MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **67** (2012) 495-504

ISSN 0340 - 6253

Some Relations Between the Second GA Index, $(Sz)_{-1}$-Index, and $(Sz)_{-1/2}$-Index of Graphs

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(Received June 24, 2011)

Abstract

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The second GA and $(Sz)_\lambda$ indices a graph G are defined as

$$GA_2(G) = \sum_{e=uv\in E(G)} \frac{2\sqrt{n_u(e)n_v(e)}}{n_u(e)+n_v(e)},\ Sz_\lambda(G) = Sz_\lambda = \sum_{e=uv\in E(G)} \left[n_u(e)n_v(e)\right]^\lambda,$$

where $n_u(e)$ is the number of vertices closer to u than v and $n_v(e)$ is the number of vertices closer to v than u. In this paper, some relations between the second GA index, $(Sz)_{-1}$ and $(Sz)_{-1/2}$ of G are studied.

1. Introduction

Let G = (V, E) be a simple molecular graph. The vertex and edge-sets of G are represented by $V(G)$ and $E(G)$, respectively. In such a graph, vertices represent atoms and edges represent bonds, see [1]. The graph G is said to be connected if for every two vertices x and y in $V(G)$ there exists a path connecting them. We denote complete, star, wheel, path and cycle graphs on n vertices by K_n, S_n, W_n, P_n, and C_n, respectively. The distance $d(u,v)$ between vertices u and v of a connected graph G is the number of edges in a minimum path from u to v.

A topological index is a real number related to a molecular graph, which is a graph invariant and which has some chemical application. There are several topological indices already defined. The Wiener index (W) is the first topological

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index that was introduced in 1947 by Harold Wiener, see for details [2]. It is defined as the sum of distances between all pairs of vertices in the graph under consideration.

The Szeged index (Sz) is another topological index which was introduced by Ivan Gutman. In order to define the Szeged index of a graph G, we assume that $e = uv$ is an edge connecting the vertices u and v. Suppose $n_u(e)$ is the number of vertices of G lying closer to u and $n_v(e)$ is the number of vertices of G lying closer to v. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e=uv\in E(G)}[n_u(e)n_v(e)]$, see [3-13] for details. Notice that vertices equidistance from u and v are not taken into account.

The second type of geometric-arithmetic and vertex PI indices of the graph G are denoted by GA_2 and PI_v, respectively. These are defined as

$$GA_2(G) = \sum_{e=uv\in E(G)} \frac{2\sqrt{n_u(e)n_v(e)}}{n_u(e)+n_v(e)} \quad \text{and} \quad PI_v(G) = \sum_{e=uv\in E(G)}[n_u(e)+n_v(e)],$$

see [14-17] for more details.

Gutman and his co-authors introduced the "modified Szeged index", $Sz_\lambda(G)$,

:

$$Sz_\lambda(G) = Sz_\lambda = \sum_{e=uv\in E(G)}[n_u(e)n_v(e)]^\lambda .$$

If $\lambda=1$ then $(Sz)_\lambda = Sz(G)$ [18-20].

In this paper, some relations between the indices GA_2, $(Sz)_{-1}$, and $(Sz)_{-1/2}$ are distinguished.

At first, we present a classic a theorem that will be used in the next section.

Theorem A. [Pólya-Szegő Inequality] Suppose a_i and b_i for i=1, 2,…,n are positive sequences of real numbers. Then

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 \le \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{i=1}^{n} a_i b_i\right)^2,$$

where M_1, M_2 and m_1, m_2 are maximum and minimum a_i's and b_i's, respectively [21].

1. Main Results

In this section, at first we compute, $Sz_{-1/2}$ for some well-known graphs, including complete graphs, stars, wheels, paths and cycles. Then some upper and lower bound for $Sz_{-1/2}$ are presented. Finally some relationships between GA_2, $Sz_{-1/2}$, PI_v, and Szeged index of any graph are proved.

Examples.

1. Sz$_{-1/2}$ $(K_n)=n(n-1)/2$,
2. Sz$_{-1/2}$ $(S_n) = \sqrt{n-1}$,
3. Sz$_{-1/2}$ $(W_n) = \begin{cases} \frac{n-1}{\sqrt{n-3}}+2 & \text{if } n \text{ is odd} \\ \frac{n-1}{\sqrt{n-3}}+\frac{2(n-1)}{n-2} & \text{if } n \text{ is even} \end{cases}$,
4. Sz$_{-1/2}$ $(P_n)= \sum_{i=1}^{n-1}\frac{1}{\sqrt{i(n-i)}}$,
5. Sz$_{-1/2}$ $(C_n)= \begin{cases} 2 & \text{if } n \text{ is even} \\ \frac{2}{n-1} & \text{if } n \text{ is odd} \end{cases}$,
6. Sz$_{-1/2}$ $(Q_n) =n$,
7. Sz$_{-1/2}$ $(K_{m,n}) =\sqrt{mn}$.

In graph theory, an edge contraction is an operation which removes an edge from a graph while simultaneously merging together the two vertices it previously connected. Edge contraction is a fundamental operation in the theory of graph minors. Vertex identification is a less restrictive form of this operation. This operation for graph G by removing the edge e, is denoted by G/e. We use this concept for proving the following lemma.

Lemma 1. Let T be a tree on n vertices and l_i be the number of edges $e=uv$, such that $\frac{1}{\sqrt{n_u(e)n_v(e)}}=\frac{1}{\sqrt{i(n-i)}}$ for $1\le i\le k=\left[\frac{n}{2}\right]$. Then, $l_1+l_2+\cdots+l_i\ge 2i$ for $1\le i\le k-1$ and $l_1+l_2+\cdots+l_k=n-1$.

Proof. By induction on the number of edges. Suppose the statement holds for all trees with n-1 edges and T is a tree with n edges. Let k_1 be the largest positive integer such that

$1\le k_1\le k$, $l_{k_1}>0$ and $l_{k_1+1}=l_{k_2}=\cdots=l_k=0$. Now we choose an edge e=uv such that $\frac{1}{\sqrt{n_u(e)n_v(e)}}=\frac{1}{\sqrt{k_1(n+1-k_1)}}$ and set $T'=T/e$. It is clear that T' is a tree with $n-1$ edges. Let l'_j be the number of edges $e'=u'v'\in E(T')$, such that

$\frac{1}{\sqrt{n_{u'}(e')n_{v'}(e')}} = \frac{1}{\sqrt{j(n-j)}}$ for $1 \le j \le k_1$. Obviously, $l'_j = l_j$ for $1 \le j \le k_1 - 1$ and $l'_{k_1} = l_k - 1$. Now by the inductive hypothesis, $l'_1 + l'_2 + \cdots + l'_i \ge 2i$ for $1 \le i \le k_1 - 1$ and $l'_1 + l'_2 + \cdots + l'_{k_1} = n - 1$. Hence $l_1 + l_2 + \cdots + l_i = l'_1 + l'_2 + \cdots + l'_i \ge 2i$ for $1 \le i \le k_1 - 1$ and since $n - 1 = l'_1 + l'_2 + \cdots + l'_{k_1} = l_1 + l_2 + \cdots + l_k - 1$, so $l_1 + l_2 + \cdots + l_k = n$.

Theorem 2. Let T be a tree on n vertices. Then $\mathrm{Sz}_{-1/2}(P_n) \le \mathrm{Sz}_{-1/2}(T) \le \mathrm{Sz}_{-1/2}(S_n)$, with left (right) equality if and only if $T = P_n$ ($T = S_n$).

Proof. We assume that l_i is the number of edges $e=uv$ of T, such that $\frac{1}{\sqrt{n_u(e)n_v(e)}} = \frac{1}{\sqrt{i(n-i)}}$ for $1 \le i \le k = \left[\frac{n}{2}\right]$. By using Lemma 1, $l_1 + l_2 + \cdots + l_i \ge 2i$ for $1 \le i \le k - 1$ and $l_1 + l_2 + \cdots + l_k = n - 1$. Let n be even number, then

$$\mathrm{Sz}_{-1/2}(P_n) = \sum_{e=uv} \frac{1}{\sqrt{n_u(e)n_v(e)}}$$
$$= 2\frac{1}{\sqrt{1(n-1)}} + 2\frac{1}{\sqrt{2(n-2)}} + \cdots + 2\frac{1}{\sqrt{(\frac{n}{2}-1)(n-\frac{n}{2}+1)}} + \frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}}$$

and

$$\mathrm{Sz}_{-1/2}(T) = \sum_{e=uv} \frac{1}{\sqrt{n_u(e)n_v(e)}}$$
$$= l_1\frac{1}{\sqrt{1(n-1)}} + l_2\frac{1}{\sqrt{2(n-2)}} + \cdots + l_{\frac{n}{2}}\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}}.$$

It is enough to prove that

$$(l_1 - 2)\frac{1}{\sqrt{1(n-1)}} + (l_2 - 2)\frac{1}{\sqrt{2(n-2)}} + \cdots + (l_{\frac{n}{2}} - 1)\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}} \ge 0.$$

$$A = (l_1 - 2)\frac{1}{\sqrt{1(n-1)}} + (l_2 - 2)\frac{1}{\sqrt{2(n-2)}} + \cdots + (l_{\frac{n}{2}} - 1)\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}}$$
$$\geq (l_1 - 2)\frac{1}{\sqrt{2(n-2)}} + (l_2 - 2)\frac{1}{\sqrt{2(n-2)}} + \cdots + (l_{\frac{n}{2}} - 1)\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}}$$
$$= (l_1 + l_2 - 4)\frac{1}{\sqrt{2(n-2)}} + (l_3 - 2)\frac{1}{\sqrt{3(n-3)}} + \ldots + (l_{\frac{n}{2}} - 1)\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}}$$
$$\geq (l_1 + l_2 - 4)\frac{1}{\sqrt{3(n-3)}} + (l_3 - 2)\frac{1}{\sqrt{3(n-3)}} + \ldots + (l_{\frac{n}{2}} - 1)\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}}$$
$$= (l_1 + l_2 + l_3 - 6)\frac{1}{\sqrt{3(n-3)}} + (l_4 - 2)\frac{1}{\sqrt{4(n-4)}} + \ldots + (l_{\frac{n}{2}} - 1)\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}}$$
$$\geq \ldots \geq (l_1 + l_2 + \ldots. + l_{\frac{n}{2}-1} - 2(\tfrac{n}{2}-1))\frac{1}{\sqrt{(\frac{n}{2}-1)(n-(\frac{n}{2}-1))}} + (l_{\frac{n}{2}} - 1)\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}}$$
$$\geq (l_1 + l_2 + \ldots. + l_{\frac{n}{2}-1} - 2(\tfrac{n}{2}-1))\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}} + (l_{\frac{n}{2}} - 1)\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}}$$
$$= (l_1 + l_2 + \ldots. + l_{\frac{n}{2}-1} + l_{\frac{n}{2}} - n + 1)\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}}$$
$$= (n - 1 - n + 1)\frac{1}{\sqrt{\frac{n}{2}(n-\frac{n}{2})}} = 0$$

By the similar argument we can prove the left inequality, when n is odd. For right inequality, it is easy to see that, for each $e = uv \in E(S_n)$, $n_u(e) = 1$ and $n_v(e) = n-1$.

Therefore $\frac{1}{\sqrt{n_u(e)n_v(e)}} = \frac{1}{\sqrt{n-1}}$, so $\mathrm{Sz}_{-1/2}(T) \leq \mathrm{Sz}_{-1/2}(S_n)$. □

Theorem 3. $GA_2(G) \geq \frac{2m^2}{n}\frac{1}{\mathrm{Sz}_{-1/2}(G)}$ with equality if and only if the graph G is bipartite.

Proof. By the Cuachy inequality,

$$GA_2(G) \geq \frac{m^2}{\sum_{e=uv}\frac{\frac{1}{2}(n_u(e)+n_v(e))}{\sqrt{n_u(e)n_v(e)}}} \geq \frac{m^2}{\frac{n}{2}\sum_{e=uv}\frac{1}{\sqrt{n_u(e)n_v(e)}}} = \frac{2m^2}{n}\frac{1}{\mathrm{Sz}_{-1/2}(G)}.$$ □

Lemma 4. Let $a_1, a_2, ..., a_m$ be real numbers, such that $1 \leq a_1 \leq a_2 \leq \ldots \leq a_m$. Then

$$m^2 a_m \geq (a_1 + a_2 + \ldots + a_m)(\frac{1}{a_1} + \frac{1}{a_2} + \ldots + \frac{1}{a_m}) \geq \frac{m(m+1)}{2}.$$

Proof. The left side inequality is clear. For right side inequality, we have

$$(a_1+...+a_m)(\frac{1}{a_1}+...+\frac{1}{a_m}) = a_1(\frac{1}{a_1}+...+\frac{1}{a_m})+...+a_m(\frac{1}{a_1}+...+\frac{1}{a_m})$$

$$\geq a_1(\frac{1}{a_1})+a_2(\frac{1}{a_1}+\frac{1}{a_2})+...+a_m(\frac{1}{a_1}+\frac{1}{a_2}+...+\frac{1}{a_m})$$

$$\geq 1+2+....+m=\frac{m(m+1)}{2}.$$ □

Theorem 5.

$$\frac{m(m+1)}{2} \leq \sum_{e=uv} \frac{\frac{1}{2}\left(n_u(e)+n_v(e)\right)}{\sqrt{n_u(e)n_v(e)}} GA_2(G) \leq m^2 \max\{\frac{\frac{1}{2}\left(n_u(e)+n_v(e)\right)}{\sqrt{n_u(e)n_v(e)}} | e=uv\} \leq m^2\frac{n}{2}.$$

Proof. By using Lemma 5, the proof is straightforward. □

Theorem 6. For any connected graph G,

$$\max\{\frac{m^2}{GA_2(G)}, 2m-GA_2(G)\} \leq \sum_{e=uv} \frac{\frac{1}{2}\left(n_u(e)+n_v(e)\right)}{\sqrt{n_u(e)n_v(e)}} \leq \frac{1}{2}|V(G)|\mathrm{Sz}_{-1/2}(G).$$

Proof. By Lemma 4, we conclude that

$$\left(\sum_{e=uv} \frac{\sqrt{n_u(e)n_v(e)}}{\frac{1}{2}\left(n_u(e)+n_v(e)\right)}\right)\left(\sum_{e=uv} \frac{\frac{1}{2}\left(n_u(e)+n_v(e)\right)}{\sqrt{n_u(e)n_v(e)}}\right) \geq m^2,$$

$$\sum_{e=uv} \frac{\sqrt{n_u(e)n_v(e)}}{\frac{1}{2}\left(n_u(e)+n_v(e)\right)} \sum_{e=uv} \frac{\frac{1}{2}\left(n_u(e)+n_v(e)\right)}{\sqrt{n_u(e)n_v(e)}} \geq 2m.$$

Then

$$\max\{\frac{m^2}{GA_2(G)}, 2m-GA_2(G)\} \leq \sum_{e=uv} \frac{\frac{1}{2}\left(n_u(e)+n_v(e)\right)}{\sqrt{n_u(e)n_v(e)}} \leq \frac{1}{2}|V(G)|\mathrm{Sz}_{-1/2}(G).$$ □

Theorem 7. $\mathrm{Sz}_{-1/2}(G) \geq \dfrac{2m^2}{PI_v}$, with equality if and only if G is the complete graph.

Proof . By the geometric-arithmetic inequality, $\sqrt{n_u(e)n_v(e)} \leq \dfrac{n_u(e)+n_v(e)}{2}$,

implying that $\dfrac{1}{\sqrt{n_u(e)n_v(e)}} \geq \dfrac{2}{n_u(e)+n_v(e)}$ with equality if and only if $n_u(e)=n_v(e)$.

By the Cauchy-Schwartz inequality,

$$\sum_{e=uv\in E(G)} \frac{2}{n_u(e)+n_v(e)} PI_v \geq 2m^2,$$

with equality if and only if $n_u(e)=n_v(e)=1$. Thus

$$\sum_{e=uv\in E(G)} \frac{2}{n_u(e)+n_v(e)} \geq \frac{2m^2}{PI_v}$$

with equality if and only if $n_u(e)=n_v(e)=1$. This proves the theorem. □

Theorem 8. $\frac{2\sqrt{m(n-1)}}{n}\sqrt{Sz_{-1}} \leq \mathrm{Sz}_{-1/2}(G) \leq \sqrt{mSz_{-1}(G)}$ with equality in right side if and only if G is K_n **.**

Proof. Suppose a_{uv}=1 and b_{uv}= $\frac{1}{\sqrt{n_u(e)n_v(e)}}$ then by the Pólya-Szegő inequality:

$$\sum_{e=uv} 1^2 \sum_{e=uv} (\frac{1}{\sqrt{n_u(e)n_v(e)}})^2 \leq \frac{1}{4}\left(\sqrt{\frac{1\times(n-1)}{1\times 1}}+\sqrt{\frac{1\times 1}{1\times(n-1)}}\right)^2 \left(\sum_{e=uv} 1\times(\frac{1}{\sqrt{n_u(e)n_v(e)}})\right)^2.$$

Therefore

$$m\sum_{e=uv} \frac{1}{n_u(e)n_v(e)} \leq \frac{1}{4}\left(\sqrt{\frac{1\times(n-1)}{1\times 1}}+\sqrt{\frac{1\times 1}{1\times(n-1)}}\right)^2 \mathrm{Sz}_{-1/2}{}^2.$$

By calculation, $\frac{2\sqrt{m}}{\sqrt{n-1}+\frac{1}{\sqrt{n-1}}}\sqrt{Sz_{-1}} \leq \mathrm{Sz}_{-1/2}(G)$. For the right hand of inequality, by definition and Cauchy-Schwarz inequality we have:

$$\begin{aligned}\mathrm{Sz}_{-1/2}(G) &= \sum_{e=uv} \frac{1}{\sqrt{n_u(e)n_v(e)}}\\ &= \sum_{e=uv} 1\times\frac{1}{\sqrt{n_u(e)n_v(e)}}\\ &\leq \sqrt{\sum \frac{m}{n_u(e)n_v(e)}}\\ &= \sqrt{mSz_{-1}(G)},\end{aligned}$$

with equality if and only if $n_u(e)n_v(e)$=1. Thus equality holds if and only if $n_u(e)=n_v(e)=1$**,** so G is a complete graph.
□

Theorem 9. Suppose G is a connected graph, then

$$\mathrm{Sz}_{-1/2}(G) \leq \left\lceil \frac{m-1}{2} \right\rceil + \sqrt{\left\lceil \frac{m-1}{2} \right\rceil^2 + Sz_{-1}(G)}$$

with equality if and only if G be K_n.

Proof . By definition,

$$[\mathrm{Sz}_{-1/2}(G)]^2 = \sum_{uv\in E}\frac{1}{n_u(e)n_v(e)} + 2\sum_{uv\neq xy}\frac{1}{\sqrt{n_u(e)n_v(e)}}.\frac{1}{\sqrt{n_x(e)n_y(e)}}$$

$$\leq Sz_{-1}(G) + 2\left\lceil\frac{m-1}{2}\right\rceil.\mathrm{Sz}_{-1/2}(G).$$

Thus

$$\left(\mathrm{Sz}_{-1/2}(G) - \left\lceil\frac{m-1}{2}\right\rceil\right)^2 \leq \left\lceil\frac{m-1}{2}\right\rceil^2 + Sz_{-1}(G).$$

Therefore $\mathrm{Sz}_{-1/2}(G) \leq \left\lceil\frac{m-1}{2}\right\rceil + \sqrt{\left\lceil\frac{m-1}{2}\right\rceil^2 + Sz_{-1}(G)}$ and equality holds if and only if G be K_n. □

Theorem 10. The following inequality is hold for a connected graph *G,*

$$\mathrm{Sz}_{-1/2}(G) \geq \sqrt{Sz_{-1}(G) + \frac{4m(m-1}{n^2}}.$$

Proof. By Theorem 8, $[\mathrm{Sz}_{-1/2}(G)]^2 = \sum_{uv\in E}\frac{1}{n_u(e)n_v(e)} + 2\sum_{uv\neq xy}\frac{1}{\sqrt{n_u(e)n_v(e)}}.\frac{1}{\sqrt{n_x(e)n_y(e)}}$

$$\geq \sum_{uv\in E}\frac{1}{n_u(e)n_v(e)} + 2\sum_{uv\neq xy}\frac{2}{n}.\frac{2}{n}$$

$$= Sz_{-1}(G) + 2(\frac{4}{n^2})(\frac{m(m-1)}{2})$$

$$= Sz_{-1}(G) + \frac{4m(m-1)}{n^2}.$$

Therefore $\mathrm{Sz}_{-1/2}(G) \geq \sqrt{Sz_{-1}(G) + \frac{4m(m-1)}{n^2}}$. □

Theorem 11. $GA_2(G)+Sz_{-1/2}(G)+PI_v(G) \geq 3m\sqrt[3]{2}$ with equality if and only if $G=K_n$.

Proof. By an easy calculation, we have

$$\prod_{e=uv}\frac{2\sqrt{n_u(e)n_v(e)}}{n_u(e)+n_v(e)}\frac{1}{\sqrt{n_u(e)n_v(e)}}(n_u(e)+n_v(e)) = 2^m.$$

Thus,

$$\sum_{e=uv} \frac{2\sqrt{n_u(e)n_v(e)}}{n_u(e)+n_v(e)} + \frac{1}{\sqrt{n_u(e)n_v(e)}} + (n_u(e)+n_v(e)) \geq 3m\sqrt[3m]{2^m} \ ,$$

with equality if and only if $n_u(e) = n_v(e) = 1$. Therefore $GA_2(G)+Sz_{-1/2}(G)+PI_v(G) \geq 3m\sqrt[3]{2}$ with equality if and only if $G=K_n$. □

Theorem 12. If G is a bipartite graph then $nGA_2(G)+2Sz_{-1/2}(G) \geq 4m$ with equality if and only if $G = K_2$.

Proof. We have

$$\prod_{e=uv} \sqrt{n_u(e)n_v(e)} \frac{1}{\sqrt{n_u(e)n_v(e)}} = 1 .$$

By a similar argument as above $\sum_{e=uv} \sqrt{n_u(e)n_v(e)} + \frac{1}{\sqrt{n_u(e)n_v(e)}} \geq 2m$ with equality if and only if $n_u(e) = n_v(e) = 1$. We know that $n_u(e) + n_v(e) = n$ for bipartite graphs. Thus $nGA_2(G)+2Sz_{-1/2}(G) \geq 4m$ with equality if and only if $G = K_2$.

□

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