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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 ith vertex(d_i is the degree of v_i), 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 ith and jth 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 $G = (V, \mathbf{E})$ be a simple connected graph with the vertex set $V(G) = \{v_1, v_2, ..., v_n\}$ and edge set $\mathbf{E}(G)$, where $|V(G)| = n$ and $|\mathbf{E}(G)| = m$. Let d_i be the degree of the ith vertex $v_i \in V$, for $i = 1, 2, ..., n$. For a graph G, the harmonic index $H(G)$ is defined in [**25**] as $H(G) = \sum_{u_iv_j \in E(G)} \frac{2}{d_i+d_j}$. 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 $v_1, v_2, \dots, v_n$. 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 $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ be the eigenvalues of its adjacency matrix $A(G)$. Then the spectrum of G is $Spec(G) = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$. These form the adjacency *spectrum* of G [**3**].

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Thus

$$detA = \prod_{i=1}^{n} \lambda_i.$$

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 $\gamma_1 \geqslant \gamma_2 \geqslant \cdots \geqslant \gamma_n$. 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 $\chi(G) \leqslant 2H(G)$ 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

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

and

$$\chi_\alpha(G) = \sum_{uv\in E(G)} (d(u) + d(v))^{\alpha}, \tag{1}$$

where α 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.,

(2) $$N_k = \sum_{j=1}^{n} (\gamma_i)^k$$

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

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

(3)
(1) $N_0 = \sum_{i=1}^{n} (\gamma_i)^0 = n,$

(4)
(2) $N_1 = tr(H) = 0,$

(5)
(3) $N_2 = tr(H^2) = 8\chi_{-2}(G),$

(6)
(4) $N_3 = tr(H^3) = 32 \sum_{i\sim j} \frac{1}{(d_i+d_j)^2} \left(\sum_{k\sim i,\, k\sim j} \frac{1}{(d_k)^2} \right),$

(7)
(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 $i \neq j$

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

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

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

wher $\sum_{k\sim i,\, k\sim j} \frac{1}{(d_k)^2} = \sum_{k\sim i,\, k\sim j} \frac{1}{(d_i+d_k)(d_k+d_j)}$.
We now calculate $tr(H^4)$. Because $tr(H^4) = \|H^2\|_F^2$, where $\|H^2\|_F^2$ denotes the *Frobenius norm* of H^2, we obtain

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

□

Remark 1. *For any real x, the power-series expansion of e^x, is the following*

(8) $$e^x = \sum_{k\geqslant 0} \frac{x^k}{k!}.$$

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

Theorem 1. *[**4**] (Chebishev inequality) Let $a_1 \leq a_2 \leqslant \cdots \leqslant a_n$ and $b_1 \leq b_2 \leqslant \cdots \leqslant b_n$ be real numbers. Then we have*

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

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 $x_1, x_2, \dots, x_n$ and $k \geqslant 2$,*

$$\sum_{i=1}^{n}(x_i)^k \leqslant (\sum_{i=1}^{n} {x_i}^2)^{\frac{k}{2}}. \tag{9}$$

Lemma 3. *[**35**] Let G be a graph with m edges. Then for $k \geqslant 4$, $M_{k+2} \geqslant M_k$ with equality for all even $k \geqslant 4$ 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 $k \geqslant 5$ 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 $\lambda_1(B) \geqslant \lambda_2(B) \leqslant \cdots \leqslant \lambda_n(B)$, then for any $X \in R^n$, $(X \neq 0)$,*

$$X^t B X \leqslant \lambda_1(B) X^t X.$$

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*

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

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:

$$E = E(G) = \sum_{i=1}^{n} \mid \lambda_i \mid . \tag{10}$$

where λ_i, $i = 1, 2, \dots, n$, 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. [**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,

e.g. [**1, 21, 26, 27, 28**]).
Therefore, by considering this, the harmonic energy defined in [**25**] as

$$HE(G) = \sum_{i=1}^{n} | \gamma_i |, \tag{11}$$

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 $n \geqslant 2$ vertices. Then the spectral radius of the harmonic matrix is bounded from below as*

$$\gamma_1 \geqslant \frac{2H(G)}{n}. \tag{12}$$

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

$$\begin{aligned} X^t H X &= \left(\sum_{j, j \sim 1}^{n} x_j h_{j1}, \sum_{j, j \sim 2}^{n} x_j h_{j2}, \ldots, \sum_{j, j \sim n}^{n} x_j h_{jn} \right)^t X \\ &= 2 \sum_{i \sim j} h_{ij} x_i x_j \end{aligned} \tag{13}$$

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

$$X^t X = \sum_{i=1}^{n} x_i^2. \tag{14}$$

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

$$\gamma_1 \geqslant \frac{2 \sum_{i \sim j} h_{ij} x_i x_j}{\sum_{i=1}^{n} x_i^2}. \tag{15}$$

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

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

□

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

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 $\gamma_1 \geqslant \gamma_2 \geqslant \cdots \geqslant \gamma_{n-1} \geqslant \gamma_n$ be the eigenvalues of G. By the $Cauchy-Schwartz$ inequality,

$$\sum_{i=1}^{n} \mid \gamma_i \mid \leqslant \sqrt{(n-1)\sum_{i=2}^{n}\gamma_i^2} = \sqrt{(n-1)(8\chi_{-2}(G)-\gamma_1^2)}.$$

Hence

$$HE(G) \leqslant \gamma_1 + \sqrt{(n-1)(8\chi_{-2}(G)-\gamma_1^2)}.$$

Note that the function $K(x) = x + \sqrt{(n-1)(8\chi_{-2}(G)-x^2)}$ decreases for $\frac{\chi(G)}{n^2} \leqslant x \leqslant \frac{\chi(G)}{n}$. By Remark 3, we have $\gamma_1 \geqslant \frac{\chi(G)}{n}$, therefore

$$\gamma_1 \geqslant \frac{\chi(G)}{n} \geqslant \frac{\chi(G)}{n^2}.$$

So $K(\gamma_1(G)) \leqslant K\left(\frac{\chi(G)}{n}\right)$, which implies that

$$HE(G) \leq \frac{\chi(G)}{n} + \sqrt{(n-1)\left(8\chi_{-2}(G) - \left(\frac{\chi(G)}{n}\right)^2\right)}.$$

□

Remark 4. *[**31**] 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*

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i, \tag{16}$$

$$\Delta = n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2. \tag{17}$$

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

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

Lemma 6. *Let G be a simple graph with $n \geqslant 2$, vertices. Then*

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

Proof. Let the characteristic polynomial of a graph G is 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 $P_n(0, -4\chi_{-2}(G))$, 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 γ_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 $\gamma_1 \geqslant \gamma_2 \geqslant \cdots \geqslant \gamma_{n-1} \geqslant \gamma_n$ be the eigenvalues of G. By the *Cauchy − Schwartz* inequality,
$$\sum_{i=1}^{n} |\, \gamma_i \,| \leqslant \sqrt{(n-1)\sum_{i=2}^{n} \gamma_i^2} = \sqrt{(n-1)(8\chi_{-2}(G) - \gamma_1^2)}.$$

Hence
$$HE(G) \leqslant \gamma_1 + \sqrt{(n-1)(8\chi_{-2}(G) - \gamma_1^2)}.$$

Note that the function $F(x) = x + \sqrt{(n-1)(8\chi_{-2}(G) - x^2)}$ decreases for $\frac{1}{n^2}\sqrt{\frac{8n\chi_{-2}(G)}{n-1}} \leqslant x \leqslant \frac{1}{n}\sqrt{\frac{8n\chi_{-2}(G)}{n-1}}$. By Lemma 6, we have $\gamma_1 \geqslant \frac{1}{n}\sqrt{\frac{8n\chi_{-2}(G)}{n-1}}$, therefore
$$\gamma_1 \geqslant \frac{1}{n}\sqrt{\frac{8n\chi_{-2}(G)}{n-1}} \geqslant \frac{1}{n^2}\sqrt{\frac{8n\chi_{-2}(G)}{n-1}}.$$

So $F(\gamma_1(G)) \leqslant F\left(\frac{1}{n}\sqrt{\frac{8n\chi_{-2}(G)}{n-1}}\right)$, 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*

$$e^{-\sqrt{8\chi_{-2}(G)}} \leqslant HE(G) \leqslant e^{\sqrt{8\chi_{-2}(G)}}. \tag{18}$$

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

$$HE(G) = \sum_{i=1}^{n} \mid \gamma_i \mid = n(\frac{1}{n}\sum_{i=1}^{n} \mid \gamma_i \mid) \geqslant n(\sqrt[n]{\mid \gamma_1 \mid\mid \gamma_2 \mid \cdots \mid \gamma_n \mid}).$$

By the geometric and harmonic mean inequality, we have

$$\begin{aligned}
n(\sqrt[n]{\mid \gamma_1 \mid\mid \gamma_2 \mid \cdots \mid \gamma_n \mid}) &\geqslant n(\frac{n}{\sum_{i=1}^{n}\frac{1}{|\gamma_i|}}) \\
&\geqslant n(\frac{n}{\sum_{i=1}^{n}\frac{1}{|\gamma_i|}\sum_{i=1}^{n}\mid \gamma_i \mid}) \\
&\geqslant n(\frac{n}{n\sum_{i=1}^{n}\frac{1}{|\gamma_i|}\mid \gamma_i \mid}), \qquad (\text{ by Theorem 1}) \\
&\geqslant n(\frac{n}{n^2\sum_{i=1}^{n}\mid \gamma_i \mid}) \\
&> n(\frac{n}{n^2\sum_{i=1}^{n} e^{|\gamma_i|}}) \\
&= \frac{1}{\sum_{i=1}^{n}\sum_{k\geqslant 0}\frac{(|\gamma_i|)^k}{k!}} \\
&= \frac{1}{\sum_{k\geqslant 0}\frac{1}{k!}(\sum_{i=1}^{n}(\mid \gamma_i \mid)^k)} \\
&\geqslant \frac{1}{\sum_{k\geqslant 0}\frac{1}{k!}(\sum_{i=1}^{n}(\mid \gamma_i \mid)^2)^{\frac{k}{2}}}, \qquad (\text{by Inequality 9}) \\
&= \frac{1}{\sum_{k\geqslant 0}\frac{1}{k!}(\sum_{i=1}^{n}(\gamma_i)^2)^{\frac{k}{2}}} \\
&= \frac{1}{\sum_{k\geqslant 0}\frac{1}{k!}\left(\sqrt{8\chi_{-2}(G)}\right)^k}, \qquad (\text{by Equality 5}) \\
&= \frac{1}{e^{\sqrt{8\chi_{-2}(G)}}}.
\end{aligned}$$

Therefore, we have

$$HE(G) \geqslant e^{-\sqrt{8\chi_{-2}(G)}}.$$

Upper bound, by definition of harmonic *energy*, we have

$$\begin{aligned}
HE(G) = \sum_{i=1}^{n} \mid \gamma_i \mid < \sum_{i=1}^{n} e^{|\gamma_i|} &= \sum_{i=1}^{n} \sum_{k\geqslant 0} \frac{(\mid \gamma_i \mid)^k}{k!} \\
&= \sum_{k\geqslant 0} \frac{1}{k!} \sum_{i=1}^{n} (\mid \gamma_i \mid)^k \\
&\leq \sum_{k\geqslant 0} \frac{1}{k!} (\sum_{i=1}^{n} (\mid \gamma_i \mid)^2)^{\frac{k}{2}}, \qquad \text{(by Inequality 9)} \\
&= \sum_{k\geqslant 0} \frac{1}{k!} (\sum_{i=1}^{n} (\gamma_i)^2)^{\frac{k}{2}} \\
&= \sum_{k\geqslant 0} \frac{1}{k!} \left(8\chi_{-2}(G)\right)^{\frac{k}{2}}, \qquad \text{(by Equality 5)} \\
&= \sum_{k\geqslant 0} \frac{1}{k!} \left(\sqrt{8\chi_{-2}(G)}\right)^{k} \\
&= e^{\sqrt{8\chi_{-2}(G)}}.
\end{aligned}$$

Therefore, we have

$$HE(G) \leqslant e^{\sqrt{8\chi_{-2}(G)}}.$$

□

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

$$\sqrt{8\chi_{-2}(G)} \leqslant HE(G) \leqslant \sqrt{8n\chi_{-2}(G)}.$$

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

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

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

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

Therefore

$$HE(G) \leqslant \sqrt{8n\chi_{-2}(G)}.$$

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

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

□

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

$$HE(G) \geqslant \sqrt{8\chi_{-2}(G) + n(n-1) \mid detH \mid^{\frac{2}{n}}}.$$

Proof. By the definition of harmonic energy, we have

$$\begin{aligned} HE(G)^2 &= \left(\sum_{i=1}^{n} \mid \gamma_i \mid\right)^2 = \sum_{i=1}^{n} \mid \gamma_i \mid^2 + 2 \sum_{1 \leqslant i \leqslant j \leqslant n} \mid \gamma_i \mid\mid \gamma_j \mid \\ &= 8\chi_{-2}(G) + 2 \sum_{1 \leqslant i \leqslant j \leqslant n} \mid \gamma_i \mid\mid \gamma_j \mid \\ &= 8\chi_{-2}(G) + 2 \sum_{i \neq j} \mid \gamma_i \mid\mid \gamma_j \mid . \end{aligned}$$

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

$$\begin{aligned} \frac{1}{n(n-1)} \sum_{i \neq j} \mid \gamma_i \mid\mid \gamma_j \mid \geqslant \left(\prod_{i \neq j} \mid \gamma_i \mid\mid \gamma_j \mid\right)^{\frac{1}{n(n-1)}} &= \left(\prod_{i=1}^{n} \mid \gamma_i \mid^{2(n-1)}\right)^{\frac{1}{n(n-1)}} \\ &= \prod_{i=1}^{n} \mid \gamma_i \mid^{\frac{2}{n}} = \mid detH \mid^{\frac{2}{n}} . \end{aligned}$$

□

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

$$HE(G) \leqslant \frac{8\chi_{-2}(G) + n}{2}.$$

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**])

$$\sum_{i=1}^{n} d_i \sum_{i=1}^{n} c_i a_i^2 + \sum_{i=1}^{n} c_i \sum_{i=1}^{n} d_i b_i^2 \geqslant 2 \sum_{i=1}^{n} a_i c_i \sum_{i=1}^{n} b_i d_i. \tag{19}$$

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

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

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

$$HE(G) \leqslant \frac{8\chi_{-2}(G) + n}{2}.$$

□

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 $\gamma_1 \geqslant \gamma_2 \geqslant \cdots \geqslant \gamma_n$. Then the harmonic Estrada index of G, denoted by HEE, is defined to be

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

Recalling Eq. (2), it follows that

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

We begin this section with theorem as follows:

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

$$HEE(G) \geqslant n + 8\chi_{-2}(G) + 32 \sum_{i\sim j} \frac{1}{(d_i+d_j)^2} \Bigg(\sum_{k\sim i,\, k\sim j} \frac{1}{(d_k)^2} \Bigg) \Big(\sinh(1) - 1 \Big) + \Big(\cosh(1) - 1 \Big) \left[\sum_{i=1}^{n} \Bigg(\sum_{i\sim j} \frac{4}{(d_i+d_j)^2} \Bigg)^2 + \sum_{i\neq j} \frac{4}{(d_i+d_j)^2} \Bigg(\sum_{k\sim i,\, k\sim j} \frac{4}{(d_k)^2} \Bigg)^2 \right].$$

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

$$\begin{aligned} HEE(G) &= n + 8\chi_{-2}(G) + \sum_{k\geqslant 1} \frac{N_{2k+1}}{(2k+1)!} + \sum_{k\geqslant 1} \frac{N_{2k+2}}{(2k+2)!} \\ &\geqslant n + 8\chi_{-2}(G) + \sum_{k\geqslant 1} \frac{N_3}{(2k+1)!} + \sum_{k\geqslant 1} \frac{N_4}{(2k+2)!} \\ &= n + 8\chi_{-2}(G) + 32 \sum_{i\sim j} \frac{1}{(d_i+d_j)^2} \Bigg(\sum_{k\sim i,\, k\sim j} \frac{1}{(d_k)^2} \Bigg) \Big(\sinh(1) - 1 \Big) \\ &+ \Big(\cosh(1) - 1 \Big) \left[\sum_{i=1}^{n} \Bigg(\sum_{i\sim j} \frac{4}{(d_i+d_j)^2} \Bigg)^2 + \sum_{i\neq j} \frac{4}{(d_i+d_j)^2} \Bigg(\sum_{k\sim i,\, k\sim j} \frac{4}{(d_k)^2} \Bigg)^2 \right]. \end{aligned}$$

□

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

$$HEE(G) \leqslant n - 1 + e^{\sqrt{8\chi_{-2}(G)-1}}. \qquad (20)$$

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

$$
\begin{aligned}
HEE = \sum_{i=1}^{n} e^{\gamma_i} < n - n_+ \sum_{i=1}^{n_+} e^{\gamma_i} &= n - n_+ \sum_{i=1}^{n_+} \sum_{k \geqslant 0} \frac{(\gamma_i)^k}{k!} \\
&= n + \sum_{k \geqslant 1} \frac{1}{k!} \sum_{i=1}^{n_+} (\gamma_i)^k \\
&\leqslant n + \sum_{k \geqslant 1} \frac{1}{k!} \Big[\sum_{i=1}^{n_+} \gamma_i^2 \Big]^{\frac{k}{2}} \\
&= n + \sum_{k \geqslant 1} \frac{1}{k!} \Big[\sum_{i=1}^{n_+} \gamma_i^2 \Big]^{\frac{k}{2}}.
\end{aligned} \tag{21}
$$

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 $\gamma_n \leqslant 1$, which implies that, $\sum_{i=n_++1}^{n} (\gamma_i)^2 \geqslant 1$. Consequently,

$$
HEE < n + \sum_{k \geqslant 1} \frac{1}{k!} \Big[8\chi_{-2}(G) - 1 \Big]^{\frac{k}{2}} = n - 1 + e^{\sqrt{8\chi_{-2}(G) - 1}}.
$$

□

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

$$
HEE(G) \geqslant \sqrt{n^2 + 8n\chi_{-2}(G) + \frac{32 \sum_{i \sim j} \frac{1}{(d_i + d_j)^2} \Big(\sum_{k \sim i,\, k \sim j} \frac{1}{(d_k)^2} \Big)}{3} + \frac{1}{12} n N_4 + 16 n^2 (\chi_{-2})^2(G)}.
$$

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

$$
\begin{aligned}
HEE(G)^2 &= \sum_{i=1}^{n} \sum_{j=1}^{n} e^{\gamma_i + \gamma_j} \\
&\geqslant \sum_{i=1}^{n} \sum_{j=1}^{n} \Big(1 + \gamma_i + \gamma_j + \frac{(\gamma_i + \gamma_j)^2}{2} + \frac{(\gamma_i + \gamma_j)^3}{6} + \frac{(\gamma_i + \gamma_j)^4}{24} \Big) \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} \Big(1 + \gamma_i + \gamma_j + \frac{\gamma_i^2}{2} + \frac{\gamma_j^2}{2} + \gamma_i \gamma_j + \frac{\gamma_i^3}{6} + \frac{\gamma_j^3}{6} + \frac{\gamma_i^2 \gamma_j}{2} + \frac{\gamma_i \gamma_j^2}{2} \\
&+ \frac{\gamma_i^4}{24} + \frac{\gamma_j^4}{24} + \frac{\gamma_i^2 \gamma_j^2}{4} + \frac{\gamma_i^3 \gamma_j}{6} + \frac{\gamma_i \gamma_j^3}{6} \Big).
\end{aligned}
$$

By equality (4)-(7), we have the following equations:

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

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

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

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

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(\frac{\gamma_i^4}{24}+\frac{\gamma_j^4}{24})=\frac{n}{24}\sum_{i=1}^{n}\gamma_i^4+\frac{n}{24}\sum_{j=1}^{n}\gamma_j^4=\frac{1}{12}nN_4.$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\gamma_i^2\gamma_j^2}{4}=16n^2\left(\sum_{i\sim j}\frac{1}{(d_i+d_j)^2}\right)^2=16n^2(\chi_{-2})^2(G).$$

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

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

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\gamma_i\gamma_j^2}{2}=\frac{1}{2}\sum_{i=1}^{n}\gamma_i\sum_{j=1}^{n}\gamma_j^3=0.$$

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

Combining the above relations, we get

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

□

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

$$HEE(G)\geqslant e^{\frac{2\mathcal{H}(G)}{n}}+\frac{n-1}{e^{\frac{\frac{2\mathcal{H}(G)}{n}}{n-1}}}.$$

Proof. By difinition of harmonic Esterada index and using arithmetic-geometric mean inequality, we obtain

$$\begin{aligned} HEE(G) &= e^{\gamma_1} + e^{\gamma_2} + \cdots + e^{\gamma_n} \\ &\geqslant e^{\gamma_1} + (n-1)\Big(\prod_{i=2}^{n} e^{\gamma_i}\Big)^{\frac{1}{n-1}} \qquad (22) \\ &= e^{\gamma_1} + (n-1)\Big(e^{-\gamma_1}\Big)^{\frac{1}{n-1}} \quad \text{by Equality (4).} \qquad (23) \end{aligned}$$

Now we consider the following function

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

for $x > 0$. We have

$$f(x) \geqslant e^x + \frac{n-1}{e^{\frac{x}{n-1}}}$$

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

$$HEE(G) \geqslant e^{\frac{2\mathcal{H}(G)}{n}} + \frac{n-1}{e^{\frac{\frac{2\mathcal{H}(G)}{n}}{n-1}}}.$$

□

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:*

$$\frac{1}{2}HE(G)(e-1) + n - n_+ \leqslant HEE(G) \leqslant n - 1 + e^{\frac{HE(G)}{2}}. \qquad (24)$$

Proof. **Lower bound**, since $e^x \geqslant 1 + x$, equality holds if and only if $x = 0$ and

$e^x \geqslant ex$, equality holds if and only if $x = 1$. We have

$$\begin{aligned} HEE(G) &= \sum_{i=1}^{n} e^{\gamma_i} = \sum_{\gamma_i>0} e^{\gamma_i} + \sum_{\gamma_i\leqslant 0} e^{\gamma_i} \\ &\geqslant \sum_{\gamma_i>0} e\gamma_i + \sum_{\gamma_i\leqslant 0}(1+\gamma_i) \\ &= e(\gamma_1+\gamma_2+\cdots+\gamma_{n_+}) + (n-n_+) + (\gamma_{n_++1}+\cdots+\gamma_n) \\ &= (e-1)(\gamma_1+\gamma_2+\cdots+\gamma_{n_+}) + (n-n_+) + \sum_{i=1}^{n}\gamma_i \\ &= \frac{1}{2}HE(G)(e-1) + n - n_+. \end{aligned}$$

Upper bound. From (21),

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

□

Theorem 14. *Let G be a graph with largest eigenvalue γ_1 and let p, τ and q be, respectively, the number of positive, zero and negative eigenvalues of G. Then*

$$HEE(G) \geqslant e^{\gamma_1} + \tau + (p-1)e^{\frac{HE(G)-2\gamma_1}{2(p-1)}} + qe^{-\frac{HE(G)}{2q}}. \tag{25}$$

Proof. Let $\gamma_1 \geqslant \cdots \geqslant \gamma_p$ 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

$$\sum_{i=2}^{p} e^{\gamma_i} \geqslant (p-1)e^{\frac{(\gamma_2+\cdots+\gamma_p)}{(p-1)}} = (p-1)e^{\frac{HE(G)-2\gamma_1}{2(p-1)}}. \tag{26}$$

Similarly,

$$\sum_{i=n-q+1}^{n} e^{\gamma_i} \geqslant qe^{-\frac{HE(G)}{2q}}. \tag{27}$$

For the zero eigenvalues, we also have

$$\sum_{i=p+1}^{n-q} e^{\gamma_i} = \tau.$$

So we obtain

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

□

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ON SIZE, ORDER, DIAMETER AND VERTEX-CONNECTIVITY

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Let G be a finite connected graph. We give an asymptotically sharp upper bound on the size of G in terms of its order, diameter and vertex-connectivity. The result is a strengthening of an old classical theorem of Ore [**5**] if vertex-connectivity is prescribed and constant.

1. Introduction

Let G be a finite connected graph with vertex set $V(G)$ and edge set $E(G)$. We denote the order of G by n and the size by m. The *distance*, $d_G(u, v)$, between vertices u and v in G is the length of a shortest $u-v$ path in G. The *eccentricity* of a vertex $v \in V(G)$ is the maximum distance between v and any other vertex in G. The *degree*, deg v, of a vertex v of G is the number of edges incident with it, and the diameter of G, d, is $\max\{d_G(u, v) : u, v \in V\}$, whilst the radius of G, r, is the minimum value of the eccentricities of vertices of G. The vertex-connectivity $\kappa(G)$ of G is defined as the minimum number of vertices whose deletion from G results in a disconnected or trivial graph. We say that G is k-vertex-connected, or simply k-connected, if $\kappa(G) \geq k$.

The diameter, apart from being an interesting graph theoretical parameter, plays an important role in analysing communication networks (see for example [**1**]). In such networks the time delay or signal disgradation for sending a message from one point to another is often proportional to the distance between the two points. The diameter can be used to indicate the worst case performance.

Several bounds on the size of a graph in terms of other graph parameters, for example, order and radius [**3, 6**], order and degree set [**7**], and order and domination

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number [**2**] have been investigated. An upper bound on the size in terms of order and diameter was determined by Ore [**5**] as early as 1968. Several authors [**6, 7**] have presented simple and short proofs to Ore's theorem. Recently one of the present authors [**4**] reported on the size, order, diameter and minimum degree. In this note we present an upper bound on the size in terms of order, diameter and vertex-connectivity. The bound, for a fixed vertex-connectivity κ, is a strengthening of Ore's theorem [**5**], which we state below

Theorem 1. *Let G be a connected graph of order n, diameter d and size m. Then* $m \leq \frac{1}{2}(n-d-1)(n-d+4)+d = \frac{1}{2}(n-d)^2 + O(n)$.

2. Results

Let G be a finite connected graph of order n, size m and diameter d. From now onwards $v_0 \in V(G)$ is a fixed vertex of eccentricity d and for each $i = 0, 1, 2, 3, \ldots, d$,

$$N_i := \{x \in V(G) | d_G(x, v_0) = i\}.$$

The following result is a strengthening of Ore's theorem if vertex-connectivity is prescribed and constant.

Theorem 2. *Let G be a κ-connected graph of order n, diameter d and size m. Then*

$$m \leq \frac{1}{2}(n - \kappa d)^2 + O(n)$$

and the bound, for fixed κ, is asymptotically tight.

Proof. Assume the notation for v_0 and N_i as above. Note that $|N_i| \geq \kappa$, for all $i = 1, 2, \ldots, d-1$. For each N_i, $i = 1, 2, \ldots, d-1$, choose any κ vertices and let this set be $N_i' = \{u_{i1}, u_{i2}, \ldots, u_{i\kappa}\}$. For each $j = 1, 2, \ldots, \kappa$, let $P_j := \{u_{1j}, u_{2j}, u_{3j}, \ldots, u_{d-1j}\}$ and $N = \cup_{j=1}^{\kappa} P_j$. Then,

$$|N| = \kappa(d-1). \tag{1}$$

Claim 1. *Let N be as above. Then* $\sum_{x \in N} \deg x \leq O(n)$.

Proof of Claim 1: First consider P_j. Partition P_j as follows: $P_j = U_1 \cup U_2 \cup U_3$, where

$$U_1 = \{u_{1j}, u_{4j}, u_{7j}, \ldots\},$$

$$U_2 = \{u_{2j}, u_{5j}, u_{8j}, \ldots\},$$

and

$$U_3 = \{u_{3j}, u_{6j}, u_{9j}, \ldots\}.$$

Note that for any $x, y \in U_i, i = 1, 2, 3$ we have $N[x] \cap N[y] = \emptyset$. It follows that

$$n \geq |\cup_{x \in U_i} N[x]| = \sum_{x \in U_i} \deg x + |U_i|, \text{for} \quad i = 1, 2, 3.$$

Therefore,

$$\begin{aligned} 3n &\geq \sum_{x \in U_1} \deg x + \sum_{x \in U_2} \deg x + \sum_{x \in U_3} \deg x + |U_1| + |U_2| + |U_3| \\ &= \sum_{x \in P_j} \deg x + |P_j| \end{aligned}$$

Thus, $\sum_{x \in P_j} \deg x \leq 3n - |P_j|$. We conclude that

$$\begin{aligned} \sum_{x \in N} \deg x &= \sum_{j=1}^{\kappa} (\sum_{x \in P_j} \deg x) \\ &\leq \sum_{j=1}^{\kappa} (3n - |P_j|) \\ &\leq 3n\kappa - |N| \\ &= O(n), \end{aligned}$$

as required.

Now let $Q = V - N$. Then from (1)

$$|Q| = n - \kappa(d-1). \tag{2}$$

Claim 2. *Let $x \in Q$. Then* $\deg x \leq n - \kappa d + O(1)$.

Proof of Claim2: Let $x \in Q$. Then x can only be adjacent to vertices from at most 3 of the sets $N_i, i = 1, 2, 3, \ldots, d-1$. Hence x is adjacent to at most 3κ vertices from N. It follows that

$$\begin{aligned} \deg x &\leq |Q| + 3\kappa \\ &= n - \kappa(d-1) + 3\kappa \\ &= n - \kappa d + 4\kappa, \end{aligned}$$

as desired.

By Claim 2, and from (2), we have

$$\begin{aligned} \sum_{x \in Q} \deg x &\leq \sum_{x \in Q} (n - \kappa d + O(1)) \\ &\leq (n - \kappa(d-1)) (n - \kappa d + O(1)) \\ &= (n - \kappa d)^2 + O(n). \end{aligned}$$

Combining this and Claim 1, we get

$$\begin{aligned}\sum_{x\in V}\deg x &= \sum_{x\in N}\deg x+\sum_{x\in Q}\deg x\\ &\le (n-\kappa d)^2+O(n).\end{aligned}$$

It follows, by the Handshaking Lemma that

$$m=\frac{1}{2}\sum_{x\in V}\deg x\le\frac{1}{2}(n-\kappa d)^2+O(n).$$

To see that the bound is asymptotically sharp, consider the graph $G_{n,d,\kappa}=G_0+G_1+\ldots+G_\kappa$ where $G_i=K_\kappa$ for $i=0,1,2,3,\cdots,d-1$ and $G_d=K_{n-\kappa d}$. □

Using the counting technique employed in Theorem 2, we obtain the following theorem which is an improvement of Vizing's Theorem [**8**] if vertex-connectivity is prescribed.

Theorem 3. *Let G be a κ-connected graph of order n, radius r and size m. Then*

$$m\le\frac{1}{2}(n-2r\kappa)^2+O(n).$$

Moreover, this inequality is, for a fixed κ, asymptotically tight. □

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The most private features of the topological index

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§ 1 Introduction

In early May of 2018 I got an astonishing e-mail from Turkey mathematician, Dr. Süleyman Ediz, asking to write an essay to a new journal MATI to be dedicated solely to those papers dealing with the mathematical aspects of the topological index (TI).

This is the most honorable and kindest offer from the group of distinguished scholars who are taking care of my beloved son bestowed to me nearly half a century ago. However, after to-and-fro net surfing I happened to know that these ladies and gentlemen don't seem to know the detailed birth and growth history of my son and his family. Then I decided to let them know the most private features of TI and the family talk around him including his godfather as honestly as I can, of course, within the scope of a scientific paper.

§ 2 Personal history of Haruo Hosoya (HH) related to TI

In 1936[*1] HH was born in Kamakura, an old capital town of Japan in 12th century, which is located to the 50 km south of Tokyo. He entered Univ. of Tokyo in 1955 to study chemistry, and in 1964 took the degree of Doctor of Science for "the research on the structure of reactive intermediates and reaction mechanism" under Prof. Saburo Nagakura. During his under-graduate age HH happened to estimate the boiling points of octane isomers reasonably well with ρ=0.942 using his own naïve conjecture. The detailed story about it is documented in his memoir "The topological index *Z* before and after 1971" [1]. However, this study is nothing related to his doctoral thesis and also to the biophysical study of vision research performed in Univ. of Michigan as a post-doctoral fellow under the direction of Prof. John Platt during 1967 and 1968.

Ironically enough, although Platt who worked with the Nobel Laureate Robert Mulliken in Chicago was the only scientist that realized the importance of the "pass number *w*" of Harry Wiener proposed in 1947 [2,3], HH did not know anything about the graph theory nor the papers by these pioneers in QSAR study during his one-year stay in Ann Arbor.

In the spring of 1969 HH became associate professor of chemistry in Ochanomizu Univ. in Tokyo. In Japan among almost one hundred national universities other than several hundred private universities, Ochanomizu and Nara are only for women students. This means that the level of the students is rather high, which, however, does not mean a good place for a professor to perform active research. Namely HH had to struggle with no research assistant, no modern instruments, no fund, but with a few master and under-graduate students.

Luckily enough he called to remember his private research note on his first QSAR (quantitative structure-activity relationship) study, and with the knowledge of Hückel molecular orbital theory he could find his own graph-theoretical recipe for obtaining the coefficients of the characteristic polynomial, $\mathrm{P_G}(x)=(-1)^N\det(\mathbf{A}-x\mathbf{E})$, for tree graph G by using the non-adjacent number, $p(\mathrm{G},k)$'s, as follows [4]:

$$\mathrm{P_G}(x) = \sum_{k=0}^{\lfloor N/2 \rfloor} (-1)^k p(\mathrm{G},k) x^{N-2k} \quad (\mathrm{G} \in \text{tree}). \tag{1}$$

Then the "topological index" Z is proposed to be defined as the sum of the $p(\mathrm{G},k)$'s as

$$Z = \sum_{k=0}^{\lfloor N/2 \rfloor} p(\mathrm{G},k). \tag{2}$$

The Z-counting polynomial $\mathrm{Q_G}(x)$ is also defined as

$$\mathrm{Q_G}(x) = \sum_{k=0}^{\lfloor N/2 \rfloor} p(\mathrm{G},k) x^k. \tag{3}$$

Naturally we have

$$Z = \mathrm{Q_G}(1). \tag{4}$$

Many years later acyclic [5], reference [6], and matching [7] polynomials $\mathrm{M_G}(x)$'s were proposed to be defined independently by several mathematical chemists and mathematicians, such as Zagreb group, Aihara, and Farrell.

$$\mathrm{M_G}(x) = \sum_{k=0}^{\lfloor N/2 \rfloor} (-1)^k p(\mathrm{G},k) x^{N-2k}. \tag{5}$$

Since all of them are using the $p(\mathrm{G},k)$ numbers of HH, these polynomials are essentially the same as $\mathrm{Q_G}(x)$.

Now let us go back to discuss our Z. HH succeeded in finding good correlation between several thermodynamic quantities, such as boiling point and entropy, and the Z obtained from the carbon atom skeleton graph of saturated hydrocarbon molecules.

In the autumn of 1970 HH read a paper on his TI at the Symposium on the Electronic Structure of Molecules held in Electro-Communication Univ. of Tokyo. Although his presentation of this new idea was welcomed by the audience at that time, HH had to be confronted by the conservative and hard wall of the societies of chemists all over the world.

First, the letter to Chemical Physics Letters was rejected severely from the following reasons. "Since such a simple proposal must have been made by some other people, try to explore document survey in other fields of science. Further, physico-chemical discussion is lacking in this letter." In 1973 when HH met the Editor E. Heilbronner in Basel, he himself betrayed this secret and made his apology to HH.

Anyway the first paper of TI, "Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons" was published in Bulletin of the Chemical Society of Japan (BCSJ) in September of 1971 [4], but later HH was told that at least two designated referees quitted their job before this official debut of TI. They must have been severely vexed by the unique idea of *Z*-index.

However, after this a number of TI papers began to be proposed by chemists all over the world especially in Eastern Europe and US, and the term TI became a common noun. Thus *Z*-index of HH is now called as "the TI" or "Hosoya index," and according to Balaban HH is the "godfather" of TI [8]. Among many reviews and monographs introducing the TI's the book by Devillers and Balaban develops the detailed historical development of TI and *Z*-index [9], especially in the chapter by Ivanciuc and Balaban [10].

The first TI paper by HH [4] is now being cited frequently not only by mathematical chemists but also by mathematicians and information scientists. According to GoogleScholar the total citation number is exceeding 1700 as of the summer of 2018, and this number is increasing weekly nearly after half a century since its debut.

Notwithstanding of dramatic debut and checkered youth, things surrounding TI was changing into warm atmosphere especially after the turn of the century.

Ramon Carbo-Dorca, Professor of the Institute of Computational Chemistry, University of Girona organized Vth Girona Seminar on Molecular Similarity dedicated to HH. The invited guests were P. Mezey, J. Galvez, J. Devillers, E. Estrada, S. Basak, J. Cioslowski, S. Iwata, K. Hirao, and H. Nakatsuji, etc.

HH retired from Ochanomizu Univ. in the spring of 2002 after serving 31 years.[*1] He invited A. T. Balaban and M. Randic to Tokyo on this occasion, where Balaban declared that HH is the godfather of TI in his lecture at Ochanomizu [8]. As a matter of fact, most of the audience there didn't know the true meaning of "godfather" in Christianity but seemed to relate HH to the famous Mafia.

In September of 2002 the special issue in honor of HH was published in Inter-electronic J. of Molecular Design for which J.-I. Aihara was nominated as the guest editor [11]. On top of this issue Ref. [1] by HH is printed. Many distinguished mathematical chemists are contributing to it, such as A. T. Balaban, J. Gasteiger, N. F. Zefirov, N. Trinajstic, O. Ivanciuc, Y. Jiang, etc. All of the 50 contributed papers can freely be downloaded.

In October of 2002 International Symposium on Thirty-First Year of the Topological Index was organized by U. Nagashima and K. Takano in Tokyo. Main Guests were: J-I Aihara, S. Fujita, A. Graovac, I. Gutman, S. Basak, and K. Funatsu.

§ 3 Topological index versus molecular descriptor

As introduced above the term "topological index" is a sloppy Japanese English invented by HH. Although there were proposed other names such as "molecular descriptor" by some groups of mathematical chemists [12,13], TI was gradually prevailing until now. The reason why HH is appreciating this big but invisible movement is as follows. If in the early stage such as in 1970's or 1980's the term molecular descriptor prevailed, almost no mathematicians got interested into such a fantastic world of TI, and as a result the new journal MATI would not be born out.

Although the Wiener index w is now known as the first TI, Wiener himself was concerned only with acyclic hydrocarbon molecules, or tree-graphs [2]. While his original definition of the path number w can be applied only to trees, HH redefined it by using the distance matrix **D**, which can commonly be applied to tree and non-tree graphs as in his first TI paper [4]. Due to this HH paper Wiener's w could gain such monumental position to date that is attracting the interest of many scientists including mathematicians.

The string of fate connecting HH and Wiener was still continuing up to 1988, when HH wrote a paper "On some counting polynomials in chemistry" in Discrete Applied Math. [14] where he proposed the following polynomial,

$$\mathrm{H}_{\mathrm{G}}(x) = \sum_{k=1}^{l} d_k x^k, \tag{6}$$

under the name of "Wiener polynomial," because the famous TI's of Wiener's w and p can formally be derived as follows.

$$w = \mathrm{H}'_G(1) \tag{7}$$

and

$$p = \mathrm{H}'''(0)/6. \tag{8}$$

However, thanks to I. Gutman et al. this polynomial (6) is now widely called as "Hosoya polynomial" [15]. They might have considered the contribution of HH who opened the Pandora's box.

Though not directly related to this topics, HH began to play with the "distance polynomial" $\mathrm{S}_\mathrm{G}(x)$ as early as 1973, when he proposed to define this polynomial by using the distance matrix **D** for a given graph as [16]

$$\mathrm{S}_{\mathrm{G}}(x) = (-1)^N \det(\mathbf{D} - x\mathbf{E}). \tag{9}$$

However, in a few years later Graham and Lovasz quite independently proposed to define the same polynomial [17]. These coincidental proposals triggered their joint work to yield a joint letter [18], which was published in the very first issue of the J. Graph Theory edited by Frank Harary.

Although this was just a short letter of only three pages, it is one of the two monumental and important papers to HH that gave him the Erdös number of 2. Another one is a joint paper of HH and his academic uncle, Harary [19] on the perfect matching numbers of some interesting graphs, which, however, is not explained here.

§ 4 Various aspects of *Z*-index

In the beginning *Z*-index was found to have good correlation with several thermodynamic properties of saturated hydrocarbon molecules [4]. However, soon after that with a little modification it was shown to be well correlated also with the π-electronic energy $E\pi$ of conjugated hydrocarbon molecules [20]. This property comes from the fact that $E\pi$ of those molecules (either tree or non-tree) is determined from the zeros of the solution of $P_G(x)=0$. For trees $P_G(x)$ is closely related to Z through (1) and (2), whereas for non-trees we need such correction terms to (1) that are dependent on the degree of the ring structure. Thus in a global sense *Z*-index correlates roughly not only with various thermodynamic properties but also with π-electronic structure of molecules.

Now let us go back to more mathematical features about the *Z*-indices of various series of graphs. The *Z*-values of the path graphs S_n's are nothing else but the Fibonacci numbers, 1, 2, 3, 5, 8, ⋯, while those of the monocyclic rings C_n's starting from a triangle are the Lucas numbers, 4, 7, 11, 18, ⋯ [21]. These interesting properties are already introduced in the famous book by Koshy [22], together with the Hosoya triangle.

These interesting properties of *Z*-index are found to come from the close relationship between the two kinds of Chebyshev polynomials and the matching polynomials of path S_n and monocyclic ring graphs C_n. The second and first kinds of Chebyshev polynomials, U_n and T_n, are defined as follows [23]:

$$U_n(\cos\theta) = \sin(n+1)\theta / \sin\theta \tag{10}$$

and

$$T_n(\cos\theta) = \cos n\theta. \tag{11}$$

The matching polynomials of S_n and C_n graphs are obtained to be as given in Tables 1 and 2, respectively, which are compared to $U_n(x)$ and $T_n(x)$, respectively. Note the following equalities,

$$M_{Sn}(x) = U_n(x/2) \tag{12}$$

and

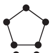
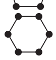
$$M_{Cn}(x) = 2\, T_n(x/2). \tag{13}$$

The sums of the absolute values of the coefficients of these two $M_G(x)$ polynomials are nothing else but the Fibonacci and Lucas numbers, respectively.

Table 1. S_n, U_n, and Fibonacci

S_n	$M_{S_n}(x) = U_n(x/2)$	$U_n(x)$	Z
ϕ	1	1	1
	x	$2x$	1
	$x^2 - 1$	$4x^2 - 1$	2
	$x^3 - 2x$	$8x^3 - 4x$	3
	$x^4 - 3x^2 + 1$	$16x^4 - 12x^2 + 1$	5
	$x^5 - 4x^3 + 3x$	$32x^5 - 32x^3 + 6x$	8
	$x^6 - 5x^4 + 6x^2 - 1$	$64x^6 - 80x^4 + 24x^2 - 1$	13

Table 2. C_n, T_n, and Lucas

C_n	$M_{C_n}(x) = 2T_n(x/2)$	$T_n(x)$	Z
ϕ	2	1	2
	x	x	1
	$x^2 - 2$	$2x^2 - 1$	3
	$x^3 - 3x$	$4x^3 - 3x$	4
	$x^4 - 4x^2 + 2$	$8x^4 - 8x^2 + 1$	7
	$x^5 - 5x^3 + 5x$	$16x^5 - 20x^3 + 5x$	11
	$x^6 - 6x^4 + 9x^2 - 2$	$32x^6 - 48x^4 + 18x^2 - 1$	18

There are two different types of Hermite polynomials as,

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \quad \text{(physicists')} \tag{14}$$

and

$$H_{e^n}(x) = (-1)^n e^{x^2/2} \frac{d^n}{dx^n} e^{-x^2/2} \quad \text{(probabilists') [24].} \tag{15}$$

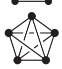
They are connected with each other as

$$H_{e^n}(x) = 2^{-n/2} H_n(x/\sqrt{2}). \tag{16}$$

According to Wolfram Mathworld, $H_{e^n}(x)$ is the independence (matching) polynomial of the complete graph K_n [25] as shown in Table 3. That is

$$M_{K_n}(x) = H_{e^n}(x). \tag{17}$$

Table 3. Complete graph K_n and Hermite polynomials.

n	K_n	$M_{K_n}(x) = H_{e^n}(x)$	$H_n(x)$	Z
0	ϕ	1	1	1
1		x	$2x$	1
2		$x^2 - 1$	$4x^2 - 2$	2
3		$x^3 - 3x$	$8x^3 - 12x$	4
4		$x^4 - 6x^2 + 3$	$16x^4 - 48x^2 + 12$	10
5		$x^5 - 10x^3 + 15x$	$32x^5 - 160x^3 + 120x$	26

In Table 3 are given the Z-values of K_n, which are found to be equal to the numbers of Young tableaux of size n, Y(n). Further, the $p(G,k)$ numbers for K_n just correspond to the partial set of $Y(n)$. For example see Fig. 1, where all the Young tableaux diagrams below n=5, are given together with the selection of non-adjacent edges for contributing to $p(G,k)$ counting in red bars. The readers can realize this property by checking the coefficients of the Z-counting polynomial $Q_{Kn}(x)$, or $M_{Kn}(x)$, for a given set of n and k.

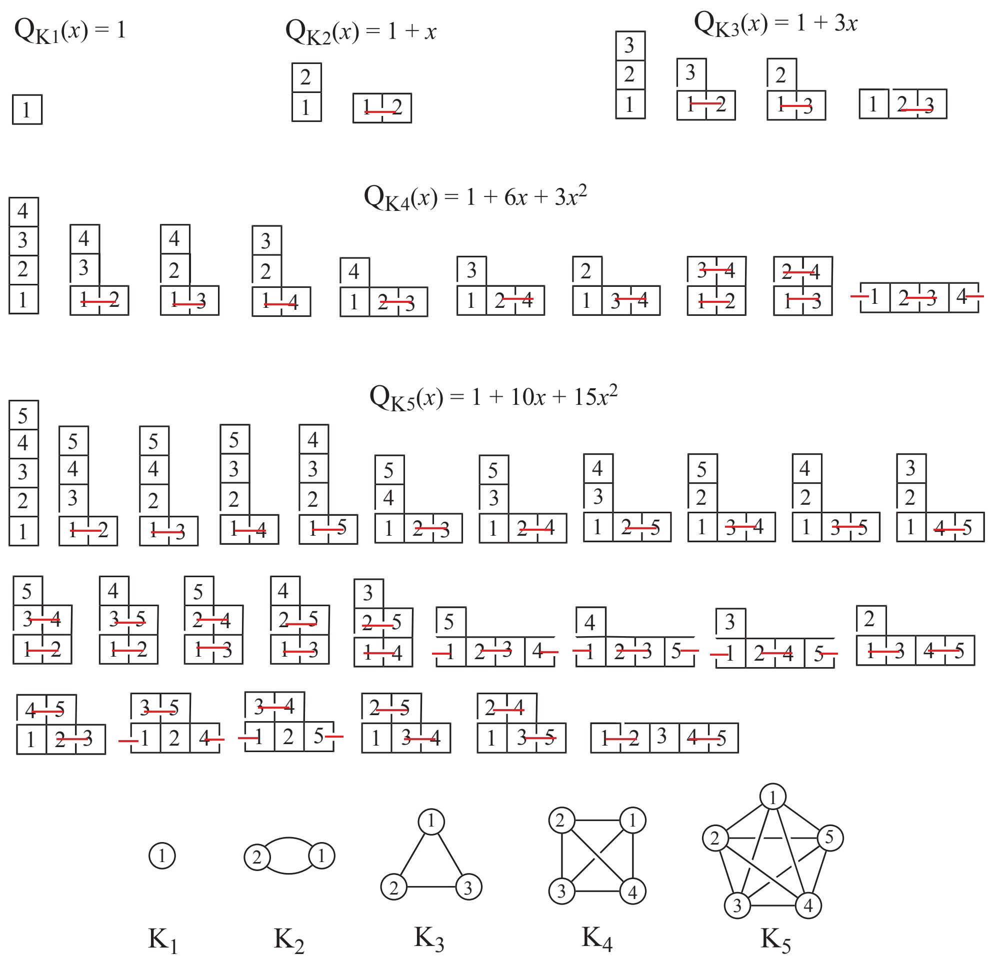


Fig. 1 Correlation between the $p(G,k)$ selection for K_n and construction of Young tableaux diagrams.

In this way matching polynomials for typical series of graphs are found to be closely related to some of the orthogonal polynomials [26]. This means that the concept of the $p(G,k)$ numbers and Z-index involves very important mathematical properties connecting between geometry and algebra. In this sense they are superior to other TI's.

On the other hand, from a global point of view Z-index can be proposed for using a rough sorting device for coding and classifying the structures of various kinds of graphs [27].

Renowned computer scientist A. Mowshowitz wrote a paper “The Hosoya entropy of a graph” with M. Dehmer, an information scientist [28]. They got a hint from the *Z*-index of HH, and defined the partial Hosoya polynomial and further Hosoya entropy. Further many other Hosoya items are introduced by them, such as, Hosoya equivalent, Hosoya profile, Hosoya graph decomposition, etc. On the other hand, T. Aurues, a medical doctor in Japan, wrote an interesting paper “The Fibonacci sequences in nature implies thermodynamic maximum entropy” in which he writes that Z-index might provide the maximum entropy values of molecular surface electrons [29]. These two papers suggest that *Z*-index has some potential features related to entropy.

Thus, in spite of its debut in the QSAR study of chemical substances *Z*-index of HH was found to be applied not only to mathematical but also to a wide variety of scientific problems. Then in 2012 HH decided to write a monograph of TI but in Nihongo dedicated solely to its mathematical aspects intentionally excluding chemical relevance [30]. For the interested readers the chapter titles will be introduced here.

§ 1 The basic series of numbers and polynomials.

§ 2 Graph theory and TI.

§ 3 Non-tree graphs and their TI’s.

§ 4 Pell equation and TI.

§ 5 Indefinite equation of Diophantos and TI.

§ 6 Pythagorean triangles and TI.

§ 7 Further development of TI.

More extensive and dramatic development is expected for TI’s. This is the final remark from HH.

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*1 $1936=44^2$. HH is declaring "I will survive at least until $2025=45^2$."

*2 HH retired Ochanomizu in 2002 after serving 31 years. Behold that $2002=2\times 7\times 11\times 13$ and $2+7+11+13=31$.

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ENERGY CONDITIONS FOR SOME HAMILTONIAN PROPERTIES OF GRAPHS

Rao Li

The energy of a graph is defined as the sum of the absolute values of the eigenvalues of the graph. In this note, we present energy conditions for some Hamiltonian properties of graphs.

1. INTRODUCTION

All the graphs considered in this note are undirected graphs without loops or multiple edges. Notation and terminology not defined here follow those in [**1**]. Let G be a graph of order n with e edges. We use $\delta = \delta(G)$ and $\Delta = \Delta(G)$ to denote the minimum and maximum degrees of G, respectively. The 2-degree, denoted $t(v)$, of a vertex v in G is defined as the sum of degrees of vertices adjacent to v. We use $T = T(G)$ to denote the maximum 2-degree of G. Obviously, $T(G) \leq (\Delta(G))^2$. A bipartite graph G is called semiregular if all the vertices in the same vertex part of a bipartition of the vertex set of G have the same degree. The independence number, denoted $\alpha = \alpha(G)$, is defined as the size of the largest independent set in G. The eigenvalues $\mu_1(G) \geq \mu_2(G) \geq ... \geq \mu_n(G)$ of the adjacency matrix $A(G)$ of G are called the eigenvalues of G. The spread, denoted $Spr(G)$, of G is defined as $\mu_1(G) - \mu_n(G)$. The energy, denoted $Eng(G)$, of G is defined as $\sum_{i=1}^{n} |\mu_i(G)|$ (see [**5**]). A cycle C in a graph G is called a Hamiltonian cycle of G if C contains all the vertices of G. A graph G is called Hamiltonian if G has a Hamiltonian cycle. A path P in a graph G is called a Hamiltonian path of G if P contains all the vertices of G. A graph G is called traceable if G has a Hamiltonian path. In this note, we will present energy conditions for Hamiltonicity and traceability of graphs. The main results are as follows.

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Keywords and Phrases. energy, Hamiltonian properties.

Theorem 1. Let G be a k-connected ($k \geq 2$) graph with $n \geq 3$ vertices and e edges. If

$$Eng(G) \geq 2\sqrt{e} + \sqrt{2(n-2)\left(e + \sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor} - \frac{2\delta^2(k+1)}{n-k-1}\right)},$$

then G is Hamiltonian or G is $K_{k,\,k+1}$ with $n = 2k+1$.

Theorem 2. Let G be a k-connected graph with $n \geq 2$ vertices and e edges. If

$$Eng(G) \geq 2\sqrt{e} + \sqrt{2(n-2)\left(e + \sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor} - \frac{2\delta^2(k+2)}{n-k-2}\right)},$$

then G is traceable.

2. LEMMAS

In order to prove Theorems 1 and 2, we need the following lemmas. Lemma 1 below is Theorem 1.5 on Page 26 in [**4**].

Lemma 1. [**4**] *For a graph G with n vertices and e edges,*

$$Spr(G) \leq \mu_1 + \sqrt{2e - \mu_1^2} \leq 2\sqrt{e}.$$

Equality holds throughout if and only if equality holds in the first inequality; equivalently, if and only if $e = 0$ or G is $K_{a,\,b}$ for some a, b with $e = ab$ and $a + b \leq n$.

Lemma 2 below is Corollary 3.4 on Page 2731 in [**7**].

Lemma 2. [**7**] *Let G be a graph. Then $Spr(G) \geq 2\delta\sqrt{\frac{\alpha(G)}{n-\alpha(G)}}$. If equality holds, then G is a semiregular bipartite graph.*

Lemma 3 is Theorem 1 on Page 5 in [**2**].

Lemma 3. [**2**] *Let G be a connected graph. Then $\mu_1 \leq \sqrt{T(G)}$ with equality if and only if G is either a regular graph or a semiregular bipartite graph.*

Lemma 4 follows from Proposition 2 on Page 174 in [**3**].

Lemma 4. [**3**] *Let G be a graph. Then $\mu_n \geq -\sqrt{\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor}$ with equality if and only if G is $K_{\lceil\frac{n}{2}\rceil,\lfloor\frac{n}{2}\rfloor}$.*

3. PROOFS

Proof of Theorem 1. Let G be a graph satisfying the conditions in Theorem 1. Suppose, to the contrary, that G is not Hamiltonian. Since G is k-connected ($k \geq 2$), G has a cycle. Choose a longest cycle C in G and give an orientation on C. Since G is not Hamiltonian, there exists a vertex $u_0 \in V(G) - V(C)$. By Menger's theorem, we can find s ($s \geq \kappa$) pairwise disjoint (except for u_0) paths P_1, P_2, ..., P_s between u_0 and $V(C)$. Let v_i be the end vertex of P_i on C, where $1 \leq i \leq s$. Without loss of generality, we assume that the appearance of v_1, v_2, ..., v_s agrees with the orientation of C. We use v_i^+ to denote the successor of v_i along the orientation of C, where $1 \leq i \leq s$. Since C is a longest cycle in G, we have that $v_i^+ \neq v_{i+1}$, where $1 \leq i \leq s$ and the index $s+1$ is regarded as 1. Moreover, $S := \{u_0, v_1^+, v_2^+, ..., v_s^+\}$ is independent (otherwise G would have cycles which are longer than C). Then $\alpha \geq s+1 \geq k+1$.

Some proof techniques in [**6**] will be used in the remainder of the proofs. From Cauchy-Schwarz inequality, we have that

$$Eng(G) = \sum_{i=1}^{n} |\mu_i| = |\mu_1| + |\mu_n| + \sum_{i=2}^{n-1} |\mu_i|$$

$$\leq \mu_1 - \mu_n + \sqrt{(n-2)\sum_{i=2}^{n-1} \mu_i^2}$$

$$= \mu_1 - \mu_n + \sqrt{(n-2)\left(\sum_{i=1}^{n} \mu_i^2 - \mu_1^2 - \mu_n^2\right)}$$

$$= \mu_1 - \mu_n + \sqrt{(n-2)(2e - (\mu_1 - \mu_n)^2 - 2\mu_1\mu_n)}.$$

Then by Lemmas 1, 2, 3, 4, $\alpha \geq k+1$ and assumptions of Theorem 1, we have that

$$2\sqrt{e} + \sqrt{2(n-2)\left(e + \sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor} - \frac{2\delta^2(k+1)}{n-k-1}\right)}$$

$$\leq Eng(G) \leq$$

$$2\sqrt{e} + \sqrt{(n-2)\left(2e + 2\sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor} - \frac{4\delta^2\alpha}{n-\alpha}\right)}$$

$$\leq 2\sqrt{e} + \sqrt{2(n-2)\left(e + \sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor} - \frac{2\delta^2(s+1)}{n-s-1}\right)}$$

$$\leq 2\sqrt{e} + \sqrt{2(n-2)\left(e + \sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor} - \frac{2\delta^2(k+1)}{n-k-1}\right)}.$$

Thus

$$Eng(G) = 2\sqrt{e} + \sqrt{2(n-2)\left(e + \sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor} - \frac{2\delta^2(k+1)}{n-k-1}\right)}.$$

Therefore, $\mu_2 = \cdots = \mu_{n-1}$, $Spr(G) = 2\sqrt{e} = 2\delta\sqrt{\frac{\alpha}{n-\alpha}}$, $\alpha = s+1 = k+1$, $\mu_1 = T$, and $\mu_n = -\sqrt{\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor}$. In view of Lemmas 1, 2, 3, 4, we have that S is a largest independent set of size $\alpha = k+1$ and G is $K_{\lceil\frac{n}{2}\rceil,\lfloor\frac{n}{2}\rfloor}$.

If n is even, then G is $K_{r,r}$ where $n = 2r$ for some integer $r \geq 2$. Thus $r = \alpha = k+1$ and G is Hamiltonian, a contradiction.

If n is odd, then G is $K_{r,r+1}$ where $n = 2r+1$ for some integer $r \geq 2$. Thus $r+1 = \alpha = k+1$ and G $K_{k,k+1}$ with $n = 2k+1$.

This completes the proof of Theorem 1. □

Proof of Theorem 2. Let G be a graph satisfying the conditions in Theorem 2. Suppose, to the contrary, that G is not traceable. Choose a longest path P in G and give an orientation on P. Let x and y be the two end vertices of P. Since G is not traceable, there exists a vertex $u_0 \in V(G) - V(P)$. By Menger's theorem, we can find s ($s \geq k$) pairwise disjoint (except for u_0) paths P_1, P_2, ..., P_s between u_0 and $V(P)$. Let v_i be the end vertex of P_i on P, where $1 \leq i \leq s$. Without loss of generality, we assume that the appearance of v_1, v_2, ..., v_s agrees with the orientation of P. Since P is a longest path in G, $x \neq v_i$ and $y \neq v_i$, for each i with $1 \leq i \leq s$, otherwise G would have paths which are longer than P. We use v_i^+ to denote the successor of v_i along the orientation of P, where $1 \leq i \leq s$. Since P is a longest path in G, we have that $v_i^+ \neq v_{i+1}$, where $1 \leq i \leq s-1$. Moreover, $S := \{u_0, v_1^+, v_2^+, ..., v_s^+, x\}$ is independent (otherwise G would have paths which are longer than P). Then $\alpha \geq s+2 \geq k+2$.

Using the proofs which are similar to the ones in Proof of Theorem 1, we have that

$$2\sqrt{e} + \sqrt{2(n-2)\left(e + \sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor} - \frac{2\delta^2(k+2)}{n-k-2}\right)}$$

$$\leq Eng(G) \leq$$

$$2\sqrt{e} + \sqrt{(n-2)\left(2e + 2\sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor} - \frac{4\delta^2\alpha}{n-\alpha}\right)}$$

$$\leq 2\sqrt{e} + \sqrt{2(n-2)\left(e + \sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor} - \frac{2\delta^2(s+2)}{n-s-2}\right)}$$

$$\leq 2\sqrt{e}+\sqrt{2(n-2)\left(e+\sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor}-\frac{2\delta^2(k+2)}{n-k-2}\right)}.$$

Thus

$$Eng(G)=2\sqrt{e}+\sqrt{2(n-2)\left(e+\sqrt{T\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor}-\frac{2\delta^2(k+2)}{n-k-2}\right)}.$$

Therefore, $\mu_2=\cdots=\mu_{n-1}$, $Spr(G)=2\sqrt{e}=2\delta\sqrt{\frac{\alpha}{n-\alpha}}$, $\alpha=s+2=k+2$, $\mu_1=T$, and $\mu_n=-\sqrt{\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor}$. In view of Lemmas 1, 2, 3, 4, we have that S is a largest independent set of size $\alpha=k+2$ and G is $K_{\lceil\frac{n}{2}\rceil,\lfloor\frac{n}{2}\rfloor}$.

If n is even, then G is $K_{r,r}$ where $n=2r$ for some integer r. Thus $r=\alpha=k+2$ and G is traceable, a contradiction.

If n is odd, then G is $K_{r,r+1}$ where $n=2r+1$ for some integer r. Thus $r+1=\alpha=k+2$ and G is $K_{k+1,k+2}$ with $n=2k+3$ and G is traceable, a contradiction.

This completes the proof of Theorem 2. □

Notice that $\mu_1\leq\sqrt{T}\leq\Delta$ and G is regular when $\mu_1=\Delta$. Thus Theorem 1 and Theorem 2 have the following Corollary 1 and Corollary 2, respectively.

Corollary 1. Let G be a k-connected ($k\geq 2$) graph with $n\geq 3$ vertices and e edges. If

$$Eng(G)\geq 2\sqrt{e}+\sqrt{2(n-2)\left(e+\sqrt{\Delta\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor}-\frac{2\delta^2(k+1)}{n-k-1}\right)},$$

then G is Hamiltonian.

Corollary 2. Let G be a k-connected graph with $n\geq 2$ vertices and e edges. If

$$Eng(G)\geq 2\sqrt{e}+\sqrt{2(n-2)\left(e+\sqrt{\Delta\lceil\frac{n}{2}\rceil\lfloor\frac{n}{2}\rfloor}-\frac{2\delta^2(k+2)}{n-k-2}\right)},$$

then G is traceable.

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NEW BOUNDS FOR THE HARARY ENERGY AND HARARY ESTRADA INDEX OF GRAPHS

Akbar Jahanbani

The harary index is defined as the sum of reciprocal distances between all pairs of vertices in a nontrivial connected graph. In this paper, we establish upper and lower bounds for the harary energy and harary Estrada index in terms of graph invariants such as the number of vertices, the number degree sequence and spectral radius.

1. INTRODUCTION

Let G be a simple, undirected, connected graph with n vertices and m edges. Let the vertices of G be labeled as $v_1, v_2, \ldots, v_n$. 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. The *eigenvalues* of $A(G)$ are the adjacency eigenvalues of G, they are labeled as $\lambda_1, \lambda_2, \ldots, \lambda_n$. These form the adjacency spectrum of G [**3**]. Thus

$$detA = \prod_{i=1}^{n} \lambda_i.$$

The *rank* matrix of A is the maximal number of linearly independent column vectors in A. The *distance* between the vertices v_i and v_j, denoted by d_{ij}, is the length of the shortest path joining v_i and v_j. The harary matrix [**13**] of a graph G is a square matrix $\mathsf{H} = [\mathsf{H}_{ij}]$ of order n, where

$$h_{ij} = \begin{cases} \frac{1}{d_{ij}} & \text{if } i \neq j \\ 0 & \text{if } i = j. \end{cases}$$

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The eigenvalues of $\mathsf{H}(G)$ labeled as $\rho_1 \geqslant \rho_2 \geqslant \cdots \geqslant \rho_n$ are said to be the harary eigenvalues or H-*eigenvalues* of G and their collection is called harary spectrum or H-*spectrum* of G. harary matrix (also called as reciprocal distance matrix [**22**]) of a graph was introduced by Ivanciuc et al. In [**13**] which has in use the study of molecules in $QSPR$ (quantitative structure property relationship) models [**13**]. Two non-isomorphic graphs are said to be H- *cospectral* if they have same H-*spectra*. The results on H-*eigenvalues* of a graph are obtained in [**2, 4, 7, 12, 26**]. The details about ordinary graph *energy* can be found in [**23**]. Bounds for the harary energy of a graph are reported in [**1, 2, 8**].
The paper is organized as follows. In Section 2, we give a list of some previously known results. In Section 3, we present bounds on the harary energy. In Section 4, we present bounds on the harary Estrada index.

2. PRELIMINARIES AND KNOWN RESULTS

In this section, we shall list some previously known results that will be needed in the next sections. Recall that [**8**] for a graph with harary eigenvalues $\rho_1, \rho_2, \ldots, \rho_n$, $N_k = tr(\mathsf{H}^k) = \sum_{i=1}^{n} (\rho_i)^k$.

$$N_0 = n, \tag{1}$$

$$N_1 = tr(\mathsf{H}) = 0, \tag{2}$$

$$N_2 = tr(\mathsf{H}^2) = 2\kappa. \tag{3}$$

Where

$$\kappa = \sum_{1\leqslant i\leqslant j\leqslant n} (\frac{1}{d_{ij}})^2.$$

Now let us present the following lemma as the first preliminary result.

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

$$N_3 = tr(\mathsf{H}^3) = 2 \sum_{1\leqslant i<j\leqslant n} \frac{1}{(d_{ij})^2} \Bigg(\sum_{\substack{1\leqslant i<k\leqslant n\\ 1\leqslant k<j\leqslant n}} \frac{1}{(d_{ik})(d_{kj})} \Bigg). \tag{4}$$

$$N_4 = tr(\mathsf{H}^4) = \sum_{i=1}^{n} \Bigg(\sum_{j=1}^{n} \frac{1}{(d_{ij})^2} \Bigg)^2 + \sum_{1\leqslant i<j\leqslant n} \frac{1}{(d_{ij})^2} \Bigg(\sum_{\substack{1\leqslant i<k\leqslant n\\ 1\leqslant k<j\leqslant n}} \frac{1}{(d_{ik})(d_{kj})} \Bigg)^2. \tag{5}$$

Proof. By definition, the diagonal elements and for $i = 1, 2, ..., n$, the (i, i)-entry of $[\mathsf{H}(G)]^2$ is equal to

$$(\mathsf{H}^2)_{ij} = \sum_{j=1}^{n} \mathsf{H}_{ij}\mathsf{H}_{ji} = \sum_{j=1}^{n} (\mathsf{H}_{ij})^2 = \sum_{j=1}^{n} (\mathsf{H}_{ij})^2 = \sum_{j=1}^{n} \frac{1}{(d_{ij})^2}.$$

Hence

$$(\mathsf{H}^2)_{ij} = \sum_{j=1}^{n} \mathsf{H}_{ij}\mathsf{H}_{ji} = \mathsf{H}_{ii}\mathsf{H}_{ij} + \mathsf{H}_{ij}\mathsf{H}_{jj} + \sum_{\substack{1 \leqslant i<k \leqslant n \\ 1 \leqslant k<j \leqslant n}} \mathsf{H}_{ik}\mathsf{H}_{kj} = \frac{1}{(d_{ij})}\Bigg(\sum_{\substack{1 \leqslant i<k \leqslant n \\ 1 \leqslant k<j \leqslant n}} \frac{1}{(d_{ik})(d_{kj})}\Bigg).$$

Since the diagonal elements of H^3 are

$$(\mathsf{H}^3)_{ii} = \sum_{j=1}^{n} \mathsf{H}_{ij}(\mathsf{H}^2)_{jk} = \sum_{1 \leqslant i<j \leqslant n} \frac{1}{(d_{ij})}(\mathsf{H}^2)_{ij} = \sum_{1 \leqslant i<j \leqslant n} \frac{1}{(d_{ij})^2}\Bigg(\sum_{\substack{1 \leqslant i<k \leqslant n \\ 1 \leqslant k<j \leqslant n}} \frac{1}{(d_{ik})(d_{kj})}\Bigg)$$

we obtain

$$tr(\mathsf{H}^3) = \sum_{i=1}^{n} \sum_{1 \leqslant i<j \leqslant n} \frac{1}{(d_{ij})^2}\Bigg(\sum_{\substack{1 \leqslant i<k \leqslant n \\ 1 \leqslant k<j \leqslant n}} \frac{1}{(d_{ik})(d_{kj})}\Bigg) = 2\sum_{1 \leqslant i<j \leqslant n} \frac{1}{(d_{ij})^2}\Bigg(\sum_{\substack{1 \leqslant i<k \leqslant n \\ 1 \leqslant k<j \leqslant n}} \frac{1}{(d_{ik})(d_{kj})}\Bigg).$$

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

$$\begin{aligned} tr(\mathsf{H}^4) &= \sum_{i,j=1}^{n} \mid (\mathsf{H}^2)_{ii} \mid^2 = \sum_{j=1}^{n} \mid (\mathsf{H}^2)_{ii} \mid^2 + \sum_{1 \leqslant i<j \leqslant n} \mid (\mathsf{H}^2)_{ij} \mid^2 \\ &= \sum_{i=1}^{n}\Bigg(\sum_{j=1}^{n} \frac{1}{(d_{ij})^2}\Bigg)^2 + \sum_{1 \leqslant i<j \leqslant n} \frac{1}{(d_{ij})^2}\Bigg(\sum_{\substack{1 \leqslant i<k \leqslant n \\ 1 \leqslant k<j \leqslant n}} \frac{1}{(d_{ik})(d_{kj})}\Bigg)^2. \end{aligned}$$

□

For any square matrix A we denote by $\rho_1(A)$ its spectral radius $\rho_1(A) = max[\mid \lambda \mid : \lambda \text{ is an eigenvalue for} A]$. We obtain lower bounds for ρ_1.

Lemma 2. *[**24**] Let A be a real matrix with $r = rank(A) \geqslant 2$. If $tr(A^2) \geqslant \frac{(tr(A))^2}{r}$, then*

$$\rho(A) \geqslant \frac{\mid tr(A) \mid}{r} + \sqrt{\frac{[tr(A^2) - (\frac{1}{r})(tr(A))^2]}{(r(r-1))}}.$$

Lemma 3. *[**25**] If $x_1, x_2, \ldots, x_n$ are real numbers such that*

$$x_n \leqslant x_{n-1} \leqslant \cdots \leqslant x_2 \leqslant x_1,$$

then

$$\frac{\sum_{i=1}^{n} x_i}{n} + \sqrt{\frac{1}{n(n-1)} \sum_{i=1}^{n} \left(x_i - \frac{\sum_{i=1}^{n} x_i}{n} \right)^2} \leqslant x_1.$$

Lemma 4. *[25] Let $y_1, y_2, \ldots, y_n$ are real numbers and k is any positive integer, then*

$$\left(\frac{\sum_{i=1}^{n} y_i^{2k}}{n} + \sqrt{\frac{1}{n(n-1)} \sum_{i=1}^{n} \left(y_i - \frac{\sum_{i=1}^{n} y_i^{2k}}{n} \right)^2} \right)^{\frac{1}{2k}} \leqslant \max_i \mid y_i \mid .$$

By equations (2), (3) and Lemma 2, we can obtain follow lemma.

Lemma 5. *Let G be a graph with n vertices, $r = rank(\mathsf{H}) \geqslant 2$ and $\rho_1 \geqslant \rho_2 \geqslant \cdots \geqslant \rho_n$ be its eigenvalues of the harary matrix H.*
If $tr(\mathsf{H}^2) \geqslant \frac{(tr(\mathsf{H}))^2}{r}$, then

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{r(r-1)}}.$$

Now equations (2), (3) and Lemma 3, we can obtain follow lemma.

Lemma 6. *Let G be a graph with n vertices and $\rho_1 \geqslant \rho_2 \geqslant \cdots \geqslant \rho_n$ be its eigenvalues of the harary matrix H. Then*

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{n(n-1)}}.$$

By equations (2), (3), (5) and Lemma 4 (for k=1) , we can obtain follow lemma.

Lemma 7. *Let G be a graph with n vertices and $\rho_1 \geqslant \rho_2 \geqslant \cdots \geqslant \rho_n$ be its eigenvalues of the harary matrix H. Then*

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)} \left(N_4 - \frac{4\kappa}{n} \right)}}.$$

Lemma 8. *Let G be a graph of order n. Then*

$$\mathsf{H}E(G) \leqslant \sqrt{2n\kappa}.$$

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

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

assuming, $a_i = 1$, $b_i = \mid \rho_i \mid$ and equation (3), we have

$$\left(\sum_{i=1}^{n} \mid \rho_i \mid \right)^2 \leqslant n \left(\sum_{i=1}^{n} \mid \rho_i \mid^2 \right) = n \sum_{i=1}^{n} (\rho_i)^2 = 2n \sum_{1 \leqslant i \leqslant j \leqslant n} (\frac{1}{d_{ij}})^2.$$

Therefore
$$\mathsf{H}E(G) \leqslant \sqrt{2n\kappa}.$$
□

3. BOUNDS FOR THE HARARY ENERGY OF GRAPHS

In this section, we obtain bounds for the harary energy in terms of number of vertices, determinant of the adjacency matrix and *distance* between the vertices of graph G.
The *energy* of the graph G is defined as:

$$E = E(G) = \sum_{i=1}^{n} \mid \lambda_i \mid . \tag{6}$$

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. [**10, 11**]. Since then, numerous other bounds for energy were found (see, e.g. [**9, 17, 18, 19**]).
The harary energy of a (molecular) graph G was introduced by Güngör et al. [**8**] as follows:
$$\mathsf{H}E(G) = \sum_{i=1}^{n} \mid \rho_i \mid,$$
where $\rho_1, \rho_2, \ldots, \rho_n$ are eigenvalues of the harary matrix. We start by proving some lower bounds for this energy of graphs.

Theorem 1. *Let G be a graph of order n with m edges such that $2m \geqslant n$. Then*
$$\mathsf{H}E(G) \geqslant \sqrt{\frac{2\kappa}{n(n-1)}} + (n-1)\left(\frac{|det\mathsf{H}|}{\sqrt{\frac{2\kappa}{n(n-1)}}}\right)^{\frac{1}{(n-1)}}.$$

Proof. Starting with the *arithmetic-geometric* mean inequality, we have
$$\mathsf{H}E(G) = \rho_1 + \sum_{i=2}^{n} \mid \rho_i \mid \geqslant \rho_1 + (n-1)\left(\prod_{i=2}^{n} \mid \rho_i \mid\right)^{\frac{1}{(n-1)}}$$
$$= \rho_1 + (n-1)\left(\frac{|det\mathsf{H}|}{\rho_1}\right)^{\frac{1}{(n-1)}}.$$

Now we consider the function
$$f(x) = x + (n-1)\left(\frac{|det\mathsf{H}|}{x}\right)^{\frac{1}{(n-1)}}.$$

Note that f is increasing for $x \geqslant \left(|det\mathsf{H}|\right)^{\frac{1}{n(n-1)}}$. As well known from Lemma 6,

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{n(n-1)}}.$$

Moreover, by Lemma 8 and the *arithmetic geometric* mean inequality, we have

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{n(n-1)}} \geqslant \frac{\mathsf{H}E(G)}{n(n-1)} = \frac{\sum_{i=1}^{n} | \rho_i |}{n(n-1)} \geqslant \left(|det\mathsf{H}|\right)^{\frac{1}{n(n-1)}}.$$

Therefore

$$\mathsf{H}E(G) \geqslant \sqrt{\frac{2\kappa}{n(n-1)}} + (n-1)\left(\frac{|det\mathsf{H}|}{\sqrt{\frac{2\kappa}{n(n-1)}}}\right)^{\frac{1}{(n-1)}}.$$

□

Theorem 2. *Let G be a graph of order n with m edges such that $2m \geqslant n$. Then*

$$\mathsf{H}E(G) \geqslant \sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)}\left(N_4 - \frac{4\kappa}{n}\right)}} + (n-1)\left(\frac{|det\mathsf{H}|}{\sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)}\left(N_4 - \frac{4\kappa}{n}\right)}}}\right)^{\frac{1}{(n-1)}}.$$

Proof. Starting with the *arithmetic*-*geometric* mean inequality, we have

$$\begin{aligned} \mathsf{H}E(G) = \rho_1 + \sum_{i=2}^{n} | \rho_i | &\geqslant \rho_1 + (n-1)\left(\prod_{i=2}^{n} | \rho_i |\right)^{\frac{1}{(n-1)}} \\ &= \rho_1 + (n-1)\left(\frac{|det\mathsf{H}|}{\rho_1}\right)^{\frac{1}{(n-1)}}. \end{aligned}$$

Now we consider the function

$$f(x) = x + (n-1)\left(\frac{|det\mathsf{H}|}{x}\right)^{\frac{1}{(n-1)}}.$$

Note that f is increasing for $x \geqslant \left(|det\mathsf{H}|\right)^{\frac{1}{n}}$. As well known from Lemma 7, for $k = 1$

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)}\left(N_4 - \frac{4\kappa}{n}\right)}}.$$

Moreover, by Lemma 8 and the *arithmetic geometric* mean inequality, we have

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)}\left(N_4 - \frac{4\kappa}{n}\right)}} \geqslant \sqrt{\frac{2\kappa}{n}}$$
$$\geqslant \frac{\mathsf{H}E(G)}{n} \geqslant \Big(|det\mathsf{H}|\Big)^{\frac{1}{n}}.$$

Therefore

$$\mathsf{H}E(G) \geqslant \sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)}\left(N_4 - \frac{4\kappa}{n}\right)}}$$
$$+ (n-1)\left(\frac{|det\mathsf{H}|}{\sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)}\left(N_4 - \frac{4\kappa}{n}\right)}}}\right)^{\frac{1}{(n-1)}}.$$

□

Theorem 3. *Let G be a graph of order n with m edges such that $2m \geqslant n$ and $rank(\mathsf{H}) = r \geqslant 2$. Then*

$$\mathsf{H}E(G) \geqslant \sqrt{\frac{2\kappa}{r(r-1)}} + (n-1)\left(\frac{|det\mathsf{H}|}{\sqrt{\frac{2\kappa}{r(r-1)}}}\right)^{\frac{1}{(n-1)}}.$$

Proof. Starting with the *arithmetic-geometric* mean inequality, we have

$$\mathsf{H}E(G) = \rho_1 + \sum_{i=2}^{n} |\ \rho_i\ | \geqslant \rho_1 + (n-1)\Big(\prod_{i=2}^{n} |\ \rho_i\ |\Big)^{\frac{1}{(n-1)}}$$
$$= \rho_1 + (n-1)\Big(\frac{|det\mathsf{H}|}{\rho_1}\Big)^{\frac{1}{(n-1)}}.$$

Now we consider the function

$$f(x) = x + (n-1)\Big(\frac{|det\mathsf{H}|}{x}\Big)^{\frac{1}{(n-1)}}.$$

Note that f is increasing for $x \geqslant \Big(|det\mathsf{H}|\Big)^{\frac{1}{n(n-1)}}$. As well known from Lemma 5,

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{r(r-1)}}.$$

Moreover, by Lemma 8 and the *arithmetic geometric* mean inequality, we have

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{r(r-1)}} \geqslant \frac{\mathsf{H}E(G)}{r(r-1)} = \frac{\sum_{i=1}^{n} |\rho_i|}{r(r-1)} \geqslant \frac{\sum_{i=1}^{n} |\rho_i|}{n(n-1)} \geqslant \Big(|det\mathsf{H}|\Big)^{\frac{1}{n(n-1)}}.$$

Therefore

$$\mathsf{H}E(G) \geqslant \sqrt{\frac{2\kappa}{r(r-1)}} + (n-1)\left(\frac{|det\mathsf{H}|}{\sqrt{\frac{2\kappa}{r(r-1)}}}\right)^{\frac{1}{(n-1)}}.$$

□

4. BOUNDS FOR THE HARARY ESTRADA INDEX OF GRAPHS

In this section, we obtain lower bounds for the harary Estrada index in terms of number of vertices and *distance* between the vertices of graph G. 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

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

In fact *Estrada index* of graphs has an important role in *Chemistry* and *Physics* and there exists a vast *litarature* that studies this special index. In addition to the Estrada's papers depicted above, we may also refer[**5, 6, 14, 15, 16, 20, 21**] to the reader for detail informations such as lower and upper bounds for EE in terms of the number of vertices and edges, and some inequalities between EE and the energy of G. The harary Estrada index of G, was introduced in [**8**] as follows:

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

We begin this section with theorem as follows:

Theorem 4. *Let G be a graph of order $n \geqslant 2$. Then*

$$\mathsf{H}EE(G) \geqslant e^{\left(\sqrt{\frac{2\kappa}{n(n-1)}}\right)} + \frac{n-1}{e^{\left(\sqrt{\frac{2\kappa}{n(n-1)}}\right)}}.$$

Proof. By definition of harary Estrada index, we have

$$\begin{aligned} \mathsf{H}EE(G) &= e^{\rho_1} + e^{\rho_2} + \cdots + e^{\rho_n} \\ &\geqslant e^{\rho_1} + (n-1)\left(\prod_{i=2}^{n}\right)^{\frac{1}{n-1}} \\ &\geqslant e^{\rho_1} + (n-1)e^{\frac{\sum_{i=2}^{n} e^{\rho_i}}{n-1}} \\ &= e^{\rho_1} + (n-1)e^{\frac{-\rho_1}{n-1}}. \end{aligned} \tag{7}$$

Now let us consider a function

$$f(x) = e^{x} + \frac{n-1}{e^{\frac{x}{n-1}}}, \qquad for \quad x > 0.$$

Therefore f is an increasing function for $x > 0$. By Lemma 6, we have

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{n(n-1)}}.$$

From Inequality (7), we get

$$\mathsf{H}EE(G) \geqslant e^{\left(\sqrt{\frac{2\kappa}{n(n-1)}}\right)} + \frac{n-1}{e^{\left(\sqrt{\frac{2\kappa}{n(n-1)}}\right)}}.$$

□

Theorem 5. *Let G be a graph of order $n \geqslant 2$ and $r = rank(A) \geq 2$. Then*

$$\mathsf{H}EE(G) \geqslant e^{\left(\sqrt{\frac{2\kappa}{r(r-1)}}\right)} + \frac{n-1}{e^{\left(\sqrt{\frac{2\kappa}{r(r-1)}}\right)}}.$$

Proof. By definition of harary Estrada index, we hav

$$\begin{aligned} \mathsf{H}EE(G) &= e^{\rho_1} + e^{\rho_2} + \cdots + e^{\rho_n} \\ &\geqslant e^{\rho_1} + (n-1)\left(\prod_{i=2}^{n}\right)^{\frac{1}{n-1}} \\ &\geqslant e^{\rho_1} + (n-1)e^{\frac{\sum_{i=2}^{n} e^{\rho_i}}{n-1}} \\ &= e^{\rho_1} + (n-1)e^{\frac{-\rho_1}{n-1}}. \end{aligned} \tag{8}$$

Now let us consider a function

$$f(x) = e^x + \frac{n-1}{e^{\frac{x}{n-1}}}, \qquad for \quad x > 0.$$

Therefore f is an increasing function for $x > 0$. By Lemma 5, we have

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{r(r-1)}}.$$

From Inequality (8), we get

$$\mathsf{H}EE(G) \geqslant e^{\left(\sqrt{\frac{2\kappa}{r(r-1)}}\right)} + \frac{n-1}{e^{\left(\sqrt{\frac{2\kappa}{r(r-1)}}\right)}}.$$

□

Theorem 6. *Let G be a graph of order $n \geqslant 2$. Then*

$$\mathsf{H}EE(G) \geqslant e^{\left(\sqrt{\frac{2\kappa}{n}+\sqrt{\frac{1}{n(n-1)}\left(N_4-\frac{4\kappa}{n}\right)}}\right)} + \frac{n-1}{e^{\left(\sqrt{\frac{2\kappa}{n}+\sqrt{\frac{1}{n(n-1)}\left(N_4-\frac{4\kappa}{n}\right)}}\right)}}.$$

Proof. By definition of harary Estrada index, we hav

$$\begin{aligned} \mathsf{H}EE(G) &= e^{\rho_1} + e^{\rho_2} + \cdots + e^{\rho_n} \\ &\geqslant e^{\rho_1} + (n-1)\left(\prod_{i=2}^{n}\right)^{\frac{1}{n-1}} \\ &\geqslant e^{\rho_1} + (n-1)e^{\frac{\sum_{i=2}^{n} e^{\rho_i}}{n-1}} \\ &= e^{\rho_1} + (n-1)e^{\frac{-\rho_1}{n-1}}. \end{aligned} \tag{9}$$

Now let us consider a function

$$f(x) = e^x + \frac{n-1}{e^{\frac{x}{n-1}}}, \qquad for \quad x > 0.$$

Therefore f is an increasing function for $x > 0$. By Lemma 7, we have

$$\rho_1 \geqslant \sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)}\left(N_4 - \frac{4\kappa}{n}\right)}}.$$

From Inequality (9), we get

$$\mathsf{H}EE(G) \geqslant e^{\left(\sqrt{\frac{2\kappa}{n}+\sqrt{\frac{1}{n(n-1)}\left(N_4-\frac{4\kappa}{n}\right)}}\right)} + \frac{n-1}{e^{\left(\sqrt{\frac{2\kappa}{n}+\sqrt{\frac{1}{n(n-1)}\left(N_4-\frac{4\kappa}{n}\right)}}\right)}}.$$

□

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