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LEAP ZAGREB INDICES OF MYCIELSKIAN OF GRAPHS

H. R. Manjunatha, Ahmed M. Naji, and Soner Nandappa D

Abstract. In a graph $G = (V, E)$, the first (second) degree of a vertex v is equal to the number of its first (second) neighbors in G and is denoted by $d(v/G)$ (resp. $d_2(v/G)$). The first, second and third leap Zagreb indices of G have been introduced by Naji et al. [**15**], and are the sum of squares of second degrees of vertices of G, the sum of products of second degrees of pairs of adjacent vertices in G and the sum of products of first and second degrees of vertices of G, respectively. In this paper, the formulaes of leap Zagreb indices for Mycielskian of G are established, and we apply these formulae for some standard graphs.

1. Introduction

In this paper, by a graph $G = (V, E)$, we mean a finite, undirected graph with neither loops nor multiple edges. The order and size of G are denoted by $n = |V|$ and $m = |E|$ respectively. The distance $d_G(u, v)$ between any two vertices u and v of a graph G is equal to the length of (number of edges in) a shortest path connecting them. For a vertex $v \in V(G)$ and a positive integer k, the open k-neighborhood of v in a graph G is denoted by $N_k(v/G)$ and is defined as $N_k(v/G) = \{u \in V(G) : d_G(u, v) = k\}$. The k-degree of a vertex v in G is denoted by $d_k(v/G)$ (or $d_k(v)$) and is defined as the number of k-neighbors of the vertex v in G, i.e., $d_k(v/G) = |N_k(v/G)|$. It is clearly that $d_1(v/G) = d(v/G)$ and $d_2(v/G) = |N_2(v/G)|$, for

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every $v \in V(G)$. We follow Harary book [**11**], for unexplained graph theoretic, terminologies and notations.

In the interdisciplinary area where chemistry, physics and mathematics meet, molecular graph based structure descriptors, usually referred to as topological indices, are of significant importance. A topological index of a graph is a graph invariant number calculated from a graph representing a molecule. Among the most important such structure descriptors are the classical first and second Zagreb indices, which introduced by Gutman and Trinajestic [**10**], in (1972), and elaborated in [**9**]. They are defined as:

$$M_1(G) = \sum_{v \in V(G)} d_1^2(v/G)$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_1(u/G)d_1(v/G).$$

These are widely studied degree based topological indices due to their applications in chemistry. For properties of the two Zagreb indices see [**5, 9, 19, 22**], and for more details see the survey [**3**] and the references cited therein. After most of the results on Zagreb indices were established, the inevitable occurred, Their various modifications have been proposed, thus opening the possibility to do analogous research and publish numerous additional papers. For these modifications see the recent survey [**8**].

In 2017, Naji et al. [**15**], have been introduced leap Zagreb indices. For a graph G, the first, second, and third leap Zagreb indices are denoted and defined respectively as:

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

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

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

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 [**2**]. For recent studying and more details on leap Zagreb indices, we refer to [**1, 2, 8, 15, 16, 17, 18, 20**].

In this paper, we establish the formulas of the leap Zagreb indices for Mycielskian of a graph G, and we apply these formulaes for some standard graphs as the path P_n, cycle C_n, complete graph K_n, complete bipartite graph $K_{r,s}$ and the star graph $K_{1,n-1}$.

The following fundamental results which will be required for many of our arguments in this paper.

LEMMA 1.1 ([**21, 23**]). *Let G be a connected graph with n vertices and m edges. Then*

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

Equality holds if and only if G is a $\{C_3, C_4\}$-free graph.

PROPOSITION 1.1 ([**15**]). *The following hold:*

(1) *For the complete graph K_n, $n \geqslant 1$,*
- $LM_i(K_n) = 0$, *for* $i = 1, 2, 3$.

(2) *For the path P_n, $n \geqslant 3$,*
- $LM_1(P_n) = \begin{cases} 2, & \text{if } n = 3; \\ 4(n-3), & \text{otherwise.} \end{cases}$
- $LM_2(P_n) = \begin{cases} 0, & \text{if } n = 3; \\ 3, & \text{if } n = 4; \\ 2(2n-7), & \text{otherwise.} \end{cases}$
- $LM_3(P_n) = 2(2n-5)$.

(3) *For the cycle C_n, $n \geqslant 3$,*
- $LM_i(C_n) = \begin{cases} 0, & \text{if } n = 3,\ i = 1,2,3; \\ 4, & \text{if } n = 4,\ i = 1,2; \\ 8, & \text{if } n = 4,\ i = 3; \\ 4n, & \text{otherwise.} \end{cases}$

(4) *For the star $K_{1,n}$, $n \geqslant 1$,*
- $LM_1(K_{1,n}) = n(n-1)^2$,
- $LM_2(K_{1,n}) = 0$,
- $LM_3(K_{1,n}) = n(n-1)$.

(5) *For the complete bipartite graph $K_{r,s}$, $s \geqslant r \geqslant 1$,*
- $LM_1(K_{r,s}) = r(r-1)^2 + s(s-1)^2$,
- $LM_2(K_{r,s}) = rs(r-1)(s-1)$,
- $LM_3(K_{r,s}) = rs(r+s-2)$.

2. Mycielskian Transformation

In this section, we present the definition of Mycielskian transformation of a graph G and we investigate some properties of degrees of vertices of Mycielskian of a graph.

DEFINITION 2.1. For a graph G with vertex set $V = \{v_1, v_2, ..., v_n\}$ the Mycielskian of G is the graph $\mu(G)$ with vertex set $V \cup U \cup \{x\}$, where $U = \{u_i : v_i \in V \textit{ and } i = 1, 2, ..., n\}$ and is disjoint from V , and $E(\mu(G)) = E(G) \cup \{v_i u_j : v_i v_j \in E(G)\} \cup \{xu : u \in U\}$. The vertices v and u are called twins of each other and x is called the root of $\mu(G)$.

The Mycielskian of G was introduced in 1955, by Mycielskian [**14**]. For recent results on the Mycielskian of a graph, we refer to [**4, 6, 7, 12, 13, 14**].

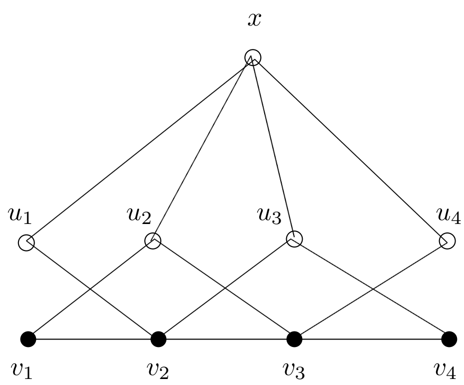

Figure 1: Mycielskian of P_4, $\mu(P_4)$

LEMMA 2.1. *Let G be a connected graph with vertex set $V = \{v_1, v_2, ..., v_n\}$ and let $\mu(G)$ be the Mycielskian of G with vertex set $V \cup U \cup \{x\}$, where $U = \{u_i : v_i \in V$ and $i = 1, 2, ..., n\}$. Then for $i = 1, 2, ..., n$*

(1) $d_1(x/\mu(G)) = d_2(x/\mu(G)) = n$.

(2) $d_1(v_i/\mu(G)) = 2d_1(v_i/G)$, *and* $d_2(v_i/\mu(G)) = 2(d_2(v_i/G) + 1)$.

(3) $d_1(u_i/\mu(G)) = d_1(v_i/G) + 1$, *and* $d_2(u_i/\mu(G)) = d_2(v_i/G) + n$.

3. Leap Zagreb Indices of Mycielskian of a graph

In this section, we obtain the expressions for the first, second and third leap Zagreb indices of Mycielskian of a graph G, and we also computing the exact values of these three leap zagreb indices for some standard graphs.

3.1. First Leap Zagreb Index of Mycielskian of Graphs.

THEOREM 3.1. *Let G be a connected graph with n vertices and m edges. Then*

$$LM_1(\mu(G)) \leqslant n^3 + n^2 + 4n + 5LM_1(G) + 2(n+4)(M_1(G) - 2m).$$

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

PROOF. Let G be a connected graph with vertex set $V = \{v_1, v_2, ..., v_n\}$ and m edges, and let $\mu(G)$ be the Mycielskian of G with vertex set $V \cup U \cup \{x\}$, where

$$U = \{u_i : v_i \in V \text{ and } i = 1, 2, ..., n\}.$$

Then by Lemma 2.1, we obtain,

$$\begin{aligned} LM_1(\mu(G)) &= \sum_{v \in V(\mu(G))} d_2^2(v/\mu(G)) \\ &= d_2^2(x/\mu(G)) + \sum_{i=1}^{n} d_2^2(v_i/\mu(G)) + \sum_{i=1}^{n} d_2^2(u_i/\mu(G)) \\ &= n^2 + \sum_{i=1}^{n} \Big(2d_2(v_i/G) + 2\Big)^2 + \sum_{i=1}^{n} \Big(d_2(v_i/G) + n\Big)^2 \end{aligned}$$

and

$$= n^2 + \sum_{i=1}^{n} 4\Big(d_2^2(v_i/G) + 2d_2(v_i/G) + 1\Big) + \sum_{i=1}^{n}\Big(d_2^2(v_i/G) + 2nd_2(v_i/G) + n^2\Big)$$

$$= n^2 + 4\Big(LM_1(G) + 2\sum_{i=1}^{n} d_2(v_i/G) + n\Big) + \Big(LM_1(G) + 2n\sum_{i=1}^{n} d_2(v_i/G) + n^3\Big)$$

$$= n^3 + n^2 + 4n + 5LM_1(G) + (8+2n)\sum_{i=1}^{n} d_2(v_i/G).$$

Hence, Lemma 1.1, led to

$$LM_1(\mu(G)) \leqslant n^3 + n^2 + 4n + 5LM_1(G) + 2(n+4)(M_1(G) - 2m),$$

with equality holds if and only if G is (C_3, C_4)-free graph. □

In the following result, we are presenting the exact values of the first leap Zagreb index for Mycielskian of some standard graphs $G \in \{P_n, C_n, K_n, K_{r,s}, K_{1,n-1}\}$. From Lemma 2.1, Proposition 1.1 and Lemma 1.1 and by applying these in Theorem 3.1, the following results immediately (by easy computing) are following. Then we left the proof to the reader.

Proposition 3.1. *For appositive integer number $n \geqslant 1$,*

(1) $LM_1(\mu(P_n)) = \begin{cases} 20, & n = 2; \\ 66, & n = 3; \\ n^3 + 5n^2 + 32n - 90, & n \geqslant 4. \end{cases}$

(2) $LM_1(\mu(C_n)) = \begin{cases} 132, & n = 3; \\ 244, & n = 4; \\ n^3 + 5n^2 + 4n, & n \geqslant 5. \end{cases}$

(3) $LM_1(\mu(K_n)) = n^3 + n^2 + 4n$.

(4) $LM_1(\mu(K_{r,s})) = 4(r^3 + s^3) + (r+s)^2 + r(2r+s-1)^2 + s(2s+r-1)^2$.

(5) $LM_1(\mu(K_{1,n-1})) = 8(n-1)^3 + 2(n^2+2)$.

3.2. Second Leap Zagreb Index of Mycielskian of Graphs.

Theorem 3.2. *Let G be a connected graph with n vertices and m edges. Then*

$$LM_2(\mu(G)) \leqslant n^3 + 8LM_2(G) + (2n+6)LM_3(G) + nM_1(G) + 2m(n+2).$$

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

Proof. Let G be a connected graph with vertex set $V = \{v_1, v_2, ..., v_n\}$ and m edges, and let $\mu(G)$ be the Mycielskian of G with vertex set

$$V(\mu(G)) = V(G) \cup U \cup \{x\},$$

where $U = \{u_i : v_i \in V \textit{ and } i = 1, 2, ..., n\}$ and from the definition of $\mu(G)$, the edge set of $\mu(G)$ is

$E(\mu(G)) =$
$E(G) \cup \{xu_j : u_j \in U, j = 1, 2, ..., n\} \cup \{v_iu_j : i, j = 1, 2, ..., n \textit{ and } i < j\}$

$\cup \{v_iu_j : i, j = 1, 2, ..., n \text{ and } i > j\}$.
Hence, by Lemma 2.1, we obtain,

$$\begin{aligned}
LM_2(\mu(G)) &= \sum_{vu \in E(\mu(G))} d_2(v/\mu(G))d_2(u/\mu(G)) \\
&= \sum_{\substack{v_iv_j \in E(G) \\ i,j=1,2,...,n, i\neq j}} d_2(v_i/\mu(G))d_2(v_j/\mu(G)) \\
&+ \sum_{\substack{xu_j \in E(\mu(G)) \\ j=1,2,...,n}} d_2(x/\mu(G))d_2(u_j/\mu(G)) \\
&+ \sum_{\substack{v_iu_j \in E(\mu(G)) \\ i,j=1,2,...,n, i<j}} d_2(v_i/\mu(G))d_2(u_j/\mu(G)) \\
&+ \sum_{\substack{v_iu_j \in E(\mu(G)) \\ i,j=1,2,...,n, i>j}} d_2(v_i/\mu(G))d_2(v_j/\mu(G))
\end{aligned}$$

and

$$\begin{aligned}
LM_2(\mu(G)) = & \sum_{\substack{v_iv_j \in E(G) \\ i,j=1,2,...,n, i\neq j}} (2d_2(v_i/G) + 2)(2d_2(v_j/G) + 2) + \sum_{i=1}^{n} n(n + d_2(v_i/G)) \\
&+ \sum_{\substack{v_iv_j \in E(G) \\ i,j=1,2,...,n, i\neq j}} (2d_2(v_i/G) + 2)(n + d_2(v_j/G)) \\
&+ \sum_{\substack{v_iv_j \in E(G) \\ i,j=1,2,...,n, i\neq j}} (2d_2(v_i/G) + 2)(n + d_2(v_j/G))
\end{aligned}$$

and

$$\begin{aligned}
LM_2(\mu(G)) = & \sum_{\substack{v_iv_j \in E(G) \\ i,j=1,2,...,n, i\neq j}} \Big[4d_2(v_i/G)d_2(v_j/G) + 2(d_2(v_i/G) + d_2(v_j/G)) + 4\Big] \\
&+ \sum_{i=1}^{n} (n^2 + nd_2(v_i/G)) \\
&+ \sum_{\substack{v_iv_j \in E(G) \\ i,j=1,2,...,n, i\neq j}} \Big[2nd_2(v_j/G) + 2n + 2d_2(v_i/G)d_2(v_j/G) + 2d_2(v_i/G)\Big] \\
&+ \sum_{\substack{v_iv_j \in E(G) \\ i,j=1,2,...,n, i\neq j}} \Big[2nd_2(v_j/G) + 2n + 2d_2(v_i/G)d_2(v_j/G) + 2d_2(v_i/G)\Big]
\end{aligned}$$

$$\begin{aligned}
LM_2(\mu(G)) &= 4LM_2(G) + 2LM_3(G) + 4m + n^3 + n\sum_{i=1}^{n} d_2(v_i/G) \\
&+ 2n\sum_{i=1}^{n} d_1(v_i/G)d_2(v_i/G) + \sum_{\substack{v_iv_j\in E(G)\\ i,j=1,2,\dots,n,i\neq j}} 4n \\
&+ 4\sum_{\substack{v_iv_j\in E(G)\\ i,j=1,2,\dots,n,i\neq j}} d_2(v_i/G)d_2(v_j/G) \\
&+ 4\sum_{\substack{v_iv_j\in E(G)\\ i,j=1,2,\dots,n,i\neq j}} d_1(v_i/G)d_2(v_j/G) \\
&= 4LM_2(G) + 2LM_3(G) + 4m + n^3 + n\sum_{i=1}^{n} d_2(v_i/G) + 2nLM_3(G) \\
&+ 4nm + 4LM_2(G) + 4LM_3(G) \\
&= n^3 + 8LM_2(G) + (2n+6)LM_3(G) + n\sum_{i=1}^{n} d_2(v_i/G) + 4m + 4nm.
\end{aligned}$$

Hence, Lemma 1.1, let to

$$\begin{aligned}
LM_2(\mu(G)) &\leqslant n^3 + 8LM_2(G) + (2n+6)LM_3(G) + n(M_1(G) - 2m) + 4m + 4nm \\
&= n^3 + 8LM_2(G) + (2n+6)LM_3(G) + nM_1(G) + 2m(n+2),
\end{aligned}$$

with equality holds if and only if G is (C_3, C_4)-free graph. □

In the following result, we are presenting the exact values of the second leap Zagreb index for Mycielskian of some standard graphs

$$G \in \{P_n, C_n, K_n, K_{r,s}, K_{1,n-1}\}.$$

From Lemma 2.1, Proposition 1.1 and Lemma 1.1 and by applying these in Theorem 3.1, the following results immediately(by easy computing) are following. Then we left the proof to the reader.

Proposition 3.2. *For appositive integer number $n \geqslant 1$,*

(1) $LM_2(\mu(P_n)) = \begin{cases} 56, & n = 3; \\ 148, & n = 4; \\ n^3 + 14n^2 + 32n - 176, & n \geqslant 5. \end{cases}$

(2) $LM_2(\mu(C_n)) = \begin{cases} 75, & n = 3; \\ 304, & n = 4; \\ n^3 + 14n^2 + 58n, & n \geqslant 5. \end{cases}$

(3) $LM_2(\mu(K_n)) = 3n^3 - 2n.$

(4) $LM_2(\mu(K_{r,s})) = 2r^3(s+1)2s^3(r+1) + 2rs(6rs + r + s) - (r+s)^2.$

(5) $LM_2(\mu(K_{1,n-1})) = 4(n-1)^2(n+2) + n^2.$

3.3. Third Leap Zagreb Index of Mycielskian of Graphs.

THEOREM 3.3. *Let G be a connected graph with n vertices and m edges. Then*

$$LM_1(\mu(G)) \leqslant 2n^2 + 5LM_3(G) + M_1(G) + 2m(n+3).$$

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

PROOF. Let G be a connected graph with vertex set $V = \{v_1, v_2, ..., v_n\}$ and m edges, and let $\mu(G)$ be the Mycielskian of G with vertex set $V(\mu(G)) = V(G) \cup U \cup \{x\}$, where $U = \{u_i : v_i \in V \ and \ i = 1, 2, ..., n\}$. Then by Lemma 2.1, we obtain

$$\begin{aligned}
LM_3(\mu(G)) = & \sum_{v \in V(\mu(G))} d_1(v/\mu(G)) d_2(v/\mu(G)) \\
& = d_1(x/\mu(G)) d_2(x/\mu(G)) + \sum_{i=1}^{n} d_1(v_i/\mu(G)) d_2(v_i/\mu(G)) \\
& + \sum_{j=1}^{n} d_1(u_j/\mu(G)) d_2(u_j/\mu(G)) \\
& = n^2 + \sum_{i=1}^{n} \Big[(2d_1(v_i/G))(2d_2(v_i/G) + 2) \Big] \\
& + \sum_{i=1}^{n} \Big[(d_1(v_i/G + 1)(d_2(v_i/G) + n) \Big] \\
& = n^2 + \sum_{i=1}^{n} 4 \Big[d_1(v_i/G) d_2(v_i/G) + d_1(v_i/G) \Big] + \sum_{i=1}^{n} \Big[d_1(v_i/G) d_2(v_i/G) \\
& + n d_1(v_i/G) + d_2(v_i/G) + n \Big] \\
& = n^2 + 4LM_3(G) + 8m + LM_3(G) + 2nm + \sum_{i=1}^{n} d_2(v_i/G) + n^2.
\end{aligned}$$

Hence, Lemma 1.1, led to

$$\begin{aligned}
LM_3(\mu(G)) &\leqslant n^2 + 4LM_3(G) + 8m + LM_3(G) + 2nm + (M_1(G) - 2m) + n^2 \\
&= 2n^2 + 5LM_3(G) + M_1(G) + 2m(n+3).
\end{aligned}$$

From Lemma1.1, equality holds if and only if G is (C_3, C_4)-free graph. □

In the following result, we are presenting the exact values of the third leap Zagreb index for Mycielskian of some standard graphs $G \in \{P_n, C_n, K_n, K_{r,s}, K_{1,n-1}\}$. From Lemma 2.1, Proposition 1.1 and Lemma 1.1 and by applying these in Theorem 3.1, the following results immediately (by easy computing) are following. Then we left the proof to the reader.

PROPOSITION 3.3. *For appositive integer number $n \geqslant 1$,*

(1) $LM_1(\mu(P_n)) = 4n^2 + 28n - 62.$

(2) $LM_1(\mu(C_n)) = \begin{cases} 60, & n = 3; \\ 140, & n = 4; \\ 2n(2n+15), & n \geqslant 5. \end{cases}$

(3) $LM_1(\mu(K_n)) = n(n^2 + 5n - 4)$.

(4) $LM_1(\mu(K_{r,s})) = (r+s)^2 + 2(r^2+s^2) + (r+s)(7rs-1)$.

(5) $LM_1(\mu(K_{1,n-1})) = 10n^2 - 12n + 4$.

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Department of Studies in Mathematics, University of Mysore, Manasagangotri, Mysore - 570 006, India
E-mail address: mnjnthhr@gmail.com

Department of Mathematics, Faculty of Education, University of Thamar, Thamar, Yemen
E-mail address: a7mnaji@gmail.com

Department of Studies in Mathematics, University of Mysore, Manasagangotri, Mysore - 570 006, India
E-mail address: ndsoner@yahoo.co.in