Computer Science Journal of Moldova, vol.**26**, no.3(78), 2018

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 $A(G)$. λ_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 λ_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 π-*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 β 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*

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

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

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

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

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

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

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 α 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 $X = (x_1, x_2, \ldots, x_n)^t$,

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

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

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

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

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

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

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 α. 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 $P_n(x) = x^n + a_1 x^{n-1} + a_2 x^{n-2} + b_3 x^{n-3} + \cdots + b_n$, 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

$$\psi_n(x) = \prod_{i=1}^{n}(x - \mid \gamma_i \mid) = x^n + a_1 x^{n-1} + a_2 x^{n-2} + b_3 x^{n-3} + \cdots + b_n.$$

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. $\square$

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 $A = B := |\gamma_1|$, $i = 1, 2, \dots n$ 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 $a_1, a_2, \dots, a_n$ and $b_1, b_2, \dots, b_n$ be real numbers for which there exist real constants R and r, so that for each $i, i = 1, 2, \dots, n$ 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 $R := |\gamma_1|$, $i = 1, 2, \dots n$, 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 $|\gamma_1| = |\gamma_2| = \cdots = |\gamma_n|$. $\square$

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

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

$\square$

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)

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

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)

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

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

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

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

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*

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

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

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

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.

Acknowledgment

The author is very grateful to the referees for helpful comments and suggestions, which improved the presentation of the original manuscript.

References

[1] C. Adiga and R. K. Zaferani, "Upper bounds for energy of a graph," *Adv. Stud. Cont. Math.*, vol. 16, pp. 279–285, 2008.

[2] N. Alawiah, N. J. Rad, A. Jahanbani, and H. Kamarulhaili, "New Upper Bounds on the Energy of a Graph," *MATCH Commun. Math. Comput. Chem.*, vol.79, pp. 287–301, 2018.

[3] J. Amalorpava Jerline and L. Benedict Michaelraj, "On a Conjecture of Harmonic Index and Diameter of Graphs," *Kragujevac Journal of Mathematics*, vol. 40, pp. 73–78, 2016.

[4] J. Amalorpava Jerline and L. Benedict Michaelraj, "On harmonic index and diameter of unicyclic graphs," *Iranian Journal of Mathematical Sciences and Informatics*, vol. 11, pp. 115–122, 2016.

[5] J. Amalorpava Jerline, L. Benedict Michaelraj, K. Dhanalakshmi, and P. Syamala, "Harmonic index of graphs with more than one cut-vertex," *Ars Combinatoria*, to be published.

[6] H. Bamdad,"New lower bounds for estrada endex," *Bull. Malays. Math. Sci. Soc.*, vol. 39, pp. 683–688, 2016.

[7] M. Biernacki, H. Pidek, and C. R. Nardzewski, "Sur une inègalitè entre des intègrales dèfinies," *Annales Universitatis Mariae Curie-Sklodowska*, vol. 4, pp. 1–4, 1950.

[8] D. Cvetkoviè, M. Doob, and H. Sachs, *Spectra of Graphs-Theory and Application*, Johann Ambrosius Barth, 1995.

[9] H. Deng, S. Balachandran, S .K.Ayyaswamy, and Y. B. Venkatakrishnan, "On harmonic indices of trees, unicyclic graphs and bicyclic graphs," *Ars Combinatoria*, to be published.

[10] H. Deng, S.Balachandran, S .K.Ayyaswamy, and Y. B.Venkatakrishnan,"Sharp bounds of the harmonic index of a graph with given girths," *Filomat*, to be published.

[11] H. Deng, S. Balachandran, S. K.Ayyaswamy, and Y. B.Venkatakrishnan, "On the harmonic index and the chromatic number of a graph," *Discrete Appl. Math.*, vol. 161, pp. 2740–2744, 2013.

[12] J. A. De la Peña, I. Gutman, and J. Rada, "Estimating the Estrada Index," *Lin. Algebra Appl.*, vol. 427, pp. 70–76, 2007.

[13] H. Deng, S. Radenkoviċ, and I. Gutman, "The Estrada Index," in *Applications of Graph Spectra*, D. Cvetkoviċ and I. Gutman, Eds. Belgrade: Math. Inst., 2009, pp. 123–140.

[14] J. B. Diaz and F. T. Metcalf, "Stronger forms of a class of inequalities of G. Pòlya - G. Szego, L. V. Kantorovich," *Bull. Amer. Math. Soc.*, vol. 69, pp. 415–418, 1963.

[15] Z. Du and B. Zhou, "On sum-connectivity index of bicyclic graphs," *Bull. Malays. Math. Sci. Soc.*, to be published.

[16] Z. Du, B. Zhou and N. Trinajstiċ, " Minimum general sum-connectivity index of unicyclic graphs," *J. Math. Chem.*, vol. 48, pp. 697–703, 2010.

[17] Z. Du, B. Zhou and N. Trinajstiċ, "Minimum sum-connectivity indices of trees and unicyclic graphs of a given matching number," *J. Math. Chem.*, vol. 47, pp. 842–855, 2010.

[18] E. Estrada and J. A. Rodrìguez-Velàzguez, "Subgraph Centrality in Complex Networks," *Phys. Rev. E.* vol 71, pp. 056103–056103-9, 2005.

[19] O. Favaron, M. Mahò, and J. F. Saclè, "Some Eigenvalue Properties in Graphs (Conjectures of Graffiti-II)," *Discrete Mathematics*, vol. 111, pp. 197–220, 1993.

[20] D. Gungor and S. B. Bozkurt, "On the distance Estrada index of graphs," *Hacettepe Journal of Mathematics and Statistics*, vol. 38, pp. 277–283, 2009.

[21] I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Berlin: Springer, 1986.

[22] I. Gutman, M. Milun, and N. Trinajstiċ, "Comment on the paper: Properties of the latent roots of a matrix. Estimation of π-electron energies by B. J. McClelland," *J. Chem. Phys.*, vol.59, pp. 2772–2774, 1973.

[23] I. Gutman, "The energy of a graph: old and new results," in *Algebraic Combinatorics and Applications*, A. Betten, A. Kohnert, R. Laue, and A. Wassermann, Eds. Berlin: Springer-Verlag, 2001, pp. 196–211.

[24] I. Gutman, "The energy of a graph," *Ber. Math. Stat. Sckt. Forschungzentrum Graz*, vol. 103, pp. 1–22, 1978.

[25] R. A. Horn and C. R. Johnson, *Matrix Analysis*, New York: Cambridge Univ. Press, 1985.

[26] L. C. Hsu and X. H. Wang, *The Methods and Examples of Mathematical Analysis*, Higher Education Press, 1988.

[27] S. M. Hosamani, B. B. Kulkarni, R. G. Boli, and V. M. Gadag, "QSPR analysis of certain graph theoretical matrices and their corresponding energy," *Appl. Math. Nonlin. Sci.*, vol.2, pp. 131–150, 2017.

[28] A. Ilic, "Note on the harmonic index of a graph," *Applied Mathematics Letters.*, vol. 25, pp. 561–566, 2012.

[29] N. Jafari Rad, A. Jahanbani, and D. A. Mojdeh, "Tetracyclic Graphs with Maximal Estrada Index," *Discrete Mathematics, Algorithms and Applications,* vol. 7, pp. 1750041, 2017.

[30] N. Jafari Rad, A. Jahanbani, and R. Hasni, "Pentacyclic Graphs with Maximal Estrada Index," *Ars Combin.*, vol. 133, pp. 133–145, 2017.

[31] N. J. Rad, A. Jahanbani, and I. Gutman, "Zagreb Energy and Zagreb Estrada Index of Graphs," *MATCH Commun. Math. Comput. Chem.*, vol. 79, pp. 371–386, 2018.

[32] A. Jahanbani, "Upper bounds for the energy of graphs," *MATCH Commun. Math. Comput. Chem.*, vol. 79, pp. 275–286, 2018.

[33] A. Jahanbani, "Some new lower bounds for energy of graphs," *Applied Mathematics and Computation*, vol. 296, no. C, pp. 233–238, 2017.

[34] A. Jahanbani, "Lower bounds for the energy of graphs," *AKCE International Journal of Graphs and Combinatorics*, vol. 15, pp. 88–96, 2018.

[35] A. Jahanbani and H. H. Raz, "On the Harmonic energy and theHarmonic Estrada index of graphs," *MATI.*, vol. 1, no. 1, pp. 1–20, 2019. Retrieved from http://dergipark.gov.tr/mati/issue/38227/425047.

[36] J. Liu, "On the Harmonic index of triangle-free graphs," *Applied Mathematics*, vol. 4, pp. 1204–1206, 2013.

[37] A. Lupas, "Inequalities for the roots of a class of polynomials," *Publ. Elektrotehn. Fak. Ser. Math. Fiz.*, vol. 594, pp. 79–85, 1977.

[38] R. Wu, Z. Tang, and H. Deng, "A Lower Bound for the Harmonic Index of a Graph with Minimum Degree at Least Two," *Filomat.*, vol. 27, pp. 51–55, 2013.

[39] L. Zhong, "The harmonic index for graphs," *Appl. Math. Lett.*, vol. 25, pp. 561–566, 2012.

[40] L. Zhong, "The harmonic index on unicyclic graphs," *Ars Combinatoria*, vol. 104, pp. 261–269, 2012.

[41] L. Zhong and K. Xu, "The harmonic index on bicyclic graphs," *Utilitas Mathematica*, vol. 90, pp. 23–32, 2013.

[42] B. Zhou and N. Trinajstiċ, "On a novel connectivity index," *J. Math. Chem.*, vol. 46, pp. 1252–1270, 2009.

[43] B. Zhou and N. Trinajstiċ, "On general sum-connectivity index," *J. Math. Chem.*, vol. 47, pp. 210–218, 2010.

Akbar Jahanbani

Received June 10, 2018

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

E–mail: akbar.jahanbani92@gmail.com