ON LOWER BOUNDS FOR THE KIRCHHOFF INDEX

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ABSTRACT. Let G be a simple graph of order $n \ge 2$ with m edges. Denote by $d_1 \ge d_2 \ge \cdots \ge d_n > 0$ the sequence of vertex degrees and by $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_{n-1} > \mu_n = 0$ the Laplacian eigenvalues of the graph G. Lower bounds for the Kirchhoff index, $Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}$, are obtained.

1 Introduction

Let G = (V, E), $V = \{1, 2, ..., n\}$, $E = \{e_1, e_2, ..., e_m\}$ be a simple connected graph of order $n \ge 3$ and size m. If vertices i and j are adjacent, we denote it as $i \sim j$. Denote by $d_1 \ge d_2 \ge \cdots \ge d_n > 0$ a sequence of vertex degrees, and by Δ and δ the greatest and the smallest vertex degrees, respectively. Let \mathbf{A} be the adjacency matrix of G, and $\mathbf{D} = \text{diag}(d_1, d_2, \ldots, d_n)$ the diagonal matrix of its vertex degrees. Then $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is the Laplacian matrix of G. Eigenvalues of \mathbf{L} , $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_{n-1} > \mu_n = 0$, are the Laplacian eigenvalues of graph G.

Some well-known properties of the Laplacian eigenvalues are (see for example [3]):

$$\sum_{i=1}^{n-1} \mu_i = \sum_{i=1}^n d_i = 2m \quad \text{and} \quad \sum_{i=1}^{n-1} \mu_i^2 = \sum_{i=1}^n d_i^2 + \sum_{i=1}^n d_i = M_1 + 2m_2$$

where

$$M_1 = M_1(G) = \sum_{i=1}^n d_i^2 = \sum_{i \sim j} (d_i + d_j) = \sum_{i=1}^m (d(e_i) + 2)$$

is the first Zagreb index introduced in [11]. In the same paper the second Zagreb index, M_2 , and so called forgotten index, F, were defined as

$$M_2 = M_2(G) = \sum_{i \sim j} d_i d_j$$
 and $F = F(G) = \sum_{i=1}^n d_i^3 = \sum_{i \sim j} (d_i^2 + d_j^2).$

More on the invariant F one can find in [7,9].

Matrix $\mathbf{L}^* = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$ is the normalized Laplacian matrix of G. Its eigenvalues, $\rho_1 \ge \rho_2 \ge \cdots \ge \rho_{n-1} > \rho_n = 0$, represent normalized Laplacian eigenvalues of G. The following is valid for ρ_i , $i = 1, 2, \ldots, n$, (see [3]):

$$\sum_{i=1}^{n-1} \rho_i = n \quad \text{and} \quad \sum_{i=1}^{n-1} \rho_i^2 = n + 2R_{-1},$$

where

$$R_{-1} = \sum_{i \sim j} \frac{1}{d_i d_j},$$

is the general Randić index (also called branching index) introduced in [27].

The Kirchhoff index of a connected graph is defined as (see [14]):

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

where r_{ij} is the effective resistance distance between vertices *i* and *j*. The following more appropriate formula from application point of view was put forward in [10]

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

This, in turn, triggered the study of this invariant and its applications in various areas, including spectral graph theory, molecular chemistry, computer science, etc. (see for example [7,9–11,14,18,27]).

Before we proceed, let us define one special class of *d*-regular graphs Γ_d (see [25]). Let N(i) be a set of all neighborhoods of the vertex *i*, i.e. $N(i) = \{k \mid k \in V, k \sim i\}$, and d(i, j) the distance between vertices *i* and *j*. Denote by Γ_d a set of all *d*-regular graphs, $1 \le d \le n-1$, with diameter D = 2 and $|N(i) \cap N(j)| = d$. Further, denote by t = t(G) a number of spanning trees of the connected graph

$$t = t(G) = \frac{1}{n} \prod_{i=1}^{n-1} \mu_i,$$

and by ID = ID(G) the graph invariant called inverse degree

$$ID = ID(G) = \sum_{i=1}^{n} \frac{1}{d_i}.$$

In this paper we are concerned with the lower bounds of Kf(G) which depend on some of the parameters n, m, Δ , and invariants R_{-1}, M_1, M_2 or F. Before going further, we recall some results from the literature needed for our subsequent consideration.

2 Preliminaries

In this section we outline some results for the invariants Kf(G), M_1 , M_2 , F, t and R_{-1} that will be needed in the remainder of the paper.

In [28] the following result was proved for the Kf(G):

Lemma 2.1. [28] Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge -1 + (n-1)\sum_{i=1}^{n} \frac{1}{d_i},$$
(1)

with equality if and only if $G \cong K_n$ or $G \cong K_{r,n-r}$, $1 \le r \le \lfloor \frac{n}{2} \rfloor$.

Remark 2.2. We believe that equality in (1) holds also when $G \in \Gamma_d$ and $G \cong K_n - e$. This only increases importance of the above inequality.

In [23] the following was proved for the general Randić index:

Lemma 2.3. [23] Let G be a simple connected graph with $n \ge 3$ vertices and m edges. Then, for any real k with the property $\rho_1 \ge k \ge \rho_{n-1}$, holds

$$2R_{-1} \ge \frac{n}{n-1} + \frac{n-1}{n-2} \left(k - \frac{n}{n-1}\right)^2,\tag{2}$$

with equality if and only if $k = \frac{n}{n-1}$ and $G \cong K_n$, or k = 2 and $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

In [13, 22, 24] for the Forgotten index the following results were established:

Lemma 2.4. [13] Let G be a simple graph with n vertices and m edges. Then

$$F \le (\Delta + \delta)M_1 - 2m\Delta\delta,\tag{3}$$

with equality if and only if G is regular or bidegreed graph.

Lemma 2.5. [24] Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$F \le 2m(\Delta^2 + \Delta\delta + \delta^2) - n\Delta\delta(\Delta + \delta), \tag{4}$$

with equality if and only if G is regular or bidegreed graph.

Lemma 2.6. [22] Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$F \le \frac{M_1}{2m} + 2m\beta(S)(\Delta - \delta)^2,\tag{5}$$

where

$$\beta(S) = \frac{1}{2m} \sum_{i \in S} d_i \left(1 - \frac{1}{2m} \sum_{i \in S} d_i \right)$$

and S is a subset of $I = \{1, 2, ..., n\}$ which minimizes the expression

$$\left|\sum_{i\in S} d_i - m\right|.$$

Equality in (5) holds if and only if L(G) is regular.

In [4] (see also [15]) for the first Zagreb index, M_1 , the following was proved:

Lemma 2.7. [4] Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$M_1 \le 2(\Delta + \delta)m - n\Delta\delta,\tag{6}$$

with equality if and only if G is regular or bidegreed graph.

For the same invariant in [21] the following was proved:

Lemma 2.8. [21] Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$M_1 \le \frac{4m^2}{n} + n\alpha(n)(\Delta - \delta)^2,\tag{7}$$

where

$$\alpha(n) = \frac{1}{4} \left(1 - \frac{(-1)^{m+1} + 1}{2n^2} \right).$$

Equality in (7) holds if and only if G is regular.

For the number of spanning trees, t, of a graph the following was proved in [5]:

Lemma 2.9. [5] Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$t \le \frac{1}{n} \left(\frac{4m^2 - M_1 - 2m}{(n-1)(n-2)} \right)^{\frac{n-1}{2}},\tag{8}$$

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

For the same invariant in [1] the following was proved:

Lemma 2.10. [1] Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$t \ge \left(\frac{\prod_{i=1}^{n} d_i}{2m}\right) \left(\frac{1}{n-1} \left(n^2 - (n-2)(n+2R_{-1})\right)\right)^{\frac{n-1}{2}},\tag{9}$$

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

3 Main results

We will first prove one general result for the lower bounds of Kf(G) in terms of one of the invariants R_{-1} , M_2 , F or M_1 .

Theorem 3.1. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \geq -1 + 2(n-1)R_{-1},$$
 (10)

$$Kf(G) \geq -1 + \frac{2(n-1)m^2}{M_2},$$
 (11)

$$Kf(G) \geq -1 + \frac{4(n-1)m^2}{F},$$
 (12)

$$Kf(G) \geq -1 + \frac{4(n-1)m^2}{\Delta M_1}.$$
 (13)

Equalities hold if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

Proof. In [19] the following inequality was proved

$$ID \ge 2R_{-1}.$$

From the inequality

$$\sum_{i \sim j} d_i d_j \sum_{i \sim j} \frac{1}{d_i d_j} \ge m^2,$$

follows that

$$R_{-1} \ge \frac{m^2}{M_2}.$$

Also, the following holds

$$2M_2 = 2\sum_{i \sim j} d_i d_j \le \sum_{i \sim j} (d_i^2 + d_j^2) = \sum_{i=1}^n d_i^3 = F,$$

and

$$F_1 = \sum_{i=1}^n d_i^3 \le \Delta \sum_{i=1}^n d_i^2 = \Delta M_1.$$

Accordingly, we have that

$$ID \ge 2R_{-1} \ge \frac{2m^2}{M_2} \ge \frac{4m^2}{F} \ge \frac{4m^2}{\Delta M_1}.$$
 (14)

From (14) and (1) inequalities (10) - (13) are obtained.

If in (10) – (13) invariants R_{-1} , M_2 , F and M_1 are replaced with corresponding lower bounds, a number of lower bounds for Kf(G) depending on various graph parameters can be obtained. In what follows we will illustrate this.

From (10) and (2) the following corollary of Theorem 3.1 is obtained.

Corollary 3.2. Let G be a simple connected graph with $n \ge 3$ vertices and m edges. Then for any real k, $\rho_1 \ge k \ge \rho_{n-1}$, holds

$$Kf(G) \ge n - 1 + \frac{(n-1)^2}{n-2} \left(k - \frac{n}{n-1}\right)^2,$$
 (15)

with equality if and only if $k = \frac{n}{n-1}$ and $G \cong K_n$, or k = 2 and $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Since

$$\rho_1 \ge \frac{\Delta+1}{\Delta} \ge \frac{n}{n-1} \ge \rho_{n-1},$$

according to (15), the following corollary of Theorem 3.1 holds.

Corollary 3.3. Let G be a simple connected graph with $n \ge 3$ vertices and m edges. Then

$$Kf(G) \ge n - 1 + \frac{(n-1)^2}{n-2} \max\left\{\left(\rho_1 - \frac{n}{n-1}\right)^2, \left(\rho_{n-1} - \frac{n}{n-1}\right)^2\right\},\$$

with equality if and only if $G \cong K_n$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Corollary 3.4. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge n - 1,\tag{16}$$

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

The inequality (16) was proved in [17]. It is not difficult to see that (16) can be obtained from (10) and inequality (see [16])

$$2R_{-1} \ge \frac{n}{n-1}.$$

Corollary 3.5. Let G be a simple connected graph with $n \ge 3$ vertices and m edges. Then

$$Kf(G) \ge n - 1 + \frac{(n - 1 - \Delta)^2}{(n - 2)\Delta^2},$$

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

Corollary 3.6. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{n(n-1) - \Delta}{\Delta},$$
(17)

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

Proof. The inequality (17) is obtained from (10) and inequality

$$R_{-1} \ge \frac{n}{2\Delta}$$

which proved in [2].

The inequality (17) was proved in [25].

According to Lemma 2.4 the following corollary of Theorem 3.1 can be obtained.

Corollary 3.7. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{4(n-1)m^2}{(\Delta+\delta)M_1 - 2m\delta\Delta} - 1,$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

Corollary 3.8. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{32(n-1)m^3\delta\Delta}{(\Delta+\delta)^2M_1^2} - 1,$$
 (18)

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

Proof. After applying the arithmetic-geometric mean (AG) inequality on (3), i.e. on

$$F + 2m\Delta\delta \le (\Delta + \delta)M_1,$$

the inequality

$$F \le \frac{(\Delta + \delta)^2 M_1^2}{8m\delta\Delta}$$

is obtained. From this and (12) we obtain (18).

From Lemma 2.5 the following corollary of Theorem 3.1 is obtained.

Corollary 3.9. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{4(n-1)m^2}{2m(\Delta^2 + \Delta\delta + \delta^2) - n\Delta\delta(\Delta + \delta)} - 1,$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

Similarly, from Lemma 5 and (12) the following corollary of Theorem 3.1 is obtained.

Corollary 3.10. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{8(n-1)m^3}{M_1^2 + 4m^2\beta(S)(\Delta-\delta)^2} - 1,$$

where

$$\beta(S) = \frac{1}{2m} \sum_{i \in S} d_i \left(1 - \frac{1}{2m} \sum_{i \in S} d_i \right)$$

and S is a subset of $I = \{1, 2, ..., n\}$ which minimizes the expression

$$\left|\sum_{i\in S} d_i - m\right|$$

Equality holds if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

Corollary 3.11. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{4(n-1)m^2}{\Delta(2m(\Delta+\delta) - n\Delta\delta)} - 1.$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

Proof. The required inequality is obtained from (6) and (13).

Corollary 3.12. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{4n(n-1)\delta}{(\Delta+\delta)^2} - 1,$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

Proof. After applying the AG inequality on (6), i.e. on

$$M_1 + n\Delta\delta \le 2m(\Delta + \delta),$$

the inequality

$$M_1 \le \frac{(\Delta + \delta)^2 m^2}{n\Delta\delta}$$

is obtained (see [6, 8, 12, 20]). The required inequality is obtained from the above inequality and (13).

From (7) and (13) the following corollary of Theorem 3.1 is obtained.

Corollary 3.13. Let G be a simple connected graph with $n \ge 2$ vertices and m edges. Then

$$Kf(G) \ge \frac{4n(n-1)m^2}{\Delta(4m^2 + n^2\alpha(n)(\Delta - \delta)^2)} - 1,$$

where

$$\alpha(n) = \frac{1}{4} \left(1 - \frac{(-1)^{n+1} + 1}{2n^2} \right).$$

Equality holds if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

$$Kf(G) \ge \frac{2m(n-1)}{\Delta^2} - 1,$$

with equality if and only if $G \cong K_n$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

Proof. The required result is obtained from (13) and inequality

$$M_1 \leq 2m\Delta$$

The following corollary of Theorem 3.1 sets up a lower bound for Kf(G) in terms of parameters n and m and the invariant t.

Corollary 3.15. Let G be a simple connected graph with $n \ge 3$ vertices and m edges. Then

$$Kf(G) \ge \frac{4(n-1)m^2}{\Delta(4m^2 - 2m - (n-1)(n-2)(nt)^{\frac{2}{n-1}})} - 1,$$
(19)

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

Proof. From inequality (8) follows

$$M_1 \le 4m^2 - 2m - (n-1)(n-2)(nt)^{\frac{2}{n-1}}.$$

From the above and inequality (13) we arrive at (19).

Similarly, the following can be proved:

Corollary 3.16. Let G be a simple connected graph with $n \ge 3$ vertices and m edges, and let t be the total number of spanning trees of G. Then

$$Kf(G) \ge \frac{n-1}{n-2} \left(2n - (n-1) \left(\frac{2mt}{\prod_{i=1}^{n} d_i} \right)^{\frac{2}{n-1}} \right) - 1,$$

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

Proof. From (9) follows

$$2R_{-1} \ge \frac{1}{n-2} \left(2n - (n-1) \left(\frac{2mt}{\prod_{i=1}^{n} d_i} \right)^{\frac{2}{n-1}} \right).$$

From the above and inequality (10) we obtain the required result.

Let us note that the connectivity condition for the graph G does not deteriorate the generality of the results. Namely, a graph G can be observed as a union of connected components as well.

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