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# New Bounds for the Harmonic Energy and Harmonic Estrada index of Graphs

Akbar Jahanbani

**Abstract**

Let $G$ be a finite simple undirected graph with $n$ vertices and $m$ edges. The Harmonic energy of a graph $G$, denoted by $\mathcal{H}E(G)$, is defined as the sum of the absolute values of all Harmonic eigenvalues of $G$. The Harmonic Estrada index of a graph $G$, denoted by $\mathcal{H}EE(G)$, is defined as $\mathcal{H}EE = \mathcal{H}EE(G) = \sum_{i=1}^{n} e^{\gamma_i}$, where $\gamma_1 \geqslant \gamma_2 \geqslant \cdots \geqslant \gamma_n$ are the $\mathcal{H}$-*eigenvalues* of $G$. In this paper we present some new bounds for $\mathcal{H}E(G)$ and $\mathcal{H}EE(G)$ in terms of number of vertices, number of edges and the sum-connectivity index.

**Keywords:** Eigenvalue of graph, Energy, sum-connectivity index, Harmonic energy, Harmonic Estrada index.

## 1 Introduction

Let $G = (V, E)$ be a simple undirected graph with vertex set $V = V(G) = \{v_1, v_2, ...., v_n\}$ and edge set $E(G), |E(G)| = m$. The *order* and *size* of G are $n = |V|$ and $m = |E|$, respectively. For a vertex $v_i \in V$ , the degree of $v_i$, denoted by $\deg(v_i)$ (or just $d_i$), is the number of edges incident to $v$. The independence number, denoted $\alpha(G)$, of graph $G$ is defined as the size of the largest independent set in $G$. The chromatic number $\chi'(G)$ of G is the smallest number of colors needed to color all vertices of $G$ in such a way that no pair of adjacent vertices get the same color. A graph $G$ is *regular* if there exists a constant $r$ such that each vertex of $G$ has degree $r$, such graphs are also called $r$-*regular*. The *adjacency matrix* $A(G)$ of $G$ is defined by its entries as $a_{ij} = 1$ if $v_iv_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ denote the *eigenvalues* of $A(G)$. $\lambda_1$ is called the *spectral radius* of the graph $G$. The *energy* of the graph $G$ is defined as:

$$\mathcal{E} = \mathcal{E}(G) = \sum_{i=1}^{n} \mid \lambda_i \mid, \tag{1}$$

where $\lambda_i$, $i = 1, 2, \ldots, n$ , are the *eigenvalues* of graph $G$. This concept was introduced by $I.$ *Gutman* and is intensively studied in *chemistry*, since it can be used to approximate the total $\pi$-*electron* energy of a *molecule* (see, e.g. [21], [23] ). Since then, numerous other bounds for *energy* were found (see, e.g. [1], [2], [22], [24], [32], [33], [34]).

For a graph $G$, the *Harmonic* index $\mathcal{H}(G)$ is defined in [19] as

$$\mathcal{H}(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)},$$

where $d(u)$ denotes the degree of a vertex $u$ in $G$. In 2012, *Zhong* reintroduced this index as *Harmonic* index and found the minimum and maximum values of the *Harmonic* index for simple connected graphs and trees [39]. To know more about this index, refer to [ [3] – [5], [11] – [10], [28], [36], [39] – [41]]. In [19], *Favaron et al.* considered the relation between *Harmonic* index and the eigenvalues of graphs. *Zhong* [39], found the minimum and maximum values of the *Harmonic* index for connected graphs and trees, and characterized the corresponding extremal graphs. Recently, Wu et al. [38], give a best possible lower bound for the *Harmonic* index of a graph (a triangle-free graph, respectively) with order $n$ and minimum degree at least two and characterize the extremal graphs.

The sum-connectivity index $\chi(G)$ and the general sum-connectivity index $\chi_\beta(G)$ were recently proposed by Zhou and Trinajstić in ( [42], [43]) and defined as

$$\chi(G) = \sum_{uv \in E(G)} (d(u) + d(v))^{\frac{-1}{2}}$$

and

$$\chi_\beta(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\beta, \tag{2}$$

where $\beta$ is a real number. Some mathematical properties of the (general) sum-connectivity index on trees, *molecular* trees, *unicyclic* graphs and *bicyclic* graphs were given in ( [42], [43], [15]- [17]). The *Harmonic* matrix of a graph $G$ is a square matrix $\mathcal{H}(G) = [h_{ij}]$ of order $n$, defined via [27]

$$h_{ij} = \begin{cases} 0 & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are not adjacent} \\ \frac{2}{(d_i+d_j)} & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent} \\ 0 & \text{if } i = j. \end{cases} \tag{3}$$

The eigenvalues of the Harmonic matrix $\mathcal{H}(G)$ are denoted by $\gamma_1, \gamma_2, \ldots, \gamma_n$ and are said to be the $\mathcal{H}$-eigenvalues of $G$ and their collection is called *Harmonic* spectrum or *$\mathcal{H}$-spectrum* of $G$. We note that since the Harmonic matrix is symmetric, its eigenvalues are real and can be ordered as $\gamma_1 \geqslant \gamma_2 \geqslant \cdots \geqslant \gamma_n$.

This paper is organized as follows. In Section 2, we give a list of some previously known results. In Section 3, we obtain lower and upper bounds for the *Harmonic energy* of graph $G$. In Section 4, we obtain lower and upper bounds for the *Harmonic Estrada* index of graph $G$. All graphs considered in this paper are simple.

## 2 Preliminaries and known results

In this section, we shall list some previously known results that will be needed in the next section. We first calculate $tr(\mathcal{H}^2)$ and $tr(\mathcal{H}^3)$, where $tr$ denotes the trace of the respective matrix.

Denote by $N_k$ the $k$-th spectral moment of the *Harmonic* matrix $\mathcal{H}$, i. e.,

$$N_k = \sum_{i=1}^{n} (\gamma_i)^k \tag{4}$$

and recall that $N_k = tr(\mathcal{H}^k)$.

**Lemma 1.** *Let $G$ be a graph with $n$ vertices and Harmonic matrix $\mathcal{H}$. Then*

$$(1)\quad N_0 = \sum_{i=1}^{n} (\gamma_i)^0 = n, \tag{5}$$

$$(2)\quad N_1 = \sum_{i=1}^{n} \gamma_i = tr(\mathcal{H}) = 0, \tag{6}$$

$$(3)\quad N_2 = \sum_{i=1}^{n} (\gamma_i)^2 = tr(\mathcal{H}^2) = 8\chi_{-2}(G), \tag{7}$$

$$(4)\quad N_3 = \sum_{i=1}^{n} (\gamma_i)^3 = tr(\mathcal{H}^3) = 32\chi_{-2}(G)\Bigg(\sum_{k\sim i,\, k\sim j} \frac{1}{(d_k)^2}\Bigg), \tag{8}$$

$$(5)\quad N_4 = \sum_{i=1}^{n} (\gamma_i)^4 = tr(\mathcal{H}^4) = \sum_{i=1}^{n} \Bigg(\sum_{i\sim j} \frac{4}{(d_i+d_j)^2}\Bigg)^2 \tag{9}$$

$$+\sum_{i\neq j} \frac{4}{(d_i+d_j)^2}\Bigg(\sum_{k\sim i,\, k\sim j} \frac{4}{(d_k)^2}\Bigg)^2. \tag{10}$$

where $\sum_{i\sim j}$ indicates summation over all pairs of adjacent vertices $v_i, v_j$ and also

$$\sum_{k\sim i,\, k\sim j} \frac{1}{(d_k)^2} = \sum_{k\sim i,\, k\sim j} \frac{1}{(d_i+d_k)(d_k+d_j)}.$$

Nowadays, $\mathcal{H}$ is referred to as the *Harmonic* index.

*Proof.* By definition, the diagonal elements of $\mathcal{H}$ are equal to zero. Therefore the trace of $\mathcal{H}$ is zero.

Next, we calculate the matrix $\mathcal{H}^2$. For $i = j$

$$(\mathcal{H}^2)_{ii} = \sum_{j=1}^{n} \mathcal{H}_{ij}\mathcal{H}_{ji} = \sum_{j=1}^{n} (\mathcal{H}_{ij})^2 = \sum_{i\sim j} (\mathcal{H}_{ij})^2 = \sum_{i\sim j} \frac{4}{(d_i+d_j)^2},$$

whereas for $i \neq j$

$$(\mathcal{H}^2)_{ij} = \sum_{j=1}^{n} \mathcal{H}_{ij}\mathcal{H}_{ji} = \mathcal{H}_{ii}\mathcal{H}_{ij} + \mathcal{H}_{ij}\mathcal{H}_{jj} + \sum_{k\sim i,\, k\sim j} \mathcal{H}_{ik}\mathcal{H}_{kj} =$$

$$= \frac{2}{(d_i + d_j)} \sum_{k\sim i,\, k\sim j} \frac{4}{(d_k)^2}.$$

Therefore

$$tr(\mathcal{H}^2) = \sum_{i=1}^{n} \sum_{i\sim j} \frac{4}{(d_i + d_j)^2} = 8 \sum_{i\sim j} \frac{1}{(d_i + d_j)^2}.$$

Hence by equality (2), we have

$$tr(\mathcal{H}^2) = 8\chi_{-2}(G).$$

Since the diagonal elements of $\mathcal{H}^3$ are

$$(\mathcal{H}^3)_{ii} = \sum_{j=1}^{n} \mathcal{H}_{ij}(\mathcal{H}^2)_{jk} = \sum_{i\sim j} \frac{2}{(d_i + d_j)} (\mathcal{H}^2)_{ij} =$$

$$= \sum_{i\sim j} \frac{4}{(d_i + d_j)^2} \left( \sum_{k\sim i,\, k\sim j} \frac{4}{(d_k)^2} \right)$$

we obtain

$$tr(\mathcal{H}^3) = \sum_{i=1}^{n} \sum_{i\sim j} \frac{4}{(d_i + d_j)^2} \left( \sum_{k\sim i,\, k\sim j} \frac{4}{(d_k)^2} \right) =$$

$$= 32 \sum_{i\sim j} \frac{1}{(d_i + d_j)^2} \left( \sum_{k\sim i,\, k\sim j} \frac{1}{(d_k)^2} \right).$$

Hence by equality (2), we have

$$tr(\mathcal{H}^3) = 32\chi_{-2}(G) \left( \sum_{k\sim i,\, k\sim j} \frac{1}{(d_k)^2} \right).$$

We now calculate $tr(\mathcal{H}^4)$. Because $tr(\mathcal{H}^4) = \|\mathcal{H}^2\|_F^2$, where $\|\mathcal{H}^2\|_F^2$ denotes the *Frobenius norm* of $\mathcal{H}^2$, we obtain

$$\begin{aligned} tr(\mathcal{H}^4) &= \sum_{i,j=1}^{n} \mid (\mathcal{H}^2)_{ii} \mid^2 = \sum_{i=j} \mid (\mathcal{H}^2)_{ii} \mid^2 + \sum_{i\neq j} \mid (\mathcal{H}^2)_{ii} \mid^2 \\ &= \sum_{i=1}^{n} \left( \sum_{i\sim j} \frac{4}{(d_i+d_j)^2} \right)^2 + \sum_{i\neq j} \frac{4}{(d_i+d_j)^2} \left( \sum_{k\sim i,\, k\sim j} \frac{4}{(d_k)^2} \right)^2 . \end{aligned}$$

□

**Remark 1.** *Recall that [8] for a graph with eigenvalues* $\lambda_1, \lambda_2, \ldots, \lambda_n$*, with* $m$ *edges and* $t$ *triangles,*

$$M_k = \sum_{i=1}^{n} (\lambda_i)^k.$$

$$M_0 = n, \quad M_1 = \sum_{i=1}^{n} (\lambda_i) = 0, \quad M_2 = \sum_{i=1}^{n} (\lambda_i)^2 = 2m,$$

$$M_3 = \sum_{i=1}^{n} (\lambda_i)^3 = 6t.$$

**Lemma 2.** *(RayleighRitz) [25] If* $\boldsymbol{B}$ *is a real symmetric* $n \times n$ *matrix with eigenvalues* $\lambda_1(\boldsymbol{B}) \geqslant \lambda_2(\boldsymbol{B}) \leqslant \cdots \leqslant \lambda_n(\boldsymbol{B})$*, then for any* $\boldsymbol{X} \in \boldsymbol{R}^n$*,* $(\boldsymbol{X} \neq 0)$*,*

$$\boldsymbol{X}^t \boldsymbol{B} \boldsymbol{X} \leqslant \lambda_1(\boldsymbol{B}) \boldsymbol{X}^t \boldsymbol{X}.$$

*Equality holds if and only if* $\boldsymbol{X}$ *is an eigenvector of* $\boldsymbol{B}$*, corresponding to the largest eigenvalue* $\lambda_1(\boldsymbol{B})$*.*

**Theorem 1.** *[11] Let* $G$ *be a simple graph with the chromatic number* $\chi'(G)$ *and the Harmonic index* $\mathcal{H}(G)$*, then*

$$\chi'(G) \leqslant 2\mathcal{H}(G),$$

*with equality if and only if* $G$ *is a complete graph, possibly with some additional isolated vertices.*

**Lemma 3.** *[36] Let $G$ be a triangle-free graph with $n$ vertices and $m$ edges, then*

$$\mathcal{H}(G) \geqslant \frac{2m}{n}.$$

**Lemma 4.** *[8] Let $G$ be a graph, where the number of eigenvalues greater than, less than, and equal to zero are $p$, $q$ and $r$, respectively. Then*

$$\alpha \leqslant r + min\{p, q\},$$

*where $\alpha$ is the independence number of $G$.*

**Remark 2.** *For non-negative $x_1, x_2, \ldots, x_n$ and $k \geqslant 2$,*

$$\sum_{i=1}^{n}(x_i)^k \leqslant (\sum_{i=1}^{n} {x_i}^2)^{\frac{k}{2}}. \tag{11}$$

**Lemma 5.** *[6] For any real $x$, one has $e^x \geqslant 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!}$. Equality holds if and only if $x = 0$.*

## 3 Bounds for the Harmonic Energy of a graph

In this section, we obtain lower and upper bounds for the Harmonic energy of graph. The *Harmonic* energy of the graph G is defined in [27] as:

$$\mathcal{H}E(G) = \sum_{i=1}^{n} \mid \gamma_i \mid . \tag{12}$$

First, we prove the following theorem that will be needed for obtaining the bounds of Harmonic energy.

**Theorem 2.** *Let $G$ be a connected graph with $n \geqslant 2$ vertices. Then the spectral radius of the Harmonic matrix is bounded from below as*

$$\lambda_1 \geqslant \frac{2\mathcal{H}(G)}{n}. \tag{13}$$

*Proof.* Let $\mathcal{H} = ||h_{ij}||$ be the Harmonic matrix corresponding to $\mathcal{H}$. By Lemma 2, for any vector $X = (x_1, x_2, \ldots, x_n)^t$,

$$X^t \mathcal{H} X = \left( \sum_{j,j\sim 1}^{n} x_j z_{j1}, \sum_{j,j\sim 2}^{n} x_j z_{j2}, \ldots, \sum_{j,j\sim n}^{n} x_j z_{jn} \right)^t X$$
$$= 2 \sum_{i\sim j} z_{ij} x_i x_j \tag{14}$$

because $h_{ij} = h_{ji}$. Also,

$$X^t X = \sum_{i=1}^{n} x_i^2. \tag{15}$$

Using Eqs. (14) and (15), by Lemma 2, we obtain

$$\gamma_1 \geqslant \frac{2 \sum_{i\sim j} z_{ij} x_i x_j}{\sum_{i=1}^{n} x_i^2}. \tag{16}$$

Since (16) is true for any vector $X$, by putting $X = (1, 1, \ldots, 1)^t$, we have

$$\gamma_1 \geqslant \frac{2\mathcal{H}(G)}{n}.$$

□

**Theorem 3.** *Let $G$ be a graph with $n$ vertices. Then*

$$\mathcal{H}E(G) \leqslant \frac{8}{n}\sqrt{\chi_{-2}(G)} + \sqrt{(n-1)\left(8\chi_{-2}(G) - \left(\frac{8}{n}\sqrt{8\chi_{-2}(G)}\right)^2\right)}.$$

*Proof.* By applying the Cauchy-Schwartz inequality to the two $(n-1)$ vectors $(1, 1, \ldots, 1)$ and $(|\gamma_1|, |\gamma_2|, \ldots, |\gamma_n|)$, we have

$$\left( \sum_{i=2}^{n} |\gamma_i| \right)^2 \leqslant (n-1)\left( \sum_{i=2}^{n} \gamma_i^2 \right).$$

By the define of Harmonic energy, we can get

$$
\begin{aligned}
(\mathcal{H}E(G)-\gamma_1)^2 &= \left(\sum_{i=2}^{n} \mid \gamma_i \mid\right)^2 \\
&\leqslant (n-1)\left(\sum_{i=1}^{n} \gamma_i^2 - \gamma_1^2\right) \\
&= (n-1)\left(8\chi_{-2}(G) - \gamma_1^2\right), \qquad \text{(by Equality 7)}
\end{aligned}
$$

then

$$
\mathcal{H}E(G) \leqslant \gamma_1 + \sqrt{(n-1)\left(8\chi_{-2}(G) - \gamma_1^2\right)}. \tag{17}
$$

Now let us define a function

$$
f(x) = x + \sqrt{(n-1)\left(8\chi_{-2}(G) - x^2\right)}.
$$

In fact, by keeping in mind $\gamma_1 \geqslant 1$, we set $\gamma_1 = x$. Using

$$
\sum_{i=2}^{n} \gamma_i^2 = 8\chi_{-2}(G),
$$

we get that

$$
x^2 = \gamma_1^2 \leqslant 8\chi_{-2}(G).
$$

In other words, $x \leqslant \sqrt{8\chi_{-2}(G)}$, meanwhile $f'(x) = 0$ implies that

$$
x = \sqrt{\frac{8}{n}\chi_{-2}(G)}.
$$

Therefore $f$ is a decreasing function in the interval

$$
\sqrt{\frac{8}{n}\chi_{-2}(G)} \leqslant x \leqslant 8\sqrt{\chi_{-2}(G)}
$$

and

$$
\sqrt{\frac{8}{n}\chi_{-2}(G)} \leqslant x \leqslant \frac{8}{n}\sqrt{\chi_{-2}(G)} \leqslant \gamma_1.
$$

Hence

$$f(\gamma_1) \leqslant f\left(\frac{8}{n}\sqrt{\chi_{-2}(G)}\right).$$

Therefore

$$\mathcal{H}E(G) \leqslant \frac{8}{n}\sqrt{\chi_{-2}(G)} + \sqrt{(n-1)\left(8\chi_{-2}(G) - (\frac{8}{n}\sqrt{8\chi_{-2}(G)})^2\right)}.$$

□

By Theorem 1 and Theorem 2, we establish the following result.

**Theorem 4.** *Let $G$ be a non-empty and non-singular graphs with $n$ vertices and chromatic number $\chi'$. Then*

$$\mathcal{H}E(G) \geqslant \frac{\chi'}{n} + ln \mid det\mathcal{H} \mid -ln\left(\frac{\chi'}{n}\right). \tag{18}$$

*Proof.* Since $G$ is non-singular, it is $\mid \gamma_i \mid > 0, i = 1, 2, \ldots, n$. Consider a function

$$f_1(x) = x - 1 - lnx,$$

for $x > 0$. It is elementary to prove that $f_1(x)$ is increasing for $x \geqslant 1$ and decreasing for $0 < x \leqslant 1$. Consequently, $f_1(x) \geqslant f_1(1) = 0$, implying that $x \geqslant 1 + lnx$ for $x > 0$, with equality holding if and only if $x = 1$. Using the above result, we get

$$\begin{aligned}
\mathcal{H}E(G) &= \gamma_1 + \sum_{i=2}^{n} \mid \gamma_i \mid \\
&\geq \gamma_1 + n - 1 + \sum_{i=2}^{n} ln \mid \gamma_i \mid \\
&= \gamma_1 + n - 1 + ln\prod_{i=2}^{n} \mid \gamma_i \mid \\
&= \gamma_1 + n - 1 + ln \mid det\mathcal{H} \mid -ln\gamma_1. \qquad (19)
\end{aligned}$$

At this point, one has to recall that, by Lemma 2, $\gamma_1 \geqslant \frac{\chi'}{n}$.
Since $x \geqslant \frac{\chi'}{n} \geqslant 1$, we have that

$$g(x) = x + n - 1 + ln \mid det\mathcal{H} \mid -lnx,$$

is an increasing function on $1 \leqslant x \leqslant n$. So we conclude that

$$g(x) \geqslant g\left(\frac{\chi'}{n}\right) = \frac{\chi'}{n} + (n-1) + ln \mid det\mathcal{H} \mid -ln\left(\frac{\chi'}{n}\right).$$

Combining the above result with (19), we arrive at (18). □

Also, by Theorem 2 and Lemma 3, we establish the following result.

**Remark 3.** *Let $G$ be a triangle-free graph with $n$ vertices and $m$ edges, then*

$$\mathcal{H}E(G) \geqslant \frac{4m}{n^2} + ln \mid det\mathcal{H} \mid -ln\left(\frac{4m}{n^2}\right).$$

*Or*

$$\mathcal{H}E(G) \leqslant \frac{4m}{n^2} + \sqrt{(n-1)(8\chi_{-2}(G) - \frac{4m}{n^2})}.$$

**Theorem 5.** *Let $G$ be a connected graph with $n \geqslant 2$ vertices and independence number $\alpha$. Then*

$$\mathcal{H}E(G) \leqslant 2\sqrt{(n-\alpha)\chi_{-2}(G)}.$$

*Proof.* Let $\gamma_1, \gamma_2, \ldots, \gamma_p$, be the $p$ positive eigenvalues of $G$ and let $\eta_1, \eta_2, \ldots, \eta_q$, be the $q$ negative eigenvalues of $G$. Then $G$ has $n-p-q$ eigenvalues which are equal to zero. From Lemma 4, we have

$$\alpha \leqslant (n-p-q) + min\{p, q\}.$$

Thus $\alpha \leqslant (n-p-q) + p$ and $\alpha \leqslant (n-p-q) + q$. Namely, $p \leqslant n - \alpha$ and $q \leqslant n - \alpha$. Since $\sum_{i=1}^{p} \gamma_i + \sum_{i=1}^{q} \eta_i = 0$, we have that

$$\mathcal{H}E(G) = 2\sum_{i=1}^{p} \gamma_i = 2\sum_{i=1}^{q} \mid \eta_i \mid.$$

From Cauchy - Schwarz inequality, we have that

$$\mathcal{H}E(G) = 2\sum_{i=1}^{p}\gamma_i \leqslant 2\sqrt{p\sum_{i=1}^{p}\gamma_i}.$$

Similarly, we have that

$$\mathcal{H}E(G) = 2\sum_{i=1}^{q}\eta_i \leqslant 2\sqrt{q\sum_{i=1}^{q}\eta_i}.$$

Therefore

$$\begin{aligned}\frac{\mathcal{H}E(G)^2}{2} = \frac{\mathcal{H}E(G)^2}{4} + \frac{\mathcal{H}E(G)^2}{4} &\leqslant p\sum_{i=1}^{p}\gamma_i^2 + q\sum_{i=1}^{q}\eta_i^2\\ &\leqslant (n-\alpha)\sum_{i=1}^{p}\gamma_i^2 + (n-\alpha)\sum_{i=1}^{q}\eta_i^2\\ &= (n-\alpha)\left(\sum_{i=1}^{p}\gamma_i^2 + \sum_{i=1}^{q}\eta_i^2\right)\\ &= 8(n-\alpha)\chi_{-2}(G).\end{aligned}$$

Hence

$$\mathcal{H}E(G) \leqslant 4\sqrt{(n-\alpha)\chi_{-2}(G)}.$$

□

**Theorem 6.** *If the graph $G$ is regular of degree $r, r > 0$ , then*

$$\mathcal{H}E(G) = \frac{1}{r}\mathcal{E}(G).$$

*If, in addition $r = 0$, then $\mathcal{H}E(G) = 0$.*

*Proof.* If $r = 0$, then $G$ is the graph without edges. Then directly from the definition (3) it follows that $\mathcal{H}_{i,j} = 0$ for all $i, j = 1, 2, \ldots, n$, i. e., that $\mathcal{H}(G) = 0$. All eigenvalues of the zero matrix 0 are equal to zero. Therefore, $\mathcal{H}E(G) = 0$.

Suppose now that $G$ is regular of degree $r > 0$, i. e., that $d_1 = d_2 = \cdots = d_n = r$. Then all non-zero terms in $\mathcal{H}(G)$ are equal to $\frac{1}{r}$, implying that $\mathcal{H}(G) = \frac{1}{r}A(G)$. Therefore, $\gamma_i = \frac{1}{r}\lambda_i$. Theorem 6 follows from the definitions of energy and Harmonic energy. □

**Theorem 7.** *Let $G$ be a graph with $n$ vertices. Then*

$$\mathcal{H}E(G) \leqslant \sqrt{8n\chi_{-2}(G) - \frac{n}{2}(\mid \gamma_1 \mid - \mid \gamma_n \mid)^2}. \tag{20}$$

*Proof.* From the Lagrange's identity (see for example [22]),

$$0 \leqslant 8n\chi_{-2}(G) - \mathcal{H}E(G)^2 = \sum_{i=1}^{n} \mid \gamma_i \mid^2 - \left( \sum_{i=1}^{n} \mid \gamma_i \mid \right)^2 =$$

$$= \sum_{1 \leqslant i \leqslant j \leqslant n} (\mid \gamma_i \mid - \mid \gamma_j \mid)^2,$$

the following inequality can be obtained

$$0 \leqslant 8n\chi_{-2}(G) - \mathcal{H}E(G)^2 \geqslant \sum_{i=2}^{n-1} \Big( (\mid \gamma_1 \mid - \mid \gamma_i \mid)^2 + (\mid \gamma_i \mid - \mid \gamma_n \mid)^2) + (\mid \gamma_1 \mid - \mid \gamma_n \mid)^2 \Big).$$

On the other hand, according to the Jennsen's inequality (see [21]), from the above inequality it follows that

$$0 \leqslant 8n\chi_{-2}(G) - \mathcal{H}E(G)^2 \geqslant \frac{n-2}{2}(\mid \gamma_1 \mid - \mid \gamma_n \mid)^2 + (\mid \gamma_1 \mid - \mid \gamma_n \mid)^2 = \frac{n}{2}(\mid \gamma_1 \mid - \mid \gamma_n \mid)^2.$$

After rearranging the above inequality, the inequality (20) is obtained. □

**Theorem 8.** *Let $G$ be a graph with $n \geqslant 2$ vertices. Then for each $T$ with the property $\gamma_1 \geqslant T \geqslant \sqrt{\frac{8\chi_{-2}(G)}{n}}$, the following is valid*

$$\mathcal{H}E(G) \leqslant T + \sqrt{(n-1)(8\chi_{-2}(G) - T^2)}. \tag{21}$$

*Proof.* In [37] a class of real polynomials $P_n(x) = x^n + a_1x^{n-1} + a_2x^{n-2} + b_3x^{n-3} + \cdots + b_n$, denoted as $P_n(a_1, a_2)$, where $a_1$ and $a_2$ are fixed real numbers, was considered. For the roots $x_1 \geqslant x_2 \geqslant \cdots \geqslant x_n$ of an arbitrary polynomial $P_n(x)$ from this class, the following values were introduced

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i, \tag{22}$$

$$\Delta = n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2. \tag{23}$$

Then upper and lower bounds for the polynomial roots, $x_i, i = 1, 2, \ldots, n$, were determined in terms of the introduced values

$$\bar{x} + \frac{1}{n}\sqrt{\frac{\Delta}{n-1}} \leqslant x_1 \leqslant \bar{x} + \frac{1}{n}\sqrt{(n-1)\Delta}, \tag{24}$$

$$\bar{x} - \frac{1}{n}\sqrt{\frac{i-1}{n-i+1}\Delta} \leqslant x_i \leqslant \bar{x} + \frac{1}{n}\sqrt{\frac{n-i}{i}\Delta}, \quad 2 \leqslant i \leqslant n-1, \tag{25}$$

$$\bar{x} - \frac{1}{n}\sqrt{(n-1)\Delta} \leqslant x_n \leqslant \bar{x} - \frac{1}{n}\sqrt{\frac{\Delta}{n-1}}. \tag{26}$$

Consider the polynomial

$$\psi_n(x) = \prod_{i=1}^{n}(x- \mid \gamma_i \mid) = x^n + a_1x^{n-1} + a_2x^{n-2} + b_3x^{n-3} + \cdots + b_n.$$

Since

$$a_1 = -\sum_{i=1}^{n} \mid \gamma_i \mid = -\mathcal{H}E$$

and

$$a_2 = \frac{1}{2}\left[\left(\sum_{i=1}^{n} \mid \gamma_i \mid\right)^2 - \sum_{i=1}^{n} \mid \gamma_i \mid^2\right] = \frac{1}{2}\mathcal{H}E^2 - 4\chi_{-2}(G),$$

the polynomial $\psi_n(x)$ belongs to a class of real polynomials $P_n(-\mathcal{H}E, \frac{1}{2}\mathcal{H}E^2 - 4\chi_{-2}(G))$. Based on the following equalities

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} \mid \gamma_i \mid = \frac{\mathcal{H}E}{n}, \tag{27}$$

$$\Delta = n\sum_{i=1}^{n} \mid \gamma_i \mid^2 - \left(\sum_{i=1}^{n} \mid \gamma_i \mid\right)^2 = 8n\chi_{-2}(G) - \mathcal{H}E^2, \tag{28}$$

for $x_1 = \gamma_1$, according to (27), (28) and the right-hand side of the first inequality in (25), we get

$$\gamma_1 \leqslant \frac{\mathcal{H}E}{n} + \sqrt{(n-1)(8n\sum_{i\sim j}\frac{1}{(d_i+d_j)^2} - \mathcal{H}E^2)}. \tag{29}$$

Now, for each real $T$ with the property $\gamma_1 \geqslant T \geqslant \sqrt{\frac{\chi_{-2}(G)}{n}}$ from (29) it follows that

$$T \leqslant \frac{\mathcal{H}E}{n} + \sqrt{(n-1)(8n\chi_{-2}(G) - \mathcal{H}E^2)}.$$

After rearranging the above inequality, the inequality (21) is obtained. □

**Theorem 9.** *Let $G$ be a simple graph with $n \geqslant 2$ vertices. Then*

$$\frac{1}{n}\sqrt{\frac{8n\chi_{-2}(G)}{n-1}} \leqslant \gamma_1 \leqslant \frac{1}{n}\sqrt{8n(n-1)\chi_{-2}(G)},$$

$$-\frac{1}{n}\sqrt{\frac{i-1}{n-i+1}8n\chi_{-2}(G)} \leqslant \gamma_i \leqslant \frac{1}{n}\sqrt{\frac{n-i}{i}8n\chi_{-2}(G)}$$

$$\textit{for} \quad 2 \leqslant i \leqslant n-1$$

$$-\frac{1}{n}\sqrt{8n(n-1)\chi_{-2}(G)} \leqslant \gamma_n \leqslant -\frac{1}{n}\sqrt{\frac{8n\chi_{-2}(G)}{n-1}}.$$

*Proof.* Let the characteristic polynomial of a graph $G$ be the following:

$$\varphi_n(x) = \prod_{i=1}^{n}(x-\gamma_i) = x^n + a_1x^{n-1} + a_2x^{n-2} + b_3x^{n-3} + \cdots + b_n.$$

Since

$$a_1 = -\sum_{i=1}^{n} \gamma_i = 0$$

and

$$a_2 = \frac{1}{2}\left[\left(\sum_{i=1}^{n} \gamma_i\right)^2 - \sum_{i=1}^{n} \gamma_i^2\right] = -4\chi_{-2}(G),$$

the polynomial $\varphi_n(x)$ belongs to a class of real polynomials $P_n(0, -4\chi_{-2}(G))$, by the equalities

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} \gamma_i = 0$$

and

$$\Delta = n\sum_{i=1}^{n} \gamma_i^2 - \left(\sum_{i=1}^{n} \gamma_i\right)^2 = 8n\chi_{-2}(G)$$

and inequalities (24), (25), (26), the proof is completed. □

**Theorem 10.** *Let $G$ be a graph with $n$ vertices and $|\gamma_1| \geqslant |\gamma_2| \geqslant \cdots \geqslant |\gamma_n|$ be a non-increasing arrangement of eigenvalues of $G$. Then, the following inequality is valid*

$$\mathcal{H}E(G) \geqslant \sqrt{8n\chi_{-2}(G) - \theta(n)(|\gamma_1| - |\gamma_n|)^2}. \tag{30}$$

*where $\theta(n) = n[\frac{n}{2}](1 - \frac{1}{n}[\frac{n}{2}])$, while $[x]$ denotes integer part of a real number $x$.*

*Proof.* Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers for which there exist real constants $a, b, A$ and $B$, so that for each $i, i = 1, 2, \ldots, n$, $a \leqslant a_i \leqslant A$ and $b \leqslant b_i \leqslant B$. Then the following inequality is valid (see [7])

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leqslant \theta(n)(A - a)(B - b). \tag{31}$$

Equality in (31) holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$.

For $a_i := |\gamma_i|$, $b_i := |\gamma_i|$, $a = b := |\gamma_n|$ and $A = B := |\gamma_1|$, $i = 1, 2, \ldots n$ inequality (31) becomes

$$\left| n \sum_{i=1}^{n} |\gamma_i|^2 - \left( \sum_{i=1}^{n} |\gamma_i| \right)^2 \right| \leqslant \theta(n)(|\gamma_1| - |\gamma_n|)^2.$$

Therefore, the above inequality becomes

$$8n\chi_{-2}(G) - \mathcal{H}E(G)^2 \leqslant \theta(n)(|\gamma_1| - |\gamma_n|)^2,$$

wherefrom the statement of Theorem 10 follows. Since equality in (31) holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$, equality in (30) holds if and only if $|\gamma_1| = |\gamma_2| = \cdots = |\gamma_n|$. □

**Theorem 11.** *Let $G$ be a graph with $n$ vertices and $|\gamma_1| \geqslant |\gamma_2| \geqslant \cdots \geqslant |\gamma_n|$ be a non-increasing arrangement of eigenvalues of $G$. Then, the following inequality is valid*

$$\mathcal{H}E(G) \geqslant \frac{|\gamma_1||\gamma_n|n + 8\chi_{-2}(G)}{|\gamma_1| + |\gamma_n|}. \tag{32}$$

*Equality in (32) holds if and only if $G \cong \bar{K}_n$.*

*Proof.* Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers for which there exist real constants $R$ and $r$, so that for each $i, i = 1, 2, \ldots, n$ there holds $ra_i \leqslant b_i \leqslant Ra_i$. Then the following inequality is valid (see [14])

$$\sum_{i=1}^{n} b_i^2 + rR \sum_{i=1}^{n} a_i^2 \leqslant (r + R) \sum_{i=1}^{n} a_i b_i. \tag{33}$$

Equality in (33) holds if and only if for at least one $i, 1 \leqslant i \leqslant n$ there holds $ra_i = bi = Ra_i$.

For $a_i := 1$, $b_i := |\gamma_i|$, $r := |\gamma_n|$ and $R := |\gamma_1|$, $i = 1, 2, \ldots n$, inequality (31) becomes

$$\sum_{i=1}^{n} |\gamma_i|^2 + |\gamma_1||\gamma_n| \sum_{i=1}^{n} 1 \leqslant (|\gamma_n| + |\gamma_1|) \sum_{i=1}^{n} |\gamma_i|.$$

Therefore, the above inequality becomes

$$8n\chi_{-2}(G) + n|\gamma_1||\gamma_n| \leqslant (|\gamma_n| + |\gamma_1|)\mathcal{H}E(G).$$

If for some $i$ there holds that $ra_i = b_i = Ra_i$, then for the same $i$ the following equality also holds: $b_i = r = R$. This means that for each $j, j \neq i$ there holds $|\gamma_i| \leqslant |\gamma_j| \leqslant |\gamma_i|$. Therefore equality in (33) holds if and only if $|\gamma_1| = |\gamma_2| = \cdots = |\gamma_n|$. □

**Theorem 12.** *Let $G$ be a non-empty graph with $n$ vertices. Then*

$$\mathcal{H}E(G) \geqslant \frac{(N_2)^2}{N_4}.$$

*Proof.* We start with the Hölder inequality

$$\sum_{i=1}^{n} a_i b_i \leqslant \left(\sum_{i=1}^{n} a_i^p\right)^{\frac{1}{p}} \left(\sum_{i=1}^{n} b_i^q\right)^{\frac{1}{q}}, \tag{34}$$

which holds for non-negative real numbers $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$. Setting $a_i = |\gamma_i|^{\frac{1}{2}}$, $b_i = |\gamma_i|^{\frac{3}{2}}$, $p = 2$ and $q = 2$, from (34), we obtain

$$\sum_{i=1}^{n} |\gamma_i|^2 = \sum_{i=1}^{n} |\gamma_i|^{\frac{1}{2}} \left(|\gamma_i|^3\right)^{\frac{1}{2}} \leqslant \left(\sum_{i=1}^{n} |\gamma_i|\right)^{\frac{1}{2}} \left(\sum_{i=1}^{n} |\gamma_i|^3\right)^{\frac{1}{2}}. \tag{35}$$

Then $\sum_{i=1}^{n} |\gamma_i|^3 \neq 0$ and (35) can be written as the following

$$\sum_{i=1}^{n} |\gamma_i| \geqslant \frac{\left(\sum_{i=1}^{n} |\gamma_i^2|\right)^2}{\sum_{i=1}^{n} |\gamma_i|^3}.$$

Hence by equalities (12), (7) and (8), we have

$$\mathcal{H}E(G) \geqslant \frac{(N_2)^2}{N_4}.$$

□

**Theorem 13.** *Let $G$ be a non-empty graph with $n$ vertices. Then*

$$\mathcal{H}E(G) \geqslant \frac{\sqrt{32n\chi_{-2}(G)\big(|\gamma_1|\gamma_n|\big)}}{|\gamma_1| + |\gamma_n|}.$$

*Proof.* Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers for which there exist real constants $m_1, m_2, M_1$ and $M_2$, so that for each $i, i = 1, 2, \ldots, n$, $m_1 \leqslant a_i \leqslant M_1$ and $m_2 \leqslant b_i \leqslant M_2$. Then the following inequality is valid by the Hölder inequality (see [26], p. 135)

$$\left[\sum_{i=1}^{n}(a_i)^2\right]\left[\sum_{i=1}^{n}(b_i)^2\right] \leqslant \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}}+\sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2\left(\sum_{i=1}^{n}a_ib_i\right)^2, \quad (36)$$

where the equality holds if and only if $a_1 = a_2 = \cdots = a_n$ , $b_1 = b_2 = \ldots = b_n$ , $m_1 = M_1 = a_1$ , $m_2 = M_2 = b_1$.

For $a_i := |\gamma_i|$, $b_i := 1$, $m_1 := |\gamma_n|$, $M_1 := |\gamma_1|$, $M_2 = m_2 := 1$, $i = 1, 2, \ldots n$, inequality (36) becomes

$$\left[\sum_{i=1}^{n}(|\gamma_i|)^2\right]\left[\sum_{i=1}^{n}(1)^2\right] \leqslant \frac{1}{4}\left(\sqrt{\frac{|\gamma_1|}{|\gamma_n|}}+\sqrt{\frac{|\gamma_n|}{|\gamma_1|}}\right)^2\left(\sum_{i=1}^{n}|\gamma_i|\right)^2. \quad (37)$$

Hence by equalities (12), (7), we have

$$8n\chi_{-2}(G) \leqslant \frac{1}{4}\left(\sqrt{\frac{|\gamma_1|}{|\gamma_n|}}+\sqrt{\frac{|\gamma_n|}{|\gamma_1|}}\right)^2\Big(\mathcal{H}E(G)\Big)^2.$$

Therefore

$$\mathcal{H}E(G) \geqslant \frac{\sqrt{32n\chi_{-2}(G)(|\gamma_1|\gamma_n|)}}{|\gamma_1| + |\gamma_n|}.$$

□

**Theorem 14.** *Let $G$ be a graph with $n$ vertices. Then*

$$\mathcal{H}E(G) \leqslant \sqrt[3]{n^2}\sqrt{8\chi_{-2}(G)}.$$

*Proof.* Let $a_1, a_2, \ldots, a_n,\ b_1, b_2, \ldots, b_n$ and $c_1, c_2, \ldots, c_n$, be positive real numbers, $i = 1, 2, \ldots, n$. Then the following inequality is valid by the Hölder inequality (see [26], p. 137)

$$\left(\sum_{i=1}^{n} a_i b_i c_i\right)^3 \leqslant \left[\sum_{i=1}^{n} (a_i)^3\right] \left[\sum_{i=1}^{n} (b_i)^3\right] \left[\sum_{i=1}^{n} (c_i)^3\right], \qquad (38)$$

where equality holds if and only if $a_i = b_i = c_i$ , $i = 1, 2, \ldots, n$. For $a_i := |\gamma_i|$, $b_i := 1$, $c_i := 1$, $i = 1, 2, \ldots n$ inequality (38) becomes

$$\begin{aligned} \left(\sum_{i=1}^{n} |\gamma_i|\right)^3 &\leqslant \left[\sum_{i=1}^{n} (|\gamma_i|)^3\right] \left[\sum_{i=1}^{n} (1)^3\right] \left[\sum_{i=1}^{n} (1)^3\right] \\ &= n^2 \left[\sum_{i=1}^{n} (|\gamma_i|)^3\right] \\ &\leqslant n^2 \left[\sum_{i=1}^{n} (|\gamma_i|)^2\right]^{\frac{3}{2}}, \quad \text{by Inequality (11 )} \\ &= n^2 \left[\sum_{i=1}^{n} (\gamma_i)^2\right]^{\frac{3}{2}} \\ &= n^2 \left[8\chi_{-2}(G)\right]^{\frac{3}{2}}, \quad \text{by Equality (7 ).} \end{aligned}$$

Therefore

$$\mathcal{H}E(G) \leqslant \sqrt[3]{n^2}\sqrt{8\chi_{-2}(G)}.$$

□

**Theorem 15.** *Let $G$ be a graph with $n$ vertices. Then*

$$\mathcal{H}E(G) \leqslant 8\chi_{-2}(G).$$

*Proof.* Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers for which there exist real constants $r$ and $s$, such that $r + s = 1$ , $r,\ s \neq 0, 1$. Then the following inequality is valid by the Hölder inequality (see [26], p. 135)

$$\sum_{i=1}^{n} a_i b_i \geqslant \left[\sum_{i=1}^{n} (a_i)^{\frac{1}{r}}\right]^r \left[\sum_{i=1}^{n} (b_i)^{\frac{1}{s}}\right]^s \quad \text{for} \quad r > 1. \qquad (39)$$

For $a_i := |\gamma_i|^{\frac{1}{2}}$, $b_i := |\gamma_i|^{\frac{1}{2}}$, $r := \frac{1}{2}$, $s := \frac{1}{2}$ inequality (39) becomes

$$\sum_{i=1}^{n} |\gamma_i|^{\frac{1}{2}} |\gamma_i|^{\frac{1}{2}} \geqslant \left[\sum_{i=1}^{n} (|\gamma_i|^{\frac{1}{2}})^2\right]^{\frac{1}{2}} \left[\sum_{i=1}^{n} (|\gamma_i|^{\frac{1}{2}})^2\right]^{\frac{1}{2}}$$

$$\sum_{i=1}^{n} |\gamma_i| \geqslant \left[\sum_{i=1}^{n} |\gamma_i|\right]^{\frac{1}{2}} \left[\sum_{i=1}^{n} |\gamma_i|\right]^{\frac{1}{2}}$$

$$\sum_{i=1}^{n} |\gamma_i|^2 \geqslant \left[\sum_{i=1}^{n} |\gamma_i|\right]^{\frac{1}{2}} \left[\sum_{i=1}^{n} |\gamma_i|\right]^{\frac{1}{2}}.$$

Hence by equalities (12) and (7), we have

$$8\chi_{-2}(G) \geqslant \mathcal{H}(G).$$

□

# 4 Bounds on the Harmonic Estrada index of a graph

In this section, we obtain lower and upper bounds for the Harmonic Estrada index of graphs. We first recall that the Estrada index of a graph $G$ is defined by

$$EE = EE(G) = \sum_{i=1}^{n} e^{\lambda_i}.$$

Denoting by $M_k = M_k(G)$ to the *k-th moment* of the graph $G$, we get

$$M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k.$$

and recalling the power-series *expansion* of $e^x$, we have

$$EE = \sum_{i=1}^{\infty} \frac{M_k(G)}{k!}.$$

It is well known that [18] $M_k(G)$ is equal to the number of *closed walks* of length $k$ of the graph $G$. In fact *Estrada index* of graphs has an important role in *Chemistry* and *Physics* and there exists a vast *literature* that studies this special index. In addition to the Estrada's papers mentioned above, we may also refer the reader to ( [12], [13], [20], [29], [30], [31]) for the detailed information, such as lower and upper bounds for *Estrada index* in terms of the number of vertices and edges, and some inequalities between *Estrada index* and the energy of $G$.

Let thus $G$ be a graph of order $n$ whose Harmonic eigenvalues are $\gamma_1 \geqslant \gamma_2 \geqslant \cdots \geqslant \gamma_n$. Then the Harmonic Estrada index of $G$, denoted by $\mathcal{H}EE(G)$, is defined as [35]

$$\mathcal{H}EE = \mathcal{H}EE(G) = \sum_{i=1}^{n} e^{\gamma_i}.$$

Recalling Eq. (4), it follows that

$$\mathcal{H}EE(G) = \sum_{i=1}^{\infty} \frac{N_k}{k!}.$$

**Theorem 16.** *Let $G$ be a graph with $n$ vertices. Then the Harmonic Estrada index of $G$ is bounded as*

$$\sqrt{n^2 + 16\chi_{-2}(G)} \leqslant \mathcal{H}EE(G) \leqslant n - 1 + e^{\sqrt{8\chi_{-2}(G)}}. \tag{40}$$

*Proof.* **Lower bound**. Directly from the definition of the Harmonic Estrada index, we get

$$\mathcal{H}EE(G)^2 = \sum_{i=1}^{n} e^{2\gamma_i} + 2\sum_{i<j} e^{\gamma_i} e^{\gamma_j}. \tag{41}$$

In view of the inequality between the arithmetic and geometric means,

$$
\begin{aligned}
2\sum_{i<j} e^{\gamma_i}e^{\gamma_j} \geqslant n(n-1)\Big(\prod_{i<j} e^{\gamma_i}e^{\gamma_j}\Big)^{\frac{2}{n(n-1)}} &= \\
= n(n-1)\left[\Big(\prod_{i=1}^{n} e^{\gamma_i}\Big)^{n-1}\right]^{\frac{2}{n(n-1)}} &= \\
= n(n-1)\Big(e^{\sum_{i=1}^{n}\gamma_i}\Big)^{\frac{2}{n}}, &\quad \text{by} \sum_{i=1}^{n}\gamma_i = 0 \\
= n(n-1). & \qquad (42)
\end{aligned}
$$

By means of a power-series expansion, and bearing in mind the properties of $N_0, N_1$ and $N_2$, we get

$$\sum_{i=1}^{n} e^{2\gamma_i} = \sum_{i=1}^{n}\sum_{k\geqslant 0}\frac{(2\gamma_i)^k}{k!} = n + 16\chi_{-2}(G) + \sum_{i=1}^{n}\sum_{k\geqslant 3}\frac{(2\gamma_i)^k}{k!}.$$

Because we are aiming at a (as good as possible) lower bound, it may look plausible to replace $\sum_{k\geqslant 3}\frac{(2\gamma_i)^k}{k!}$ by $8\sum_{k\geqslant 3}\frac{(\gamma_i)^k}{k!}$. However, instead of $8 = 2^3$ we shall use a multiplier $\omega \in [0, 8]$, so as to arrive at

$$
\begin{aligned}
\sum_{i=1}^{n} e^{2\gamma_i} &\geqslant n + 16\chi_{-2}(G) + \omega\sum_{i=1}^{n}\sum_{k\geqslant 3}\frac{(\gamma_i)^k}{k!} \\
&= n + 16\chi_{-2}(G) - \omega n - 4\omega\chi_{-2}(G) + \omega\sum_{i=1}^{n}\sum_{k\geqslant 0}\frac{(\gamma_i)^k}{k!},
\end{aligned}
$$

i.e.,

$$\sum_{i=1}^{n} e^{2\gamma_i} \geqslant (1-\omega)n + 4(4-\omega)\chi_{-2}(G) + \omega\mathcal{H}EE(G). \qquad (43)$$

By substituting (42) and (43) back into (41), and solving for $\mathcal{H}EE$ we obtain

$$\mathcal{H}EE \geqslant \frac{\omega}{2} + \sqrt{(n-\frac{\omega}{2})^2 + 4(4-\omega)\chi_{-2}(G)}. \qquad (44)$$

It is elementary to show that for $n \geqslant 2$ and $4\chi_{-2}(G) \geqslant 1$ the function

$$f(x) := \frac{x}{2} + \sqrt{(n - \frac{x}{2})^2 + (4 - x)4\chi_{-2}(G)}$$

monotonically decreases in the interval $[0, 8]$. Consequently, the best lower bound for $\mathcal{H}EE$ is attained not for $\omega = 8$, but for $\omega = 0$. Setting $\omega = 0$ into (44 ) we arrive at the first half of Theorem 16.

**Upper bound**. By definition of the Harmonic Estrada index, we have

$$\begin{aligned}
\mathcal{H}EE &= n + \sum_{i=1}^{n} \sum_{k \geqslant 1} \frac{(\gamma_i)^k}{k!} \leqslant n + \sum_{i=1}^{n} \sum_{k \geqslant 1} \frac{(\mid \gamma_i \mid)^k}{k!} \\
&= n + \sum_{k \geqslant 1} \frac{1}{k!} \sum_{i=1}^{n} \left[(\gamma_i)^2\right]^{\frac{k}{2}} \leqslant n + \sum_{k \geqslant 1} \frac{1}{k!} \left[\sum_{i=1}^{n} (\gamma_i)^2\right]^{\frac{k}{2}} \\
&= n + \sum_{k \geqslant 1} \frac{1}{k!} \left(8\chi_{-2}(G)\right)^{\frac{k}{2}} = n - 1 + \sum_{k \geqslant 0} \frac{\left(\sqrt{8\chi_{-2}(G)}\right)^k}{k!},
\end{aligned}$$

which directly leads to the right-hand side inequality in (40). By this the proof of Theorem 16 is completed. □

**Theorem 17.** *Let $G$ be a graph with $n$ vertices.*

$$\mathcal{H}EE(G) \leqslant n - 1 + e^{\sqrt[4]{N_4}}.$$

*Proof.* By definition of the Harmonic Estrada index, we have

$$\begin{aligned}
\mathcal{H}EE(G) = \sum_{i=1}^{n} e^{\gamma_i} = \sum_{i=1}^{n}\sum_{k=0}^{\infty}\frac{\gamma_i^k}{k!} \leqslant n + \sum_{i=1}^{n}\sum_{k=1}^{\infty}\frac{\mid \gamma_i \mid^k}{k!} &= \\
&= n + \sum_{k=1}^{\infty}\frac{1}{k!}\sum_{i=1}^{n}(\gamma_i^4)^{\frac{k}{4}} \\
&\leqslant n + \sum_{k=1}^{\infty}\frac{1}{k!}\left(\sum_{i=1}^{n}\gamma_i^4\right)^{\frac{k}{4}} = \\
&= n + \sum_{k=1}^{\infty}\frac{1}{k!}H^{\frac{k}{4}} = \\
&= n - 1 + \sum_{k=0}^{\infty}\frac{\sqrt[4]{N_4^k}}{k!} = \\
&= n - 1 + e^{\sqrt[4]{N_4}}.
\end{aligned}$$

□

**Theorem 18.** *Let $G$ be a graph with $n$ vertices. Then*

$$\mathcal{H}EE(G) \leqslant e^{\sqrt{8\chi_{-2}(G)}}. \tag{45}$$

*Proof.* By definition of Harmonic Estrada index, we have

$$\begin{aligned}\mathcal{H}EE(G) = \sum_{i=1}^{n} e^{\gamma_i} \leqslant \sum_{i=1}^{n} e^{|\gamma_i|} &= \sum_{i=1}^{n}\sum_{k\geqslant 0} \frac{(|\ \gamma_i\ |)^k}{k!} = \sum_{k\geqslant 0}\frac{1}{k!}\sum_{i=1}^{n}(|\ \gamma_i\ |)^k \\ &\leq \sum_{k\geqslant 0}\frac{1}{k!}(\sum_{i=1}^{n}(|\ \gamma_i\ |)^2)^{\frac{k}{2}} \qquad \text{(by Inequality 11)} \\ &= \sum_{k\geqslant 0}\frac{1}{k!}(\sum_{i=1}^{n}(\gamma_i)^2)^{\frac{k}{2}} \\ &= \sum_{k\geqslant 0}\frac{1}{k!}(8\chi_{-2}(G))^{\frac{k}{2}} \qquad (\text{ by Equality 7}) \\ &= \sum_{k\geqslant 0}\frac{1}{k!}(\sqrt{8\chi_{-2}(G)})^k = e^{\sqrt{8\chi_{-2}(G)}}.\end{aligned}$$

□

**Theorem 19.** *Let $G$ be a graph with $n$ vertices. Then*

$$\mathcal{H}EE(G) \geqslant \sqrt{n^2 + 8n\chi_{-2}(G) + \frac{32n\chi_{-2}(G)\left(\sum_{k\sim i,\, k\sim j}\frac{1}{(d_k)^2}\right)}{3}}. \tag{46}$$

*Proof.* Suppose that $\gamma_1, \gamma_2, \dots, \gamma_n$ is the spectrum of $G$. Using the definition of the Harmonic Estrada index and Lemma 5 we have

$$\begin{aligned}\mathcal{H}EE(G)^2 &= \sum_{i=1}^{n}\sum_{j=1}^{n} e^{\gamma_i+\gamma_j} \\ &\geqslant \sum_{i=1}^{n}\sum_{j=1}^{n}\left(1+\gamma_i+\gamma_j+\frac{(\gamma_i+\gamma_j)^2}{2}+\frac{(\gamma_i+\gamma_j)^3}{6}\right) \\ &= \sum_{i=1}^{n}\sum_{j=1}^{n}\Bigg(1+\gamma_i+\gamma_j+\frac{\gamma_i^2}{2}+\frac{\gamma_j^2}{2}+\gamma_i\gamma_j+ \\ &+\frac{\gamma_i^3}{6}+\frac{\gamma_j^3}{6}+\frac{\gamma_i^2\gamma_j}{2}+\frac{\gamma_i\gamma_j^2}{2}\Bigg).\end{aligned}$$

Now, by Equality (6), $\sum_{i=1}^{n}\sum_{j=1}^{n}(\gamma_i + \gamma_j) = n\sum_{i=1}^{n}\gamma_i + n\sum_{j=1}^{n}\gamma_j = 0$, $\sum_{i=1}^{n}\sum_{j=1}^{n}\gamma_i\gamma_j = (\sum_{i=1}^{n}\gamma_i)^2 = 0$.
By Equality (7),

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(\frac{\gamma_i^2}{2} + \frac{\gamma_j^2}{2}) = \frac{n}{2}\sum_{i=1}^{n}\gamma_i^2 + \frac{n}{2}\sum_{j=1}^{n}\gamma_j^2 = 8n\chi_{-2}(G).$$

Similarly by Equality (8),

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(\frac{\gamma_i^3}{6}+\frac{\gamma_j^3}{6}) = \frac{n}{6}\sum_{i=1}^{n}\gamma_i^3+\frac{n}{6}\sum_{j=1}^{n}\gamma_j^3 = \frac{32n\chi_{-2}(G)\left(\sum_{k\sim i,\, k\sim j}\frac{1}{(d_k)^2}\right)}{3}.$$

By Equality (6),

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\gamma_i\gamma_j^2}{2} = \frac{1}{2}\sum_{i=1}^{n}\gamma_i\sum_{j=1}^{n}\gamma_j^2 = 0,$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\gamma_i^2\gamma_j}{2} = \frac{1}{2}\sum_{i=1}^{n}\gamma_i^2\sum_{j=1}^{n}\gamma_j = 0.$$

Combining the above relations, the proof is completed. □

## 5 Summary and conclusions

For a graph of order $n$, the Harmonic matrix is defined as the square matrix whose $(i, j)$- element is equal to the sum $\frac{2}{d(u)+d(v)}$ of degrees of adjacent vertices $u$ and $v$ , and zero otherwise. In this paper we obtain some new bounds for the Harmonic Energy and Harmonic Estrada index of graphs.

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Akbar Jahanbani

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Department of Mathematics,
Shahrood University of Technology,
Shahrood, Iran

E–mail: akbar.jahanbani92@gmail.com