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Comparing Variable Zagreb Indices of Graphs *

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Abstract

The variable first and second Zagreb indices are defined to be ${}^{\lambda}M_1(G) = \sum_{u \in V}(d(u))^{2\lambda}$ *and* ${}^{\lambda}M_2(G) = \sum_{uv \in E}(d(u)d(v))^{\lambda}$, where λ is any real number. In this paper, we prove that when $\lambda \in [0,\ 1]$ (*resp.* $\lambda \in (-\infty,\ 0)$), ${}^{\lambda}M_1(G)/n \leq {}^{\lambda}M_2(G)/m$ (*resp.* ${}^{\lambda}M_1(G)/n \geq {}^{\lambda}M_2(G)/m$) holds for graphs G satisfying one of the following conditions: $\Delta(G)-\delta(G) \leq 2$; $\Delta(G)-\delta(G) \leq 3$ and $\delta(G) \neq 2$; G is a chemical graph. When $\lambda \in (1, +\infty)$, the relationship of numerical value between ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ is indefinite for distinct graphs G even if $\Delta(G) - \delta(G) \leq 2$.

1 Introduction

A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are usually used in the study of molecular graphs, and they are defined in [2] as follows:

$$M_1(G) = \sum_{u \in V}(d(u))^2 \text{ and } M_2(G) = \sum_{uv \in E} d(u)d(v),$$

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where V is the set of vertices, E is the set of edges and $d(u)$ is degree of the vertex u of G. The research of Zagreb indices and their generalization are often found in chemistry and mathematical chemistry.

A natural issue is to compare the values of the Zagreb indices on the same graph. In [1], the AutoGraphiX system proposed the following conjecture:

Conjecture 1.1 *([1]) For all simple connected graphs G,*

$$M_1(G)/n \le M_2(G)/m$$

and the bound is tight for complete graphs.

However, this conjecture does not hold for all general graphs ([3]), while it is proved to be true for chemical graphs ([3]), trees ([10]) and unicyclic graphs([7]), and connected bicyclic graphs except one class ([9]). Besides, its generalization to the variable Zagreb indices has already been discussed (see e.g. [5, 6, 13]). The variable first and the variable second Zagreb indices are defined as:

$$^{\lambda}M_1(G) = \sum_{u \in V} (d(u))^{2\lambda} \text{ and } {}^{\lambda}M_2(G) = \sum_{uv \in E} (d(u)d(v))^{\lambda},$$

where λ is any real number. Clearly, $^{1}M_1(G) = M_1(G)$ and $^{1}M_2(G) = M_2(G)$.

Similarly as Conjecture 1.1, many mathematicians showed that

$$^{\lambda}M_1(G)/n \le {}^{\lambda}M_2(G)/m \tag{1}$$

is true for the following cases: all chemical graphs and $\lambda \in [0, 1]$ ([11]), all trees and $\lambda \in [0, 1]$ ([12]), all unicyclic graphs and $\lambda \in [0, 1]$ ([4]).

On the other hand, the inequality

$$^{\lambda}M_1(G)/n \ge {}^{\lambda}M_2(G)/m \tag{2}$$

is true for the following cases: all unbalanced bipartite graphs and $\lambda \in R\backslash[0, 1]$ ([11]), all unicyclic graphs and $\lambda \in (-\infty, 0]$ ([14]).

Let G be an undirected, simple graph. Let $\Delta(G)$ and $\delta(G)$ denote the maximum and minimum degrees of G, respectively. A graph G is called a chemical graph if $\Delta(G) \le 4$. A graph G is called k-regular if $d(v) = k$ for all $v \in V(G)$.

It is known to all that there are many molecular graphs with small difference between the maximum and minimum degrees. In [8], it has been proved that $M_1(G)/n \le M_2(G)/m$ holds for graphs G with small difference between the maximum and minimum degrees, which implies the results in [3].

In this paper, we investigate the relationship of ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ in the graphs G with small difference between the maximum and minimum degrees for $\lambda \in R$. When $\lambda \in [0, 1]$ (*resp.* $\lambda \in (-\infty, 0)$), we show that (1) (*resp.* (2)) holds for graphs satisfying one of the following conditions: $\Delta(G) - \delta(G) \leq 2$; $\Delta(G) - \delta(G) \leq 3$ and $\delta(G) \neq 2$; all chemical graphs. Moreover, the extremal graphs (with the equality (1) or (2) holds) are characterized completely. When $\lambda \in (1, +\infty)$, the relationship of numerical value between ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ is indefinite for distinct graphs even if $\Delta(G) - \delta(G) \leq 2$.

2 Preliminaries

In this section, we introduce some notations and lemmas which are useful in the presentations and proofs of our main results.

Let $\{i, j\}, \{k, l\} \in (Z^{+})^2$ and $\lambda \in R$. Suppose

$$f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} = i^{\lambda+1}j^{\lambda+1}l + i^{\lambda+1}j^{\lambda+1}k + jk^{\lambda+1}l^{\lambda+1} + ik^{\lambda+1}l^{\lambda+1} - i^{2\lambda}jkl - ij^{2\lambda}kl - ijk^{2\lambda}l - ijkl^{2\lambda}.$$

In the following lemmas, let a, b, c, d be distinct positive integers.

Lemma 2.1 $f^{\lambda}_{\{a,\ a\},\ \{a,\ a\}} = 0.$

Proof. Obviously, we have $f^{\lambda}_{\{a,\ a\},\ \{a,\ a\}} = 4a^{2\lambda+3} - 4a^{2\lambda+3} = 0.$ □

Lemma 2.2 $f^{\lambda}_{\{a,\ a\},\ \{a,\ b\}} \begin{cases} > 0, & if\ 0 < \lambda \leq 1, \\ < 0, & if\ \lambda < 0. \end{cases}$

Proof. Note that $f^{\lambda}_{\{a,\ a\},\ \{a,\ b\}} = a^{2\lambda+2}b + a^{2\lambda+3} + 2a^{\lambda+2}b^{\lambda+1} - 3a^{2\lambda+2}b - a^3b^{2\lambda}$

$$= a^2(b^{\lambda} - a^{\lambda})[(b - a)a^{\lambda} + ab(a^{\lambda-1} - b^{\lambda-1})].$$

Case 1. $0 < \lambda \leq 1$.
If $b > a > 0$, then $b^{\lambda} - a^{\lambda} > 0$, $(b - a)a^{\lambda} + ab(a^{\lambda-1} - b^{\lambda-1}) > 0$.
If $a > b > 0$, then $b^{\lambda} - a^{\lambda} < 0$, $(b - a)a^{\lambda} + ab(a^{\lambda-1} - b^{\lambda-1}) < 0$.
Therefore, we always have $f^{\lambda}_{\{a,\ a\},\ \{a,\ b\}} > 0$.
Case 2. $\lambda < 0$.
If $b > a > 0$, then $b^{\lambda} - a^{\lambda} < 0$, $(b - a)a^{\lambda} + ab(a^{\lambda-1} - b^{\lambda-1}) > 0$.
If $a > b > 0$, then $b^{\lambda} - a^{\lambda} > 0$, $(b - a)a^{\lambda} + ab(a^{\lambda-1} - b^{\lambda-1}) < 0$.
It can be seen that $f^{\lambda}_{\{a,\ a\},\ \{a,\ b\}} < 0$. □

Lemma 2.3 $f^{\lambda}_{\{a,\,a\},\,\{b,\,b\}}\begin{cases} > 0, & if\ 0 < \lambda \le 1, \\ < 0, & if\ \lambda < 0. \end{cases}$

Proof. Note that $f^{\lambda}_{\{a,\,a\},\,\{b,\,b\}} = 2a^{2\lambda+2}b + 2ab^{2\lambda+2} - 2a^{2\lambda+1}b^2 - 2a^2b^{2\lambda+1}$

$$= 2ab(b-a)(b^{2\lambda} - a^{2\lambda}).$$

Case 1. $0 < \lambda \le 1$. Without loss of generality, suppose $b > a > 0$. Then

$$b - a > 0,\ b^{2\lambda} - a^{2\lambda} > 0.$$

Thus we have $f^{\lambda}_{\{a,\,a\},\,\{b,\,b\}} > 0$.

Case 2. $\lambda < 0$. Without loss of generality, suppose $b > a > 0$. Then

$$b - a > 0,\ b^{2\lambda} - a^{2\lambda} < 0.$$

It follows that $f^{\lambda}_{\{a,\,a\},\,\{b,\,b\}} < 0$. □

Lemma 2.4 $f^{\lambda}_{\{a,\,b\},\,\{a,\,b\}}\begin{cases} = 0, & if\ \lambda = 1, \\ > 0, & if\ 0 < \lambda < 1, \\ < 0, & if\ \lambda < 0. \end{cases}$

Proof. Note that $f^{\lambda}_{\{a,\,b\},\,\{a,\,b\}} = 2a^{\lambda+1}b^{\lambda+2} + 2a^{\lambda+2}b^{\lambda+1} - 2a^{2\lambda+1}b^2 - 2a^2b^{2\lambda+1}$

$$= 2a^2b^2(b^{\lambda} - a^{\lambda})(a^{\lambda-1} - b^{\lambda-1}).$$

Without loss of generality, suppose $b > a > 0$.

Case 1. $\lambda = 1$. Then $b^{\lambda} - a^{\lambda} > 0,\ a^{\lambda-1} - b^{\lambda-1} = 0$. Hence $f^{\lambda}_{\{a,\,b\},\,\{a,\,b\}} = 0$.

Case 2. $0 < \lambda < 1$. Then $b^{\lambda} - a^{\lambda} > 0,\ a^{\lambda-1} - b^{\lambda-1} > 0$. So $f^{\lambda}_{\{a,\,b\},\,\{a,\,b\}} > 0$.

Case 3. $\lambda < 0$. Then $b^{\lambda} - a^{\lambda} < 0,\ a^{\lambda-1} - b^{\lambda-1} > 0$. Thus $f^{\lambda}_{\{a,\,b\},\,\{a,\,b\}} < 0$. □

Lemma 2.5 $f^{\lambda}_{\{a,\,b\},\,\{a,\,c\}}\begin{cases} > 0, & if\ 0 < \lambda \le 1, \\ < 0, & if\ \lambda < 0. \end{cases}$

Proof. Notice that $f^{\lambda}_{\{a,\,b\},\,\{a,\,c\}}$

$$= a^{\lambda+1}b^{\lambda+1}c + a^{\lambda+2}b^{\lambda+1} + a^{\lambda+1}bc^{\lambda+1} + a^{\lambda+2}c^{\lambda+1} - 2a^{2\lambda+1}bc - a^2b^{2\lambda}c - a^2bc^{2\lambda}$$

$$= a^2bc[(a^{\lambda-1} - b^{\lambda-1})(b^{\lambda} - a^{\lambda}) + (a^{\lambda-1} - c^{\lambda-1})(c^{\lambda} - a^{\lambda})] + a^{\lambda+2}(c-b)(c^{\lambda} - b^{\lambda}).$$

Case 1. $0 < \lambda \le 1$. Without loss of generality, suppose $c > b > 0$.

If $c > b > a > 0$, then

$$a^{\lambda-1} - b^{\lambda-1} \geq 0,\ b^{\lambda} - a^{\lambda} > 0,\ a^{\lambda-1} - c^{\lambda-1} \geq 0,\ c^{\lambda} - a^{\lambda} > 0,\ c^{\lambda} - b^{\lambda} > 0.$$

If $a > c > b > 0$, then

$$a^{\lambda-1} - b^{\lambda-1} \leq 0,\ b^{\lambda} - a^{\lambda} < 0,\ a^{\lambda-1} - c^{\lambda-1} \leq 0,\ c^{\lambda} - a^{\lambda} < 0,\ c^{\lambda} - b^{\lambda} > 0.$$

If $c > a > b > 0$, then

$$a^{\lambda-1} - b^{\lambda-1} \leq 0,\ b^{\lambda} - a^{\lambda} < 0,\ a^{\lambda-1} - c^{\lambda-1} \geq 0,\ c^{\lambda} - a^{\lambda} > 0,\ c^{\lambda} - b^{\lambda} > 0.$$

All in all, we always have $f^{\lambda}_{\{a,\ b\},\ \{a,\ c\}} > 0$.
Case 2. $\lambda < 0$. Without loss of generality, suppose $c > b > 0$.
If $c > b > a > 0$, then

$$a^{\lambda-1} - b^{\lambda-1} > 0,\ b^{\lambda} - a^{\lambda} < 0,\ a^{\lambda-1} - c^{\lambda-1} > 0,\ c^{\lambda} - a^{\lambda} < 0,\ c^{\lambda} - b^{\lambda} < 0.$$

If $a > c > b > 0$, then

$$a^{\lambda-1} - b^{\lambda-1} < 0,\ b^{\lambda} - a^{\lambda} > 0,\ a^{\lambda-1} - c^{\lambda-1} < 0,\ c^{\lambda} - a^{\lambda} > 0,\ c^{\lambda} - b^{\lambda} < 0.$$

If $c > a > b > 0$, then

$$a^{\lambda-1} - b^{\lambda-1} < 0,\ b^{\lambda} - a^{\lambda} > 0,\ a^{\lambda-1} - c^{\lambda-1} > 0,\ c^{\lambda} - a^{\lambda} < 0,\ c^{\lambda} - b^{\lambda} < 0.$$

Therefore, it can be conclude that $f^{\lambda}_{\{a,\ b\},\ \{a,\ c\}} < 0$. □

Lemma 2.6 *Let $c > b > 0$. If $c > a > b$, we suppose $bc \leq a^2$. Then*

$$f^{\lambda}_{\{a,\ a\},\ \{b,\ c\}} \begin{cases} \geq 0, & if\ \lambda = 1, \\ > 0, & if\ 0 < \lambda < 1, \\ < 0, & if\ \lambda < 0. \end{cases}$$

Proof. $f^{\lambda}_{\{a,\ a\},\ \{b,\ c\}} = a^{2\lambda+2}c + a^{2\lambda+2}b + 2ab^{\lambda+1}c^{\lambda+1} - 2a^{2\lambda+1}bc - a^2b^{2\lambda}c - a^2bc^{2\lambda}$

$$= a^2bc(c^{\lambda} - b^{\lambda})(b^{\lambda-1} - c^{\lambda-1}) + a(2bc - ab - ac)(b^{\lambda}c^{\lambda} - a^{2\lambda}).$$

Case 1. $0 < \lambda \leq 1$.
If $c > b > a > 0$, then

$$c^{\lambda} - b^{\lambda} > 0,\ b^{\lambda-1} - c^{\lambda-1} \geq 0,\ 2bc - ab - ac > 0,\ b^{\lambda}c^{\lambda} - a^{2\lambda} > 0.$$

If $a > c > b > 0$, then

$$c^{\lambda} - b^{\lambda} > 0,\ b^{\lambda-1} - c^{\lambda-1} \geq 0,\ 2bc - ab - ac < 0,\ b^{\lambda}c^{\lambda} - a^{2\lambda} < 0.$$

If $c > a > b > 0$, then $c^{\lambda} - b^{\lambda} > 0,\ b^{\lambda-1} - c^{\lambda-1} \begin{cases} > 0, & if\ 0 < \lambda < 1, \\ = 0, & if\ \lambda = 1. \end{cases}$

Since $bc \leq a^2$. Hence $b^{\lambda}c^{\lambda} - a^{2\lambda} \leq 0$, and

$$2bc - ab - ac \leq bc + a^2 - ab - ac = (c - a)(b - a) < 0.$$

It can be seen that $f^{\lambda}_{\{a,\ a\},\ \{b,\ c\}} \begin{cases} > 0, & if\ 0 < \lambda < 1, \\ \geq 0, & if\ \lambda = 1. \end{cases}$

Case 2. $\lambda < 0$.

If $c > b > a > 0$, then

$$c^{\lambda} - b^{\lambda} < 0,\ b^{\lambda-1} - c^{\lambda-1} > 0,\ 2bc - ab - ac > 0,\ b^{\lambda}c^{\lambda} - a^{2\lambda} < 0.$$

If $a > c > b > 0$, then

$$c^{\lambda} - b^{\lambda} < 0,\ b^{\lambda-1} - c^{\lambda-1} > 0,\ 2bc - ab - ac < 0,\ b^{\lambda}c^{\lambda} - a^{2\lambda} > 0.$$

If $c > a > b > 0$, then $c^{\lambda} - b^{\lambda} < 0,\ b^{\lambda-1} - c^{\lambda-1} > 0$.

Note that $bc \leq a^2$. Hence $b^{\lambda}c^{\lambda} - a^{2\lambda} \geq 0$, and

$$2bc - ab - ac \leq bc + a^2 - ab - ac = (c - a)(b - a) < 0.$$

Consequently, we conclude that $f^{\lambda}_{\{a,\ a\},\ \{b,\ c\}} < 0$. □

Lemma 2.7 *Let $c > b > 0$. If $c > a > b$, we suppose $a,\ b,\ c \in \{p,\ p+1,\ p+2,\ p+3\}$ and $p \neq 2$. Then*

$$f^{\lambda}_{\{a,\ a\},\ \{b,\ c\}} \begin{cases} \geq 0, & if\ \lambda = 1, \\ > 0, & if\ 0 < \lambda < 1, \\ < 0, & if\ \lambda < 0. \end{cases}$$

Proof. From the proof of Lemma 2.6, we need to discuss the case $c > a > b$.

Case 1. $0 < \lambda \leq 1$. Thus $c^{\lambda} - b^{\lambda} > 0,\ b^{\lambda-1} - c^{\lambda-1} \begin{cases} > 0, & if\ 0 < \lambda < 1, \\ = 0, & if\ \lambda = 1. \end{cases}$

Subcase 1.1 $a = p + 1,\ b = p,\ c = p + 2.$

Subcase 1.2 $a = p + 2,\ b = p,\ c = p + 3.$

Subcase 1.3 $a = p + 2,\ b = p + 1,\ c = p + 3.$

For Subcase 1.1-1.3, since $bc \le a^2$, by Lemma 2.6, the results are obtained.

Subcase 1.4 $a = p+1,\ b = p,\ c = p+3$. Then

$$b^\lambda c^\lambda - a^{2\lambda} = p^\lambda (p+3)^\lambda - (p+1)^{2\lambda} \begin{cases} > 0, & if\ p \ge 3, \\ = 0, & if\ p = 1. \end{cases}$$

$$2bc - ab - ac = p - 3 \ge 0\ if\ p \ge 3.$$

All in all, we obtain the results as desired.

Case 2. $\lambda < 0$. Then $c^\lambda - b^\lambda < 0,\ b^{\lambda-1} - c^{\lambda-1} > 0$.

Similarly, for Subcase 1.1-1.3, since $bc \le a^2$, it follows from Lemma 2.6 that the results are obtained as desired.

If $a = p+1,\ b = p,\ c = p+3$, then

$$b^\lambda c^\lambda - a^{2\lambda} = p^\lambda (p+3)^\lambda - (p+1)^{2\lambda} \begin{cases} < 0, & if\ p \ge 3, \\ = 0, & if\ p = 1. \end{cases}$$

$$2bc - ab - ac = p - 3 \ge 0\ if\ p \ge 3.$$

Therefore, we always have $f^\lambda_{\{a,\ a\},\ \{b,\ c\}} < 0$ if $\lambda < 0$. □

Lemma 2.8 *Let $d > c$ and $a = \min\{a,\ b,\ c,\ d\}$. If $b > d > c > a$, we suppose $a + b \ge c + d,\ ab \le cd$. Thus*

$$f^\lambda_{\{a,\ b\},\ \{c,\ d\}} \begin{cases} \ge 0, & if\ \lambda = 1, \\ > 0, & if\ 0 < \lambda < 1, \\ < 0, & if\ \lambda < 0. \end{cases}$$

Proof. Note that $f^\lambda_{\{a,\ b\},\ \{c,\ d\}}$

$= a^{\lambda+1}b^{\lambda+1}d + a^{\lambda+1}b^{\lambda+1}c + bc^{\lambda+1}d^{\lambda+1} + ac^{\lambda+1}d^{\lambda+1} - a^{2\lambda}bcd - ab^{2\lambda}cd - abc^{2\lambda}d - abcd^{2\lambda}$

$= abcd[(a^{\lambda-1} - b^{\lambda-1})(b^\lambda - a^\lambda) + (c^{\lambda-1} - d^{\lambda-1})(d^\lambda - c^\lambda)] + [ac(d-b) + bd(c-a)](c^\lambda d^\lambda - a^\lambda b^\lambda)$.

Case 1. $0 < \lambda \le 1$.

If $d > c > b > a > 0$ or $d > b > c > a > 0$, then

$$a^{\lambda-1} - b^{\lambda-1} \ge 0,\ b^\lambda - a^\lambda > 0,\ c^{\lambda-1} - d^{\lambda-1} \ge 0,\ d^\lambda - c^\lambda > 0,$$

$$ac(d-b) + bd(c-a) > 0,\ c^\lambda d^\lambda - a^\lambda b^\lambda > 0.$$

If $b > d > c > a > 0$, since $a + b \geq c + d$ and $ab \leq cd$, then

$$a^{\lambda-1} - b^{\lambda-1} \begin{cases} > 0, & if\ 0 < \lambda < 1, \\ = 0, & if\ \lambda = 1. \end{cases},\ b^\lambda - a^\lambda > 0,\ c^{\lambda-1} - d^{\lambda-1} \geq 0,\ d^\lambda - c^\lambda > 0,$$

$$c^\lambda d^\lambda - a^\lambda b^\lambda \geq 0,\ ac(d-b)+bd(c-a) = cd(a+b)-ab(c+d) \geq ab(a+b-c-d) \geq 0.$$

Therefore, we always have $f^\lambda_{\{a,\ b\},\ \{c,\ d\}} \begin{cases} > 0, & if\ 0 < \lambda < 1, \\ \geq 0, & if\ \lambda = 1. \end{cases}$

Case 2. $\lambda < 0$.

If $d > c > b > a > 0$ or $d > b > c > a > 0$, then

$$a^{\lambda-1} - b^{\lambda-1} > 0,\ b^\lambda - a^\lambda < 0,\ c^{\lambda-1} - d^{\lambda-1} > 0,\ d^\lambda - c^\lambda < 0,$$

$$ac(d-b) + bd(c-a) > 0,\ c^\lambda d^\lambda - a^\lambda b^\lambda < 0.$$

If $b > d > c > a > 0$, note that $a + b \geq c + d$ and $ab \leq cd$, then

$$a^{\lambda-1} - b^{\lambda-1} > 0,\ b^\lambda - a^\lambda < 0,\ c^{\lambda-1} - d^{\lambda-1} > 0,\ d^\lambda - c^\lambda < 0,$$

$$c^\lambda d^\lambda - a^\lambda b^\lambda \leq 0,\ ac(d-b) + bd(c-a) \geq ab(a+b-c-d) \geq 0.$$

Therefore, it can be seen that $f^\lambda_{\{a,\ b\},\ \{c,\ d\}} < 0$. □

3 Main results

Let G be a finite, undirected and simple graph. If $xy \in E(G)$, we say that y is a neighbor of x and denote by $N(x)$ the set of neighbors of x. And $d(x) = |N(x)|$ is called the degree of x. We denote the number of vertices of degree i in G by n_i and the number of edges that connect vertices of degree i and j by m_{ij}, where we do not distinguish m_{ij} and m_{ji}. Similarly as in paper [11] we show that:

Lemma 3.1 *Let G be a graph with n vertices and m edges. Let N denote the set of the degrees of vertices in G. Let $\mu = \sum_{k\leq l\in N} m_{kl} \cdot \sum_{k\leq l\in N} m_{kl}(\frac{1}{k} + \frac{1}{l})$. Then*

$$^\lambda M_2(G)/m - {}^\lambda M_1(G)/n = \frac{1}{\mu} \cdot \sum_{\substack{i\leq j,\ k\leq l,\\ \{i,\ j\},\ \{k,\ l\}\subseteq N^2}} (f^\lambda_{\{i,\ j\},\ \{k,\ l\}} \cdot \frac{m_{ij}m_{kl}}{i \cdot j \cdot k \cdot l}).$$

Theorem 3.2 *Let G be a graph with n vertices, m edges and* $\Delta(G) - \delta(G) \le 2$.

$$If\ \lambda \in [0,\ 1],\ then\ {}^{\lambda}M_1(G)/n \le {}^{\lambda}M_2(G)/m. \tag{3}$$

$$If\ \lambda \in (-\infty,\ 0),\ then\ {}^{\lambda}M_1(G)/n \ge {}^{\lambda}M_2(G)/m. \tag{4}$$

Moreover, if $\lambda = 0$*, the equality of* (3) *always holds.*

If $\lambda = 1$*, the equality of* (3) *holds if and only if all edges* ij *have the same pair* $(d_i,\ d_j)$ *of degrees.*

If $\lambda \in (0,\ 1)$ ($resp.\ \lambda \in (-\infty,\ 0)$)*, the equality of* (3) ($resp.$ (4)) *holds if and only if G is a regular graph.*

Proof. For simplicity, let $\delta(G) = p$ and $N = \{p,\ p+1,\ p+2\}$.

Case 1. If $\lambda = 0$, it is obvious that

$${}^{0}M_1(G)/n = (\sum_{v \in V}[d(v)]^{2\cdot 0})/n = 1 = (\sum_{uv \in E}[d(u)d(v)]^{0})/m = {}^{0}M_2(G)/m.$$

Case 2. If $\lambda \in (0,\ 1]$ ($resp.\ \lambda \in (-\infty,\ 0)$), by Lemma 3.1,

$${}^{\lambda}M_2(G)/m - {}^{\lambda}M_1(G)/n = \frac{1}{\mu} \cdot \sum_{\substack{i \le j,\ k \le l, \\ \{i,\ j\},\ \{k,\ l\} \subseteq N^2}} (f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} \cdot \frac{m_{ij}m_{kl}}{i \cdot j \cdot k \cdot l}).$$

Note that all $i,\ j,\ k$ and l can not be distinct numbers, we need to show that $f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} \ge 0$ ($resp.\ \le 0$) for each $\{i,\ j\},\ \{k,\ l\} \subseteq N^2$. Let $a,\ b,\ c$ be distinct elements of N. Then we have the following subcases.

Subcase 2.1 $\{\{i,\ j\},\ \{k,\ l\}\} = \{\{a,\ a\},\ \{a,\ a\}\}$. By Lemma 2.1, $f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} = 0$.

Subcase 2.2 $\{\{i,\ j\},\ \{k,\ l\}\} = \{\{a,\ a\},\ \{a,\ b\}\}$. By Lemma 2.2,

$$f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} \begin{cases} > 0, & if\ 0 < \lambda \le 1, \\ < 0, & if\ \lambda < 0. \end{cases}$$

Subcase 2.3 $\{\{i,\ j\},\ \{k,\ l\}\} = \{\{a,\ a\},\ \{b,\ b\}\}$. By Lemma 2.3,

$$f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} \begin{cases} > 0, & if\ 0 < \lambda \le 1, \\ < 0, & if\ \lambda < 0. \end{cases}$$

Subcase 2.4 $\{\{i,\ j\},\ \{k,\ l\}\} = \{\{a,\ b\},\ \{a,\ b\}\}$. By Lemma 2.4,

$$f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} \begin{cases} = 0, & if\ \lambda = 1, \\ > 0, & if\ 0 < \lambda < 1, \\ < 0, & if\ \lambda < 0. \end{cases}$$

Subcase 2.5 $\{\{i,\ j\},\ \{k,\ l\}\} = \{\{a,\ b\},\ \{a,\ c\}\}$. By Lemma 2.5,

$$f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}}\begin{cases} > 0, & if\ 0 < \lambda \leq 1, \\ < 0, & if\ \lambda < 0. \end{cases}$$

Subcase 2.6 $\{\{i,\ j\},\ \{k,\ l\}\} = \{\{a,\ a\},\ \{b,\ c\}\}$. Without loss of generality, suppose $i = j$ and $l > k$. If $k < i = j < l$, since $N = \{p,\ p+1,\ p+2\}$, then $kl = p(p+2) \leq (p+1)^2 = i^2$. By Lemma 2.6,

$$f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}}\begin{cases} \geq 0, & if\ \lambda = 1, \\ > 0, & if\ 0 < \lambda < 1, \\ < 0, & if\ \lambda < 0. \end{cases}$$

All in all, the inequality (3) (*resp.* (4)) is proved.

Moreover, if $\lambda = 0$, then the equality of (3) always holds.

If $\lambda = 1$, from the proof of Case 2, the equality of (3) holds if and only if $f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} = 0$ for all $m_{ij} \cdot m_{kl} > 0$, which implies that all edges ij have the same pair $(d_i,\ d_j)$ of degrees (also see [8]).

If $\lambda \in (0,\ 1)$ (*resp.* $\lambda \in (-\infty,\ 0)$), from the foregoing proof, the equality of (3) (*resp.* (4)) holds if and only if $f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} = 0$ for all $m_{ij} \cdot m_{kl} > 0$, which means $i = j = k = l$ for each $\{i,\ j\},\ \{k,\ l\} \subseteq N^2$, that is, G is a regular graph. □

From Theorem 3.2, we obtain the main result in [8] immediately.

Corollary 3.3 *([8]) Let G be a graph with n vertices, m edges and* $\Delta(G) - \delta(G) \leq 2$. *Then* $M_1(G)/n \leq M_2(G)/m$, *with the equality holds if and only if all edges* ij *have the same pair* $(d_i,\ d_j)$ *of degrees.*

Let G^* denote the graphs with each edge connecting a 3-degree vertex and a 6-degree vertex. The star graph S_n is a tree on n vertices with one vertex having degree $n-1$ and the other vertices having degree 1.

Theorem 3.4 *Let G be a graph with n vertices and m edges such that* $\Delta(G) - \delta(G) \leq 3$ *and* $\delta(G) \neq 2$.

$$If\ \lambda \in [0,\ 1],\ then\ {}^{\lambda}M_1(G)/n \leq {}^{\lambda}M_2(G)/m. \tag{5}$$

$$If\ \lambda \in (-\infty,\ 0),\ then\ {}^{\lambda}M_1(G)/n \geq {}^{\lambda}M_2(G)/m. \tag{6}$$

Moreover, if $\lambda = 0$, *the equality of* (5) *always holds.*

If $\lambda = 1$, the equality of (5) *holds if and only if all edges ij have the same pair $(d_i,\ d_j)$ of degrees or if the graph is composed of disjoint stars S_5 and cycles of any length or if the graph is composed of disjoint G^* and* 4*-regular graphs ([8]).*

If $\lambda \in (0,\ 1)$ (resp. $\lambda \in (-\infty,\ 0)$), the equality of (5) *(resp.* (6)*) holds if and only if G is a regular graph.*

Proof. For simplicity, let $\delta(G) = p$ and $N = \{p,\ p+1,\ p+2,\ p+3\}$. Let $a,\ b,\ c,\ d$ be distinct elements of N. If $\lambda = 0$, it is obvious that ${}^0M_1(G)/n = {}^0M_2(G)/m$.

If $\lambda \in (0,\ 1]$ (resp. $\lambda \in (-\infty,\ 0)$), by Lemma 3.1, we just need to show that $f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} \geq 0$ (resp. ≤ 0) for each $\{i,\ j\},\ \{k,\ l\} \subseteq N^2$ $(i \leq j,\ k \leq l)$.

In the proof of Theorem 3.2, we found that $f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} = 0$ holds for the case $\{\{i,\ j\},\ \{k,\ l\}\} = \{\{a,\ a\},\ \{a,\ a\}\}$, and $f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} \begin{cases} \geq 0, & if\ \lambda = 1, \\ > 0, & if\ 0 < \lambda < 1, \\ < 0, & if\ \lambda < 0 \end{cases}$ holds for the cases $\{\{i,\ j\},\ \{k,\ l\}\} = \{\{a,\ a\},\ \{a,\ b\}\}$, $\{\{a,\ a\},\ \{b,\ b\}\}$, $\{\{a,\ b\},\ \{a,\ b\}\}$ and $\{\{a,\ b\},\ \{a,\ c\}\}$. We only need to discuss the following two cases.

Case 1. $\{\{i,\ j\},\ \{k,\ l\}\} = \{\{a,\ a\},\ \{b,\ c\}\}$. Without loss of generality, suppose $i = j$ and $l > k$. It follows from Lemma 2.7 that

$$f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} \begin{cases} \geq 0, & if\ \lambda = 1, \\ > 0, & if\ 0 < \lambda < 1, \\ < 0, & if\ \lambda < 0. \end{cases}$$

Case 2. $\{\{i,\ j\},\ \{k,\ l\}\} = \{\{a,\ b\},\ \{c,\ d\}\}$. Without loss of generality, suppose $l > k$ and $i = min\{i,\ j,\ k,\ l\}$. If $i < k < l < j$, then $i = p,\ k = p+1,\ l = p+2,\ j = p+3$, and it follows that

$$i + j = 2p + 3 = k + l,\ and\ ij = p^2 + 3p \leq p^2 + 3p + 2 = kl.$$

Then by Lemma 2.8, we obtain that $f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} \begin{cases} \geq 0, & if\ \lambda = 1, \\ > 0, & if\ 0 < \lambda < 1, \\ < 0, & if\ \lambda < 0. \end{cases}$

Therefore, the inequality (5) and (6) are proved.

Moreover, if $\lambda = 0$, the equality of (5) always holds.

If $\lambda = 1$, the equality of (5) in this case had been proved in [8].

If $\lambda \in (0,\ 1)$ (*resp.* $\lambda \in (-\infty,\ 0)$), from the foregoing proof, the equality of (5) (*resp.* (6)) holds if and only if $f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} = 0$ for all $m_{ij} \cdot m_{kl} > 0$, which means $i = j = k = l$ for each $\{i,\ j\},\ \{k,\ l\} \subseteq N^2$, that is, G is a regular graph. □

If $\lambda = 1$, Hansen and Vukičević in [3] proved that $M_1(G)/n \leq M_2(G)/m$ for chemical graphs. Now we consider the case $\lambda \in (0,\ 1)$ (*resp.* $\lambda \in (-\infty,\ 0)$).

Corollary 3.5 *Let G be a chemical graph with n vertices and m edges.*

$$If\ \lambda \in (0,\ 1),\ then\ {}^{\lambda}M_1(G)/n \leq {}^{\lambda}M_2(G)/m.\ ([11]) \tag{7}$$

$$If\ \lambda \in (-\infty,\ 0),\ then\ {}^{\lambda}M_1(G)/n \geq {}^{\lambda}M_2(G)/m. \tag{8}$$

Moreover, if $\lambda \in (0,\ 1)$) (*resp.* $\lambda \in (-\infty,\ 0)$)*, the equality of* (7) (*resp.* (8)) *holds if and only if G is a regular graph.*

Proof. Note that G is a chemical graph, thus $\Delta \leq 4$. If $\delta = 1$, then $\Delta - \delta \leq 3$, by Theorem 3.4, the results are proved. If $\delta \geq 2$, we have $\Delta - \delta \leq 2$, and it follows from Theorem 3.2 that the results are obtained as desired. □

Let $e_i,\ e_j \in E$, where the degrees of their end vertices are $\{d_{i_1},\ d_{i_2}\}$ $(d_{i_1} \leq d_{i_2})$ and $\{d_{j_1},\ d_{j_2}\}$ $(d_{j_1} \leq d_{j_2})$, respectively. A pair of edges $[e_i,\ e_j]$ is called a degrees-nested edges pair if $d_{i_1} < d_{j_1} \leq d_{j_2} < d_{i_2}$ or $d_{j_1} < d_{i_1} \leq d_{i_2} < d_{j_2}$.

Corollary 3.6 *Let G be a graph with n vertices, m edges, and G contains no degrees-nested edges pairs.*

$$If\ \lambda \in (0,\ 1),\ then\ {}^{\lambda}M_1(G)/n \leq {}^{\lambda}M_2(G)/m. \tag{9}$$

$$If\ \lambda \in (-\infty,\ 0),\ then\ {}^{\lambda}M_1(G)/n \geq {}^{\lambda}M_2(G)/m. \tag{10}$$

Moreover, if $\lambda \in (0,\ 1)$ (*resp.* $\lambda \in (-\infty,\ 0)$)*, the equality of* (9) (*resp.* (10)) *holds if and only if G is a regular graph.*

Proof. If $\lambda \in (0,\ 1]$ (resp. $\lambda \in (-\infty,\ 0)$), by Lemma 3.1, we just need to show that $f^{\lambda}_{\{i,\ j\},\ \{k,\ l\}} \geq 0$ (resp. ≤ 0) for each $\{i,\ j\},\ \{k,\ l\} \subseteq N^2$ $(i \leq j,\ k \leq l)$ $(*)$.

Since G contains no degrees-nested edges pairs, from the proof of Lemma 2.1-2.8, we conclude that $(*)$ always holds, and this completes the proof. □

Finally, we consider the relationship of ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ for $\lambda > 1$. A simple graph on n vertices in which each pair of distinct vertices is joined by an edge is called a complete graph, and denoted by K_n. A complete bipartite graph is a simple bipartite graph with bipartition $(X,\ Y)$ in which each vertex of X is joined to each vertex of Y; if $|X| = n_1$ and $|Y| = n_2$, such a graph is denoted by $K_{n_1,\ n_2}$. The disjoint union of k copies of G is often written by kG.

Example 1 *Let G_1 be a graph of order 9 created from K_3 and $3K_2$ by connecting each vertex of K_3 to a vertex of a K_2. Thus $\Delta(G_1) - \delta(G_1) = 3 - 1 = 2$, and*

$$^{\lambda}M_2(G_1)/m - {}^{\lambda}M_1(G_1)/n = \frac{6^{\lambda} + 2^{\lambda} - 4^{\lambda} - 1}{3} > 0 \ for\ \lambda > 1.$$

Example 2 *Let $G_2 = K_{4,\,5}$. Obviously, $\Delta(G_2) - \delta(G_2) = 5 - 4 = 1$, and*

$$^{\lambda}M_2(G_2)/m - {}^{\lambda}M_1(G_2)/n = \frac{9 \cdot 20^{\lambda} - 4 \cdot 25^{\lambda} - 5 \cdot 16^{\lambda}}{9} < 0 \ for\ \lambda > 1.$$

Remark 1 *It is known that the inequality $^{\lambda}M_2(G)/m - {}^{\lambda}M_1(G)/n < 0$ is true for all unbalanced bipartite graphs G and $\lambda \in R\backslash[0,\ 1]$ ([11]).*

Combining Example 1 and 2, when $\lambda > 1$, we can find a suitable graph G_1 such that $^{\lambda}M_2(G_1)/m - {}^{\lambda}M_1(G_1)/n > 0$, and a suitable graph G_2 such that $^{\lambda}M_2(G_2)/m - {}^{\lambda}M_1(G_2)/n < 0$. Besides, note that $\Delta(G_i) - \delta(G_i) \leq 2$ $(i = 1,\ 2)$ and $|V(G_1)| = |V(G_2)|$, we conclude that when $\lambda \in (1, +\infty)$, the relationship of $^{\lambda}M_1(G)/n$ and $^{\lambda}M_2(G)/m$ is indefinite for distinct graphs G even if $\Delta(G) - \delta(G) \leq 2$.

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