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First Zagreb Index, k-Connectivity, β-Deficiency and k-Hamiltonicity of Graphs

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Abstract

The first Zagreb index $M_1(G)$ is equal to the sum of squares of the degrees of the vertices of the underlying molecular graph G. Finding sufficient conditions for graphs possessing certain properties are important problems. In this paper, we give sufficient conditions in terms of the first Zagreb index for a graph to be k-connected, β-deficient or k-hamiltonian.

1 Introduction

All graphs considered in this paper are finite, undirected and simple connected graphs. Let $G = (V(G), E(G))$ be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$, $|E(G)| = m$. Let $\deg_G(v_i)$ or d_i be the degree of a vertex v_i in G. When the graph is clear from the context, we will omit the subscript G from the notation. For other undefined terminology and notations from graph theory, the readers are referred to [5].

Gutman and Trinajstić [12] derived a formula for estimating total π-electron energy of conjugated systems. Their formula contained two terms that later became known as the

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Zagreb indices M_1 and M_2. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of graph G are among the oldest and most studied topological indices. They are defined as:

$$M_1(G) = \sum_{v_i \in V(G)} \deg(v_i)^2 \quad \text{and} \quad M_2(G) = \sum_{v_i v_j \in E(G)} \deg(v_i)\deg(v_j).$$

We encourage the reader to consult [1, 6, 10, 17, 20, 21] for historical background, computational techniques and mathematical properties of Zagreb indices.

The problem of deciding whether a given graph possesses certain properties is often difficult. For example, determining whether a given graph is Hamiltonian or traceable is NP-complete [14]. Thus, finding these sufficient conditions for graphs becomes meaningful in graph theory. Up to now, there are lots of existing results. For example, in [3, Page 4], it is stated that if G is a simple graph of order $n \geq k+1$, and if its minimum degree $\delta(G) \geq \frac{1}{2}(n+k-2)$, then G is k-connected. It is known that [7], for a graph G, if $\delta(G) \geq \frac{n+k}{2}$, then G is k-hamiltonian. In [5, Page 15], it declares that for a connected graph G, if $\delta(G) \geq n-\beta-1$, then G contains a cycle of length at least $n-\beta$, and hence G has a matching of size at least $\frac{n-\beta}{2}$. However, there are only few such conditions in terms of the topological indices. Hua and Wang [13] presented a sufficient condition for a graph to be traceable by using the Harary index. By using the Wiener index, Yang [19] gave a sufficient condition for a graph to be traceable. The above results are further generalized by Liu et al. [15, 16]. Recently, in terms of the Wiener index or Harary index, Feng et al. [9] presented several sufficient conditions for a graph to be k-connected, β-deficient, k-hamiltonian, k-path-coverable or k-edge-hamiltonian. In this paper, we continue this program to the first Zagreb index, and give sufficient conditions in terms of the first Zagreb index for a graph to be k-connected, β-deficient or k-hamiltonian.

The paper is organized as follows. In the next section we give the necessary definitions and some lemmas. Section 3 contains our main results. The last section is concerned with possible directions of future research.

2 Preliminaries

In this section, we first give some definitions and notations which will be used throughout the paper. A connected graph G is said to be *k-connected* (or *k-vertex connected*) if it has more than k vertices and remains connected whenever fewer than k vertices are removed. The *deficiency* of a graph G, denoted by $\mathrm{def}(G)$, is the number of vertices unmatched under a maximum matching in G. In particular, G has a 1-factor if and only if def(G) $= 0$. We call G, β-deficient if def(G)$\leq \beta$. Thus a β-deficient graph G of order n has matching number $\frac{n-\beta}{2}$. A graph G is *k-hamiltonian* if for all $|X| \leq k$, the subgraph induced by $V(G) \setminus X$ is hamiltonian.

An integer sequence $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ is called *graphical* if there exists a graph G having π as its vertex degree sequence; in that case, G is called a *realization* of π. If P is a graph property, such as k-connectivity or hamiltonicity, we call a graphical sequence π *enforces* P if every realization of π has property P.

For two vertex-disjoint graphs G_1 and G_2, we use $G_1 \cup G_2$ to denote their union. The *join* $G_1 \vee G_2$ of graphs G_1 and G_2 is the graph obtained from the disjoint union of G_1 and G_2 by adding all edges between $V(G_1)$ and $V(G_2)$. Given a graph G, a subset S of $V(G)$ is said to be an *independent set* of G if the subgraph $G[S]$, induced by S, is a graph with $|S|$ isolated vertices. The *independence number* $\alpha(G)$ of G is the number of vertices in the largest independent set of G. As usual, K_n denotes, the complete graph on n vertices.

Next, we give some lemmas which will be used later.

Lemma 2.1. [4] *Let $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ be a graphical sequence with $n \geq 2$ and $1 \leq k \leq n-1$. If*

$$d_i \leq i + k - 2 \Rightarrow d_{n-k+1} \geq n - i \text{ for } 1 \leq i \leq \frac{1}{2}(n-k+1),$$

then π is enforces k-connected.

Lemma 2.2. [18] *Let $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ be a graphical sequence, and also let $0 \leq \beta \leq n$ with $n \equiv \beta \,(mod\ 2)$. If*

$$d_{i+1} \leq i - \beta \Rightarrow d_{n+\beta-i} \geq n - i - 1 \text{ for } 1 \leq i \leq \frac{1}{2}(n+\beta-2),$$

then π is enforces β-deficient.

Lemma 2.3. [8] *Let $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ be a graphical sequence and $0 \leq k \leq n-3$. If*

$$d_i \leq i + k \Rightarrow d_{n-i-k} \geq n - i \text{ for } 1 \leq i < \frac{1}{2}(n-k),$$

then π is enforces k-hamiltonian.

Lemma 2.4. [2] *Let $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ be a graphical sequence and $k \geq 1$. If $d_{k+1} \geq n-k$, then π is enforces $\alpha(G) \leq k$.*

3 Main results

In this section we present sufficient conditions in terms of the first Zagreb index for a graph to be k-connected, β-deficient or k-hamiltonian.

Theorem 3.1. *Let G be a connected graph of order $n \geq k+1$. If*

$$M_1(G) > f(n,\, k), \quad \textit{where} \quad f(n,\, k) = (k-1)^2 + (n-k)(n-2)^2 + (k-1)(n-1)^2,$$

then G is k-connected. Moreover, $M_1(G) = f(n,\, k)$ if and only if $G \cong K_{k-1} \vee (K_1 \cup K_{n-k})$.

Proof: Suppose that G is not k-connected. Then by Lemma 2.1, there exists an integer i $\big(1 \leq i \leq \frac{1}{2}(n-k+1)\big)$ such that $d_i \leq i+k-2$ and $d_{n-k+1} \leq n-i-1$. Note that $1 \leq k \leq n-1$. Then by the definition of the first Zagreb index, we have

$$\begin{aligned} M_1(G) &= \sum_{i=1}^{n} d_i^2 \\ &\leq i(i+k-2)^2 + (n-k-i+1)(n-i-1)^2 + (k-1)(n-1)^2 \\ &= (3n+k-5)i^2 - (3n+k-5)(n-k+1)i + n(n-1)^2. \end{aligned}$$

Denote

$$f(x) = (3n+k-5)\big[x^2 - (n-k+1)x\big]$$

with $1 \leq x \leq \frac{1}{2}(n-k+1)$. By taking the first derivative of $f(x)$ on $1 \leq x \leq \frac{1}{2}(n-k+1)$, we have

$$f'(x) = (3n+k-5)\big[2x - (n-k+1)\big].$$

Evidently, $f'(x) \leq 0$ when $1 \leq x \leq \frac{1}{2}(n-k+1)$. Thus $f(x)$ is a decreasing function on $x \in [1,\, \frac{n-k+1}{2}]$, and consequently $f(x) \leq f(1)$. Thus

$$M_1(G) \leq (k-1)^2 + (n-k)(n-2)^2 + (k-1)(n-1)^2 = f(n,\, k),$$

which contradicts to the assumption, and the conclusion follows.

If $G \cong K_{k-1} \vee (K_1 \cup K_{n-k})$, then one can easily see that $M_1(G) = f(n,\, k)$. Conversely, let $M_1(G) = f(n,\, k)$. Then all the inequalities in the proof should be equalities. So $i = 1$, and hence $d_1 = k-1$, $d_2 = \cdots = d_{n-k+1} = n-2$, $d_{n-k+2} = \cdots = d_n = n-1$. Thus $G = K_{k-1} \vee (K_1 \cup K_{n-k})$. ■

Remark 3.2. *By [2], graph $K_{k-1} \vee (K_1 \cup K_{n-k})$ is not k-connected.*

Theorem 3.3. *Let G be a connected graph of order $n \geq 10$ with $n \equiv \beta\,(mod\ 2)$ and $0 \leq \beta \leq n$. If*

$$M_1(G) > g(n,\beta), \quad \textit{where} \quad g(n,\beta) = 2(\beta-1)^2 + (n+\beta-3)(n-3)^2 - (\beta-1)(n-1)^2,$$

then G is β-deficient. Moreover, $M_1(G) = g(n,\beta)$ if and only if $G \cong K_1 \vee (2K_1 \cup K_{n-3})$.

Proof: Suppose that G is not β-deficient. Then from Lemma 2.2, there exists an integer i ($1 \leq i \leq \frac{n+\beta-2}{2}$) such that $d_{i+1} \leq i-\beta$ and $d_{n+\beta-i} \leq n-i-2$. Again from the definition of the first Zagreb index, we have

$$\begin{aligned} M_1(G) &= \sum_{i=1}^{n} d_i^2 \\ &\leq (i+1)(i-\beta)^2 + (n+\beta-2i-1)(n-i-2)^2 + (i-\beta)(n-1)^2 \\ &= -i^3 + (5n-\beta-8)i^2 + (\beta^2+2\beta-3n^2-2n\beta+12n-11)i + \beta^2 \\ &\qquad + (n-2)^2(n+\beta-1) - \beta(n-1)^2. \end{aligned}$$

Denote

$$\begin{aligned} g(x) &= -x^3 + (5n-\beta-8)x^2 + (\beta^2+2\beta-3n^2-2n\beta+12n-11)x + \beta^2 \\ &\qquad + (n-2)^2(n+\beta-1) - \beta(n-1)^2 \end{aligned}$$

with $1 \leq x \leq \frac{1}{2}(n+\beta-2)$ and $0 \leq \beta \leq n$. Then the first and second derivative of $g(x)$, respectively, are

$$g'(x) = -3x^2 + 2(5n-\beta-8)x + \beta^2 + 2\beta - 3n^2 - 2n\beta + 12n - 11,$$

and

$$g''(x) = 2(-3x+5n-\beta-8).$$

Since $n \geq 10$, $n \geq \beta$ and $x \leq \frac{1}{2}(n+\beta-2)$, we have

$$\begin{aligned} g''(x) &= 3(-2x+n+\beta-2) + 7n - 5\beta - 10 \\ &\geq 5(n-\beta) + 2(n-5) > 0. \end{aligned}$$

Therefore $g(x)$ is a convex function on $x \in [1, \frac{n+\beta-2}{2}]$. So $g(x) \leq \max\Big\{g(1),\, g(\frac{n+\beta-2}{2})\Big\}$. Direct calculations yield

$$g(1) = 2\beta^2 + 4(1-n)\beta + n^3 - 8n^2 + 25n - 24,$$

$$g\left(\frac{n+\beta-2}{2}\right)=\frac{1}{8}\beta^3-\frac{1}{8}(n-6)\beta^2-\frac{1}{8}(5n^2-4n-8)\beta+\frac{5}{8}n^3-\frac{9}{4}n^2+2n.$$

After subtraction,

$$g\left(\frac{n+\beta-2}{2}\right)-g(1)=\frac{1}{8}\Big[\beta^3-(n+10)\beta^2-(5n^2-36n+24)\beta-3n^3+46n^2-184n+192\Big].$$

Define $\phi(\beta)=\beta^3-(n+10)\beta^2-(5n^2-36n+24)\beta-3n^3+46n^2-184n+192$ as a function of β on the interval $[0, n]$. Then

$$\phi'(\beta)=3\beta^2-2(n+10)\beta-(5n^2-36n+24),$$

and

$$\phi''(\beta)=2\big(3\beta-n-10\big).$$

Case 1 : $\beta\in[0, \frac{n+10}{3}]$. Then $\phi''(\beta)\le 0$. So $\phi'(\beta)$ is a decreasing function on $\beta\in[0, \frac{n+10}{3}]$, and consequently $\phi'(\beta)\le\phi'(0)$. Note that $\phi'(0)=-(5n^2-36n+24)<0$ as $n\ge 10$. Therefore $\phi'(\beta)<0$ for $\beta\in[0, \frac{n+10}{3}]$.

Case 2 : $\beta\in(\frac{n+10}{3}, n]$. Then $\phi''(\beta)>0$. So $\phi'(\beta)$ is an increasing function on $\beta\in(\frac{n+10}{3}, n]$, and consequently $\phi'(\beta)\le\phi'(n)$. Note that $\phi'(n)=-4(n^2-4n+6)<0$ as $n\ge 10$. Therefore $\phi'(\beta)<0$ for $\beta\in(\frac{n+10}{3}, n]$.

From **Case 1** and **Case 2**, we conclude that $\phi(\beta)$ is a decreasing function on $\beta\in[0, n]$. Thus $\phi(\beta)\le\phi(0)$. An elementary calculation gives $\phi(0)=-3n^3+46n^2-184n+192<0$ as $n\ge 10$, that is, $\phi(\beta)<0$. Implying that $g\big(\frac{n+\beta-2}{2}\big)-g(1)<0$, and consequently $g(x)\le g(1)$. Hence

$$M_1(G)\le 2(\beta-1)^2+(n+\beta-3)(n-3)^2-(\beta-1)(n-1)^2=g(n, \beta),$$

a contradiction. So the result follows.

If $G\cong K_1\vee(2K_1\cup K_{n-3})$, then one can easily see that $M_1(G)=g(n, \beta)$. Conversely, let $M_1(G)=g(n, \beta)$. Then $i=1$. Since $\beta\le i$, either $\beta=0$ or $\beta=1$. If $\beta=1$, then $d_1=d_2=0$ and therefore graph G is disconnected, a contradiction. Otherwise, $\beta=0$. Then $d_1=d_2=1$, $d_3=\cdots=d_{n-1}=n-3$, $d_n=n-1$. Thus $G\cong K_1\vee(2K_1\cup K_{n-3})$. ∎

Theorem 3.4. *Let G be a connected graph of order $n\ge 5$ and $0\le k\le n-3$. If*

$$M_1(G)>h(n, k),\quad \text{where}\quad h(n, k)=(k+1)^2+(n-k-2)(n-2)^2+(k+1)(n-1)^2, \tag{1}$$

then G is k-hamiltonian. Moreover, $M_1(G)=h(n, k)$ if and only if $G\cong K_{k+1}\vee(K_1\cup K_{n-k-2})$.

Proof: Suppose that G is not k-hamiltonian. Then by Lemma 2.3, there exists an integer i $(1 \le i < \frac{n-k}{2})$ such that $d_i \le i+k$ and $d_{n-i-k} \le n-i-1$. From the definition of the first Zagreb index of graph G, we have

$$\begin{aligned} M_1(G) &= \sum_{i=1}^{n} d_i^2 \\ &\le i(i+k)^2 + (n-2i-k)(n-i-1)^2 + (i+k)(n-1)^2 \\ &= -i^3 + (5n+k-4)i^2 + \big[k^2 - 2(n-k)(n-1) - (n-1)^2\big]i + n(n-1)^2. \end{aligned}$$

Since i is an integer with $1 \le i < \frac{n-k}{2}$, we have $1 \le i \le \frac{n-k-1}{2}$. Denote

$$h(x) = -x^3 + (5n+k-4)x^2 + \big[k^2 - 2(n-k)(n-1) - (n-1)^2\big]x$$

with $1 \le x \le \frac{1}{2}(n-k-1)$ and $0 \le k \le n-3$. Since x is an integer, we have to consider $n-k-1$ is odd or even.

Case 1 : $n-k-1$ is odd. Then $1 \le x \le \frac{1}{2}(n-k-2)$ and $0 \le k \le n-4$. Hence

$$h'(x) = -3x^2 + 2(5n+k-4)x + k^2 - 2(n-k)(n-1) - (n-1)^2,$$

and

$$\begin{aligned} h''(x) = 2\big(-3x+5n+k-4\big) &= 3\left(\frac{10n}{3} - 2x + \frac{2k}{3} - \frac{8}{3}\right) \\ &\ge 7n+5k-2 > 0 \quad \text{as} \quad n-2x-k-2 \ge 0, \end{aligned}$$

and consequently $h(x)$ is a convex function on $1 \le x \le \frac{1}{2}(n-k-2)$. It implies that $h(x) \le \max\Big\{h(1),\, h(\frac{n-k-2}{2})\Big\}$. Direct calculations yield

$$h(1) = k^2 + (2n-1)k - 3n^2 + 9n - 6,$$

and

$$h\left(\frac{n-k-2}{2}\right) = -\frac{1}{8}k^3 - \frac{1}{8}(n-6)k^2 + \frac{1}{8}(5n^2-4n+8)k - \frac{3}{8}n^3 - \frac{1}{4}n^2 + 3n - 2.$$

After subtraction,

$$h\left(\frac{n-k-2}{2}\right) - h(1) = -\frac{1}{8}\Big[k^3 + (n+2)k^2 - (5n^2-20n+16)k + 3n^3 - 22n^2 + 48n - 32\Big].$$

Define $\phi(k) = k^3 + (n+2)k^2 - (5n^2-20n+16)k + 3n^3 - 22n^2 + 48n - 32$ as a function of k on the interval $[0, n-4]$. By taking the first and second derivative of $\phi(k)$, respectively, we have

$$\phi'(k) = 3k^2 + 2(n+2)k - (5n^2-20n+16),$$

and

$$\phi''(k) = 6k + 2(n+2).$$

Since $0 \le k \le n-4$ and $n \ge 5$, we have $\phi''(k) \ge 0$. So $\phi'(k)$ is an increasing function on $k \in [0,\, n-4]$, and consequently $\phi'(k) \le \phi'(n-4)$. Note that $\phi'(n-4) = -8n+16 < 0$ as $n \ge 5$, thus $\phi'(k) < 0$ for $k \in [0,\, n-4]$. It follows that $\phi(k)$ is a decreasing function on $k \in [0,\, n-4]$. Thus $\phi(k) \ge \phi(n-4)$. Note that $\phi(n-4) = 0$, so $\phi(k) \ge 0$, implying that $h\big(\frac{n-k-2}{2}\big) - h(1) \le 0$. Therefore, $h(x) \le h(1)$. Hence

$$M_1(G) \le (k+1)^2 + (n-k-2)(n-2)^2 + (k+1)(n-1)^2 = h(n,\, k),$$

a contradiction, by (1). Hence G is k-hamiltonian.

Case 2 : $n-k-1$ is even. Then $1 \le x \le \frac{1}{2}(n-k-1)$. In this case $k = n-3$ or $k \in [0,\, n-5]$.

Subcase 2.1 : $k = n-3$. Then $n-k-1 = 2$ and $x = 1$. Thus

$$M_1(G) \le (n-2)\big[2(n-2) + (n-1)^2\big] = h(n,\, n-3),$$

a contradiction, by (1). Hence G is k-hamiltonian.

Subcase 2.2 : $k \in [0,\, n-5]$. Then similar to **Case 1**, we get that $h(x)$ is a convex function on $1 \le x \le \frac{1}{2}(n-k-1)$. Therefore $h(x) \le \max\Big\{h(1),\, h(\frac{n-k-1}{2})\Big\}$. Note that the value of $h(1)$ is already known in **Case 1**, so we only need to calculate $h(\frac{n-k-1}{2})$. Direct calculations yield

$$h\left(\frac{n-k-1}{2}\right) = \frac{1}{8}\Big[-k^3 - (n-3)k^2 + (5n^2-6n+1)k - 3n^3 + 3n^2 + 3n - 3\Big].$$

After subtraction,

$$h\left(\frac{n-k-1}{2}\right) - h(1) = -\frac{1}{8}\Big[k^3 + (n+5)k^2 - (5n^2-22n+9)k + 3n^3 - 27n^2 + 69n - 45\Big].$$

Define $\psi(k) = k^3 + (n+5)k^2 - (5n^2-22n+9)k + 3n^3 - 27n^2 + 69n - 45$ is a function of k on the interval $[0,\, n-5]$. Then

$$\psi'(k) = 3k^2 + 2(n+5)k - (5n^2-22n+9),$$

and

$$\psi''(k) = 2\big(3k+n+5\big).$$

Since $0 \le k \le n-5$ and $n \ge 5$, $\psi''(k) > 0$. So $\psi'(k)$ is an increasing function on $k \in [0,\, n-5]$, and consequently $\psi'(k) \le \psi'(n-5)$. Note that $\psi'(n-5) = -8n+16 < 0$ as

$n \geq 5$. Thus $\psi'(k) < 0$ for $k \in [0,\, n-5]$. It follows that $\psi(k)$ is a decreasing function on $k \in [0,\, n-5]$. Thus $\psi(k) \geq \psi(n-5)$. Note that $\psi(n-5) = 0$, so $\psi(k) \geq 0$ on $k \in [0,\, n-5]$, implying that $h\left(\frac{n-k-1}{2}\right) - h(1) \leq 0$. Therefore $h(x) \leq h(1)$. Similarly, by **Case 1**, G is k-hamiltonian.

Second Part: If $G \cong K_{k+1} \vee (K_1 \cup K_{n-k-2})$, then one can easily see that $M_1(G) = h(n,\, k)$. Conversely, let $M_1(G) = h(n,\, k)$. Then for each **Case 1**, **Subcase 2.1** and **Subcase 2.2**, we have $i = 1$. Hence $d_1 = k+1$, $d_2 = \cdots = d_{n-k-1} = n-2$, $d_{n-k} = \cdots = d_n = n-1$. Thus $G \cong K_{k+1} \vee (K_1 \cup K_{n-k-2})$. ■

Let $k = 0$ in Theorem 3.4, then we immediately obtain the following corollary:

Corollary 3.5. *Let G be a connected graph of order $n \geq 5$. If*

$$M_1(G) > n^3 - 5n^2 + 10n - 6,$$

then G is hamiltonian. Moreover, $M_1(G) = n^3 - 5n^2 + 10n - 6$ if and only if $G \cong K_1 \vee (K_1 \cup K_{n-2})$.

Theorem 3.6. *Let G be a connected graph of order n. If*

$$M_1(G) > \zeta(n,\, k), \quad \text{where} \quad \zeta(n,\, k) = (n-1)^3 + (n-1)^2 - 2(n-1)k(k+1) + k^2(k+1),$$

then G satisfies $\alpha(G) \leq k$. Moreover, $M_1(G) = \zeta(n,\, k)$ if and only if $G \cong \overline{K_{k+1}} \vee K_{n-k-1}$.

Proof: Suppose that $\alpha(G) > k$. Then by Lemma 2.4, $d_{k+1} \leq n-k-1$. From the definition of the first Zagreb index, we have

$$\begin{aligned} M_1(G) &= \sum_{i=1}^{n} d_i^2 \\ &\leq (k+1)(n-k-1)^2 + (n-k-1)(n-1)^2 \\ &= (n-1)^3 + (n-1)^2 - 2(n-1)k(k+1) + k^2(k+1), \end{aligned}$$

a contradiction. So the result follows.

If $G \cong \overline{K_{k+1}} \vee K_{n-k-1}$, then one can easily see that $M_1(G) = \zeta(n,\, k)$. Conversely, let $M_1(G) = \zeta(n,\, k)$. Then from the above $M_1(G) = (n-1)^3 + (n-1)^2 - 2(n-1)k(k+1) + k^2(k+1)$, that is, $d_1 = \cdots = d_{k+1} = n-k-1$, $d_{k+2} = \cdots = d_n = n-1$. Therefore $G \cong \overline{K_{k+1}} \vee K_{n-k-1}$. ■

4 Conclusion

In this paper, by using the first Zagreb index, we provide sufficient conditions for a graph to possess certain properties. Can these results be extended for the other popular Zagreb index, named the second Zagreb index, and for other properties such as toughness and the thickness? We will leave them for further studies.

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