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ON LEAP ZAGREB COINDICES OF GRAPHS

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Abstract

The leap Zagreb indices of a graph G are a distance-degree-based topological indices conceived depending on the second degrees of vertices (number of its second neighbors). In the last years, these attract the attention of many researchers in Graph Theory and also in other sciences including chemistry. In this paper, we are interested in studying leap Zagreb coincidces of graphs. The exact formulas for some standard graphs are estimated. The relations between the leap Zagreb coindices and each of the leap Zagreb indices, Zagreb indices and Zagreb coindices are determined. Finally, lower and upper bounds on leap Zagreb coindices are established.

1. Introduction

In this paper, we consider only with a finite simple graph, that is undirected with no loops, weighted and multiple edges. As usual, we denote by $m = |E|$, where $V = V(G)$ and $E = E(G)$ are the vertex and edge sets of a graph G, respectively and by a symbol $|X|$, we mean a cardinality of a set X.

The distance $d(u, v)$ between any two vertices u and v of G is the length of a minimum path connecting them. The eccentricity of $v \in vV(G)$ is $e(v) = \max\{d(u, v) : u \in V(G)\}$, the radius of G is $rad(G) = \min\{e(v) : u \in V(G)\}$ and the diameter of G is $diam(G) = \max\{e(v) : v \in V(G)\}$.

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For a vertex $v \in V(G)$ and a positive integer k, the open k-distance neighborhood of v in a graph G, denote $N_k(v/G)$ $(or N_k(v)$, if no misunderstanding), is $N_k(v/G) = \{u \in V(G) : d(u, v) = k\}$. The k-distance degree of a vertex v, denote $d_k(v/G)$ $(or d_k(v))$, and is $d_k(v) = |N_k(v)|$. The k-maximum and k-minimum degrees among the vertices of a graph G, are denoted by $\Delta_k = \Delta_k(G)$ and $\delta_k = \delta_k(G)$, respectively. We denote $E_k(G) = \{e_k = uv : u, v \in V(G)$, and $d(u, v) = k\}$. To write less, when $k = 1$, the symbols d_k, N_k, $E_k, \ldots$, will be write without index, e. g., $d_1(v)$ will be write $d(v)$ and etc.

A graph G is called a trivial graph if it has only one vertex. The complement graph of a graph G, denoted $\overline{G}$, is a graph with vertex set V and edge set $\overline{E}$, such that $e \in \overline{E}$, if and only if $e \notin E$. Two graphs G and H are isomorphic, if there are bijections $f : V(G) \to V(H)$ and $g : E(G) \to E(H)$ such that $e = uv \in E(G)$, if and only if $g(e) = f(u)f(v) \in E(H)$. A graph G is said to be a self-complementary (in short sc-graph) if G is isomorphic to its complement. $\overline{K}_n$ is the empty or total disconnected graph with n vertices, i.e., the graph with n vertices no two of which are adjacent. An r-regular graph G is a graph which in the degree $d(v/G)$ of each vertex $v \in V(G)$ is equal to r. A graph G is called F-free graph if no induced subgraph of G is isomorphic to F. If a graph G consists of p disjoint components of a graph H, then we write $G = pH$. $diam(G) = rad(G)$, then G is called a self-centered graph. For any terminology or notation not mention here, we refer the reader to the books [5, 11].

A topological index (or a graph invariant) is a fixed invariant number for two isomorphic graphs, where a graph invariant is any function on a graph that does not depend on a labeling of its vertices. These indices are especially useful in the study of molecular graphs. In mathematical chemistry, particularly in QSPR/QSAR investigation, a large number of topological indices were introduced and extensively studied in an attempt to characterize the physical-chemical properties of molecules. Some of topological indices are defined by means of the vertex degrees and can be generally represented as the sum of a real function f associated with the edges of G. Their general formula is

$$TI = TI(G) = \sum_{uv \in E(G)} f(d(u), d(v))$$

where $f(x, y)$ is some function with the property $f(x, y) = f(y, x)$.

In the current mathematical and mathematico-chemical literature a large number of vertex-degree-based graph invariants are being studied [10, 14]. Among them, the so-called first $M_1(G)$ and second $M_2(G)$ Zagreb indices are the far most extensively investigated ones. These have been introduced more than forty years ago [15, 16], and are defined as:

$$M_1(G) = \sum_{v \in V(G)} d^2(v) = \sum_{uv \in E(G)} (d(v) + d(d)),$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

For more properties of the two Zagreb indices see [13] and the papers cited therein.

Analogously, the Zagreb coindices was put forward in [9], in the hope that it will improve our ability to quantify the contributions of pairs of non-adjacent vertices to various properties of molecules. As a bonus, the new invariants allowed for more compact expressions for the vertex-weighted Wiener polynomials of the considered composite graphs. Whereas the Zagreb indices can be considered as consisting of the contributions of pairs of adjacent vertices to additively and multiplicative weighted versions of Wiener numbers and polynomials. The Zagreb coindices are defined as:

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} (d(u) + d(v)),$$

$$\overline{M_2}(G) \sum_{uv \notin E(G)} d(u)d(v).$$

For more details on the Zagreb coindices, we refer the reader to [1, 2, 8, 12]. The reader should note that Zagreb coindices of G are not Zagreb indices of $\overline{G}$, the defining sums run over the edges of the complement graph $\overline{G}$, but the degrees are with respect to G. However, those quantities are closely related.

In 2017, Naji et al. [20], introduced three new distance-degree-based topological indices conceived depending on the second degrees of vertices, and are so-called leap Zagreb indices of a graph G and are defined as:

$$LM_1(G) = \sum_{v \in V(G)} d_2^2(v)$$

$$LM_2(G) = \sum_{uv \in E(G)} d_2(u) d_2(v)$$

$$LM_3(G) = \sum_{v \in V(G)} d(v) d_2(v).$$

The leap Zagreb indices have several chemical applications. Surprisingly, the first leap Zagreb index has very good correlation with physical properties of chemical compounds like boiling point, entropy, DHVAP, HVAP and accentric factor [4], hence attract the attention of many graph theorists and also other scientists including chemists. For properties and more details of leap Zagreb indices, we refer the readers to [3, 4, 17-21, 23-26].

In this paper, motivated by the Zagreb coindices of a graph, we introduce the leap Zagreb coindices of a graph G. The exact formulas of them for some standard graphs as the complete graph K_n, path P_n, cycle C_n, complete bipartite $K_{r,s}$, star $K_{1,n-1}$ and wheel graph W_n, will be derive. Lower and upper bounds will be establish. Furtherer, We wish to investigate the relationships between leap Zagreb coindices and each of Zagreb coindices, Zagreb indices and leap Zagreb indices.

The following fundamental results which will be used in many of our subsequent considerations are found in the earlier papers [26] and [20].

Lemma 1.1. *Let G be a connected graph with n vertices and m edges. Then*

$$d_2(v) \leq \left(\sum_{u \in N(v)} d(u) \right) - d(v)$$

Equality holds if and only if G is a C_3, C_4-free graph.

Lemma 1.2. *Let G be a connected graph with n vertices. Then for any vertex $v \in V(G)$*

$$d_2(v) \leq n + 1 - d(v) - e(v).$$

Equality holds if and only if G is a Moore graph with diameter at most two.

Lemma 1.3. *Let G be a connected graph with n vertices. Then for any vertex $v \in V(G)$*

$$d_2(v/G) \leq d(v/\overline{G}) = n - 1 - d(v/G).$$

Equality holds if and only if G has diameter at most two.

From Lemma 1.1, it follows,

Corollary 1.4. *Let G be a graph with n vertices and m edge. Then*

$$\sum_{v \in V(G)} d_2(v) \leq M_1(G) - 2m.$$

Equality holds if and only if G is C_3, C_4-free graph.

Corollary 1.5. *Let G be a C_3, C_4-free k-regular graph with n vertices. Then*

$$d_2(v) = k(k-1).$$

2. Leap Zagreb Coindices of a graph

To simplify the definition of leap Zagreb coindices of a graph, we will rewrite the expressions of leap Zagreb indices (namely, first and third) such that the sum run over the edges of the graph G. It is easy to show that the first and third leap Zagreb indices can also be expressed as:

$$LM_1(G) = \sum_{uv \in E(G)} \left(\frac{d_2^2(v)}{d(v)} + \frac{d_2^2(u)}{d(u)} \right) = \sum_{uv \in E_2(G)} (d_2(v) + d_2(u)),$$

$$LM_3(G) = \sum_{uv \in E(G)} (d_2(v) + d_2(u)).$$

where, E_2 is denoted to the set of all pairs of vertices $u, v \in V(G)$, with $d(u, v) = 2$. In other word, E_2 is the edge set of G^2, where G^2 is the graph with $V(G^2) = V(G)$ and $uv \in E_2 = E(G^2)$ if and only if $d(u, v) = 2$ in a graph G.

Definition 1. For *a* graph $G = (V, E)$, the leap Zagreb coindices of G are defined as

$$\overline{LM_1}(G) = \sum_{uv \notin E_2(G)} (d_2(v) + d_2(u))$$

$$\overline{LM_2}(G) = \sum_{uv \notin E(G)} d_2(v) d_2(v),$$

$$\overline{LM_3}(G) = \sum_{uv \notin E(G)} (d_2(v) + d_2(u))$$

In what following, to write less, we will be writing $L_i(G), \overline{L}_i(G)$ (or in short L_i, $\overline{L}_i$) instead of $LM_i(G)$ and $\overline{LM}_i(G)$, for $i = 1, 2, 3$.

The following result is straightforward consequence of Definition 1:

Theorem 2.1. *For integer number $k \geq 2$, let $G_1, G_2, \ldots, G_k$ be pairwise vertex-disjoint graphs. Then for $G = G_1 \cup G_2 \cup \ldots \cup G_k$ and for $i = 1, 2, 3$,*

$$\overline{L_i}(G) = \overline{L_i}(G_1) + \overline{L_i}(G_2) + \ldots + \overline{L_i}(G_k).$$

3. Leap Zagreb Coindices for Some Standard Graphs

In this section, we are interested in computing the exact formulas of leap Zagreb coindices of some standard graphs.

1. For the complete graph K_n and the totally disconnected graph $\overline{K_n}$, $n \leq 1$,

$$\overline{L_i}(K_n) = \overline{L_i}(\overline{K_n}) = 0, \text{ for } i = 1, 2, 3,$$

2. For the path P_n, $n \geq 3$,

- $\overline{L_1}(P_n) = \begin{cases} 2, & \text{for } n = 3, \\ 2n(n-1)+16, & \text{otherwise.} \end{cases}$

- $\overline{L_2}(P_n) = \begin{cases} 2, & \text{if } n = 3, \\ 8, & \text{if } n = 4, \\ 2n(n-7)+28, & \text{otherwise.} \end{cases}$

- $\overline{L_3}(P_n) = 2n(n-5)$.

3. For the cycle C_n, $n \geq 3$,

- $\overline{L_1}(C_n) = 2n(n-3)$.

- $\overline{L_2}(C_n) = \begin{cases} 0, & \text{if } n = 3, \\ 4, & \text{if } n = 4, \\ 2n(n-3), & \text{otherwise.} \end{cases}$

- $\overline{L_3}(C_n) = \begin{cases} 0, & \text{if } n = 3, \\ 4, & \text{if } n = 4, \\ 2n(n-3), & \text{otherwise.} \end{cases}$

4. For the complete bipartite $K_{r,s,}$ for $2 \leq r \leq s$,

- $\overline{L_1}(K_{r,s}) = rs(r+s-2)$.

- $\overline{L_2}(K_{r,s}) = \frac{1}{2}(r(r-1)^3 + s(s-1)^3)$.

- $\overline{L_3}(K_{r,s}) = r(r-1)^2 + s(s-1)^2$.

5. For the star $K_{1,n-1}$, $n \geq 3$

- $\overline{L_1}(K_{1,n-1}) = (n-1)(n-2)$.

- $\overline{L_1}(K_{1,n-1}) = \frac{1}{2}(n-1)(n-2)^3$.

- $\overline{L_1}(K_{1,n-1}) = (n-1)(n-2)^2$.

6. For the wheel $W_{1,n}$, $n \geq 4$,

- $\overline{L_1}(W_{1,n}) = 3n(n-3)$.

- $\overline{L_2}(W_{1,n}) = \frac{1}{2}n(n-3)^3$.

- $\overline{L_3}(W_{1,n}) = n(n-3)^2$.

4. Some properties of leap Zagreb coindices of graphs

In this section, we investigate to determine all relationships between the leap Zagreb indices and coindices of a graph G and of its complement $\overline{G}$.

Theorem 4.1. *Let G be a graph with n vertices and m edges. Then*

$$\overline{L_1}(G) \leq (n-1)[M_1(G) - 2m] - L_1(G), \tag{1}$$

$$\overline{L_2}(G) \leq \frac{(n-1)}{2n}[M_1(G) - 2m]^2 - L_2(G), \tag{2}$$

$$\overline{L_3}(G) \leq (n-1)[M_1(G) - 2m] - L_3(G). \tag{3}$$

Equalities holds if and only if G is C_3, C_4*-free.*

Proof. We start with the proof of the inequality (1), by using the following famous identity which is found in [12],

$$\sum_{u \in v(G)} \sum_{u \in v(G)} [d(u) + d(v)] = 4nm.$$

Where the summation in the left-hand-side can be partitioned as follows

$$\sum_{uv \in E(G)} + \sum_{uv \notin E(G)} + \sum_{v = u \in V(G)} 4nm.$$

Which is a direct consequence of the fact that the sum of degrees of all vertices is equal to $4nm$. To make it consistent with the sum of the second degrees and to used it without repeat in the computations, we rewrite it as follows

$$\sum_{uv\in E_2(G)} + \sum_{uv\notin E_2(G)} = (n-1)\sum_{v\in V(G)} d_2(v).$$

Which in view of the definitions of $L_1(G)$ and $\overline{L_1}(G)$ yields

$$L_1(G) + \overline{L_1}(G) = (n-1)\sum_{v\in V(G)} d_2(v)$$

which led by using Corollary 1.4, to

$$\overline{L_1}(G) \leq (n-1)[M_1(G) - 2m] - L_1(G)$$

and again by Corollary 1.4, the equality holds if and only if G is a C_3, C_4-free graph.

To prove the inequality (2), we again using the following identity, which also found in [12],

$$\sum_{u\in v(G)}\sum_{u\in v(G)}[d(u)d(v)] = 4m^2.$$

Where the summation in the left-hand-side can be partitioned as follows

$$2\sum_{uv\in E(G)} + 2\sum_{uv\notin E(G)} + \sum_{v=u\in V(G)} = 4m^2$$

and hence

$$2\sum_{uv\in E} d_2(v)d_2(u) + 2\sum_{uv\notin E} d_2(v)d_2(u) + \sum_{v\in V(G)} d_2^2(v) = \left(\sum_{v\in V(G)} d_2(v)\right)^2.$$

Which in view of the definitions of $L_2(G)$ and $\overline{L_2}(G)$ yields

$$2L_2(G) + 2\overline{L_2}(G) + \sum_{v\in V(G)} d_2^2(v) = \left(\sum_{v\in V(G)} d_2(v)\right)^2$$

and by using Corollary 1.4, and bearing in the mind Theorem 5, in [21],

which state that, $L_1(G) \geq \frac{1}{2}(M_1(G) - 2m)^2$, with equality holds if and only if G is a C_3, C_4-free, we get

$$\overline{L_2}(G) \leq \frac{1}{2}(M_1(G) - 2m)^2 - \frac{1}{2}L_1(G) - L_2(G)$$

$$\leq \frac{1}{2}(M_1(G) - 2m)^2 - \frac{1}{2n}(M_1(G) - 2m)^2 - L_2(G).$$

$$= \frac{n-1}{2n}(M_1(G) - 2m)^2 - L_2(G).$$

and equality holds if and only if G is a C_3, C_4-free.

Finally, the proof of the inequality (3), is analogous to the proof of the inequality (1).

Corollary 4.2. *Let G be a C_3, C_4-free graph with n vertices and m edges. Then*

$$L_1(G) + \overline{L_1}(G) = (n-1)[M_1(G) - 2m],$$

$$L_2(G) + \overline{L_2}(G) = \frac{(n-1)}{2n}[M_1(G) - 2m]^2,$$

$$L_3(G) + \overline{L_3}(G) = (n-1)[M_1(G) - 2m].$$

In the following result, we determine the relationships between the first and third leap Zagreb indices and coindices of a graph.

Theorem 4.3. *For a connected graph G,*

$$\overline{L_1}(G) \geq L_3(G) \tag{4}$$

$$\overline{L_3}(G) \geq L_1(G). \tag{5}$$

Equalities holds if and only if G has a diameter at most two.

Proof. We prove only the inequality (4). The proof of the inequality (5) is analogous.

Let G be a connected graph with n vertices and $diam(G) = D$, and let the set of all k-edge of G, for $1 \leq k \leq D$, is denoted and defined as

$$\varepsilon = \varepsilon(G) = E_1(G) \cup E_2(G) \cup \ldots \cup E_D(G).$$

It is clear, that $E_1, E_2, \ldots, E_D$ are pairwise edge-disjoint and the complement set of E_k is $\overline{E_k}(G) = \varepsilon - E_k(G)$. Thus, for any two vertices $u, v \in V(G)$, if $uv \in E_1 = E(G)$, then $uv \in \overline{E_2}$, and so, $uv \notin E_2$, which implies that $E(G) \subseteq \overline{E_2}$. Moreover, for any fixed number $k, 1 \leq k \leq D$, the following inequality yields

$$\sum_{uv \in E} [d_k(u) + d_k(v)] \leq \sum_{uv \in \overline{E_2}} [d_k(u) + d_k(v)].$$

Hence,

$$L_3(G) = \sum_{uv \in E(G)} (d_2(u) + d_2(v)) \leq \sum_{uv \in \overline{E_2}} (d_2(u) + d_2(v))$$

$$= \sum_{uv \notin E_2(G)} (d_2(u) + d_2(v)) = \overline{L_1}(G).$$

To prove the equality in (4), firstly, it is easy to see that, $E(G) = \overline{E_2}(G)$, if and only if $\varepsilon = E \cup E_2$, if and only if G has a diameter $D = 2$. Then, if $diam(G) = 1$ or $G = K_1$, then $d_2(v) = 0$, for every $v \in V(G)$, and hence, $L_3(G) = \overline{L_1}(G) = 0$. Therefore, $\overline{L_1}(G) = L_3(G)$, if and only if $diam(G) \leq 2$.

From the Definitions of leap Zagreb indices and condices, and by using the identity

$$\sum_{uv \in E_k} [d_j(u) + d_j(v)] + \sum_{uv \notin E_k} [d_j(u) + d_j(v)] = (n-1) \sum_{v \in V(G)} d_j(v)$$

where, $j, k = 1, 2, \ldots, diam(G)$, the following result is straightforward.

Observation 4.4. For any graph G,

$$L_1(G) + \overline{L_1}(G) = L_3(G) + \overline{L_3}(G).$$

Recall, the Leap graph [18], that is a graph G in which $d(v) = d_2(v)$, for every $v \in V(G)$, and by using the above Observation, we directly arrive at the following result.

Observation 4.5. For $n \leq 1$, if G, is a leap graph or $G = K_1 + 2K_n$, then

$$L_1(G) = L_3(G) \, and \, \overline{L_1}(G) = \overline{L_3}(G).$$

Furthermore*, if* G is a leap graph with $diam(G) = 2$, *or* $G = K_1 + 2K_n$, then

$$L_1(G) = \overline{L_1}(G) = L_3(G) = \overline{L_3}(G).$$

5. Relations between Leap Zagreb Coindices and Zagreb Indices and Coindices

In this section we determine the relationships between leap Zagreb coindices and both of Zagreb indices and coindices of a graph.

Firstly, for the first leap coindex, in general case, we can compare between the first leap Zagreb coindex and any one of the first Zagreb indices and coindices. For instance,

$$\overline{L_1}(P_4) < M_1(P_4), \overline{L_1}(P_5) = M_1(P_5), \overline{L_1}(P_6) > M_1(P_6),$$

$$\overline{L_1}(P_5) < \overline{M_1}(P_5), \overline{L_1}(P_4) = \overline{M_1}(P_4), \overline{L_1}(B_{3,3}) > \overline{M_1}(B_{3,3}),$$

where $B_{3,3}$ is a graph formed by join $\overline{K_3}$ to an end vertex of P_3. Similarly, for the complement graph, we have,

$$\overline{L_1}(\overline{P_6}) < \overline{M_1}(P_6) = \overline{M_1}(\overline{P_6}), \overline{L_1}(\overline{P_4}) = \overline{M_1}(P_4), \overline{L_1}(\overline{P_5}) > \overline{M_1}(P_5).$$

However, we have the following special case,

Observation 5.1. Let G be a graph diameter at most two. Then

$$\overline{L_1}(G) = \overline{L_1}(\overline{G}) = \overline{M_1}(G) = \overline{M_1}(\overline{G}).$$

Then, for the second leap Zagreb coindex, we have

Proposition 5.2. *Let G be a connected graph*. Then

$$\overline{L_2}(G) \leq M_2(\overline{G}) \tag{6}$$

$$\overline{L_2}(\overline{G}) \leq M_2(G). \tag{7}$$

Equalities hold if and only if G has diameter at most two.

Proof. By Lemma 1.3, and the definition of the complement graph, the proof is immediately consequence.

Observation 5.3. If G is a leap graph, or $G = K_1 + 2K_n,\ n \geq 1,$ then

$$\overline{L_2}(G) = \overline{M_2}(G) \tag{8}$$

$$L_2(G) = M_2(G). \tag{9}$$

From Theorem 3, in [18], and by combine the above results on $\overline{L_2}(G),$ we arrive at,

Observation 5.4. If G is a connected leap graph with $diam(G) = 2,$ then

$$L_2(G) = L_2(\overline{G}) = \overline{L_2}(G) = \overline{L_2}(\overline{G}) = \overline{M_2}(G) = M_2(G) = \frac{m(n-1)^2}{4}.$$

Finally, similar to the results of the second leap Zagrb coindex above, for the third leap Zagreb coindex, we have,

Proposition 5.5. *Let G be a connected graph. Then*

$$\overline{L_3}(G) \leq M_1(\overline{G}) \tag{10}$$

$$\overline{L_3}(\overline{G}) \leq M_1(G) \tag{11}$$

Equalities hold if and only if G has diameter at most two.

Observation 5.6. If G is a leap graph, or $G = K_1 + 2K_n,\ n \geq 1,$ then

$$\overline{L_3}(G) = \overline{M_1}(G) \tag{12}$$

$$L_1(G) = M_1(G). \tag{13}$$

Observation 5.7. If G is a connected leap graph with $diam(G) = 2,$ then

$$L_3(G) = L_3(\overline{G}) = \overline{L_3}(G) = \overline{L_3}(\overline{G}) = \overline{M_1}(G) = M_1(G) = \frac{m(n-1)^2}{4}.$$

6. Bounds on Leap Zagreb Coindices of Graphs

In this section, some lower and upper bounds on leap Zagreb coindices of a graph will be established.

Theorem 6.1. *Let G be a graph with n vertices and m edges. Then*

$$\overline{L_2}(G) \leq (n-1)^2\left(\frac{n(n-1)-2m}{2}\right) - (n-1)\overline{M_1}(G) + M_2(G),$$

$$\overline{L_3}(G) \leq n(n-1)^2 - 2m(n-1) - \overline{M_1}(G).$$

Equalities hold if and only if G has diameter at most two.

Proof. We prove only the inequality (14). Similar arguments can be applied on the inequality (15). From Corollary 1.4, and by using the definitions of the Zagreb coindices, we get

$$\begin{aligned}
\overline{L_2}(G) &= \sum_{uv \notin E(G)} d_2(u) d_2(v) \\
&\leq \sum_{uv \notin E(G)} (n-1-d(u))(n-1-d(v)) \\
&= \sum_{uv \notin E(G)} [(n-1)^2 - (n-1)(d(u)+d(v)) + d(u)d(v)] \\
&= \sum_{uv \notin E(G)} (n-1)^2 - (n-1) \sum_{uv \notin E(G)} (d(u)+d(v)) + \sum_{uv \notin E(G)} d(u)d(v) \\
&= \left[\frac{n(n-1)}{2} - m\right](n-1)^2 - (n-1)\overline{M_1}(G) + \overline{M_2}(G) \\
&= (n-1)^2\left(\frac{n(n-1)-2m}{2}\right) - (n-1)\overline{M_1}(G) + \overline{M_2}(G).
\end{aligned}$$

By Corollary 1.4, $d_2(v) = n-1-d(v)$, for every $v \in V(G)$ if and only if $diam(G) \leq 2$. This completes the proof.

Throughout the proof of the next result, $\xi^c(G)$ denotes the eccentric connectivity index of a graph, which introduced by Sharma at el., [22], and defined as

$$\xi^c(G) = \sum_{v \in V(G)} d(v)e(v) = \sum_{uv \in E(G)} e(v)e(u).$$

Theorem 6.2. *Let G be a connected graph with n vertices, m edges and diam(G) = D. Then*

$$\overline{L_2}(G) \leq (n+1)^2\left(\frac{n(n-1)-2m}{2}\right) + (D-n-1)\overline{M_1}(G) + \overline{M_2}(G) - (n+1)\overline{\xi^c}(G) \tag{16}$$

$$\overline{L_3}(G) \leq n(n^2-1) - 2m(n+1) - \overline{M_1}(G) - \overline{\xi^c}(G). \tag{17}$$

Equalities hold if and only if G is a Moore graph with diameter two.

Proof. Let us start proving the inequality (16). By Lemma 1.2, and using the fact $e(v) \leq D$, for every $v \in V(G)$, we get

$$\overline{L_2}(G) = \sum_{uv \notin E(G)} d_2(u) d_2(v)$$

$$\leq \sum_{uv \notin E(G)} [n+1-d(u)-e(u)][n+1-d(v)-e(v)]$$

$$= \sum_{uv \notin E(G)} [(n+1)^2 - (n+1)[d(u)+d(v)+e(u)+e(v)] + d(u)d(v) + d(u)e(v) + d(v)e(u)]$$

$$\leq \sum_{uv \notin E(G)} (n+1)^2 - (n+1)\left[\sum_{uv \notin E(G)} [d(u)+d(v)] + \sum_{uv \notin E(G)} [e(u)+e(v)]\right]$$

$$+ \sum_{uv \notin E(G)} d(u)d(v) + D \sum_{uv \notin E(G)} [d(u)+d(v)]$$

$$\overline{L_2}(G) \leq (n+1)^2\left[\frac{n(n-1)}{2} - m\right] - (n+1)[\overline{M_1}(G) + \overline{\xi^c}(G)] + \overline{M_2}(G) + D\overline{M_1}(G)$$

$$= (n+1)^2\left(\frac{n(n-1)-2m}{2}\right) + (D-n-1)\overline{M_1}(G) + \overline{M_2}(G) - (n+1)\overline{\xi^c}(G).$$

Then, by Lemma 1.2, $d_2(v) = n+1-d(v)-e(v)$, for every $v \in V(G)$ if and only if G is a more graph with $diam(G) \leq 2$, and since all Moore graph with diameter two are the pentagon, Petersen graph, Hoffman singleton graph, and possibly a 57-regular with $572+1$ vertices (see [7]). Moreover, every one of them is a self-centered graph, which is our assertion.

The proof of the inequality (17), is similar in sprite.

Proposition 6.3. *Let G be a connected graph with n vertices and m edges Then*

$$\overline{L_1}(G) \le \frac{m(m-1)}{n^2}[n^2(n-1) - 2m(2m-n)], \tag{18}$$

$$\overline{L_3}(G) \le \frac{m(m-1)}{n}[n(n-1) - 2m]. \tag{19}$$

Proof. For the inequality (18), by Theorem 1.4, and bearing in the mind the facts that, $M_1(G) \ge \frac{4m^2}{n}$, for any connected graph G with $n \ge 2$ vertices, (see [6, 27]), and $M_1(G) \ge m(m+1)$ (see [6]) and by using the inequality

$$L_1(G) \ge \frac{(M_1(G) - 2m)^2}{n} \text{ (see [20]), we get that}$$

$$\overline{L_1}(G) \le (n-1)[M_1(G) - 2m] - L_1(G)$$

$$\le (n-1)[M_1(G) - 2m] - \frac{(M_1(G) - 2m)^2}{n}$$

$$\le (M_1(G) - 2m)\left[(n-1) - \frac{(M_1(G) - 2m)}{n}\right]$$

$$\le (m(m+1) - 2m)\left[(n-1) - \frac{4m^2/n - 2m}{n}\right]$$

$$= \left(m^2 - m\right)\left[(n-1) - \frac{2m}{n^2}(2m-n)\right]$$

$$= \frac{m(m-1)}{n^2}\left[n^2(n-1) - 2m(2m-n)\right].$$

Similar arguments can be applied for the proof of the inequality (19), with using the inequality $L_3(G) \ge \frac{2m}{n}(M_1(G) - 2m)$ (see [20]), which complete the proof.

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