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Bounds on Szeged and PI Indexes in terms of Second Zagreb Index

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Abstract: In this short note, we studied the *vertex version* and the *edge version* of the *Szeged index* and the *PI index* and obtained bounds for these indices in terms of the Second Zagreb index. Also, established the connections of bounds to the above sighted indices.

Key Words: Simple graph, Smarandache-Zagreb index, Szeged index, PI index, Zagreb index.

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§1. Introduction and Terminologies

Graph theory has provided chemists with a variety of useful tools, such as topological indices [9]. Let $G = (V, E)$ be a simple graph with $n = |V|$ vertices and $e = |E = E(G)|$ edges. For the vertices u, $v \in V$, the distance $d(u, v)$ is defined as the length of the shortest path between u and v in G. In theoretical Chemistry, molecular structure descriptors, the topological indices are used for modeling physic - chemical, toxicologic, biological and other properties of chemical compounds. Arguably, the best known of these indices is the *Wiener index* W [10], defined as the sum of the distances between all pairs of vertices of the graph G.

$$W(G) = \sum d(u, v).$$

The various extensions and generalization of the *Wiener index* are recently put forward.

Let $e = (u, v)$ be an edge of the graph G. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of G whose distance to the vertex v is smaller than the distance to the vertex u. Similarly $m_u(e)$ denotes the number of edges of G whose distance to the vertex u is smaller than the distance to the vertex v. The topological indices *vertex version* and the *edge version* of the *Szeged Index* and the *PI Index* [4,8] of G is defined as

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$$PI_v(G) = \sum [n_u(e) + n_v(e)]$$
$$PI_e(G) = \sum [m_u(e) + m_v(e)]$$
$$SZ_v(G) = \sum [n_u(e)n_v(e)]$$
$$SZ_e(G) = \sum [m_u(e)m_v(e)].$$

The structure-descriptor the *Zagreb index* [3,5,6-7], more precisely, the *first Zagreb index* is

$$M_1(G) = \sum d(u)^2$$

and the *second Zagreb index* is

$$M_2(G) = \sum d(u).d(v)$$

where $(u, v) \in E(G)$. Generally, let G be a graph and H its a subgraph. The *Smarandache-Zagreb index of G relative to H* is defined by

$$M^S(G) = \sum_{u \in V(H)} d^2(u) + \sum_{(u,v) \in E(G \setminus H)} d(u)d(v).$$

Particularly, if $H = G$ or $H = \emptyset$, we get the first or second Zagreb index $M_1(G)$ and $M_2(G)$, respectively.

The outline of the paper is as follows: Introduction and terminologies are described in the first section. In forthcoming section, we concentrate our efforts on initiate a systematic study on the vertex version and the edge version of the *Szeged index* and the *PI index* and obtained some bounds for these indices in terms of the *Second Zagreb index*. For other undefined notations and terminology from graph theory, the readers are referred to J.A. Bondy and et al [1].

§2. Relations of the Szeged Index and PI Index in Terms of Second Zagreb Index

In this section, we derived the relations connecting the Zagreb index on Compliment Graph of various graph operators with respect to the ladder graph, complete graph and wheel graph.

Theorem 2.1 *For a simple graph G with the first and the second Zagreb indices $M_1(G)$ and $M_2(G)$ respectively, then, $M_2(G) \leq \frac{1}{2}\sqrt{M_1(G)}$.*

Proof For an edge $(u, v) \in E(G)$,

$$[d(u) + d(v)]^2 \geq 4d(u)d(v)Rightarrow \sum [d(u) + d(v)]^2 \geq 4 \sum d(u)d(v)].$$

Summing up similar inequalities of all the edges $e \in E(G)$ then,

$$4 \sum d(u)d(v) \leq \sum [(d(u))^2]^{\frac{1}{2}} + \sum [(d(v))^2]^{\frac{1}{2}}$$
$$\Rightarrow 4M_2(G) \leq 2\sqrt{M_1(G)} \Rightarrow M_2(G) \leq \frac{1}{2}\sqrt{M_1(G)}.$$

This completes the proof. □

Remark The equality holds in the above relation only for the regular graph.

Theorem 2.2 *For a simple graph G with e edges and n vertices then,*

$$M_2(G) \leq SZ_v \leq en^2 + M_2(G)(1-n).$$

Proof For an edge $e = (u, v)\epsilon E(G)$, $n_u(e) \geq d(v)$ and $n_v(e) \geq d(v)$. Hence,

$$\begin{aligned} &\Rightarrow d(u)d(v) \leq n_u(e)n_v(e) \\ &\Rightarrow \sum d(u)d(v) \leq \sum n_u(e)n_v(e) \\ &\Rightarrow M_2(G) \leq SZ_v(G). \end{aligned} \tag{2.1}$$

Also $n_u(e) \leq n - d(v)$ and $n_v(e) \leq n - d(u)$. From these

$$\begin{aligned} &n_u(e)n_v(e) \leq n^2 - n[d(u) + d(v)] + d(u)d(v) \\ &\Rightarrow \sum [n_u(e)n_v(e)] \leq en^2 - n[d(u)d(v)] + d(u)d(v) \\ &\Rightarrow SZ_v(G) \leq en^2 + M_2(G)(1-n). \end{aligned} \tag{2.2}$$

From equations (2.1) and (2.2),

$$M_2(G) \leq SZ_v(G) \leq en^2 + M_2(G)(1-n). \qquad \square$$

Theorem 2.3 *For a simple graph G with the vertex version of the PI index $PI_v(G)$ then,*

$$PI_v(G) \leq 2ne - M_2(G).$$

Proof We have

$$\begin{aligned} &[n_u(e) + n_v(e)] \leq 2n - [d(u) + d(v) \\ &\Rightarrow \sum [n_u(e) + n_v(e)] \leq 2ne - \sum [d(u)d(v)] \\ &\Rightarrow PI_v(G) \leq 2ne - M_2(G). \qquad \square \end{aligned}$$

Theorem 2.4 *For a simple graph G with the edge version of the szeged index $SZ_e(G)$ then,*

$$SZ_e(G) \geq M_2(G).$$

Proof For any edge $e = (u, v) \in E(G)$, $m_u(e) \geq d(u) - 1$ and $m_v(e) \geq d(v) - 1$. Hence,

$$\begin{aligned} &m_u(e)m_v(e) \geq [d(u) - 1][d(v) - 1] \\ &\Rightarrow m_u(e)m_v(e) \geq d(u)d(v) - [d(u) + d(v)] + 1 \\ &\Rightarrow \sum [m_u(e)m_v(e)] \geq \sum [d(u)d(v)] - \sum [d(u) + d(v)] + e \\ &\text{(where e is the number of edges)} \\ &\Rightarrow SZ_e(G) \geq M_2(G). \qquad \square \end{aligned}$$

Theorem 2.5 *For a graph G with the vertex version and the edge version of the PI index as $PI_v(G)$ and $PI_e(G)$ respectively, then*

$$PI_v(G) \geq PI_e(G) + 2e.$$

Proof For an edge $e = (u, v) \in E(G)$,

$$n_u(e) \geq m_u(e) + 1 \tag{2.3}$$

and

$$n_v(e) \geq m_v(e) + 1 \tag{2.4}$$

Hence,

$$\begin{aligned}
&(n_u(e) + n_v(e)) \geq (m_u(e) + m_v(e)) + 2 \\
&\Rightarrow \sum(n_u(e) + n_v(e)) \geq \sum(m_u(e) + m_v(e)) + 2e \\
&\Rightarrow PI_v(G) \geq PI_e(G) + 2e. \qquad \square
\end{aligned}$$

Theorem 2.6 *For a simple graph G then,*

$$SZ_v(G) \geq SZ_e(G) + PI_e(G) + e.$$

Proof From equations 2.3 and 2.4, we have,

$$n_u(e)n_v(e) \geq m_u(e)m_v(e) + [m_u(e) + m_v(e)] + 1.$$

Whence,

$$\begin{aligned}
&\sum[n_u(e)n_v(e)] \geq \sum[m_u(e)m_v(e)] + \sum[m_u(e) + m_v(e)] + e \\
&\Rightarrow SZ_v(G) \geq SZ_e(G) + PI_e(G) + e. \qquad \square
\end{aligned}$$

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