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Some New Bounds for a Real Power of the Normalized Laplacian Eigenvalues

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***Abstract*—**For a given a simple connected graph, we present some new bounds via a new approach for a special topological index given by the sum of the real number power of the non-zero normalized Laplacian eigenvalues. To use this approach presents an advantage not only to derive old and new bounds on this topic but also gives an idea how some previous results in similar area can be developed.

***Keywords*—**Degree Kirchhoff index, normalized Laplacian eigenvalue, spanning tree.

I. INTRODUCTION

THROUGHOUT this paper G will denote a simple connected graph with n vertices (labelled by $v_1, v_2, ..., v_n$) and m edges. Moreover, for $1 \le i \le n$, the degree of each vertex v_i will be denoted by d_i.

Among various indices in mathematical chemistry, *the Kirchhoff index* $K_f(G)$ and a relative of it, the close *degree Kirchhoff index* $K'_f(G)$, have received a great deal of attention, recently. For a connected undirected graph G, the *Kirchhoff index* was defined by Klein and Randic ([16]) as

$$K_f(G) = \sum_{i<i} r_{ij},$$

where r_{ij} is the effective resistance of the edge $v_i v_j$. We refer the reader to [1], [16], [17], [21], and their bibliographies, to get a taste of the variety of approaches used to study this descriptor. In [28], Zhou et al. studied the extremal graphs with given matching number, connectivity and the minimal Kirchhoff index. Also in [23], [25] and [26] the authors determined independently the extremality on the unicyclic graphs with respect to the Kirchhoff index. Moreover, in [27], Zhou et al. presented some lower bounds for the Kirchhoff index of a connected (molecular) graph via the number of vertices (atoms), the number of edges (bands), valency (maximum vertex degree), connectivity and chromatic number.

The *degree Kirchhoff index* was proposed by Chen and Zhang in [7], defined as

$$K'_f(G) = \sum_{i \sim j} d_i d_j r_{ij}.$$

The *degree Kirchhoff index* has been taken attention as much as the *Kirchhoff index*. For instance, in [12], the authors have been recently characterized unicyclic graphs having maximum, second-maximum, minimum and second-minimum degree Kirchhoff index. One can depict [7] for some bounds over the degree Kirchhoff index and for some relations between degree Kirchhoff and Kirchhoff indices. We finally refer [19] for further studies over degree Kirchhoff index.

For the *adjacency matrix* $A(G)$ and the diagonal matrix $D(G)$ of the vertex degrees of G, let us consider the *Laplacian matrix* $L(G) = D(G) - A(G)$. It is known that the eigenvalues of $L(G)$ are named as the *Laplacian eigenvalues* of G. Suppose $\mu_1 \ge \mu_2 \ge ... \ge \mu_{n-1} \ge \mu_n = 0$ are the Laplacian eigenvalues of G. By [13], we know that the multiplicity of $\mu_n = 0$ is equal to the number of connected components of G. We refer [6], [18] for more and some other details on Laplacian eigenvalues. We just want to remind the expression of Kirchhoff index in terms of the Laplacian eigenvalues (see [15], [22], [29]) as in the equality

$$K_f(G) = n\sum_{i=1}^{n-1} \frac{1}{\mu_i}. \tag{1}$$

Other than Laplacian matrix, there also exists the *normalized Laplacian matrix* $l(G) = D(G)^{-\frac{1}{2}} L(G) D(G)^{-\frac{1}{2}}$ of G, where $D(G)^{-\frac{1}{2}}$ is the matrix obtained by taking $\left(-\frac{1}{2}\right)$-power of the each entry of $D(G)$. Similarly as Laplacian eigenvalues, the *normalized Laplacian eigenvalues* of G are the eigenvalues of $l(G)$. So let $\lambda_1 \ge \lambda_2 \ge ... \ge \lambda_{n-1} \ge \lambda_n = 0$ be the normalized Laplacian eigenvalues matrix of G. By [8], the multiplicity of $\lambda_n = 0$ is actually equal to the number of connected components of G. We may refer [8], [11] for whole detailed information on normalized Laplacian eigenvalues. In [7], by considering normalized Laplacian eigenvalues, the degree Kirchhoff index is defined as

$$K'_f(G) = 2m\sum_{i=1}^{n-1} \frac{1}{\lambda_i}. \tag{2}$$

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Hence, by taking into account (1) and (2), we can easily conclude that the degree Kirchhoff index is the normalized Laplacian analogue of the ordinary Kirchhoff index.

This latter expression was the source of inspration for a whole new family of descriptors, in terms of the sum of the α-th powers of normalized Laplacian eigenvalues as in the form

$$s'_\alpha = s'_\alpha(G) = \sum_{i=1}^{h} \lambda_i^\alpha , \tag{3}$$

defined in [5]. These authors found a number of bounds for arbitrary α and particularly for $\alpha = -1$, which is the case of the degree Kirchhoff index. We note that $\alpha = 1$ implies the trivial case $s'_1 = n$, and for $\alpha = 2$, we obtain

$$s'_2 = trace(l^2). \tag{4}$$

There exists a closed relation between s'_α and the general *Randic index* of G defined by

$$R_\alpha = R_\alpha(G) = \sum_{i\sim j} \left(d_i d_j\right)^\alpha ,$$

where the summation is over all (unordered) edges $v_i v_j$ in G and $\alpha \neq 0$ is a fixed real number (see [4]). By (4), it is shown that

$$s'_2 = n + 2\sum_{i\sim j} \frac{1}{d_i d_j} = n + 2R_{-1}$$

(cf. [30]). We may refer [2], [9], [24] for the detailed knowledge of the parameter R_{-1} and the useage of this into the normalized Laplacian eigenvalues.

For a non-zero real number α, one can think about the sum of the $\alpha -$th powers of non-zero Laplacian eigenvalues. In fact this sum has been defined by Zhou in [27] as in the form

$$s_\alpha(G) = \sum_{i=1}^{h} \mu_i^\alpha ,$$

where h is the number of non-zero Laplacian eigenvalues of G.

In this paper, for the graph G, we present some lower and upper bounds on $s'_\alpha(G)$ (where $\alpha \neq 0,1$) in terms of mainly n, m, t (the number of spanning trees), Δ (see Lemma 1) and R_{-1}.

II. Preliminary Results

We seperate this section to express some assistant results which will be needed to construct our main theories.

Lemma 1 ([10]): The number of spanning trees of G is given by

$$t = \frac{\Delta}{2m}\prod_{i=1}^{n-1} \lambda_i ,$$

where $\Delta = \prod_{i=1}^{n} d_i$.

Lemma 2 ([8]): Suppose that the normalized Laplacian eigenvalues of G are given by $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n = 0$. Then

$$\lambda_1 \geq \frac{n}{n-1}. \tag{5}$$

Moreover the equality holds in (5) if and only if $G \cong K_n$.

Under the same assumptions on G as in Lemma 2, Chung also presented the following lemma about the normalized Laplacian eigenvalues.

Lemma 3 ([8]): Let the normalized Laplacian eigenvalues of G be given as $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n = 0$. Then

$$0 \leq \lambda_i \leq 2.$$

Moreover $\lambda_1 = 2$ if and only if G has a connected bipartite and nontrivial component.

Lemma 4 ([11]): Let us consider again the normalized Laplacian eigenvalues in Lemma 2, and let

$$P = 1 + \sqrt{\frac{2}{n(n-1)} R_{-1}} .$$

We then have

$$\lambda_1 \geq P. \tag{6}$$

Moreover the equality holds in (6) if and only if $G \cong K_n$.

We note that Lemma 4 implies the lower bound expressed in (6) is always better than the bound in (5).

Again, by according to the [11], we have the following two lemmas.

Lemma 5([11]): For a connected graph G of order $n > 2$, it is true that $\lambda_2 = \lambda_3 = \ldots = \lambda_{n-1}$ if and only if $G \cong K_n$ or $G \cong K_{p,q}$.

Lemma 6([11]): Let G be a graph of order n without isolated vertices. Then $\lambda_1 = \lambda_2 = \lambda_3 = \ldots = \lambda_{n-1}$ if and only if $G \cong K_n$.

Let $a_1, a_2, \ldots, a_r$ 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:

$$P_1 = \frac{a_1 + a_2 + \ldots + a_r}{r},$$

$$P_2 = \frac{a_1a_2 + a_1a_3 + \ldots + a_1a_r + a_2a_3 + \ldots + a_{r-1}a_r}{\frac{1}{2}r(r-1)},$$

$$\vdots$$

$$P_{r-1} = \frac{a_1a_2\ldots a_{r-1} + a_1a_2\ldots a_{r-2}a_r + \ldots + a_2a_3\ldots a_{r-1}a_r}{r},$$

$$P_r = a_1a_2\ldots a_r .$$

Hence the *arithmetic mean* is simply P_1 while the *geometric mean* is $P_r^{1/r}$. In fact the following famous lemma (see [3],[14],[20]) gives a relationship among them.

Lemma 7: (Maclaurin's Symmetric Mean Inequality) For $a_1, a_2, ..., a_r \in \mathbb{R}^+$, it is true that

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

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

We purpose to obtain some better bounds by using this fruitful inequality (in Lemma 7) technique on this new family of descriptors (given before this lemma).

After all above material, we are ready to present our results on the bounds of the sum of the α-th power of normalized Laplacian eigenvalues $s'_\alpha(G)$ as defined in (3).

III. Main Results

We recall that

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

The first result of this paper is the following.

Theorem 1: Let α be a real number with $\alpha \neq 0,1$, and let G be a connected graph with $n \geq 3$ vertices, m edges and having t spanning trees. Thus we have a lower bound

$$s'_\alpha(G) \geq P^\alpha + (n-2)\left(\frac{2mt}{\Delta P}\right)^{\alpha/(n-2)}, \tag{7}$$

where P is defined as in Lemma 4. Moreover equality in (7) holds if and only if $G \cong K_n$.

Proof: By Lemma 1, we have

$$\frac{\Delta \lambda_1^{n-1}}{2mt} = \prod_{i=2}^{n-1} \frac{\lambda_1}{\lambda_i} \quad as \quad \lambda_1 \geq \lambda_i, i = 2,3,...,n-1,$$

that is,

$$\lambda_1^{n-1} \geq \frac{2mt}{\Delta}. \tag{8}$$

Setting $r = n-2$ and $a_i = \lambda_i^{-\alpha}$ in Lemma 7, we obtain

$$P_{n-3}^{1/(n-3)} \geq P_{n-2}^{1/(n-2)}$$

such that $P_{n-2} = \prod_{j=2}^{n-1} \lambda_j^{-\alpha}$ and

$$P_{n-3} = \frac{\sum_{i=2}^{n-1} \sum_{j=2, j \neq n-i+1}^{n-1} \lambda_j^{-\alpha}}{n-2} = \frac{\prod_{j=2}^{n-1} \lambda_j^{-\alpha}}{n-2} \times \sum_{i=2}^{n-1} \frac{1}{\lambda_j^{-\alpha}} = \frac{\left(\frac{\Delta\lambda_1}{2mt}\right)^\alpha}{n-2}\left(s'_\alpha - \lambda_1^\alpha\right).$$

From this, we then get

$$\frac{\left(\frac{\Delta\lambda_1}{2mt}\right)^\alpha}{n-2}\left(s'_\alpha - \lambda_1^\alpha\right) \geq \left(\frac{\Delta\lambda_1}{2mt}\right)^\alpha.$$

In other words,

$$s'_\alpha \geq \lambda_1^\alpha + (n-2)\left(\frac{2mt}{\Delta\lambda_1}\right)^{\alpha/(n-2)}.$$

Let us now consider a function

$$g(x) = x^\alpha + (n-2)\left(\frac{2mt}{\Delta x}\right)^{\alpha/(n-2)}$$

such that $x \geq P$ and $x^{n-1} \geq \frac{2mt}{\Delta}$. It is clear that

$$\begin{aligned} g'(x) &= \alpha\left[x^{\alpha-1} - x^{-\frac{\alpha+n-2}{n-2}}\left(\frac{2mt}{\Delta}\right)^{\alpha/(n-2)}\right] \\ &\geq \alpha\left[x^{\alpha-1} - x^{-\frac{\alpha+n-2}{n-2}} x^{\frac{\alpha(n-1)}{n-2}}\right] = 0 \quad as \quad x^{n-1} \geq \frac{2mt}{\Delta}, \end{aligned}$$

and so $g(x)$ is an increasing function on $x \geq P$ and $x^{n-1} \geq \frac{2mt}{\Delta}$. Hence we have

$$g(x) \geq P^\alpha + (n-2)\left(\frac{2mt}{\Delta}\right)^{\alpha/(n-2)}$$

which gives the required lower bound in (7).

Now let us suppose that the equalities in both sides of (7) hold. Then all inequalities in the above processes must become equalities. The lower bound equality will be implied that $\lambda_1 = P$ and $\lambda_2 = \lambda_3 = ... = \lambda_{n-1}$ by Lemma 7. In addition, by Lemmas 4 and 5, we have $G \cong K_n$, as required. The converse part is quite clear.

For $i = 1,2,3,...,n-1$, by taking $a_i = \lambda_i$ in Lemma 7, and using similar technique as in the proof of Theorem 1, we obtain the following result.

Theorem 2: Let G be a connected graph with $n \geq 3$ vertices, m edges and t spanning trees. Also let P be assumed as in Theorem 1. Thus we have a lower bound

$$K'_f(G) \geq \frac{2m}{P} + 2(n-2)m\left(\frac{\Delta P}{2mt}\right)^{1/(n-2)}$$

with equality if and only if $G \cong K_n$.

The next two corollaries are the consequences of Theorem 1 and 2.

Corollary 1: Let T be a tree of order n. Then

$$s'_\alpha(T) \geq P^\alpha + (n-2)\left(\frac{2m}{\Delta P}\right)^{\alpha/(n-2)}$$

and

$$K'_f(T) \geq \frac{2m}{P} + 2(n-2)m\left(\frac{\Delta P}{2m}\right)^{1/(n-2)}.$$

Proof: Since T is a tree, it is clear that $t = 1$. Thus, from Theorems 1 and 2, we get the result.

Corollary 2: Let U be a connected unicyclic graph of order n. Then

$$s'_\alpha(U) \geq P^\alpha + (n-2)\left(\frac{6m}{\Delta P}\right)^{\alpha/(n-2)}$$

and

$$K'_f(U) \geq \frac{2m}{P} + 2(n-2)m\left(\frac{\Delta P}{2mn}\right)^{1/(n-2)}.$$

Equalities hold if and only if $U \cong K_3$.

Proof: For any unicyclic graph U of order n, we certainly have $3 \leq t \leq n$. Again by Theorems 1 and 2, we obtain the required lower bounds. On the other hand, the same theorems imply the necessary and sufficient equality condition on these lower bounds.

Remark 1: Let us point out that in Theorems 1 and 2, we recover the same bounds as in Theorem 1 and Corollary 2 in the paper [5], throught a different approach. We actually improve them in the next theorem (see Theorem 3).

Theorem 3: Let G be a connected graph with $n \geq 3$ vertices, m edges and t spanning trees. Hence we have the lower and upper bounds

$$\left.\begin{array}{l} s'_\alpha(G) \geq (n-1)\left[\left(\frac{2mt}{\Delta}\right)^\alpha \frac{\left(s'_{-\alpha}\right)^2 - s'_{-2\alpha}}{(n-1)(n-2)}\right]^{1/(n-3)} \\ \text{and} \\ s'_\alpha(G) \leq \sqrt{s'_{2\alpha} + (n-1)(n-2)\left(\frac{2mt}{\Delta}\right)^\alpha \left(\frac{s'_{-\alpha}}{n-1}\right)^{n-3}} \end{array}\right\}, \quad (9)$$

respectively.

Moreover, equality holds if and only if $G \cong K_n$.

Proof: Setting $r = n-1$ and $a_i = \lambda_i^\alpha$ (for $i = 1,2,...,n-1$) in Lemma 7, we obtain

$$P_1 \geq P_{n-3}^{1/(n-3)},$$

where $P_1 = \frac{\sum_{i=1}^{n-1} \lambda_i^\alpha}{n-1}$, and also

$$P_{n-3} = \frac{\prod_{i=1}^{n-1} \lambda_i^\alpha}{(n-1)(n-2)} \left\{ \left(\sum_{i=1}^{n-1} \frac{1}{\lambda_i^\alpha} \right)^2 - \sum_{i=1}^{n-1} \frac{1}{\lambda_i^{2\alpha}} \right\}.$$

We hence obtain

$$s'_\alpha(G) \geq (n-1)\left[\left(\frac{2mt}{\Delta}\right)^\alpha \frac{\left(s'_{-\alpha}\right)^2 - s'_{-2\alpha}}{(n-1)(n-2)}\right]^{1/(n-3)}.$$

On the other hand, by taking $r = n-1$ and $a_i = \lambda_i^{-\alpha}$ (for $i = 1,2,...,n-1$) in Lemma 7, we get

$$s'_\alpha(G) \leq \sqrt{s'_{2\alpha} + (n-1)(n-2)\left(\frac{2mt}{\Delta}\right)^\alpha \left(\frac{s'_{-\alpha}}{n-1}\right)^{n-3}}.$$

The equality holds in (9) if and only if $\lambda_1 = \lambda_2 = \lambda_3 = ... = \lambda_{n-1}$ from Lemma 7. Also, by Lemma 6, $G \cong K_n$. Conversely the equality follows easily.

Remark 2: Although we managed to see that the equalities in (9) always hold on special examples (see Example 1), it is still remained to see it in the general case.

Using similar arguments as in Theorem 3, one can see the truthness of the following result for $K'_f(G)$.

Theorem 4: Under the same assumptions with Theorem 3, we have

$$\left.\begin{array}{l} K'_f(G) \geq 2m(n-1)\left[\left(\frac{2mt}{\Delta}\right)^\alpha \frac{n^2 - n - 2R_{-1}}{(n-1)(n-2)}\right]^{n-3} \\ \text{and} \\ K'_f(G) \leq 2m\sqrt{s_{2\alpha} + (n-1)(n-2)\left(\frac{2mt}{\Delta}\right)^\alpha \left(\frac{n}{n-1}\right)^{n-3}} \end{array}\right\} \quad (10)$$

respectively, with equality holding if and only if $G \cong K_n$.

Notice that bounds $K'_f(G) = 2ms'_{-1}$ can be also easily derived by taking into account the bounds for s'_α with $\alpha = -1$.

Remark 3: As a first consequence of Theorems 3 and 4, we can easily express the results on a tree T and an unicyclicgraph U.

Remark 4: Note that if G is a k-regular graph, then $\lambda_i = \frac{\mu_i}{k}$ for $i = 1,2,...,n$ (see [8]). Hence we have $s_\alpha = k^\alpha s'_\alpha$ for any k-regular graph. Therefore, in the case of G is regular, results obtained for s'_α can be immediately re-stated for s_α.

In the following, we give a lower and an upper bound over s'_α for connected bipartite graphs.

Theorem 5: Let G be a connected bipartite graphs with $n > 2$ vertices, m edges and t spanning trees. Then

$$s'_\alpha \geq 2^\alpha + \left(\frac{mt}{\Delta}\right)^{\alpha/(n-2)} (n-2)$$

and

$$s'_\alpha \leq 2^\alpha + \left(s'_{-\alpha} - \frac{1}{2^\alpha}\right)^{n-3} \frac{1}{(n-2)^{n-4}} \left(\frac{mt}{\Delta}\right)^\alpha$$

with equality if and only if $G \cong K_{p,q}$.

Proof:

Lower Bound: Now, in Lemma 7, let us take $r = n-2$ for both cases $a_i = \lambda_i^\alpha$ and $a_i = \lambda_i^{-\alpha}$ such that $i = 1,2,...,n-1$, respectively. Therefore we write

$$P_1 \geq P_{n-2}^{1/(n-2)} \text{ for } a_i = \lambda_i^\alpha$$

and

$$P_1 \geq P_{n-3}^{1/(n-3)} \text{ for } a_i = \lambda_i^{-\alpha},$$

where

$$P_1 = \frac{\sum_{i=2}^{n-1} \lambda_i^\alpha}{n-2} = \frac{s'_\alpha - \lambda_1^\alpha}{n-2},$$

$$P_{n-2} = \prod_{i=2}^{n-1} \lambda_i^\alpha = \left(\frac{2mt}{\Delta\lambda_1}\right)^\alpha$$

and

$$P_{n-3} = \frac{\prod_{j=2}^{n-1} \lambda_j^{-\alpha}}{n-2} \sum_{i=2}^{n-1} \lambda_i^\alpha = \left(\frac{\Delta\lambda_1}{2mt}\right)^\alpha \frac{s'_\alpha - \lambda_1^\alpha}{n-2}.$$

Since G is connected bipartite graph, we have $\lambda_1 = 2$ and hence the result follows. All equalities hold if and only if $\lambda_2 = \lambda_3 = ... = \lambda_{n-1}$.

Now we suppose that all equalities hold. Then, by Lemma 5, we conclude that $G \cong K_{p,q}$.

Conversely, we can easily see that the equalities hold for the complete bipartite graph $K_{p,q}$.

As a consequence of Theorem 5, we obtain the following corollary.

Corollary 3: There exist the lower and upper bounds

$$m + 2m(n-2)\left(\frac{\Delta}{mt}\right)^{1/(n-2)} \leq K'_f(G) \leq m + \frac{2\Delta}{t(n-2)}$$

with equality if and only if $G \cong K_{p,q}$.

Example 1: For the complete bipartite graph $K_{1,3}$, the normalized Laplacian spectrum is $\{0,1,1,2\}$. For $\alpha = 2$, while the lower bound in (7) gives $s'_2 \geq 5.98$, the both lower and upper bounds in (9) gives a unique value $s'_2 = 6$. Even this example itself enough to show that the bounds obtained in Theorem 3 would be better than the bounds in Theorem 1 and so [5].

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