ON THE HARMONIC ENERGY AND THE HARMONIC ESTRADA INDEX OF GRAPHS

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Let $G$ be a graph with $n$ vertices and $d_i$ is the degree of its $i$th vertex, then the harmonic matrix of $G$ is the square matrix of order $n$ whose $(i, j)$-entry is equal to $\frac{2}{d_i + d_j}$ if the $i$th and $j$th vertex of $G$ are adjacent, and zero otherwise. The main purpose of this paper is to introduce the harmonic Estrada index of a graph. Moreover we establish upper and lower bounds for these energy and index separately also we investigate the relations between the harmonic Estrada index and the harmonic energy.

1. INTRODUCTION

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G) = \{v_1, v_2, ..., v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let $d_i$ be the degree of the $i$th vertex $v_i \in V$, for $i = 1, 2, ..., n$. For a graph $G$, the harmonic index $H(G)$ is defined in \cite{25} as $H(G) = \sum_{u, v_j \in E(G)} \frac{2}{d_u + d_j}$. 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. Let the vertices of $G$ be labeled as $v_1, v_2, ..., v_n$. The adjacency matrix of a graph $G$ is the square matrix $A = A(G) = [a_{ij}]$, in which $a_{ij} = 1$ if $v_i$ is adjacent to $v_j$ and $a_{ij} = 0$, otherwise. For a graph $G$, its characteristic polynomial $P(G, x)$ is the characteristic polynomial of its adjacency matrix, that is, $P(G, x) = det(xI - A(G))$. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of its adjacency matrix $A(G)$. Then the spectrum of $G$ is $Spec(G) = \{\lambda_1, \lambda_2, ..., \lambda_n\}$. These form the adjacency spectrum of $G$ \cite{3}.

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Thus
\[ \det A = \prod_{i=1}^{n} \lambda_i. \]

The harmonic matrix of a graph \( G \) is a square matrix \( H(G) = [h_{ij}] \) of order \( n \), defined in [25] as
\[
    h_{ij} = \begin{cases} 
    0 & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are not adjacent} \\
    \frac{2}{(d_i+d_j)} & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent} \\
    0 & \text{if } i = j.
    \end{cases}
\]

The eigenvalues of the harmonic matrix \( H(G) \) are denoted by \( \gamma_1, \gamma_2, \ldots, \gamma_n \) and are said to be the \( H \)-eigenvalues of \( G \) and their collection is called harmonic spectrum or \( H \)-spectrum of \( G \). We note that since the harmonic matrix is symmetric, its eigenvalues are real and can be ordered as \( \gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_n \). Favaron et al. [20] considered the relation between harmonic index and the eigenvalues of graphs. Zhong [36] found the minimum and maximum values of the harmonic index for simple connected graphs and trees, and characterized the corresponding extremal graphs. Deng, Balachandran, Ayyaswamy, Venkatakrishnan [8] considered the relation relating the harmonic index \( H(G) \) and the chromatic number and proved that \( \chi(G) \leq 2H(G) \) by using the effect of removal of a minimum degree vertex on the harmonic index. Deng, Tang, Zhang [6] considered the harmonic index \( H(G) \) and the radius \( r(G) \). Deng, Balachandran, Ayyaswamy, Venkatakrishnan [7] determined the trees with the second-the sixth maximum harmonic indices, and unicyclic graphs with the second-the fifth maximum harmonic indices, and bicyclic graphs with the first-the fourth maximum harmonic indices.

The sum-connectivity index \( \chi'(G) \) and the general sum-connectivity index \( \chi_\alpha(G) \) were recently proposed by Zhou and Trinajstić in [37, 38] and defined as
\[
    \chi'(G) = \sum_{uv \in E(G)} \frac{(d(u)+d(v))^{\frac{1}{2}}}{2}
\]
and
\[
    \chi_\alpha(G) = \sum_{uv \in E(G)} (d(u)+d(v))^{\alpha}, \tag{1}
\]
where \( \alpha \) 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 [12, 13, 14].

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 put forward the concept of harmonic Estrada index, and obtain lower and upper bounds for it. In Section 5, we investigate the relations between the harmonic Estrada index and the harmonic energy. 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 sections. In this section we first calculate $tr(H^2)$, $tr(H^3)$ and $tr(H^4)$, where $tr$ denotes the trace of a matrix. Now let us present the following lemma as the first preliminary result. Denote by $N_k$ the $k$-th spectral moment of the harmonic matrix $H$, i. e.,

\[ N_k = \sum_{j=1}^{n} (\gamma_j)^k \]

and recall that $N_k = tr(H^k)$.

**Lemma 1.** Let $G$ be a graph with $n$ vertices and harmonic matrix $H$. Then

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

(2) $N_1 = tr(H) = 0,$

(3) $N_2 = tr(H^2) = 8\chi-2(G),$  

(4) $N_3 = tr(H^3) = 32 \sum_{i<j} \frac{1}{(d_i + d_j)^2} \left( \sum_{k \sim i, k \sim j} \frac{1}{(d_k)^2} \right),$  

(5) $N_4 = tr(H^4) = \sum_{i=1}^{n} \left( \sum_{i \sim j} \frac{4}{(d_i + d_j)^2} \right)^2 + \sum_{i \neq j} \frac{4}{(d_i + d_j)^2} \left( \sum_{k \sim i, k \sim j} \frac{4}{(d_k)^2} \right)^2.$

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

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

Next, we calculate the matrix $H^2$. For $i = j$

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

whereas for $i \neq j$

\[(H^2)_{ij} = \sum_{j=1}^{n} H_{ij} H_{ji} = H_{ii} H_{jj} + H_{ij} H_{ji} + \sum_{k \sim i, k \sim j} H_{ik} H_{kj} = \frac{2}{(d_i + d_j)} \sum_{k \sim i, k \sim j} \frac{4}{(d_k)^2}.\]
Therefore,
\[ tr(H^2) = \sum_{i=1}^{n} \sum_{i\sim j} \frac{4}{(d_i + d_j)^2} = 8 \sum_{i\sim j} \frac{1}{(d_i + d_j)^2}. \]

Hence by Equality (1), we have
\[ tr(H^2) = 8 \chi_2(G). \]

Since the diagonal elements of \( H^3 \) are
\[ (H^3)_{ii} = \sum_{j=1}^{n} H_{ij}(H^2)_{jk} = \sum_{i\sim j} \frac{2}{(d_i + d_j)} (H^2)_{ij} = \sum_{i\sim j} \frac{4}{(d_i + d_j)^2} \left( \sum_{k\sim i, k\sim j} \frac{4}{(d_k)^2} \right) \]
we obtain
\[ tr(H^3) = \sum_{i=1}^{n} \sum_{i\sim j} \frac{4}{(d_i + d_j)^2} \left( \sum_{k\sim i, k\sim j} \frac{4}{(d_k)^2} \right) = 32 \sum_{i\sim j} \frac{1}{(d_i + d_j)^2} \left( \sum_{k\sim i, k\sim j} \frac{1}{(d_k)^2} \right), \]

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

We now calculate \( tr(H^4) \). Because \( tr(H^4) = \|H^2\|_F^2 \), where \( \|H^2\|_F \) denotes the Frobenius norm of \( H^2 \), we obtain
\[ tr(H^4) = \sum_{i,j=1}^{n} |(H^2)_{ii}|^2 = \sum_{i,j=1}^{n} |(H^2)_{ij}|^2 + \sum_{i\neq j} |(H^2)_{ii}|^2 \]
\[ = \sum_{i=1}^{n} \left( \sum_{i\sim j} \frac{4}{(d_i + d_j)^2} \right)^2 + \sum_{i\neq j} \frac{4}{(d_i + d_j)^2} \left( \sum_{k\sim i, k\sim j} \frac{4}{(d_k)^2} \right)^2. \]

\[ \square \]

Remark 1. For any real \( x \), the power-series expansion of \( e^x \), is the following
\[ (8) \]
\[ e^x = \sum_{k\geq 0} \frac{x^k}{k!}. \]

Lemma 2. For any non-negative real \( x \), \( e^x \geq 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{4} \). Equality holds if and only if \( x = 0 \).

Theorem 1. [4] (Chebishev inequality) Let \( a_1 \leq a_2 \leq \cdots \leq a_n \) and \( b_1 \leq b_2 \leq \cdots \leq b_n \) be real numbers. Then we have
\[ \left( \sum_{i=1}^{n} a_i \right) \left( \sum_{i=1}^{n} b_i \right) \leq n \sum_{i=1}^{n} a_i b_i, \]
equality occurs if and only if \( a_1 = a_2 = \cdots = a_n \) or \( b_1 = b_2 = \cdots = b_n \).
Remark 2. For nonnegative $x_1, x_2, \ldots, x_n$ and $k \geq 2$,

$$
\sum_{i=1}^{n} (x_i)^k \leq \left( \sum_{i=1}^{n} x_i^2 \right)^{\frac{k}{2}}.
$$

Lemma 3. [35] Let $G$ be a graph with $m$ edges. Then for $k \geq 4$, $M_{k+2} \geq M_k$ with equality for all even $k \geq 4$ if and only if $G$ consists of $m$ copies of complete graph on two vertices and possibly isolated vertices, and with equality for all odd $k \geq 5$ if and only if $G$ is a bipartite graph.

Lemma 4. (Rayleigh-Ritz) [24] If $B$ is a real symmetric $n \times n$ matrix with eigenvalues $\lambda_1(B) \geq \lambda_2(B) \leq \cdots \leq \lambda_n(B)$, then for any $X \in \mathbb{R}^n$, ($X \neq 0$),

$$
X^t BX \leq \lambda_1(B)X^t X.
$$

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

Theorem 2. [8] Let $G$ be a simple graph with the chromatic number $\chi(G)$ and the harmonic index $H(G)$, then

$$
\chi(G) \leq 2H(G),
$$

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

3. BOUNDS FOR THE HARMONIC ENERGY

In this section, we study energy and harmonic energy of graph $G$. We also give lower and upper bounds for it.

The energy of the graph $G$ is defined as:

$$
E = E(G) = \sum_{i=1}^{n} | \lambda_i | .
$$

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. [22, 23]). After 1978 the graph-energy concept was presented to the mathematico-chemical community on several other occasions [23, 29]. Initially, the response of other colleagues was almost nil. However, around the turn of the century the study of $E$ suddenly became a rather popular topic both in mathematical chemistry and in pure mathematics. Of the numerous papers on graph energy that recently appeared, since then, the numerous bounds for energy were found (see,
Therefore, by considering this, the harmonic energy defined in \[25\] as

\[
(11) \quad HE(G) = \sum_{i=1}^{n} |\gamma_i|, \]

where \(\gamma_1, \gamma_2, \ldots, \gamma_n\) are eigenvalues of the harmonic matrix.

Bearing this in mind, we immediately arrive at the following estimates:

**Lemma 5.** Let \(G\) be a connected graph with \(n \geq 2\) vertices. Then the spectral radius of the harmonic matrix is bounded from below as

\[
(12) \quad \gamma_1 \geq \frac{2H(G)}{n}. \]

**Proof.** Let \(H = ||h_{ij}||\) be the harmonic matrix corresponding to \(H\). By Lemma 4, for any vector \(X = (x_1, x_2, \ldots, x_n)^t\),

\[
X^tHX = \left(\sum_{j,j \sim 1} x_j h_{j1}, \sum_{j,j \sim 2} x_j h_{j2}, \ldots, \sum_{j,j \sim n} x_j h_{jn}\right)^t X
\]

\[
(13) \quad = 2 \sum_{i \sim j} h_{ij} x_i x_j
\]

because \(h_{ij} = h_{ji}\). Also,

\[
(14) \quad X^tX = \sum_{i=1}^{n} x_i^2.
\]

Using Eqs. (13) and (14), by Lemma 4, we obtain

\[
(15) \quad \gamma_1 \geq \frac{2 \sum_{i \sim j} h_{ij} x_i x_j}{\sum_{i=1}^{n} x_i^2}. \]

Since (15) is true for any vector \(X\), by putting \(X = (1, 1, \ldots, 1)^t\), we have

\[
\gamma_1 \geq \frac{2H(G)}{n}.
\]

**Remark 3.** Let \(G\) be a graph with \(n\) vertices, by Theorem 2 and Lemma 5, we have \(\gamma_1 \geq \frac{\chi(G)}{n}\).

**Theorem 3.** Let \(G\) be a non-empty graph with \(n\) vertices. Then

\[
HE(G) \leq \frac{\chi(G)}{n} + \sqrt{(n-1) \left(8\chi_{-2}(G) - \frac{\chi(G)}{n}\right)^2}. \]
Proof. Let $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_{n-1} \geq \gamma_n$ be the eigenvalues of $G$. By the Cauchy-Schwartz inequality,
\[
\sum_{i=1}^{n} |\gamma_i| \leq \sqrt{(n-1) \sum_{i=2}^{n} \gamma_i^2} = \sqrt{(n-1)(8\chi_{-2}(G) - \gamma_1^2)}.
\]
Hence
\[
HE(G) \leq \gamma_1 + \sqrt{(n-1)(8\chi_{-2}(G) - \gamma_1^2)}.
\]
Note that the function $K(x) = x + \sqrt{(n-1)(8\chi_{-2}(G) - x^2)}$ decreases for $\frac{\chi(G)}{n} \leq x \leq \chi(G)$. By Remark 3, we have $\gamma_1 \geq \frac{\chi(G)}{n}$, therefore
\[
\gamma_1 \geq \frac{\chi(G)}{n} \geq \frac{\chi(G)}{n^2}.
\]
So $K(\gamma_1(G)) \leq K\left(\frac{\chi(G)}{n}\right)$, which implies that
\[
HE(G) \leq \frac{\chi(G)}{n} + \sqrt{(n-1)\left(8\chi_{-2}(G) - \left(\frac{\chi(G)}{n}\right)^2\right)}.
\]
\[
\Box
\]

Remark 4. [31] For the roots $x_1 \geq x_2 \geq \cdots \geq x_n$ of an arbitrary polynomial $P_n(x)$ from this class, the following values were introduced
\[
(16) \quad \bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i,
\]
\[
(17) \quad \Delta = n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2.
\]
Then upper and lower bounds for the polynomial roots, $x_i, i = 1, 2, \ldots, n$, were determined in terms of the introduced values
\[
\bar{x} + \frac{1}{\sqrt{n-1}} \Delta \leq x_1 \leq \bar{x} + \frac{1}{\sqrt{n-1}n} \Delta.
\]

Lemma 6. Let $G$ be a simple graph with $n \geq 2$, vertices. Then
\[
\frac{1}{n} \sqrt{\frac{8n\chi_{-2}(G)}{n-1}} \leq \gamma_1 \leq \frac{1}{n} \sqrt{8n(n-1)\chi_{-2}(G)}.
\]

Proof. Let the characteristic polynomial of a graph $G$ is the following:
\[
\varphi_n(x) = \prod_{i=1}^{n} \left(x - \gamma_i\right) = x^n + a_1 x^{n-1} + a_2 x^{n-2} + b_3 x^{n-3} + \cdots + b_n.
\]
Since
\[ a_1 = -\sum_{i=1}^{n} \gamma_i = 0 \]
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 \( P_n(0, -4\chi_{-2}(G)) \). From 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 Remark (4), we obtain that for the eigenvalues \( \gamma_1 \).

**Theorem 4.** Let \( G \) be a non-empty graph with \( n \) vertices. Then
\[
HE(G) \leq \frac{1}{n} \sqrt{\frac{8n\chi_{-2}(G)}{n-1}} + \sqrt{(n-1) \left( 8\chi_{-2}(G) - \left( \frac{1}{n} \sqrt{\frac{8n\chi_{-2}(G)}{n-1}} \right)^2 \right)}.
\]

**Proof.** Let \( \gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_{n-1} \geq \gamma_n \) be the eigenvalues of \( G \). By the Cauchy–Schwartz inequality,
\[
\sum_{i=1}^{n} |\gamma_i| \leq \sqrt{(n-1) \sum_{i=2}^{n} \gamma_i^2} = \sqrt{(n-1)(8\chi_{-2}(G) - \gamma_1^2)}.
\]
Hence
\[
HE(G) \leq \gamma_1 + \sqrt{(n-1)(8\chi_{-2}(G) - \gamma_1^2)}.
\]
Note that the function \( F(x) = x + \sqrt{(n-1)(8\chi_{-2}(G) - x^2)} \) decreases for \( x \leq \frac{1}{n} \sqrt{\frac{8n\chi_{-2}(G)}{n-1}} \). By Lemma 6, we have \( \gamma_1 \geq \frac{1}{n} \sqrt{\frac{8n\chi_{-2}(G)}{n-1}} \), therefore
\[
\gamma_1 \geq \frac{1}{n} \sqrt{\frac{8n\chi_{-2}(G)}{n-1}} \geq \frac{1}{n^2} \sqrt{\frac{8n\chi_{-2}(G)}{n-1}}.
\]
So \( F(\gamma_1(G)) \leq F\left( \frac{1}{n} \sqrt{\frac{8n\chi_{-2}(G)}{n-1}} \right) \), which implies that
\[
HE(G) \leq \frac{1}{n} \sqrt{\frac{8n\chi_{-2}(G)}{n-1}} + \sqrt{(n-1) \left( 8\chi_{-2}(G) - \left( \frac{1}{n} \sqrt{\frac{8n\chi_{-2}(G)}{n-1}} \right)^2 \right)}.
\]
Theorem 5. Let $G$ be a non-empty graph with $n$ vertices. Then

\begin{equation}
\varepsilon^{-\sqrt{8\chi -2(G)}} \leq HE(G) \leq e^{\sqrt{8\chi -2(G)}}.
\end{equation}

**Proof.** Lower bound, by definition of harmonic energy and by the arithmetic-geometric mean inequality, we have

\[
HE(G) = \sum_{i=1}^{n} |\gamma_i| = n\left(\frac{1}{n} \sum_{i=1}^{n} |\gamma_i|\right) \geq n\left(\sqrt{\sum_{i=1}^{n} |\gamma_i|}\right).
\]

By the geometric and harmonic mean inequality, we have

\[
n\left(\sqrt[|\gamma_1|]{|\gamma_2| \cdots |\gamma_n|}\right) \geq n\left(\frac{n}{\sum_{i=1}^{n} |\gamma_i|}\right), \quad \text{(by Theorem 1)}
\]

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

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

\[
= \frac{1}{\sum_{i=1}^{n} \sum_{k \geq 0} \frac{(|\gamma_i|)^k}{k!}}
\]

\[
= \frac{1}{\sum_{k \geq 0} \frac{1}{k!} (\sum_{i=1}^{n} |\gamma_i|)^k}
\]

\[
\geq \frac{1}{\sum_{k \geq 0} \frac{1}{k!} (\sum_{i=1}^{n} |\gamma_i|)^k}
\]

\[
= \frac{1}{\sum_{k \geq 0} \frac{1}{k!} \left(\sum_{i=1}^{n} (|\gamma_i|)^{2k}\right)^{\frac{1}{2k}}}
\]

\[
= \frac{1}{e^{\sqrt{8\chi -2(G)}}}.
\]

Therefore, we have

\[
HE(G) \geq e^{-\sqrt{8\chi -2(G)}}.
\]
Upper bound, by definition of harmonic energy, we have

$$HE(G) = \sum_{i=1}^{n} |\gamma_i| < \sum_{i=1}^{n} e^{\gamma_i} = \sum_{i=1}^{n} \sum_{k=0}^{n} \frac{(\gamma_i)^k}{k!}$$

$$= \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{i=1}^{n} (\gamma_i)^k$$

$$\leq \sum_{k=1}^{\infty} \frac{1}{k!} \left( \sum_{i=1}^{n} (\gamma_i)^2 \right)^{\frac{k}{2}}, \text{ (by Inequality 9)}$$

$$= \sum_{k=1}^{\infty} \frac{1}{k!} \left( \sum_{i=1}^{n} \gamma_i^2 \right)^{k}, \text{ (by Equality 5)}$$

$$= \sum_{k=1}^{\infty} \frac{1}{k!} \sqrt{8\chi - 2(G)}^k$$

$$= e^{\sqrt{8\chi - 2(G)}}.$$ 

Therefore, we have

$$HE(G) \leq e^{\sqrt{8\chi - 2(G)}}.$$

\[ \square \]

**Theorem 6.** Let $G$ be a graph with $n$ vertices. Then

$$\sqrt{8\chi - 2(G)} \leq HE(G) \leq \sqrt{8n\chi - 2(G)}.$$ 

**Proof.** By Cauchy-Schwarz inequality, for real numbers $a_i$ and $b_i$, we have

$$\left( \sum_{i=1}^{n} a_i b_i \right)^2 \leq \left( \sum_{i=1}^{n} a_i^2 \right) \left( \sum_{i=1}^{n} b_i^2 \right),$$

assuming, $a_i = 1$, $b_i = |\gamma_i|$, we have

$$\left( \sum_{i=1}^{n} |\gamma_i| \right)^2 \leq n \left( \sum_{i=1}^{n} |\gamma_i|^2 \right) = n \sum_{i=1}^{n} (\gamma_i)^2 = 8n\chi - 2(G).$$

Therefore

$$HE(G) \leq \sqrt{8n\chi - 2(G)}.$$ 

Therefore this gives the upper bound for $HE(G)$. Now for the lower bound of $HE(G)$, we can easily obtain the inequality

$$HE(G)^2 = \left( \sum_{i=1}^{n} |\gamma_i| \right)^2 \geq \sum_{i=1}^{n} |\gamma_i|^2 = 8\chi - 2(G).$$
Theorem 7. Let $G$ be a connected graph with $n$ vertices. Then

$$HE(G) \geq \sqrt{8\chi^{-2}(G) + n(n-1) | detH |^\frac{2}{n}}.$$ 

Proof. By the definition of harmonic energy, we have

$$HE(G)^2 = \left( \sum_{i=1}^{n} |\gamma_i| \right)^2 = \sum_{i=1}^{n} |\gamma_i|^2 + 2 \sum_{1 \leq i < j \leq n} |\gamma_i||\gamma_j|$$

$$= 8\chi^{-2}(G) + 2 \sum_{1 \leq i < j \leq n} |\gamma_i||\gamma_j|$$

$$= 8\chi^{-2}(G) + 2 \sum_{i \neq j} |\gamma_i||\gamma_j|.$$

Since, for nonnegative numbers, the arithmetic mean is not smaller than the geometric mean, we then have

$$\frac{1}{n(n-1)} \sum_{i \neq j} |\gamma_i||\gamma_j| \geq \left( \prod_{i \neq j} |\gamma_i||\gamma_j| \right)^\frac{1}{n(n-1)} = \left( \prod_{i=1}^{n} |\gamma_i|^{2(n-1)} \right)^\frac{1}{n(n-1)} = \prod_{i=1}^{n} |\gamma_i|^{\frac{2}{n}} = |detH|^{\frac{2}{n}}.$$

Theorem 8. Let $G$ be a graph with $n$ vertices. Then

$$HE(G) \leq \frac{8\chi^{-2}(G) + n}{2}.$$ 

Proof. Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be sequences of real numbers, and $c_1, c_2, \ldots, c_n$ and $d_1, d_2, \ldots, d_n$ are nonnegative, then Then the following inequality is valid (see [11])

$$\sum_{i=1}^{n} a_i^2 + \sum_{i=1}^{n} b_i^2 \geq 2 \sum_{i=1}^{n} a_i c_i \sum_{i=1}^{n} b_i d_i.$$

For $a_i := |\gamma_i|$, $b_i := c_i = d_i = 1$, $i = 1, 2, \ldots, n$, inequality () becomes

$$\sum_{i=1}^{n} |\gamma_i|^2 + \sum_{i=1}^{n} 1 \geq 2 \sum_{i=1}^{n} |\gamma_i| \sum_{i=1}^{n} 1.$$

Therefore, by equalities (5) and (11), we have

$$HE(G) \leq \frac{8\chi^{-2}(G) + n}{2}.$$
4. BOUNDS FOR THE HARMONIC ESTRADA INDEX

In this section, we consider the harmonic estrada index of graph $G$. We also give lower and upper bounds for it. As a new direction for the studying on indexes and their bounds, we will introduce and investigate harmonic estrada index and its bounds. A graph-spectrum-based graph invariant, recently put forward by Estrada [10], is defined as

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

$EE$ is usually referred as the Estrada index. Although invented in 2000, the Estrada index has found numerous applications. The Estrada index has been successfully employed to quantify the degree of folding of long-chain molecules, especially proteins, and to measure the centrality of complex (reaction, metabolic, communication, social, etc.) networks. There is also a connection between the Estrada index and the extended atomic branching of molecules.

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

Where $M_k = M_k(G)$ is the $k$-th spectral moment of the graph $G$. Some mathematical properties of the Estrada index were established. One of most important properties is the following:

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

It is well known that [18] $M_k(G)$ is equal to the number of closed walks of length $k$ of the graph $G$. There have been found a lot of chemical and physical applications, including quantifying the degree of folding of long-chain proteins,[15, 16, 17] and complex networks [18]. Mathematical properties of this invariant can be found in e.g. [35, 33, 34]. Recently, the analogous concepts of Estrada indices of this kind are the:

- Zagreb Estrada Index, $ZEE = ZEE(G) = \sum_{i=1}^{n} e^{\zeta_i}$ [32],
- Harary Estrada index, $H'EE = H'EE(G) = \sum_{i=1}^{n} e^{\mu_i}$ [19],
- Resolvent Estrada index, $EE_r = EE_r(G) = \sum_{i=1}^{n} \left( 1 - \frac{\lambda_i}{n-1} \right)^{-1}$ [9],
- Randić Estrada index $REE = REE(G) = \sum_{i=1}^{n} e^{\rho_i}$ [2].
Let thus $G$ be a graph of order $n$ whose harmonic eigenvalues are $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_n$. Then the harmonic Estrada index of $G$, denoted by $\text{HEE}$, is defined to be

$$\text{HEE} = \text{HEE}(G) = \sum_{i=1}^{n} e^{\gamma_i}.$$ 

Recalling Eq. (2), it follows that

$$\text{HEE}(G) = \sum_{i=1}^{\infty} \frac{N_k}{k!}.$$ 

We begin this section with theorem as follows:

**Theorem 9.** Let $G$ be a graph with $n$ vertices. Then

$$\text{HEE}(G) \geq n + 8\chi_{-2}(G) + 32 \sum_{i \sim j} \left( \frac{1}{d_i + d_j} \right)^2 \left( \sum_{k \sim i, k \sim j} \frac{1}{(d_k)^2} \right) \left( \sinh(1) - 1 \right)$$

$$+ \left( \cosh(1) - 1 \right) \left[ \sum_{i=1}^{n} \left( \sum_{i \sim j} \frac{4}{(d_i + d_j)^2} \right)^2 + \sum_{i \sim j} \frac{4}{(d_i + d_j)^2} \left( \sum_{k \sim i, k \sim j} \frac{4}{(d_k)^2} \right)^2 \right].$$

**Proof.** Note that $N_2 = 8\chi_{-2}(G)$. By Lemma 3,

$$\text{HEE}(G) = n + 8\chi_{-2}(G) + \sum_{k \geq 1} \frac{N_{2k+1}}{(2k+1)!} + \sum_{k \geq 1} \frac{N_{2k+2}}{(2k+2)!}$$

$$\geq n + 8\chi_{-2}(G) + \sum_{k \geq 1} \frac{N_3}{(2k+1)!} + \sum_{k \geq 1} \frac{N_4}{(2k+2)!}$$

$$= n + 8\chi_{-2}(G) + 32 \sum_{i \sim j} \left( \frac{1}{d_i + d_j} \right)^2 \left( \sum_{k \sim i, k \sim j} \frac{1}{(d_k)^2} \right) \left( \sinh(1) - 1 \right)$$

$$+ \left( \cosh(1) - 1 \right) \left[ \sum_{i=1}^{n} \left( \sum_{i \sim j} \frac{4}{(d_i + d_j)^2} \right)^2 + \sum_{i \sim j} \frac{4}{(d_i + d_j)^2} \left( \sum_{k \sim i, k \sim j} \frac{4}{(d_k)^2} \right)^2 \right].$$

**Theorem 10.** Let $G$ be a graph with $n$ vertices. Then

$$\text{HEE}(G) \leq n - 1 + e^{\sqrt{8\chi_{-2}(G)-1}}.$$ 

**Proof.** Let $n_+$ be the number of positive harmonic eigenvalues of $G$. Since $f(x) = e^x$...
monotonically increases in the interval \((\infty, +\infty)\) and \(m \neq 0\), we get

\[
\text{HEE} = \sum_{i=1}^{n} e^\gamma_i < n - n + \sum_{i=1}^{n} e^\gamma_i = n - n + \sum_{i=1}^{n} \sum_{k \geq 0} (\gamma_i)^k
\]

\[
= n + \sum_{k \geq 1} \frac{1}{k!} \sum_{i=1}^{n} (\gamma_i)^k
\]

\[
\leq n + \sum_{k \geq 1} \frac{1}{k!} \left[ \sum_{i=1}^{n} \gamma_i^2 \right]^\frac{k}{2}
\]

\[
= n + \sum_{k \geq 1} \frac{1}{k!} \left[ \sum_{i=1}^{n} \gamma_i^2 \right]^\frac{k}{2}.
\]

Since every \((n,m)\)-graph with \(m \neq 0\) has \(K_2\) as its induced subgraph and the spectrum of \(K_2\) is \(1, -1\) it follows from the interlacing inequalities that \(\gamma_n \leq 1\), which implies that, \(\sum_{i=n+1}^{n} (\gamma_i)^2 \geq 1\). Consequently,

\[
\text{HEE} < n + \sum_{k \geq 1} \frac{1}{k!} \left[ 8\chi_2(G) - 1 \right]^\frac{k}{2} = n - 1 + e\sqrt{8\chi_2(G) - 1}.
\]

\[\square\]

**Theorem 11.** Let \(G\) be a graph with \(n\) vertices. Then

\[
\text{HEE}(G) \geq \sqrt{n^2 + 8n\chi_2(G) + \frac{32}{3} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{(d_i + d_j)^2} \left( \sum_{k \sim i, k \sim j} \frac{1}{(d_k)^2} \right) + \frac{1}{12} nN_4 + 16n^2(\chi_2)^2(G)}.
\]

**Proof.** Suppose that \(\gamma_1, \gamma_2, \ldots, \gamma_n\) is the spectrum of \(G\). Using Lemma 2 we have

\[
\text{HEE}(G)^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} e^{\gamma_i + \gamma_j}
\]

\[
\geq \sum_{i=1}^{n} \sum_{j=1}^{n} \left( 1 + \gamma_i + \gamma_j + \frac{(\gamma_i + \gamma_j)^2}{2} + \frac{(\gamma_i + \gamma_j)^3}{6} + \frac{(\gamma_i + \gamma_j)^4}{24} \right)
\]

\[
= \sum_{i=1}^{n} \sum_{j=1}^{n} \left( 1 + \gamma_i + \gamma_j + \frac{\gamma_i^2}{2} + \frac{\gamma_j^2}{2} + \gamma_i \gamma_j + \frac{\gamma_i^3}{6} + \frac{\gamma_j^3}{6} + \frac{\gamma_i^2 \gamma_j}{2} + \frac{\gamma_i \gamma_j^2}{2} + \frac{\gamma_i^4}{24} + \frac{\gamma_j^4}{24} + \frac{\gamma_i^2 \gamma_j^2}{4} + \frac{\gamma_i^3 \gamma_j}{6} + \frac{\gamma_i \gamma_j^3}{6} \right).
\]
By equality (4)-(7), we have the following equations:

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} (\gamma_i + \gamma_j) = n \sum_{i=1}^{n} \gamma_i + n \sum_{j=1}^{n} \gamma_j = 0.
\]

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \gamma_i \gamma_j = \left( \sum_{i=1}^{n} \gamma_i \right)^2 = 0.
\]

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \left( \frac{\gamma_i^2}{2} + \frac{\gamma_j^2}{2} \right) = \frac{n}{2} \sum_{i=1}^{n} \gamma_i^2 + \frac{n}{2} \sum_{j=1}^{n} \gamma_j^2 = 8n\chi(G) - 2.
\]

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \left( \frac{\gamma_i^3}{6} + \frac{\gamma_j^3}{6} \right) = \frac{n}{6} \sum_{i=1}^{n} \gamma_i^3 + \frac{n}{6} \sum_{j=1}^{n} \gamma_j^3 = \frac{32}{3} \sum_{i \sim j} \frac{1}{(d_i + d_j)^2} \left( \sum_{k \sim i, k \sim j} \frac{1}{(d_k)^2} \right).
\]

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\gamma_i^4}{24} + \frac{\gamma_j^4}{24} = \frac{n}{24} \sum_{i=1}^{n} \gamma_i^4 + \frac{n}{24} \sum_{j=1}^{n} \gamma_j^4 = \frac{1}{6} nN_4.
\]

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\gamma_i \gamma_j^3}{6} = \frac{1}{6} \sum_{i=1}^{n} \gamma_i \sum_{j=1}^{n} \gamma_j^3 = 0.
\]

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\gamma_i^3 \gamma_j}{6} = \frac{1}{6} \sum_{i=1}^{n} \gamma_i^3 \sum_{j=1}^{n} \gamma_j = 0.
\]

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

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

Combining the above relations, we get

\[
HEE(G) \geq \sqrt{n^2 + 8n\chi(G) + \frac{32}{3} \sum_{i \sim j} \frac{1}{(d_i + d_j)^2} \left( \sum_{k \sim i, k \sim j} \frac{1}{(d_k)^2} \right) + \frac{1}{12} nN_4 + 16n^2(\chi(G))^2}.
\]

\[\square\]

**Theorem 12.** Let \( G \) be a graph with \( n \) vertices. Then

\[
HEE(G) \geq e^{\frac{2N(G)}{n}} + \frac{n - 1}{e^{\frac{2N(G)}{n}}}.
\]
Proof. By definition of harmonic Estrada index and using arithmetic-geometric mean inequality, we obtain

\[
HEE(G) = e^{\gamma_1} + e^{\gamma_2} + \cdots + e^{\gamma_n}
\]

(22) \[\geq e^{\gamma_1} + (n - 1)\left(\prod_{i=2}^{n} e^{\gamma_i}\right)^{\frac{1}{n-1}}\]

(23) \[= e^{\gamma_1} + (n - 1)\left(e^{-\gamma_1}\right)^{\frac{1}{n-1}}\] by Equality (4).

Now we consider the following function

\[
f(x) = e^x + \frac{n - 1}{e^{\frac{x}{n-1}}}
\]

for \(x > 0\). We have

\[
f(x) \geq e^x + \frac{n - 1}{e^{\frac{x}{n-1}}}
\]

for \(x > 0\). It is easy to see that \(f\) is an increasing function for \(x > 0\). From the Equation (23) and Lemma 5, we obtain

\[
HEE(G) \geq e^{-\frac{2H(G)}{n}} + \frac{n - 1}{e^{-\frac{2H(G)}{n-1}}}.
\]

\[
\square
\]

5. BOUND FOR THE HARMONIC ESTRADA INDEX INVOLVING THE HARMONIC ENERGY

In this section, we investigate the relations between the harmonic Estrada index and the harmonic energy.

Theorem 13. The harmonic Estrada index \(HEE(G)\) and the graph harmonic energy \(HE(G)\) satisfy the following inequality:

(24) \[
\frac{1}{2}HE(G)(e - 1) + n - n_+ \leq HEE(G) \leq n - 1 + e^{\frac{HE(G)}{2}}.
\]

Proof. Lower bound, since \(e^x \geq 1 + x\), equality holds if and only if \(x = 0\) and
$e^x \geq ex$, equality holds if and only if $x = 1$. We have

$$HEE(G) = \sum_{i=1}^{n} e^\gamma_i = \sum_{\gamma_i > 0} e^\gamma_i + \sum_{\gamma_i \leq 0} e^\gamma_i \geq \sum_{\gamma_i > 0} e\gamma_i + \sum_{\gamma_i \leq 0} (1 + \gamma_i) \geq e(\gamma_1 + \gamma_2 + \cdots + \gamma_{n_+}) + (n - n_+) + (\gamma_{n_+ + 1} + \cdots + \gamma_n) = (e - 1)(\gamma_1 + \gamma_2 + \cdots + \gamma_{n_+}) + (n - n_+) + \sum_{i=1}^{n} \gamma_i = \frac{1}{2}HE(G)(e - 1) + n - n_+.$$

**Upper bound.** From (21),

$$HEE(G) \leq n + \sum_{k \geq 1} \frac{n!}{k!} \sum_{i=1}^{n_+} (\gamma_i)^k \leq n + \sum_{k \geq 1} \frac{1}{k!} \left( \sum_{i=1}^{n_+} \gamma_i \right)^k = n - 1 + e^{HE(G)/2}.$$

**Theorem 14.** Let $G$ be a graph with largest eigenvalue $\gamma_1$ and let $p, \tau$ and $q$ be, respectively, the number of positive, zero and negative eigenvalues of $G$. Then

$$HEE(G) \geq e^{\gamma_1} + \tau + (p - 1)e^{\frac{HE(G) - 2\gamma_1}{2(p - 1)}} + q e^{\frac{HE(G)}{2q}}.$$

**Proof.** Let $\gamma_1 \geq \cdots \geq \gamma_p$ be the positive, and $\gamma_{n-q+1}, \ldots, \gamma_n$ be the negative eigenvalues of $G$. As the sum of eigenvalues of a graph is zero, one has

$$HE(G) = 2 \sum_{i=1}^{n} \gamma_i = -2 \sum_{i=n-q+1}^{n} \gamma_i.$$

By the arithmetic-geometric mean inequality, we have

$$\sum_{i=2}^{p} e^{\gamma_i} \geq (p - 1)e^{\frac{\gamma_2 + \cdots + \gamma_p}{p - 1}} = (p - 1)e^{\frac{HE(G) - 2\gamma_1}{2(p - 1)}}.$$

Similarly,

$$\sum_{i=n-q+1}^{n} e^{\gamma_i} \geq q e^{\frac{HE(G)}{2q}}.$$

For the zero eigenvalues, we also have

$$\sum_{i=p+1}^{n} e^{\gamma_i} = \tau.$$
So we obtain

\[ HEE(G) \geq e^{\gamma_1} + \tau + (p - 1)e^{\frac{H_E(G) - 2\gamma_1}{2(p - 1)}} + qe^{\frac{H_E(G)}{2q}}. \]

\[ \square \]

REFERENCES


11. S. S. Dragomir: On some inequalities (Romanian), Caiete Metodico Stiintific, Faculty of Mathematics, Timisoara University, Romania, 13, 1984.


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