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New Bounds on the Incidence Energy, Randić Energy and Randić Estrada Index

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Abstract

For a simple graph G and a real number α $(\neq 0, 1)$ the graph invariant s_α is equal to the sum of powers of signless Laplacian eigenvalues of G. In this paper, we present some new bounds on s_α of graphs and improve some results which was obtained on bipartite graphs. As a result of these bounds, we also obtain the some improved results on incidence energy. In addition, we study on Randić energy (RE) and Randić Estrada index (REE) of (bipartite) graphs.

1 Introduction

Let G be a finite, simple and undirected graph with n vertices. Let $V(G) = \{v_1, v_2, ..., v_n\}$ be the vertex set of G.If any vertices v_i and v_j are adjacent, then we use the notation $v_i \sim v_j$. For $v_i \in V(G)$, the degree of the vertex v_i, denoted by d_i, is the number of the vertices adjacent to v_i.

The matrix $L(G) = D(G) - A(G)$ (resp., $Q(G) = D(G) + A(G)$) is called the Laplacian matrix [51, 52] (resp., the signless Laplacian matrix ([13]- [16])) of G, where

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$A(G)$ is the adjacency matrix and $D(G)$ is the diagonal matrix of the vertex degrees. Since $A(G)$, $L(G)$ and $Q(G)$ are all real symmetric matrices, their eigenvalues are real numbers. So, we can assume that $\lambda_1(G) \geq \lambda_2(G) \geq ... \geq \lambda_n(G)$ (resp., $\mu_1(G) \geq \mu_2(G) \geq ... \geq \mu_n(G)$, $q_1(G) \geq q_2(G) \geq ... \geq q_n(G)$) are the adjacency (resp., Laplacian, signless Laplacian) eigenvalues of G. It follows from the Geršgorin disc theorem that $L(G)$ and $Q(G)$ are semidefinite. Therefore, all Laplacian (resp., signless Laplacian) eigenvalues of G are nonnegative. If the graph G is a connected non-bipartite graph, then $\mu_i(G) > 0$ for $i = 1, 2, ..., n$ [13]. Moreover, G is bipartite graph if and only if $q_n = 0$ [12].

On one of the most remarkeble chemical applications of graph theory is based on the close correspondence between the graph eigenvalues and the molecular orbital energy levels of $\pi-$electrons in conjugated hydrocarbons. For the Hüchkel molecular orbital approximation, the total $\pi-$electron energy in conjugated hydrocarbons is given by the sum of absolute values of the eigenvalues corresponding to the molecular graph G in which the maximum degree is not more than four in general. The energy of G was defined by Gutman in [29] as

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

Research on graph energy is nowadays very active, as seen from the recent papers ([27, 28, 30, 31, 38, 39, 41, 44, 56, 61]), monograph [42], the references quoted therein.

The singular values of a real matrix (not necessarily square) M are the square roots of the eigenvalues of the matrix MM^T, where M^T denotes the transpose of M. Recently, Nikiforov [53] extended the concept of graph energy to any matrix M by defining the energy $E(M)$ to be the sum of singular values of M. Obviously, $E(G) = E(A(G))$.

Let $I(G)$ be the (vertex-edge) incidence matrix of the graph G. For a graph G with vertex set $\{v_1, v_2, ..., v_n\}$ and edge set $\{e_1, e_2, ..., e_n\}$, the (i, j)-entry of $I(G)$ is 0 if v_i is not incident with e_j and 1 if v_i is incident with e_j. Jooyandeh et al. [40] introduced the incidence energy IE of G, which is defined as the sum of the singular values of the incidence matrix of G. Gutman et al. [32] showed that

$$IE = IE(G) = \sum_{i=1}^{n} \sqrt{q_i(G)}\ .$$

Some basic properties of IE may be found in [32, 33, 40].

From (1), one can immediately get the incidence energy of a graph by computing the signless Laplacian eigenvalues of the graph. However, even for special graphs, it is still complicated to find the signless Laplacian eigenvalues of them. Hence, it makes sense to establish lower and upper bounds to estimate the invariant for some classes of graphs. Zhou [59] obtained the upper bounds for the incidence energy using the first Zagreb index. Gutman et al. [33] gave several lower and upper bounds for IE.

In [45] Liu and Lu introduced a new graph invariant based on Laplacian eigenvalues

$$LEL = LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i}$$

and called it Laplacian energy like invariant. At first it was considered that [45] LEL shares similar properties with Laplacian energy [34]. Then it was shown that it is much more similar to the ordinary graph energy [35]. For survey and details on LEL, see [46].

For a graph G with n vertices and a real number α, to avoid trivialities it may be required that $\alpha \neq 0, 1$, the sum of the αth powers of the non-zero Laplacian eigenvalues is defined as [60]

$$\sigma_\alpha = \sigma_\alpha(G) = \sum_{i=1}^{n-1} \mu_i^\alpha .$$

The cases $\alpha = 0$ and $\alpha = 1$ are trivial as $\sigma_0 = n - 1$ and $\sigma_1 = 2m$, where m is the number of edges of G. Note that $\sigma_{1/2}$ is equal to LEL. It is worth noting that $n\sigma_{-1}$ is also equal to the Kirchhoff index of G (one can refer to the papers [4, 36, 54] for its definition and extensive applications in the theory of electric circuits, probabilistic theory and chemistry). Recently, various properties and the estimates of σ_α have been well studied in the literature. For details, see [17, 47, 57, 59, 60].

Motivating the definitions of IE, LEL and σ_α, Akbari et al. [1] introduced the sum of the αth powers of the signless Laplacian eigenvalues of G as

$$s_\alpha = s_\alpha(G) = \sum_{i=1}^{n} q_i^\alpha \tag{1}$$

and they also gave some relations between σ_α and s_α. In this sum, the cases $\alpha = 0$ and $\alpha = 1$ are trivial as $s_0 = n$ and $s_1 = 2m$. Note that $s_{1/2}$ is equal to the incidence energy IE. Note further that Laplacian eigenvalues and signless Laplacian eigenvalues of bipartite graphs coincide [13, 51, 52]. Therefore, for bipartite graphs σ_α is equal to s_α [9] and LEL is equal to IE [32]. Recently some properties and the lower and upper bounds of s_α have been established in [1, 9, 43, 48].

The Randić matrix of G is the $n \times n$ matrix

$$\mathbf{R} = \mathbf{R}(G) = \begin{cases} \frac{1}{\sqrt{d_i d_j}}, \text{ if } v_i \sim v_j \\ 0, \text{ otherwise.} \end{cases}$$

The Randić eigenvalues $\rho_1, \rho_2, ..., \rho_n$ of the graph G are the eigenvalues of its Randić matrix. Since $R(G)$ is real symmetric matrix, its eigenvalues are real number. So we can order them so that $\rho_1 \geq \rho_2 \geq ... \geq \rho_n$.

The Randić energy of the graph G is defined in [5, 6] as:

$$RE = RE(G) = \sum_{i=1}^{n} |\rho_i| . \tag{2}$$

The Estrada index of the graph G is defined in [22]- [25] as:

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

The Estrada index of graphs has an important role in Chemistry an Physics. For more detailed information we refer to the reader [22]- [25]. In addition, there exist a vast literature that studies Estrada index and its bounds. For detailed information we may also refer to the reader [19], [21], [49], [55].

Then the Randić Estrada index of the graph G is defined in [7] as:

$$REE = REE(G) = \sum_{i=1}^{n} e^{\rho_i}. \tag{3}$$

Research on graph energy is nowadays very active, as seen from the recent papers [39]- [44], [53]- [61] monograph [42], the references quoted therein. Moreover properties of Randić energy can be found in [5]- [7], [19], [26], [37].

At the outset we note that

$$REE = REE(G) = \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{i=1}^{n} \rho_i^k,$$

where the standard notational convention that $0^0 = 1$ is used.

Recall that the general Randić index of a graph G is defined in [3] as

$$R_\alpha = R_\alpha(G) = \sum_{v_i \sim v_j} (d_i d_j)^\alpha ,$$

where the summation is over all edges $v_i v_j$ in G, and $\alpha \neq 0$ is a fixed real number.

The general Randić index when $\alpha = -1$ is

$$R_{-1} = R_{-1}(G) = \sum_{v_i \sim v_j} \frac{1}{d_i d_j}.$$

Some properties on $R_{-1}(G)$ can be founded in [10].

Let $a_1, a_2, ..., a_r$ be positive real numbers. For a positive number k among the values $1 \leq k \leq r$, let us suppose that each P_k is defined as in the following:

$$\begin{aligned}
P_1 &= \frac{a_1 + a_2 + \cdots + a_r}{r}, \\
P_2 &= \frac{a_1a_2 + a_1a_3 + \cdots + a_1a_r + a_2a_3 + \cdots + a_{r-1}a_r}{\frac{1}{2}r(r-1)}, \\
&\vdots \\
P_{r-1} &= \frac{a_1a_2\cdots a_{r-1} + a_1a_2\cdots a_{r-2}a_r + \cdots + a_2a_3\cdots a_{r-1}a_r}{r}, \\
P_r &= a_1a_2\cdots a_r\,.
\end{aligned}$$

Hence the arithmetic mean is simply P_1 while the geometric mean is $P_r^{1/r}$. In fact the following famous lemma (see [2]) gives a relationship among them.

Lemma 1.1 (Maclaurin's Symmetric Mean Inequality) *For* $a_1, a_2, \cdots, a_r \in \mathbb{R}^+$, *it is true that*

$$P_1 \geq P_2^{1/2} \geq P_3^{1/3} \geq \cdots \geq P_r^{1/r}\,.$$

Equality among them holds if and only if $a_1 = a_2 = \cdots = a_r$.

We purpose to obtain some better bounds this fruitful inequality (in Lemma 1.1) tecnique on our main results.

In this paper, we obtain some new bounds on s_α of graphs and improve some results which was obtained on bipartite graphs. As a result of these bounds, we also obtain the some improved results on incidence energy. In addition, we study on RE and REE of (bipartite) graphs, and get some bounds for RE and REE in term of the vertex number (n), general Randić index (R_{-1}), the maximum degree (Δ) and the minimum degree (δ) , and also find some inequalities between RE and REE.

2 New bounds for s_α and IE

The following lemmas will be used later for our main results in this section.

Let $t = t(G)$ be the number of spanning trees of a graph G. Let $G_1 \times G_2$ denotes the Cartesian product of the graphs G_1 and G_2 [12].

Now we introduce the following two auxiliary quantities for a graph G as

$$t_1 = t_1(G) = \frac{2t(G \times K_2)}{t(G)} \text{ and } T = T(G) = \frac{\Delta + \delta + \sqrt{(\Delta - \delta)^2 + 4\Delta}}{2} \tag{4}$$

where Δ and δ are the maximum and minimum vertex degree of G, respectively.

Lemma 2.1 *[15] If G is a connected bipartite graph of order n, then $\prod_{i=1}^{n-1} \mu_i = \prod_{i=1}^{n-1} q_i = nt(G)$. If G is a connected non-bipartite graph of order n, then $\prod_{i=1}^{n} q_i = t_1$.*

Lemma 2.2 *[11, 58] Let G be a connected graph with $n \geq 3$ vertices and Δ be the maximum vertex degree of G. Then $q_1 \geq T \geq \Delta + 1$ with either equalities if and only if G is a star graph $K_{1,n-1}$.*

Lemma 2.3 *[13, 51, 52]The spectra of $L(G)$ and $Q(G)$ coincide if and only if the graph G is bipartite.*

After all above material, we are ready to present our main results.

Theorem 2.4 *Let G be a connected graph with n vertices and m edges. Thus we have an upper bound $IE \leq \sqrt{2mn}$. Equality holds if and only if $q_1 = q_2 = \cdots = q_n$.*

Proof. If we take $r = n$ and $a_i = \sqrt{q_i}$ for $i = 1, 2, ..., n$, by Lemma 1.1 , then we obtain $P_1 \geq P_2^{1/2}$ such that

$$P_1 = \frac{\sum_{i=1}^{n} \sqrt{q_i}}{n} = \frac{IE}{n}$$

and

$$\begin{aligned} P_2 &= \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j=1,\, j \neq i}^{n} \sqrt{q_i q_j} \\ &= \frac{1}{n(n-1)} \left[\left(\sum_{i=1}^{n} \sqrt{q_i} \right)^2 - \sum_{i=1}^{n} (\sqrt{q_i})^2 \right] \\ &= \frac{1}{n(n-1)} \left[IE^2 - 2m \right] \end{aligned}$$

as $\sum_{i=1}^{n} \sqrt{q_i} = IE$ and $\sum_{i=1}^{n} q_i = 2m$.

From this, we then get $IE \leq \sqrt{2mn}$.

From Lemma 1.1, the equality holds if and only if $q_1 = q_2 = \cdots = q_n$. ■

Remark 2.5 *Let us point out that in Theorem* 2.4*, we recover the same upper bound as in Theorem* 5 *in the paper [40], throught a different approach and equality condition.*

Theorem 2.6 *Let G be a connected graph with n vertices and t_1 be given by (4).*

(i) If G is non-bipartite graph, then

$$s_\alpha = \sigma_\alpha \geq \sqrt{n\,(n-1)\, t_1^{2\alpha/n} + s_{2\alpha}}\ .$$

(ii) If G is bipartite graph, then

$$s_\alpha = \sigma_\alpha \geq \sqrt{s_{2\alpha}}.$$

Equalities hold if and only if $q_1 = q_2 = \cdots = q_n$.

Proof. If we take $r = n$ and $a_i = q_i^\alpha$ for $i = 1, 2, ..., n$, by Lemma 1.1 , then we obtain $P_2^{1/2} \geq P_n^{1/n}$ such that

$$\begin{aligned} P_2 &= \frac{1}{n\,(n-1)} \sum_{i=1}^{n} \sum_{j=1,\, j\neq i}^{n} q_i^\alpha q_j^\alpha \\ &= \frac{1}{n\,(n-1)} \left[\left(\sum_{i=1}^{n} q_i^\alpha \right)^2 - \sum_{i=1}^{n} (q_i^\alpha)^2 \right] \\ &= \frac{1}{n\,(n-1)} \left[s_\alpha^2 - s_{2\alpha} \right] \end{aligned}$$

and

$$P_n = \prod_{i=1}^{n} q_i^\alpha = t_1^\alpha$$

as $s_\alpha = \sum\limits_{i=1}^{n} q_i^\alpha$ by (1). From this, we then get the result.

If G is bipartite graph, then it is well known that $q_n = 0$ [12]. Thus, $t_1 = 0$. As a result, the inequality in (ii) is obvious.

By Lemma 2.3, $s_\alpha = \sigma_\alpha$.

From Lemma 1.1, the equalities hold if and only if $q_1 = q_2 = \cdots = q_n$. ∎

Taking $\alpha = 1/2$ in Theorem 2.4, we actually improve the bounds (13) and (14) which was obtained in [8] in the next corollary.

Corollary 2.7 *Let G be a connected graph with n vertices and m edges. Let t_1 be given by (4).*

(i) If G is non-bipartite, then

$$IE \geq \sqrt{n\,(n-1)\,t_1^{1/n} + 2m}. \tag{5}$$

(ii) If G is bipartite, then

$$LEL = IE \geq \sqrt{2m}. \tag{6}$$

The equalities (5) and (6) hold if and only if $q_1 = q_2 = \cdots = q_n$.

Remark 2.8 *By some basic elementary calculations, one may see that the bounds (5) and (6) are better than the bounds* (13) *and* (14) *in [8].*

In addition, for bipartite graphs, we know that $nt = \prod_{i=1}^{n-1} q_i$ where t is the number of spanning trees of a graph G by Lemma 2.1.

Using Arithmetic-Geometric Mean inequality, we have

$$(nt)^{1/n-1} \leq \left(\frac{\prod_{i=1}^{n-1} q_i}{n-1}\right)^{1/n-1} \leq \frac{\sum_{i=1}^{n-1} q_i}{n-1} = \frac{2m}{n-1}.$$

From this, it is easily to see that the lower bound (6) is greater than the lower bound (13)*. That is,*

$$\sqrt{2m} \geq \sqrt{\left(\frac{n-1}{n-2}\right)\left[(n-1)^2\,(nt)^{1/n-1} - 2m\right]}\;.$$

Now we will present new and important a lower bound for s_α.

Theorem 2.9 *Let G be a connected graph with n vertices. Let t_1 and T be given by (4).*

(i) If G is non-bipartite graph, then

$$s_\alpha \geq T^\alpha + (n-1)\left(\frac{t_1}{T}\right)^{\alpha/(n-1)} \tag{7}$$

(ii) If G is bipartite graph, then

$$s_\alpha = \sigma_\alpha \geq T^\alpha \tag{8}$$

The equalities in (7) and (8) hold if and only if G is isomorphic to $K_{1,n-1}$.

Proof. Now taking $r = n-1$ and $a_i = q_i^{-\alpha}$ for $i = 2, ..., n$, in Lemma 1.1, we have

$$P_{n-2}^{1/(n-2)} \geq P_{n-1}^{1/(n-1)}, \tag{9}$$

where

$$P_{n-1} = \prod_{i=2}^{n} \frac{1}{\sqrt{q_i}} = \left(\frac{q_1}{t_1}\right)^{\alpha}$$

and also

$$P_{n-2} = \frac{\sum\limits_{i=2}^{n}\sum\limits_{j=2}^{n} \frac{1}{q_j^{\alpha}}}{n-1} = \frac{\prod\limits_{j=2}^{n} \frac{1}{q_j^{\alpha}}}{n-1} \times \sum_{i=2}^{n} q_i^{\alpha}.$$

We hence obtain

$$s_{\alpha} \geq q_1^{\alpha} + (n-1)\left(\frac{t_1}{q_1}\right)^{\alpha/(n-1)}, \tag{10}$$

by (9).

Let us consider the function

$$f(x) = x + (n-1)\left(\frac{t_1^{\alpha}}{x}\right)^{1/(n-1)},$$

where $x = q_1^{\alpha}$ in (10).

One can see that $f(x)$ is increasing for $x > t_1^{1/n}$. By Lemma 2.2, we have $q_1 \geq T \geq \Delta + 1 > \Delta \geq \frac{2m}{n}$. Using Arithmetic-Geometric Mean inequality and Lemma 2.1, we get

$$t_1^{1/n} \leq \left(\prod_{i=1}^{n} q_i\right)^{1/n} \leq \frac{\sum\limits_{i=1}^{n} q_i}{n} = \frac{2m}{n}.$$

Therefore $f(x) \geq f(T^{\alpha}) = T^{\alpha} + (n-1)\left(\frac{t_1}{T}\right)^{\alpha/(n-1)}$.

Combining this with (10), (7) is obtained.

If G is bipartite graph, then it is well known that $q_n = 0$ [12]. Thus, $t_1 = 0$. Hence, the inequality in (ii) is obvious.

Now we assume that the equalities in (7) and (8) hold. Then all inequalities in the corresponding arguments must be equalities. Then, $q_1 = T$. By Lemma 2.2, we conclude that $G \cong K_{1,n-1}$. ■

Remark 2.10 *We should note that the bound (8) improves the results in [17, Theo. 3.4, Cor. 3.5, Cor. 3.7, Lemma 3.8, Theo. 3.9, Theo. 3.11] for bipartite graphs.*

Corollary 2.11 *Let G be a connected graph of order n and t_1 and T be as given in (4).*

(i) If G is non-bipartite graph, then

$$IE \geq \sqrt{T} + (n-1)\left(\frac{t_1}{T}\right)^{1/2(n-1)} \tag{11}$$

(ii) If G is bipartite graph, then

$$IE = LEL \geq \sqrt{T} \tag{12}$$

The equalities in (11) and (12) hold if and only if G is isomorphic to $K_{1,n-1}$.

Remark 2.12 *We should note that the lower bound in (11) is the same with one which was obtained in [9, Theorem 4.8]. Moreover, in the same paper, it was also stated that it can not become an equality for the same bound. But, as seen in Theorem 2.9, using different method, we gave this lower bound with an equality condition.*

Morever, one can easily see that the lower bound in (12) is better than the results in [8, Theo. 3.1 (i) and Theo. 3.3 (i)] and in [9, Theo. 4.8]. This bound also improves the results in [18, Theo. 2.5 and Theo. 2.12] for bipartite graphs.

2.1 New bounds for RE and REE

Firstly, we select some basic properties on the Randi ć eigenvalues of G and the other materials which will be used in this section.

Lemma 2.13 *[5] Let G be a graph with n vertices and Randić matrix R. Then*

$$tr\left(\mathbf{R}\right) = \sum_{i=1}^{n} \rho_i = 0$$

and

$$tr\left(\mathbf{R}^2\right) = \sum_{i=1}^{n} \rho_i^2 = 2\sum_{v_i \sim v_j} \frac{1}{d_i d_j} = 2R_{-1}.$$

Lemma 2.14 *[50] The Randić spectral radius $\rho_1 = 1$.*

Lemma 2.15 *[6] A simple connected graph G has two distinct Randić eigenvalues if and only if G is complete.*

Lemma 2.16 *[10] Let G be a connected graph of order n with maximum degree Δ and minimum degree δ. Then*

$$\frac{n}{2\Delta} \leq R_{-1} \leq \frac{n}{2\delta}.$$

Equality occurs in both bounds if and only if G is a regular graph.

The first result of this section is the following.

Theorem 2.17 *Let G be a connected graph with n vertices and P be the absolute value of the determinant of the Randić matrix R. Thus we have*

$$1+\sqrt{(n-1)(n-2)P^{2/(n-1)}+2R_{-1}-1} \le RE \le 1+\sqrt{(n-1)(2R_{-1}-1)}.$$

The equality occurs in both bounds if and only if G is a complete graph.

Proof. Now taking $r=n-1$ and $a_i=|\rho_i|$ for $i=2,...,n$, in Lemma 1.1, we have

$$P_1 \ge P_2^{1/2}, \tag{13}$$

where

$$P_1=\frac{\sum_{i=2}^{n}|\rho_i|}{n-1}=\frac{RE-1}{n-1}$$

and also

$$\begin{aligned} P_2 &= \frac{1}{(n-1)(n-2)}\sum_{i=2}^{n}\sum_{j=2,\, j\neq i}^{n}|\rho_i|\,|\rho_j| \\ &= \frac{1}{(n-1)(n-2)}\left[\left(\sum_{i=2}^{n}|\rho_i|\right)^2-\sum_{i=2}^{n}(\rho_i)^2\right] \\ &= \frac{1}{(n-1)(n-2)}\left[(RE-1)^2-(2R_{-1}-1)\right] \end{aligned}$$

We hence obtain the right-hand side of inequality by (13).

Similarly setting $r=n-1$ and $a_i=|\rho_i|$ for $i=2,...,n$, in Lemma 1.1, we get

$$P_2^{1/2} \ge P_{n-1}^{1/(n-1)}, \tag{14}$$

where

$$P_{n-1}=\prod_{i=2}^{n}|\rho_i|=P.$$

and P_2 is as given in above. From (14), we obtain the left-hand side of inequality.

The equalities hold in both bounds if and only if G is complete graph by Lemma 2.14, 2.15 and 1.1. ■

Remark 2.18 *It can be easily to see that the lower bound in Theorem 2.17 is better than (12) in [7] on many special examples. We consider the graph $G=(V,E)$ with the vertex set $V=\{v_1,v_2,v_3,v_4\}$ and the edge set $E=\{v_1v_2,v_2v_3,v_1v_3,v_3v_4\}$. For this graph, $RE=2.4574$. While the lower bound in Theorem 2.17 gives $RE\ge 2.406$, the lower bound in (12) gives $RE\ge 2.301$. But our upper bound in Theorem 2.17 is not better than (13) in [7] for this graph.*

Using Lemma 2.16, we can give the following corollary for Theorem 2.17.

Corollary 2.19 *Let G be a connected graph with n vertices. Then*

$$1+\sqrt{(n-1)(n-2)P^{2/(n-1)}+\frac{n-\Delta}{\Delta}} \leq RE \leq 1+\sqrt{(n-1)\left(\frac{n-\delta}{\delta}\right)}$$

with equaliy if and only if G is complete graph.

Remark 2.20 *Let us point out that in Corollary 2.19, we recover the same lower and upper bounds as in Theorem 3.5 and Theorem 4.1 in the paper [19].*

Now we consider the bipartite graph case of the above theorem (Theorem 2.17).

Theorem 2.21 *Let G be a connected bipartite graph and P be the absolute value of the determinant of the Randić matrix R. Thus we have*

$$2+\sqrt{(n-2)(n-3)P^{2/(n-2)}+2R_{-1}-2} \leq RE \leq 2+\sqrt{(n-2)(2R_{-1}-2)}.$$

The equality occurs in both bounds if and only if G is a complete bipartite graph.

Proof. Since G is a bipartite graph, we have $\rho_1 = -\rho_n$, that is, $\rho_1 = 1$ and $\rho_n = -1$, from [12, p.109] and Lemma 2.16. The rest of the proof is similar to the proof of Theorem 2.17, taking $r = n-2$. ■

Corollary 2.22 *Let G be a connected bipartite graph with n vertices. Then*

$$2+\sqrt{(n-2)(n-3)P^{2/(n-2)}+\frac{n-2\Delta}{\Delta}} \leq RE \leq 2+\sqrt{(n-2)\left(\frac{n-2\delta}{\delta}\right)}.$$

with equaliy if and only if G is complete bipartite regular graph.

For REE, we give the important result in the following.

Theorem 2.23 *Let G be a connected graph of order n.Then*

$$REE \geq e+\frac{n-1}{e^{1/(n-1)}}. \tag{15}$$

Moreover, the equality holds if and only if G is complete graph.

Proof. Recall that $\rho_1 = 1$. Directly from (3), we have

$$\begin{aligned} REE &= e^1 + e^{\rho_2} + ... + e^{\rho_n} \\ &\geq e + (n-1)\left[\prod_{i=2}^{n} e^{\rho_i}\right]^{1/(n-1)} \\ &= e + \frac{n-1}{e^{1/(n-1)}} \quad \text{as} \quad \sum_{i=1}^{n} \rho_i = 0. \end{aligned}$$

Suppose that the equality in (15) holds. Then all inequalities in the above argument must be equalities, i. e., $\rho_2 = ... = \rho_n$. Hence by Lemma 2.15, we have G is complete graph.

Conversely, it is easy to check that the equality in (15) holds for complete graph, which completes the proof. ■

If G is a bipartite graph, it is known that $\rho_1 = -\rho_n$. Using the same way as in Theorem 2.23, we then have the following bound.

Theorem 2.24 *Let G be a connected bipartite graph of order n.Then*

$$REE \geq e + \frac{1}{e}.$$

Moreover, the equality holds if and only if G is a complete bipartite graph.

Remark 2.25 *In fact, Theorem 2.23 concludes that among all graphs of order n, the complete graph K_n with minimum Randić Estrada index; and Theorem 2.24 concludes that among all bipartite graphs of order n, the complete bipartite graphs with minimum Randić Estrada index.*

Moreover, the result in (15) is better than the lower bound (15) which was obtained for REE in [7]. While (15) in [7] was obtained taking the lower bound of ρ_1,we obtain the result (15) taking $\rho_1 = 1$.

We now deduce some bounds for the Randić Estrada index of a (bipartite) graph and obtain some inequalities between REE and RE.

Theorem 2.26 *Let G be a connected bipartite graph of order n.Then*

$$\begin{aligned} e + e^{-1} + \sqrt{(n-2)^2 + 2\,(2R_{-1} - 2)} &\leq REE \qquad (16) \\ &\leq e + e^{-1} + (n-3) - \sqrt{2R_{-1} - 2} + e^{\sqrt{2R_{-1}-2}}. \end{aligned}$$

Equality occurs in both bounds if and only if G is a complete bipartite graph.

Proof. Note that $\rho_1 = 1$ and $\rho_n = -1$ for any bipartite graph G. Directly from (3), we get

$$\left(REE - e - e^{-1}\right)^2 = \sum_{i=2}^{n-1} e^{2\rho_i} + 2 \sum_{2\le i<j\le n-1} e^{\rho_i} e^{\rho_j}. \tag{17}$$

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

$$\begin{aligned} 2 \sum_{2\le i<j\le n-1} e^{\rho_i} e^{\rho_j} &\ge (n-2)(n-3) \left[\prod_{2\le i<j\le n-1} e^{\rho_i} e^{\rho_j} \right]^{2/[(n-2)(n-3)]} \\ &= (n-2)(n-3) \left[\left(\prod_{i=2}^{n-1} e^{\rho_i} \right)^{n-3} \right]^{2/[(n-2)(n-3)]} \\ &= (n-2)(n-3) \quad \text{as} \quad \sum_{i=2}^{n-1} \rho_i = 0. \end{aligned} \tag{18}$$

Note that $\sum\limits_{i=2}^{n-1} \rho_i^0 = n-2$, $\sum\limits_{i=2}^{n-1} \rho_i = 0$ and $\sum\limits_{i=2}^{n-1} \rho_i^2 = 2R_{-1} - 2$. By means of a power-series expansion, we get

$$\begin{aligned} \sum_{i=2}^{n-1} e^{2\rho_i} &= \sum_{k\ge 0}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} (2\rho_i)^k \\ &= (n-2) + 4(R_{-1} - 1) + \sum_{k\ge 3}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} (2\rho_i)^k \\ &\ge (n-2) + 4(R_{-1} - 1) + t \sum_{k\ge 3}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} \rho_i^k \quad \text{for } t \in [0,4] \\ &= (1-t)(n-2) + (4-t)(R_{-1} - 1) + t\left(REE - e - e^{-1}\right). \end{aligned} \tag{19}$$

By substituting (18)and (19) back into (17), and solving for $REE - e - e^{-1}$, we have

$$REE - e - e^{-1} \ge \frac{t}{2} + \frac{\sqrt{[t - 2(n-2)]^2 + 2(2R_{-1} - 2)(4-t)}}{2}.$$

It is elementary to show that for $n \ge 2$ and $R_{-1} \ge \begin{cases} 1, \text{if } n \text{ is even} \\ \frac{n}{n+1}, \text{ if } n \text{ is odd} \end{cases}$, the function

$$f(x) = \frac{x}{2} + \frac{\sqrt{[x - 2(n-2)]^2 + 2(2R_{-1} - 2)(4-x)}}{2}$$

monotonically decreases in the interval $[0,4]$. Consequently, the best lower bound for $REE - e - e^{-1}$ is attained for $t = 0$. Then we arrive at the first half of Theorem 2.26.

Starting from the following inequality, we get

$$\begin{aligned}
REE - e - e^{-1} &= n-2+\sum_{k\geq 2}^{\infty}\frac{1}{k!}\sum_{i=2}^{n-1}\rho_i^k \\
&\leq n-2+\sum_{k\geq 2}^{\infty}\frac{1}{k!}\sum_{i=2}^{n-1}|\rho_i|^k \\
&= n-2+\sum_{k\geq 2}^{\infty}\frac{1}{k!}\sum_{i=2}^{n-1}\left(\rho_i^2\right)^{k/2} \\
&\leq n-2+\sum_{k\geq 2}^{\infty}\frac{1}{k!}\left[\sum_{i=2}^{n-1}\rho_i^2\right]^{k/2} \\
&= n-2+\sum_{k\geq 2}^{\infty}\frac{(2R_{-1}-2)^{k/2}}{k!} \\
&= n-3-\sqrt{2R_{-1}-2}+\sum_{k\geq 0}^{\infty}\frac{\left(\sqrt{2R_{-1}-2}\right)^k}{k!} \\
&= n-3-\sqrt{2R_{-1}-2}+e^{\sqrt{2R_{-1}-2}}.
\end{aligned}$$

From derivation of (16) and Lemma 2.14 it is evident that equality will be attained if and only if $\rho_2 = ... = \rho_{n-1} = 1$. By Lemma 2.15, this happens only in the case of G is complete bipartite. The proof now is completed. ■

Using Lemma 2.16, we give the following corollary for above theorem (Theorem 2.26)

Corollary 2.27 *Let G be a connected bipartite graph with n vertices. Then*

$$\begin{aligned}
e+e^{-1}+\sqrt{(n-2)^2+\frac{2(n-2\Delta)}{\Delta}} &\leq REE \qquad (20)\\
&\leq e+e^{-1}+(n-3)-\sqrt{\frac{n-2\delta}{\delta}}+e^{\sqrt{\frac{n-2\delta}{\delta}}}.
\end{aligned}$$

Equality holds in both bounds if and only if G is a complete bipartite regular graph.

Recall that for a general graph G, we have $\rho_1 = 1$, by Lemma 2.14. If we consider $REE - e = \sum_{i=2}^{n} e^{\rho_i}$ in the same way as in Theorem 2.26, we then have the following bounds for general graphs.

Theorem 2.28 *Let G be a graph of order n with the Randić index R_{-1}. Then the Randić Estrada index of G is bounded as*

$$REE \leq e+(n-3)-\sqrt{2R_{-1}-1}+e^{\sqrt{2R_{-1}-1}} \qquad (21)$$

and

$$REE \geq e + \sqrt{(n-1)\left(1 + \frac{n-2}{e^{2/(n-1)}}\right) + 2\left(4R_{-1} - 3\right)}. \qquad (22)$$

Equality occurs in both bounds if and only if G *is a complete bipartite graph.*

Remark 2.29 *We should note that the bounds in (21) and (22) for* REE *is better than the bounds (21) in [7] on many special examples. We consider the graph* G *in Remark 2.18. For this graph, while* $4.78 \leq REE \leq 5.26$ *in (21) and (22), the bounds in (21) give* $4.08 \leq REE \leq 6.38$ *in [7].*

Corollary 2.30 *Let* G *be a graph of order* n *with maximum degree* Δ *and minimum degree* δ*. Then the Randić Estrada index of* G *is bounded as*

$$REE \leq e + (n-3) - \sqrt{\frac{n-\delta}{\delta}} + e^{\sqrt{\frac{n-\delta}{\delta}}}$$

and

$$REE \geq e + \sqrt{(n-1)\left(1 + \frac{n-2}{e^{2/(n-1)}}\right) + 2\left(\frac{2n}{\Delta} - 3\right)}.$$

Equality holds in both bounds if and only if G *is a complete bipartite regular graph.*

Recall that the Randić energy of a graph G is defined in [5,6] as:

$$RE = RE(G) = \sum_{i=1}^{n} |\rho_i|.$$

Some properties on RE can be found in [5,6]. In what follows, we give inequalities between REE and RE.

Theorem 2.31 *Let* G *be a bipartite graph of order* n *with minimum degree* δ*. Then*

$$REE - RE \leq (n-5) + e + e^{-1} - \sqrt{\frac{n-2\delta}{\delta}} + e^{\sqrt{\frac{n-2\delta}{\delta}}} \qquad (23)$$

or

$$REE + RE \leq n - 1 + e + e^{-1} + e^{(RE-2)}. \qquad (24)$$

Equality (23) or (24) is attained if and only if G *is a complete bipartite regular graph.*

Proof. Note that $\rho_1 = 1$ and $\rho_n = -1$. Then we get

$$REE - e - e^{-1} = n - 2 + \sum_{k\geq 1}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} \rho_i^k \leq n - 2 + \sum_{k\geq 1}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} |\rho_i|^k.$$

Taking into accout the definition of graph Randić energy (2), we have

$$REE - e - e^{-1} \leq (n-2) + (RE-2) + \sum_{k\geq 2}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} |\rho_i|^k \,,$$

which, as in Theorem 2.26, leads to

$$\begin{aligned} REE - RE &\leq (n-4) + e + e^{-1} + \sum_{k\geq 1}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} |\rho_i|^k \\ &\leq (n-5) + e + e^{-1} - \sqrt{2R_{-1}-2} + e^{\sqrt{2R_{-1}-2}} \\ &\leq (n-5) + e + e^{-1} - \sqrt{2R_{-1}-2} + e^{\sqrt{2R_{-1}-2}}. \end{aligned}$$

The equality holds if and only if G is a complete bipartite regular graph.

Another route to connect REE and RE, is the following:

$$\begin{aligned} REE - e - e^{-1} &= n-2 + \sum_{k\geq 2}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} \rho_i^k \\ &\leq n-2 + \sum_{k\geq 2}^{\infty} \frac{1}{k!} \sum_{i=2}^{n-1} |\rho_i|^k \\ &\leq n-2 + \sum_{k\geq 2}^{\infty} \frac{\left[\sum_{i=2}^{n-1} |\rho_i|^k\right]}{k!} \\ &= (n-2) - 1 - (RE-2) + \sum_{k\geq 0}^{\infty} \frac{(RE-2)^k}{k!} \\ &= (n-1) - RE + e^{(RE-2)} \end{aligned}$$

implying

$$REE + RE \leq n - 1 + e + e^{-1} + e^{(RE-2)}.$$

Also on this formula equality occurs if and only if G is a complete bipartite regular graph.

This completes the proof. ■

Similary, if we consider $REE - e = \sum_{i=2}^{n} e^{\rho_i}$ in the same way as in Theorem 2.31, we then have the following inequalities for general graphs.

Theorem 2.32 *Let G be a graph of order n with the minimum degree δ. Then*

$$REE - RE \leq n - 3 + e - \sqrt{\frac{n-\delta}{\delta}} + e^{\sqrt{\frac{n-\delta}{\delta}}} \tag{25}$$

or

$$REE + RE \leq n - 2 + e + e^{(RE-2)}. \tag{26}$$

Equality (25) or (26) is attained if and only if G is a complete bipartite regular graph.

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