A SHORT NOTE ON ZAGREB INDICES AND HYPER ZAGREB INDICES OF GRAPHS

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Let G be a simple graph with n vertices and m edges. The first hyper Zagreb index of G is defined as $HM_1(G) = \sum_{uv\in E(G)} (d(u) + d(v))^2$, where $d(v)$ denotes the degree of a vertex v in G. The aim of this paper is to correct some of the inequalities that were derived in [9] and characterize the extremal graphs.

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1. INTRODUCTION

Throughout this paper, we only consider simple and connected graph $G = (V(G), E(G))$ with n vertices and m edges. We use the notations $d(v)$, $\Delta = \Delta(G)$ and $\delta = \delta(G)$ to denote the degree of a vertex v, the maximum vertex degree of G and the minimum vertex degree of G, respectively. A vertex $v \in V(G)$ is said to be *pendant* if its neighborhood contains exactly one vertex, i.e., $d(v) = 1$. As usual $K_{1,n-1}$, P_n and C_n denotes a star, path and cycle on n vertices, respectively. Let $K^*_{1,n-1}$ be a graph that obtained from $K_{1,n-1}$ by adding an edge between any two vertices with $d(v) = \delta$. The Line graph $L(G)$ obtained from G in which $V(L(G)) = E(G)$, where two vertices of $L(G)$ are adjacent if and only if they are adjacent edges of G. Note that $L(G)$ has m vertices and $(\frac{1}{2}\sum_{v\in V(G)} d(v)^2 - m)$ edges. We use Δ_e and δ_e to denote the maximum and the minimum vertex degree of $L(G)$, respectively.

Mathematical calculations are quite necessary to analyze essential concepts in chemistry because molecules are often modeled by graph structures named molecular graphs. A *molecular graph* is a simple graph in which vertices represent the atoms and edges represent the linking bonds among them. By IUPAC terminology, a *topological index* is a numerical value for the correlation of a chemical structure with various physical properties, chemical reactivity, or biological activity.

In chemical graph theory, a *graphical invariant* is a number related to a graph which is structurally invariant. These invariant numbers are also known as the topological indices. In 1972, Gutman and Trinajstić [5] examined the study of total π-electron energy on the molecular structure and introduced two vertex-degree based graph invariants. These invariants are defined as $M_1(G) = \sum_{v\in V(G)} d(v)^2$ and $M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$. In 2004, Miličević, Nikolić and Trinajstić [7] reformulated the first Zagreb index in terms of edge-degree instead of vertex-degree as $EM_1(G) = \sum_{uv\in E(G)} (d(u) + d(v) - 2)^2$. In 2013, Shirdel et al. [8] defined the first hyper Zagreb index as

$$HM_1(G) = \sum_{uv\in E(G)} [d(u) + d(v)]^2.$$

For the recent results, see [1, 3, 4] and references therein. In 2016, Wang et al. [9] defined the second hyper Zagreb index as

$$HM_2(G) = \sum_{uv\sim xy} (d(u) + d(v))(d(x) + d(y)),$$

where $uv \sim xy$ represents the adjacent edges of G.

The aim of this paper is to characterize the extremal graphs in addition to correcting some of the inequalities derived in [9]. More precisely, in the next section, we correct and comment on Theorems 3, 4, and 7 in [9].

2. MAIN RESULTS

In 2010, Zhou and Trinajstić [10] obtained the following result on genereal sum connectivity index.

Lemma 1. (see [10]) *Let G be a graph with $m \geq 1$ edges. If $0 < \alpha < 1$, then*

$$\chi_\alpha(G) \leq M_1(G)^\alpha m^{1-\alpha},$$

and if $\alpha > 1$ or $\alpha < 0$, then

$$\chi_\alpha(G) \geq M_1(G)^\alpha m^{1-\alpha}, \tag{1}$$

and either equality holds if and only if $d(u) + d(v)$ is constant for any edge uv.

In [9], Wang et al. gave a lower bound for the Hyper Zagreb index of graph G:

$$HM_1(G) \geq \frac{M_1(G)^2}{m}, \tag{2}$$

where the equality holds if and only if G is edge degree regular. Note that by Lemma 1, it is easy to see that (2) is a special case of (1) with $\alpha = 2$.

Comments on Theorem 3 in [9]: Wang et al. [9] gave an upper bound for the *first hyper Zagreb index* of graph G:

$$HM_1(G) \leq M_1(G)(m + 2\delta - 1) - 2m(m - 1)\delta, \tag{3}$$

where the equality holds if and only if G is regular. Note that sometimes the upper bound in (3) is not true. For example, if $G \cong K_{1,n-1}$ with n vertices, then we have $m = n-1$, $\delta = 1$ and $HM_1(G) = n^2(n-1)$, while

$$\begin{aligned} M_1(G)(m+2\delta-1) - 2m(m-1)\delta &= n^2(n-1) - 2(n-1)(n-2) \\ &= (n-1)(n^2-2n+4) \\ &< n^2(n-1), \text{ for } n > 2. \end{aligned}$$

Also, if $G \cong K^*_{1,n-1}$, then we have $m = n$, $\delta = 1$ and

$$HM_1(G) = n^3 - n^2 + 4n + 18,$$

while

$$\begin{aligned} M_1(G)(m+2\delta-1) - 2m(m-1)\delta &= (n+1)\left(n^2-n+6\right) - 2n(n-1) \\ &= n^3 - 2n^2 + 7n + 6. \\ &< n^3 - n^2 + 4n + 18, \quad \text{for } n > 3. \end{aligned}$$

We now present some preliminary results that will be needed to achieve our main goal. From [2], we have that $d_i\mu_i =$ sum of the degrees of the vertices adjacent to vertex v_i:

$$(4) \quad \sum_{i=1}^{n} d_i\mu_i = \sum_{v\in V(G)} d(v)^2 \le \sum_{v\in V(G)} [2m - d(v) - (n-1-d(v))\delta].$$

LEMMA 2. (see [6]) *Let G be a simple graph with n vertices and m edges. Then*

$$M_1(G) \le 2m(\Delta+\delta) - n\Delta\delta.$$

The equality holds if and only if G is regular or bidegreed graph.

Note that in the proof of Theorem 3 of [9] picking the erroneous value for m, that is, the edge version as of $d(e)$, resulted in an incorrect inequality. We now present the corrected version of the result.

THEOREM 1. *Let G be a simple connected graph with n vertices and m edges. Then*

$$HM_1(G) < (m+2\delta+1)M_1(G) - 2m(m-1) - 2(3m-1)(\delta-1).$$

Proof. The edge version of the inequality (4) can be expressed as $d(e_i)\mu_i =$ sum of the degrees of the edges adjacent to edge e_i.

$$\sum_{i=1}^{m} d(e_i)\mu_i = \sum_{e\in E(G)} d(e)^2 = EM_1(G),$$

where $d(e) = d(u) + d(v) - 2$ is the edge degree of any edge $e \in E(G)$, with $\delta_e = 2(\delta - 1) \leq d(e) \leq 2(\Delta - 1) = \Delta_e$. Note that $EM_1(G)$ is simply the first Zagreb index of the line graph of G. Thus

(5)

$$\sum_{e \in E(G)} d(e)^2 \leq \sum_{e \in E(G)} \left[2\left(\frac{1}{2} \sum_{v \in V(G)} d(v)^2 - m \right) - d(e) - (m - 1 - d(e))(2\delta - 2) \right]$$

From the definition of $EM_1(G)$, we have

$$EM_1(G) = \sum_{uv \in E(G)} (d(u) + d(v))^2 - 4 \sum_{uv \in E(G)} d(u) + d(v) + 4 \sum_{uv \in E(G)} 1.$$

By using (5), we complete the proof. $\square$

Furthermore, the following corollary is established in [9] using Lemma 2 and Theorem 3 in [9].

$$HM_1(G) \leq (2m(\Delta + \delta) - n\Delta\delta)(m + 2\delta - 1) - 2m(m-1)(\delta - 1), \tag{6}$$

where the equality holds if and only if G is regular. Note that (6) is correct due to the choice in Lemma 2, i.e., the R.H.S is always larger than the L.H.S, but still, the equality is not correct. The equality never holds for the regular graphs. But it holds only for the star $K_{1,n-1}$.

Comments on Theorem 4 in [9]: Theorem 4 in [9] is obtained from Pólya-Szegó inequality:

$$HM_1(G) \leq \frac{(\Delta + \delta)^2}{4m\Delta\delta} M_1(G)^2 \tag{7}$$

with equality holds if and only if G is regular or there are exactly $\dfrac{m\delta}{\Delta + \delta}$ edges of degree 2Δ and $\dfrac{m\Delta}{\Delta + \delta}$ edges of degree 2δ such that $(\Delta + \delta)$ divides $m\delta$. The following inequalities are obtained from the above result with $\delta \geq 2$:

$$HM_1(G) \leq \frac{(n+1)^2}{8m(n-1)} M_1(G)^2 \tag{8}$$

with equality holds if and only if G has exactly $\frac{m}{n-1}$ edges of degree $2(n-2)$ and $\frac{n(n-2)}{n-1}$ edges of degree 2 such that $(n-1)$ divides m, and hence

$$HM_1(G) \leq \frac{m^3(n+1)^6}{16n^2(n-1)^2} \tag{9}$$

with equality holds if and only if $G \cong K_3$.

The characterization of extremal graphs in (7) and (8) is incorrect. If n is even, then both $\frac{m\delta}{\Delta+\delta}$ edges of degree 2Δ and $\frac{m\Delta}{\Delta+\delta}$ edges of degree 2δ are possible if and only if G is regular. If n is odd, then $\frac{m\delta}{\Delta+\delta}$ and $\frac{m\Delta}{\Delta+\delta}$ are not integers. This concludes that (7) holds if and only if G is regular.

Suppose $G \cong C_3$, then the equality of (8) holds, but C_3 doesn't satisfy the given equality class. Also, C_3 is the unique graph that satisfies the equality case. It is easy to see that, the equality of (9) does not hold for any class of graphs.

Comments on Theorem 7 in [9]: In [9], Wang et al. gave a lower bound for the *second hyper Zagreb index* of graph G:

$$HM_2(G) \geq \frac{M_1(G)^3}{2m^2} \tag{10}$$

with equality holds if and only if G is regular.

For $G \cong P_2$, (10) is true. Suppose $G \cong K_{1,n-1}$ with $n > 2$, then $m = n-1$ and $HM_2(G) = \frac{n^2(n-1)(n-2)}{2}$, so

$$\frac{M_1(G)^3}{2m^2} = \frac{\left((n-1)^2 + (n-1).1^2\right)^3}{2(n-1)^2} = \frac{n^3(n-1)}{2} > \frac{n^2(n-1)(n-2)}{2}, \quad n > 2.$$

For $G \cong C_n$, then $m = n$ and $HM_2(G) = 16n$, while $\frac{M_1(G)^3}{2m^2} = 64n > 16n$, which is a contradiction to (10). Note that the choice of $N = \frac{1}{2}M_1(G)$ in the proof of Theorem 7 [9], leads to wrong inequality. By choosing $d(e) = d(u) + d(v) - 2$ and $N = \frac{1}{2}M_1(G) - m$, we get $EM_2(G) \geq \frac{(M_1(G)-2m)^3}{2m^2}$. It is easy to see that $HM_2(G) > EM_2(G)$, so we have the following result.

THEOREM 2. *Let G be a simple graph with n vertices and m edges, then*

$$HM_2(G) > \frac{(M_1(G) - 2m)^3}{2m^2}.$$

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