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On Relations Between Kirchhoff Index, Laplacian Energy, Laplacian-Energy-Like Invariant and Degree Deviation of Graphs

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Abstract. Let G be a simple connected graph of order n and size m, vertex degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, and let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ be the eigenvalues of its Laplacian matrix. Laplacian energy LE, Laplacian-energy-like invariant LEL and Kirchhoff index Kf, are graph invariants defined in terms of Laplacian eigenvalues. These are, respectively, defined as $LE(G) = \sum_{i=1}^{n} \left|\mu_i - \frac{2m}{n}\right|$, $LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i}$ and $Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}$. A vertex–degree–based topological index referred to as degree deviation is defined as $S(G) = \sum_{i=1}^{n} \left|d_i - \frac{2m}{n}\right|$. Relations between Kf and LE, Kf and LEL, as well as Kf and S are obtained.

1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, be a simple connected graph with n vertices, m edges, vertex degree sequence $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(i)$. Denote by $\mathbf{A}$ the adjacency matrix of G, and by $\mathbf{D} = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ the diagonal matrix of its vertex degrees. Then Laplacian matrix of G is defined as $\mathbf{L} = \mathbf{D} - \mathbf{A}$. Eigenvalues of matrix $\mathbf{L}$, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$, form the so-called Laplacian spectrum of G.

A graph invariant, or topological index, is a numeric quantity associated with a graph which characterize the topology of graph and is invariant under graph automorphism. Very often in chemistry the aim is the construction of chemical compounds with certain properties, which not only depend on the chemical formula but also strongly on the molecular structure. That's where various topological indices come into consideration.

The Wiener index, $W(G)$, originally termed as a "path number", is a topological graph index defined by

$$W(G) = \sum_{i<j} d_{ij},$$

where d_{ij} is the the shortest path between vertices i and j in G. The first investigations into the Wiener index were made by Harold Wiener in 1947 [32] who realized that there are correlations between the boiling points of paraffin and the structure of the molecules. Since then it has become one of the most frequently

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used topological indices in chemistry, as molecules are usually modeled as undirected graphs. Based on its success, many other topological indices of chemical graphs have been developed.

In [16], Klein and Randić, introduced the notion of resistance distance, r_{ij}, as the second distance function on the vertex set of a graph. It is defined as the resistance between the nodes i and j in an electrical network corresponding to the graph G in which all edges are replaced by unit resistors. The sum of resistance distances of all pairs of vertices of a graph G is named as the Kirchhoff index, i.e.

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

There are several equivalent ways to define the resistance distance. As Gutman and Mohar in [14] (see also [34]) proved, the Kirchhoff index can also be represented as

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

which is more appropriate formula from the computational point of view.

In 2006 Gutman and Zhou [10] introduced another quantity based on the eigenvalues of the Laplacian matrix of G and called it Laplacian energy, LE. It is defined as

$$LE = LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|.$$

In 2008, Liu and Liu [18] conceived a new Laplacian-spectrum-based graph invariant

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

and named it Laplacian-energy-like invariant.

Details of the theory of these Laplacian-spectrum-based invariants can be found, for example, in [11, 17, 19, 21–25, 30].

Historically, the first vertex-degree-based (VDB) structure descriptors were the graph invariants that nowadays are called Zagreb indices. The first Zagreb index, M_1, is defined as [12]

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2\,.$$

Since

$$M_1 = \sum_{i=1}^{n-1} \mu_i(\mu_i - 1),$$

M_1 can be also considered as Laplacian-spectrum-based graph invariant.

A modification of the first Zagreb index, defined as the sum of third powers of vertex degrees, that is

$$F = F(G) = \sum_{i=1}^{n} d_i^3\,,$$

was first time encountered in 1972, in the paper [12], but was eventually disregarded. Recently, it was re-considered in [9] and named the forgotten index.

The inverse degree of a graph G with no isolated vertices is defined as [8]

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

The inverse degree first attracted attention through conjectures of the computer program Graffiti [8].

A graph is said to be regular if all its vertices are of the same degree. Otherwise, it is irregular. As the quantitative topological characterization of irregularity of graphs Nikiforov [27] proposed a measure defined as

$$S(G) = \sum_{i=1}^{n} \left| d_i - \frac{2m}{n} \right|.$$

which is usually referred to as the degree deviation. More on this and other irregularity measures of graph one can find, for example in [1–3, 15].

Before we proceed, let us define one special class of d-regular graphs Γ_d (see [28]). Let $N(i)$ be a set of all neighbors of the vertex i, i.e. $N(i) = \{k \,|\, k \in V,\, k \sim i\}$, 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 2, and $|N(i) \cap N(j)| = d$ for $i \nsim j$. With $C_k(G)$, $3 \le k \le n$, we denote the number of cycles of length k in graph G.

In this paper we obtain relations between $Kf(G)$ and $LE(G)$, $Kf(G)$ and $LEL(G)$, $Kf(G)$ and $S(G)$.

2. Preliminary results

In this section we recall some results from the literature that are of interest for our work.

In [6] Das and Gutman proved the following result.

Lemma 2.1. [6] *Let G be a graph of order n with m edges. Then*

$$\left(LE(G) - \frac{2m}{n} \right)^2 \le 4m^2 \left(\frac{2m}{n^3} Kf(G) - \frac{n-2}{n} \right) \tag{1}$$

with equality if and only if $G \cong K_n$, or $\mu_1 = \mu_2 = \cdots = \mu_p$, $\mu_{p+1} = \mu_{p+2} = \cdots = \mu_{n-1}$ $(1 \le p \le n-2)$ with $\frac{1}{\mu_1} + \frac{1}{\mu_{n-1}} = \frac{n}{m}$.

Lemma 2.2. [6] *Let G be a graph of order $n > 2$ and size m. Then*

$$Kf(G)\,(M_1(G) + 2m) \ge nLEL^2(G) \tag{2}$$

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

Let us note that inequality (2) is a corollary of one more general result proven in [6].

Wang and Luo [31] proved the following result.

Lemma 2.3. [31] *If G has n vertices, $m \ge 1$ edges and maximum vertex degree Δ, then*

$$LEL(G) \ge \sqrt{\frac{8m^3}{n\Delta^2 + 2m}}, \tag{3}$$

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

In [13] (see also [19]) the following lower bound for LEL was established.

Lemma 2.4. *For a graph G with n vertices and m edges*

$$LEL(G) \ge \frac{2m}{\sqrt{n}}, \tag{4}$$

with equality if and only if $G \cong K_n$ or $G \cong \overline{K}_n$.

As observed in [31], the lower bounds given by (3) and (4) are not comparable. Therefore, it follows

$$LEL(G) \geq \max\left\{\frac{2m}{\sqrt{n}}, \frac{2m\sqrt{2m}}{\sqrt{n\Delta^2+2m}}\right\}. \tag{5}$$

This lower bound is correct, but we will show that it is not optimal in the class of lower bounds depending on parameters n, m and Δ.

Zhou and Trinajstić [33] determined the following lower bound for $Kf(G)$.

Lemma 2.5. [33] *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$Kf(G) \geq -1 + (n-1)\sum_{i=1}^{n}\frac{1}{d_i} = -1 + (n-1)ID(G). \tag{6}$$

Equality holds if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$.

Let us note that equality in (6) also holds if $G \in \Gamma_d$.

In [29] Radon proved the following analytic inequality for real number sequences.

Lemma 2.6. [29] *Let $x = (x_i)$ and $a = (a_i)$, $i = 1, 2, \ldots, n-1$, be positive real number sequences. Then for any r, $r \geq 0$, holds*

$$\sum_{i=1}^{n-1}\frac{x_i^{r+1}}{a_i^r} \geq \frac{\left(\sum_{i=1}^{n-1}x_i\right)^{r+1}}{\left(\sum_{i=1}^{n-1}a_i\right)^r}. \tag{7}$$

Equality holds if and only if $\frac{x_1}{a_1} = \frac{x_2}{a_2} = \cdots = \frac{x_{n-1}}{a_{n-1}}$ or $r = 0$.

3. Main results

In the following theorem we prove the inequality that establishes relation between the Kirchhoff index and Laplacian energy in terms of parameters n, m, invariants F, M_1 and number of cycles C_3.

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

$$\begin{aligned} & n\left(LE(G) - \frac{2m}{n}\right)^2 \\ & \leq Kf(G)\left(F(G) + \frac{3n-4m}{n}M_1(G) - 6C_3(G) + \frac{8m^2(m-n)}{n^2}\right). \end{aligned} \tag{8}$$

Equality holds if and only if $G \cong K_n$, or $\mu_1 = \mu_2 = \cdots = \mu_p$, $\mu_{p+1} = \mu_{p+2} = \cdots = \mu_{n-1}$ $(1 \leq p \leq n-2)$ with $n(\mu_1^2 + \mu_{n-1}^2) = 2m(\mu_1 + \mu_{n-1})$.

Proof. For $r = 1$, $x_i := \left|\mu_i - \frac{2m}{n}\right|$, $a_i := \frac{1}{\mu_i}$, $i = 1, 2, \ldots, n-1$, the inequality (7) becomes

$$\sum_{i=1}^{n-1}\left(\mu_i - \frac{2m}{n}\right)^2\mu_i = \sum_{i=1}^{n-1}\frac{\left|\mu_i - \frac{2m}{n}\right|^2}{\frac{1}{\mu_i}} \geq \frac{\left(\sum_{i=1}^{n-1}\left|\mu_i - \frac{2m}{n}\right|\right)^2}{\sum_{i=1}^{n-1}\frac{1}{\mu_i}},$$

that is

$$\sum_{i=1}^{n-1}\left(\mu_i-\frac{2m}{n}\right)^2\mu_i \ge \frac{n\left(LE(G)-\frac{2m}{n}\right)^2}{Kf(G)}. \tag{9}$$

The following identities are valid for the Laplacian eigenvalues μ_i

$$\sum_{i=1}^{n-1}\mu_i = 2m, \quad \sum_{i=1}^{n-1}\mu_i^2 = tr(D-A)^2 = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i = M_1(G)+2m,$$

and

$$\sum_{i=1}^{n-1}\mu_i^3 = tr(D-A)^3 = tr(D^3+3DA^2-A^3) = F(G)+3M_1(G)-6C_3(G)\,.$$

Therefore it follows

$$\sum_{i=1}^{n-1}\left(\mu_i-\frac{2m}{n}\right)^2\mu_i = F(G)+3M_1(G)-6C_3(G)-\frac{4m}{n}(M_1(G)+2m)+\frac{8m^3}{n^2}.$$

From the above and (9) we arrive at (8).

Since the equality in (9) holds if and only if $\left|\mu_i-\frac{2m}{n}\right|\mu_i = \left|\mu_j-\frac{2m}{n}\right|\mu_j$, for every $1\le i\ne j\le n-1$, we conclude that the equality in (8) holds if and only if $\mu_1=\mu_2=\cdots=\mu_{n-1}$, or $\mu_1=\mu_2=\cdots=\mu_p$, $\mu_{p+1}=\mu_{p+2}=\cdots=\mu_{n-1}$ $(1\le p\le n-2)$ with $n(\mu_1^2+\mu_{n-1}^2)=2m(\mu_1+\mu_{n-1})$.
□

Since for the graph without triangles, i.e. cycles of length 3, holds $C_3(G)=0$, we have the following corollary of Theorem 3.1.

Corollary 3.2. *Let G be a simple connected graph with $n\ge 3$ vertices and m edges without triangles. Then*

$$n\left(LE(G)-\frac{2m}{n}\right)^2 \le Kf(G)\left(F(G)+\frac{3n-4m}{n}M_1(G)+\frac{8m^2(m-n)}{n^2}\right).$$

Equality holds if and only if $G\cong K_n$, or $\mu_1=\mu_2=\cdots=\mu_p$, $\mu_{p+1}=\mu_{p+2}=\cdots=\mu_{n-1}$ $(1\le p\le n-2)$ with $n(\mu_1^2+\mu_{n-1}^2)=2m(\mu_1+\mu_{n-1})$.

Theorem 3.3. *Let G be a simple connected graph with $n\ge 2$ vertices and m edges. Then*

$$nLEL^4(G)\le 8m^3Kf(G). \tag{10}$$

Equality holds if and only if $G\cong K_n$.

Proof. Setting $r=3$, $x_i:=\sqrt{\mu_i}$, $a_i:=\mu_i$, $i=1,2,\ldots,n-1$, in (7), we get

$$\sum_{i=1}^{n-1}\frac{1}{\mu_i}=\sum_{i=1}^{n-1}\frac{\mu_i^2}{\mu_i^3}=\sum_{i=1}^{n-1}\frac{\left(\sqrt{\mu_i}\right)^4}{\mu_i^3}\ge\frac{\left(\sum_{i=1}^{n-1}\sqrt{\mu_i}\right)^4}{\left(\sum_{i=1}^{n-1}\mu_i\right)^3},$$

i.e.

$$\frac{1}{n}Kf(G)\ge\frac{LEL^4(G)}{8m^3}, \tag{11}$$

wherefrom (10) is obtained.

Equality in (11) holds if and only if $\frac{\sqrt{\mu_1}}{\mu_1}=\frac{\sqrt{\mu_2}}{\mu_2}=\cdots=\frac{\sqrt{\mu_{n-1}}}{\mu_{n-1}}$, that is if and only if $\mu_1=\mu_2=\cdots=\mu_{n-1}$. Therefore equality in (10) is attained if and only if $G\cong K_n$ (see [7]). □

Remark 3.4. *In* [13] *it was proven*

$$LEL^2(G) \geq \frac{8m^3}{M_1(G)+2m}. \tag{12}$$

It can be easily verified that this inequality can simply be obtained from the inequality (see e.g. [26])

$$\left(\sum_{i=1}^{n-1} p_i\right)^2 \sum_{i=1}^{n-1} p_i a_i b_i c_i \geq \sum_{i=1}^{n-1} p_i a_i \sum_{i=1}^{n-1} p_i b_i \sum_{i=1}^{n-1} p_i c_i$$

by setting $p_i = a_i = b_i = c_i = \sqrt{\mu_i}$, $i = 1, 2, \ldots, n-1$.

From (12) *follows*

$$\frac{nLEL^4(G)}{8m^3} \geq \frac{nLEL^2(G)}{M_1(G)+2m},$$

therefore the inequality (10) *is stronger than* (2).

Remark 3.5. *Since*

$$M_1(G) + 2m \leq n\Delta^2 + 2m,$$

the inequality (3) *is a direct consequence of* (12).

Also, since

$$M_1(G) + 2m = \sum_{i=1}^{n} d_i^2 + 2m \leq \Delta \sum_{i=1}^{n} d_i + 2m = 2m(\Delta+1) \leq n\Delta^2 + 2m,$$

according to (12) *we get*

$$LEL(G) \geq \frac{2m}{\sqrt{1+\Delta}}. \tag{13}$$

The inequality (13) *is stronger than the inequalities* (3) *and* (4). *Therefore it is stronger than the inequality* (5). *This means that lower bound of LEL given by* (5) *is not optimal.*

In the next theorems we prove several inequalities that establish relationships between $S(G)$ and $Kf(G)$.

Theorem 3.6. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$Kf(G) \geq \frac{n^2(n-1)-2m}{2m} + \frac{n-1}{4m^2}\left(\frac{(n\Delta-2m)^2}{\Delta} + \frac{(nS(G)+2m-n\Delta)^2}{2m-\Delta}\right). \tag{14}$$

Equality holds if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \in \Gamma_d$.

Proof. The inequality (7) can be considered as

$$\sum_{i=2}^{n} \frac{x_i^{r+1}}{a_i^r} \geq \frac{\left(\sum_{i=2}^{n} x_i\right)^{r+1}}{\left(\sum_{i=2}^{n} a_i\right)^{r}}.$$

For $r = 1$, $x_i := \left|d_i - \frac{2m}{n}\right|$, $a_i := d_i$, $i = 2, 3, \ldots, n$, this inequality transforms into

$$\sum_{i=2}^{n} \frac{\left|d_i - \frac{2m}{n}\right|^2}{d_i} \geq \frac{\left(\sum_{i=2}^{n}\left|d_i - \frac{2m}{n}\right|\right)^2}{\sum_{i=2}^{n} d_i},$$

that is

$$\sum_{i=2}^{n} \frac{\left|d_i - \frac{2m}{n}\right|^2}{d_i} \geq \frac{\left(S(G) - \Delta + \frac{2m}{n}\right)^2}{2m - \Delta}. \tag{15}$$

On the other hand we have

$$\sum_{i=2}^{n} \frac{\left(d_i - \frac{2m}{n}\right)^2}{d_i} = \sum_{i=1}^{n} \frac{\left(d_i - \frac{2m}{n}\right)^2}{d_i} - \frac{\left(\Delta - \frac{2m}{n}\right)^2}{\Delta}$$
$$= \frac{4m^2}{n^2} ID(G) - 2m - \frac{(n\Delta - 2m)^2}{n^2\Delta}.$$

According to the above and (15) we get

$$\frac{4m^2}{n^2} ID(G) \geq 2m + \frac{(n\Delta - 2m)^2}{n^2\Delta} + \frac{(nS(G) + 2m - n\Delta)^2}{n^2(2m - \Delta)},$$

i.e.

$$ID(G) \geq \frac{n^2}{2m} + \frac{(n\Delta - 2m)^2}{4m^2\Delta} + \frac{(nS(G) + 2m - n\Delta)^2}{4m^2(2m - \Delta)}.$$

From the above and (6) follows

$$Kf(G) \geq -1 + \frac{n^2(n-1)}{2m} + \frac{n-1}{4m^2}\left(\frac{(n\Delta - 2m)^2}{\Delta} + \frac{(nS(G) + 2m - n\Delta)^2}{2m - \Delta}\right),$$

wherefrom (14) is obtained.

Equality in (6) holds if and only if $G \cong K_n$, or $G \cong K_{t,n-t}$, $1 \leq t \leq \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$. Equality in (15) is attained if and only if $d_2 = d_3 = \cdots = d_n$, or $d_2 = d_3 = \cdots = d_p$, $d_{p+1} = d_{p+2} = \cdots = d_n$, $2 \leq p \leq n-1$, with $\frac{\left|d_2 - \frac{2m}{n}\right|}{d_2} = \frac{\left|d_n - \frac{2m}{n}\right|}{d_n}$. These conditions together give that equality in (14) holds if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \in \Gamma_d$.

□

Since $\frac{(n-1)(nS(G) + 2m - n\Delta)^2}{4m^2(2m - \Delta)} \geq 0$, we have the following corollary of Theorem 3.6.

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

$$Kf(G) \geq \frac{n^2(n-1) - 2m}{2m} + \frac{(n-1)(n\Delta - 2m)^2}{4m^2\Delta}. \tag{16}$$

Equality holds if and only if $G \cong K_n$, or $G \in \Gamma_d$.

Remark 3.8. *The inequality* (16) *is stronger than inequalities*

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

and

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

proven in [21].

In the case of d-regular graphs, $1 \leq d \leq n-1$, the inequality (16) *transforms into*

$$Kf(G) \geq \frac{n(n-1) - d}{d},$$

which was proven in [28].

By the similar arguments as in case of Theorem 3.6, the following results can be proved.

Theorem 3.9. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$Kf(G) \geq \frac{n^2(n-1)-2m}{2m} + \frac{n-1}{4m^2}\left(\frac{(n\delta-2m)^2}{\delta} + \frac{(nS(G)-2m+n\delta)^2}{2m-\delta}\right).$$

Equality holds if and only if $G \cong K_n$, or $G \in \Gamma_d$.

Theorem 3.10. *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

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

Equality holds if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \in \Gamma_d$.

Theorem 3.11. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$8m^3(Kf(G)+1) - n^2(n-1)S^2(G) \geq 4n^2(n-1)m^2.$$

Equality holds if and only if $G \cong K_n$, or $G \in \Gamma_d$.

Theorem 3.12. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$(Kf(G)+1)\left(F(G) - \frac{4m}{n}M_1(G) + \frac{8m^3}{n^2}\right) \geq (n-1)S^2(G). \tag{17}$$

Equality holds if and only if G is a regular graph.

Proof. For $r = 1$, $x_i := \left|d_i - \frac{2m}{n}\right|$, $a_i := \frac{1}{d_i}$, $i = 1, 2, \dots, n$, the inequality (7) becomes

$$\sum_{i=1}^{n}\left|d_i - \frac{2m}{n}\right|^2 d_i \geq \frac{\left(\sum_{i=1}^{n}\left|d_i - \frac{2m}{n}\right|\right)^2}{\sum_{i=1}^{n}\frac{1}{d_i}},$$

that is

$$\sum_{i=1}^{n}\left|d_i - \frac{2m}{n}\right|^2 d_i \geq \frac{S^2(G)}{ID(G)}. \tag{18}$$

On the other hand we have

$$\sum_{i=1}^{n}\left|d_i - \frac{2m}{n}\right|^2 d_i = \sum_{i=1}^{n}\left(d_i^3 - \frac{4m}{n}d_i^2 + \frac{4m^2}{n^2}d_i\right) = F(G) - \frac{4m}{n}M_1(G) + \frac{8m^3}{n^2}.$$

According to the above and (18) we get

$$\left(F(G) - \frac{4m}{n}M_1(G) + \frac{8m^3}{n^2}\right)ID(G) \geq S^2(G). \tag{19}$$

From (6) follows

$$ID(G) \leq \frac{Kf(G)+1}{n-1}. \tag{20}$$

Now, (17) is obtained from (19) and (20).

Equality in (19) holds if and only if G is a regular graph for any value of invariant $ID(G)$. Therefore equality in (17) is attained if and only if G is a regular graph.

□

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