frac{4(n-3)}{3m+1} + \frac{2(m-1)(n-2)}{2m+3} \\ &+ \frac{(m-1)(m-2)}{m} + \frac{4(m-1)}{m+3} + \frac{4(m-1)}{3m-1} + \frac{(m-4)}{2m} \\ &+ \frac{4(m-1)}{3m+1} + \frac{4(n-3)(m-1)}{3m+2} + \frac{4(n-3)(m-1)}{m+6} + \frac{4(m-1)}{m+5} + \frac{4}{4m-1} \\ &+ \frac{(n-2)(m-1)(m-2)}{2m+4} \\ &+ \frac{4(m-1)}{m+2} + \frac{2(m-1)(n-2)}{m+4} + \frac{4}{2m+1} + \frac{2(n-3)}{2m+2} \\ &= \frac{8(m-1)}{m+2} + \frac{2n(m-1)}{m+5} + \frac{6m^2-9m+2}{6m} + \frac{(m-1)(485n-368)}{420} \\ &+ \frac{4}{3m-1} + \frac{4(n-3)}{3m+1} + \frac{2(m-1)(n-2)}{2m+3} + \frac{4(m-1)}{m+3} + \frac{4(m-1)}{3m-1} \\ &+ \frac{4(m-1)}{3m+1} + \frac{4(n-3)(m-1)}{3m+2} + \frac{4(n-3)(m-1)}{m+6} + \frac{4}{4m-1} \\ &+ \frac{(n-2)(m-1)(m-2)}{2m+4} + \frac{2(m-1)(n-2)}{m+4} + \frac{4}{2m+1} + \frac{2(n-3)}{2m+2}. \end{aligned}$$

□

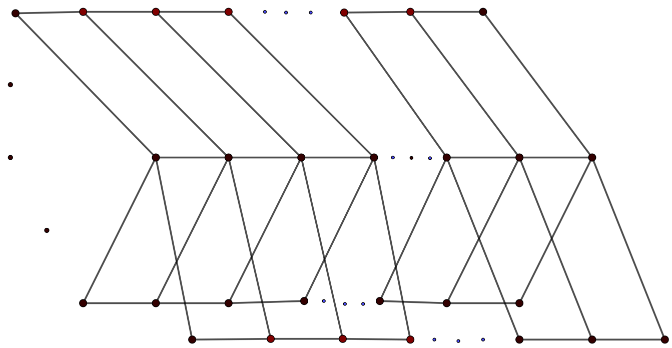

Figure 5. Stacked Book Graph.

5. Relationships between the Entire Harmonic Index and Other Indices

Proposition 5. *For any nontrivial connected graph G, $H^{\mathcal{E}}(G) \leq R^{\mathcal{E}}(G)$. The equality holds, if and only if G is a cycle C_n.*

Proof. Let G be any nontrivial connected graph, and let $G = (V, E)$ be a simple graph. Then, for any element $\{x, y\}$ in $B(G)$, obviously, $deg(x) + deg(y) \geq 2(deg(x)deg(y))^{1/2}$. Then,

$$H^{\mathcal{E}}(G) = 2\sum_{\{x,y\}\in B(G)}(deg(x) + deg(y))^{-1} \leq \sum_{\{x,y\}\in, B(G)}(deg(x)deg(y))^{-1} = R^{\mathcal{E}}(G).$$

If the graph is a cycle C_n, then, clearly, $H^{\mathcal{E}}(G) = R^{\mathcal{E}}(G) = 2n$. Suppose that $H^{\mathcal{E}}(G) = R^{\mathcal{E}}(G)$. Then, $2\sum_{\{x,y\}\in B(G)}(deg(x) + deg(y))^{-1} = 2\sum_{\{x,y\}\in, B(G)}(deg(x)deg(y))^{-1/2}$, which implies that $deg(x) = deg(y)$, and the only nontrivial connected graph with edges and vertices all of the same degree is the cycle graph C_n. □

Theorem 6. *For the graph G, which has m edges, we obtain*

$$H^{\mathcal{E}}(G) \leq (2m + \frac{M_1(G)}{2})\alpha,$$

where $\alpha = \sum_{\{x,y\}\ \in\ B(G)} \frac{1}{deg(x)+deg(y)}$, and $M_1(G)$ is the first Zagreb index of G.

Proof. For the graph G with n, m vertices and edges, we obtain

$$H^{\mathcal{E}}(G) = \sum_{\{x,y\}\in B(G)} \frac{2}{deg(x) + deg(y)}.$$

Leveraging the Cauchy–Schwarz inequality, we can deduce

$$\begin{aligned} H^{\mathcal{E}}(G) &= \textstyle\sum_{\{x,y\}\in B(G)} \frac{2}{deg(x) + deg(y)} \\ &\leq |B(G)| \textstyle\sum_{\{x,y\}\in B(G)} \frac{2}{deg(x) + deg(y)} \\ &= |B(G)| M_1^{\mathcal{E}*}(G) \\ &= (2m + \frac{M_1(G)}{2})\alpha. \end{aligned}$$

□

6. Conclusions

In this article, we introduced a new version of the Randić index referred to as the entire Harmonic index, along with its associated polynomial. This index was conceptualized, and its discriminating power was investigated with regard to the predictability of the boiling point, enthalpy of formation, and π electronic energy of the chemical substances; the correlation coefficients between 0.909 and 1 were acquired, higher than the ones received in the case of the Harmonic index and the Randić index in terms of the enthalpy of formation and π-electronic energy. Furthermore, it was higher than the one achieved in the case of the Harmonic index for the boiling point. Specific formulae for some families of graphs and graph operations were achieved; bounds and some important results were found.

Finally, as this represents the initial introduction of the entire Harmonic Index (EHI), several intriguing open problems and potential research avenues require further exploration. These include:

1. More mathematical study for this new index to discover its relations with the other graph parameters;
2. Investigation of the broader applicability of this new index across diverse network types, including social networks, biological networks, and technological networks;
3. Exploration of the potential of this index in various domains, such as drug discovery in medicine and material design in engineering.

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