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ON SZEGED INDEX OF STANDARD GRAPHS

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ABSTRACT

A recently introduced graph-invariant is 'Szeged Index' and it has considerable applications in molecular chemistry. In this paper, the Szeged indices of standard graphs are calculated. A modified Szeged index of a graph is also introduced in which all the vertices of the graph are taken into consideration; thereby the variations in these indices of standard graphs are identified.

Keywords: *Wiener number, Szeged index, modified Szeged index.*

1. INTRODUCTION

An important concept of a molecular graph associated with alkanes or more generally of a simple, connected graph is termed as the Wiener number (see [5]). A refined concept of this is coined as Szeged index (see [2]) & [3]). As in the case of Wiener number, no standard formula is available to calculate the Szeged index of a connected graph. In §2, we calculate the Szeged index of standard graphs and in §3, we introduce a modified Szeged index and observe the variations in these indices for the standard graphs.

For the standard notation and results we refer Bondy & Murthy [1].

For ready reference, we give the following:

Definition: 1.1 [2]: G is a connected graph. Then the Wiener number W(G) of G is defined to be 1/2 $\sum_{u,v\in V(G)} d(u,v)$, where V(G) is the vertex set of G and d(u, v) = d_G (u, v) is the shortest distance between the vertices u,v of G.

Observations 1.2 [4]:

a) For the complete graph K_n ($n\geq 2$), $W(K_n) = n\,(n-1)/2$.
b) For the path P_n ($n\geq 2$), $W(P_n) = n\,(n^2 - 1)/6$.
c) For the cycle C_n ($n\geq 3$), $W(C_n) = n\,[n/2]^2$.
d) For the star graph $K_{1,n}$, $W(K_{1,n}) = n^2$ ($n \geq 1$).
e) For the complete bipartite graph $K_{m,n}$ ($m, n \geq 1$), $W(K_{m,n}) = (m^2 + mn+n^2) - (m+n)$.
f) For the wheel $K_1 \vee C_n$($n\geq 3$), $W(K_1 \vee C_n) = n\,(n-1)$.

Throughout this paper, we consider only non-empty, simple, finite and connected graph to avoid trivialities.

2. SZEGED INDEX OF STANDARD GRAPHS

For convenience, we recollect the following:

Definition 2.1 [3]: Let G be a graph (i.e., nonempty, simple, finite and connected graph). Let e = uv be any edge of G. Denote

$N_1(e \mid G) = \{w\in V(G): d(w, u) < d(w, v)\}$ (w is closer to u than v in G),

$N_2(e \mid G) = \{w\in V(G): d(w, v) < d(w, u)\}$(w is closer to v than to u in G);

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and $n_1(e \mid G) = \mid N_1(e \mid G) \mid$, $n_2(e \mid G) = \mid N_2(e \mid G)$. ($\mid \mid$ denotes the cardinality function).

The Szeged index of G, denoted by Sz(G) (in the earlier works denoted by $W^*(G)$), is defined as

$\sum_{e \in E(G)} n_1(e \mid G) \cdot n_2(e \mid G)$ (E (G) being the edge set of G).

Theorem 2.2: For the path P_n ($n \geq 2$)

$$Sz(P_n) = \frac{n(n^2-1)}{6} \ (= W(P_n)).$$

Proof: Let n be any integer ≥ 2 and $V(P_n) = \{v_1, v_2, ..., v_n\}$.

Any edge of P_n is of the form v_iv_{i+1}, i being any positive integer, $\leq n-1$. Now

$N_1(v_i v_{i+1} \mid P_n) = \{w \in V(P_n) : d(w, v_i) < d(w, v_{i+1})\} = \{v_1, ..., v_i\}$

And

$N_2(v_i v_{i+1} \mid P_n) = \{w \in V(P_n) : d(w, v_{i+1}) < d(w, v_i)\} = \{v_{i+1}, ..., v_n\}$

$\Rightarrow n_1(v_i v_{i+1} \mid P_n) = \mid \{v_1, ..., v_i\} \mid = i$ and $n_2(v_i v_{i+1} \mid P_n) = \mid \{ v_{i+1}, ..., v_n\} \mid = n-i$.

This is true for all the (n-1) edges v_iv_{i+1} of P_n. So

$$Sz(P_n) = \sum_{i=1}^{n-1} n_1(v_i v_{i+1} \mid P_n) \cdot n_2(v_i v_{i+1} \mid P_n) = \sum_{i=1}^{n-1} i(n-i) = \frac{n(n^2-1)}{6}.$$

Theorem 2.3: For $n \geq 2$, $Sz(K_n) = \dfrac{n(n-1)}{2}$ $(= W(K_n))$.

Proof: Let $V(K_n) = \{v_1, v_2, ..., v_n\}$. Let e = uv be any edge of K_n. Since

d(u, u) = d(v, v) = 0, d(u, v) = 1 and

$d(w, u) = d(w, v) = 1$ for $w \in V(K_n) \setminus \{u, v\}$, follows that

$N_1(e = uv \mid K_n) = \{w \in V(G): d(w, u) < d(w, v)\} = \{u\}$ and

$N_2(e = uv \mid K_n) = \{w \in V(G): d(w, v) < d(w, u)\} = \{v\}$.

So, $n_1(e \mid K_n) = n_2(e \mid K_n) = 1$. This is true for all the edges e of K_n.

Since any two vertices in K_n are adjacent ($\Rightarrow K_n$ has ${}^nc_2 = \dfrac{n(n-1)}{2}$ edges) follows that

$$S_z(K_n) = = \sum_{e \in E(K_n)} n_1(e \mid K_n) \cdot n_2(e \mid K_n) = \sum_{e \in E(K_n)} 1.1 = \frac{n(n-1)}{2}.$$

Theorem 2.4: For any star $K_{1,n}$ (n being any positive integer),

$Sz(K_{1,n})$ $(= Sz(K_{n,1})) = n^2 = (W(K_{1,n}) = W(K_{n,1}))$.

Proof: Let n = 1. $K_{1,1} = K_2$ and so $Sz(K_{1,1}) = Sz(K_2) = {}^2c_2 = 1^{2.}$

Let n be any integer ≥ 2 and $V(K_{1,n}) = \{u_0, v_1, v_2, \ldots, v_n\}$.

Now $E(K_{1,n}) = \{e_i = u_o v_i : I = 1,2,\ldots,n\}$.So

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$N_1(e_i \mid K_{1,n}) = V(K_{1,n}) \setminus \{v_i\}$ and $N_2(e_i \mid K_{1,n}) = \{v_i\}$

$\Rightarrow n_1(e_i \mid K_{1,n}) = (n+1) - 1 = n$ and $n_2(e_i \mid K_{i,n}) = \{v_i\}$.

This is true for all the n edges e_i of $K_{1,n}$. So

$$S_z(K_{1,n}) = \sum_{e_i \in E(K_{1,n})} n_1(e_i \mid K_{1,n}) \,.\, n_2(e_i \mid K_{1,n}) = \sum_{e_i \in E(K_{1,n})} n(1) = n^2$$

Since the graph $K_{n,1}$ is isomorphic to $K_{1,n}$ it follows that $Sz(K_{n,1}) = Sz(K_{1,n}) = n^2$.

Theorem 2.5: For the complete bipartite graph, $K_{m,n}(m,n \geq 1)$, $Sz(K_{m,n}) = (mn)^2$.

Proof: Case (i): $m = n = 1 \Rightarrow K_{m,n} = K_{1,1} = K_2$.

$S_z(K_{1,1}) = S_z(K_2) = 1 = (1.1)^2$.

Case (ii): Let one of m,n is 1 and the other is ≥ 2.

Without loss of generality, we can assume that m = 1 and so $n \geq 2$. Now

$W(K_{m,n}) = W(K_{1,n}) = n^2 = (1.n)^2$

Case (iii): Let $m, n \geq 2$.

Since $K_{m,n}$ is bipartite we can write $V(K_{m,n}) = V_1 \cup V_2$ where

$V_1 = \{u_i : i = 1,\ldots,m\}$ and $V_2 = \{v_j : j = 1,2,\ldots,n\}$

and $E(K_{m,n}) = \{e_{i,j} = u_i v_j : i = 1,2,\ldots.m,\ j = 1,2,\ldots,n\}$.

Since $d(u_i, u_{i'}) = \begin{cases} 0 & if \;\; i' = i \\ 2 & if \;\; i' \neq i \end{cases}$

and

$$d(v_j, v_{j'}) = \begin{cases} 0 & if \;\; j' = j \\ 2 & if \;\; j' \neq j \end{cases}$$

follows that

$N_1(e_{i,j} \mid K_{m,n}) = \{u_i\} \cup (V_2 \setminus \{v_j\})$ and $N_2(e_{i,j} \mid K_{m,n}) = \{v_j\} \cup (V_1 \setminus \{u_i\})$

$\Rightarrow n_1(e_{i,j} \mid K_{m,n}) = 1 + (n-1) = n$, $n_2(e_{i,j} \mid K_{m,n}) = 1 + (m-1) = m$.

This is true for all the mn edges $e_{i,j}$ of $K_{m,n}$.

$$\therefore\ Sz(K_{m,n}) = \sum_{e_{i,j} \in E(K_{m,n})} n_1\left(e_{i,j} \middle| K_{m,n}\right) .\, n_2\left(e_{i,j} \middle| K_{m,n}\right) = \sum_{e_{i,j} \in E(K_{m,n})} n.m = nm \;\left| E\left(K_{m,n}\right) \right| = (mn)^2$$

(observe that $Sz_{m,n} > W(K_{m,n})$ where $m, n \geq 2$).

Theorem 2.6: For any integer $n \geq 2$,

a) $Sz(C_{2n}) = 2n^3 = 2n(n^2)$ and
b) $Sz(C_{2n-1}) = (2n-1)(n-1)^2$

i.e. $Sz(C_k) = k\,[k/2]^2$ for any integer $k \geq 3$.

Proof: Let n be any integer ≥ 2.

Case (i): Let $V(C_{2n}) = \{v_1,v_2,\ldots,v_{2n}\}$.

Any edge of C_{2n} is of the form v_iv_{i+1} for i = 1, 2,…, 2n with the convention $v_{2n+1} = v_1$.

Now $N_1(v_1v_2 \mid C_{2n}) = \{v_1,v_2,\ldots,v_{2n-(n-2)} = v_{n+2}\}$ and $N_2(v_1v_2 \mid C_{2n}) = \{v_2,v_3,\ldots,v_{n+1}\}$.

For $2 \le i < n$
$N_1(v_iv_{i+1} \mid C_{2n}) = \{v_i,v_{i+1},\ldots,v_1,v_{2n},\ldots,v_{2n-(n-i-1)}\}$ and $N_2(v_iv_{i+1} \mid C_{2n}) = \{v_{i+1},\ldots,v_{i+1}\}$.

For i = n
$N_1(v_iv_{n+1} \mid C_{2n}) = \{v_i, v_{i+1}, \ldots, v_{i+(n-1)}\}$ and $N_2(v_iv_{n+1} \mid C_{2n}) = \{v_{i+n}, v_{i+n+1}, \ldots, v_{2n}, v_1, \ldots, v_{i-1}\}$

For n < i < 2n,
$N_1(v_iv_{i+1} \mid C_{2n}) = \{v_i,v_{i-1},\ldots,v_{i-n+1}\}$ and $N_2(v_iv_{i+1} \mid C_{2n}) = \{v_{i+1},v_{i+2},\ldots,v_{2n},v_1,\ldots,v_{i-n}\}$.

For i = 2n,
$N_1(v_{2n}v_1 \mid C_{2n}) = \{v_{2n},v_{2n-1},\ldots,v_{2n-(n-1)} = v_{n+1}\}$ and $N_2(v_{2n}v_1 \mid C_{2n}) = \{v_1,v_2,\ldots,v_n\}$.

So follows that
$n_1(v_iv_{i+1} \mid C_{2n}) = n = n_2(v_iv_{i+1} \mid C_{2n})$ for i = 1, ..., 2n.

Hence $Sz\,(C_{2n}) = \sum_{i=1}^{2n} n_1(v_iv_{i+1} \mid C_{2n}).\, n_2(v_iv_{i+1} \mid C_{2n}) = \sum_{i=1}^{2n} (n)\,(n)$

$$= 2n^3 = 2n\,(n^2) = 2n\,[(\frac{2n}{2})]^2.$$

Case (ii). Let $V(C_{2n-1}) = \{v_1, v_2, \ldots, v_{2n-1}\}$

Any edge of C_{2n-1} is of the form v_iv_{i+1}, for i = 1, 2, ..., 2n-1 with the convention $v_{2n} = v_1$.

Now
$N_1(v_1v_2 \mid C_{2n-1}) = \{v_1,v_{2n-1},\ldots,v_{2n-(n-2)} = v_{n+2}\}$ and $N_2(v_1v_2 \mid C_{2n-1}) = \{v_2,v_3,\ldots,v_n\}$.

For $2 \le i < n-1$
$N_1(v_iv_{i+1} \mid C_{2n-1}) = \{v_i,v_{i-1},\ldots,v_1,v_{2n-1},\ldots,v_{2n-(n-i-1)} = v_{n+i+1}\}$ and $N_2(v_iv_{i+1} \mid C_{2n-1}) = \{v_{i+1},\ldots,v_{i+n-1}\}$.

For i = n-1
$N_1(v_{n-1}v_n \mid C_{2n-1}) = \{v_{n-1},\ldots,v_1\}$ and $N_2(v_{n-1}v_n \mid C_{2n-1}) = \{v_n, v_{n+1}, v_{n+2},\ldots,v_{2n-2}\}$.

For i = n
$N_1(v_nv_{n+1} \mid C_{2n-1}) = \{v_n, v_{n-1},\ldots,v_2\}$ and $N_2(v_nv_{n+1} \mid C_{2n-1}) = \{v_{n+1}, v_{n+2},\ldots, v_{n+(n-1)} = v_{2n-1}\}$.

For $n+1 \le i \le 2n-1$
$N_1(v_iv_{i+1} \mid C_{2n-1}) = \{v_i, v_{i-1},\ldots,v_{i-(n-2)}\}$ and $N_2(v_iv_{i+1} \mid C_{2n-1}) = \{v_{i+1},\ldots, v_{2n-1}, v_2, \ldots, v_{i-n}\}$.

Finally, for i = 2n-1
$N_1(v_{2n-1}v_1 \mid C_{2n-1}) = \{v_{2n-1}, v_{2n-2},\ldots,v_{2n-(n-1)} = v_{n+1}\}$ and $N_2(v_{2n-1}v_1 \mid C_{2n-1}) = \{v_1, v_2,\ldots, v_{n-1}\}$.

So follows that

$N_1(v_iv_{i+1} \mid C_{2n-1}) = n - 1 = N_2(v_iv_{i+1} \mid C_{2n-1})$ for i = 1, 2, ..., 2n-1.

$\therefore\ Sz\,(C_{2n-1}) = \sum_{i=1}^{2n-1} (n-1)(n-1) = (2n-1)(n-1)^2 = (2n-1)([\frac{2n-1}{2}])^2.$

This proves the result.

Theorem 2.7: For the wheel $K_1 v\, C_n$ $(n \ge 3)$,

$Sz\,(K_1 \text{ v } C_n) = n\,(n-2 + [\frac{n}{2}]^2)$.

Proof: Let n be any integer ≥ 3 and $V(K_1 \text{ v } C_n) = \{u_0, v_1, v_2, \ldots, v_n\}$.

Now $E(K_1 \text{ v } C_n) = \{u_0v_i : i = 1, \ldots, n\} \bigcup \{v_iv_{i+1} : i = 1, \ldots, n\}$ (with the convention $v_{n+1} = v_1$).

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Denote $e_i = u_0v_i$ and $f_i = u_iv_{i+1}$ (i=1,..., n}.

Now $N_1(e_i \mid K_1 \vee C_n) = V(K_1 \vee C_n) \setminus \{v_{i-1}, v_i, v_{i+1}\}$(with the convention $v_0 = v_n$)

and $N_2(e_i \mid K_1 \vee C_n) = \{v_i\}$.

$\therefore$ $N_1(e_i \mid K_1 \vee C_n) = (n+1) - 3 = (n-2)$ and $N_2(e_i \mid K_1 \vee C_n) = 1$.

So $\sum_{i=1}^{n} n_1(e_i \mid K_1 \vee C_n) \,.\, n_2(e_i \mid K_1 \vee C_n) = \sum_{i=1}^{n} (n-2).1 = n(n-2)$ (i)

Further,

$N_j (f_i \mid K_1 \vee C_n) = N_j(f_i \mid C_n)$ (j = 1, 2) (ii)

(u_0 is ignored since $d(u_0, v_{i-1}) = 1 = d(u_0, v_i)$).

(ii), by virtue of Theorem (2.6) implies that

$$\sum_{i=1}^{n} n_1(f_i \mid K_1 \vee C_n) \,.\, n_2(f_i \mid K_1 \vee C_n) = Sz(C_n) = n[\frac{n}{2}]^2 . \qquad \text{(iii)}$$

Now, from (i) and (iii) follows that $Sz(K_1 \vee C_n) = n(n-2) + n[\frac{n}{2}]^2 = n\{(n-2) + [\frac{n}{2}]^2\}$.

(Observe that for $n \geq 4$, $S_z (K_1 \vee C_n) > W (K_1 \vee C_n)$).

3. MODIFIED SZEGED INDEX OF STANDARD GRAPHS

In the calculation of Szeged Index of $K_n(n \geq 2)$, $K_1 V C_n$ $(n \geq 3)$, the contribution of all the vertices of the connected graph is not there. To avoid this, we propose the following modified index that involves all the vertices.

Definition 3.1: Let G be a graph (i.e., nonempty, simple, finite and connected graphs). Let e = {u, v} be any edge of G. Denote

$N_1^*(e \mid G) = \{w \in V(G) : d(w,u) \leq d(u,v)$, $N_2^*(e \mid G) = \{w \in V(G) : d(w,v) < d(w,u)$;

and

$n_1^*(e \mid G) = \mid N_1^*(e \mid G \mid$, $n_2^*(e \mid G) = \mid N_2^*(e \mid G) \mid$.

The refined Szeged index of G, denoted by $Sz^*(G)$ is defined as,

$$\sum_{e \in E(G)} n_1^*\left(e \mid G\right).n_2^*\left(e \mid G\right)$$

(Another way of defining this modified index is to keep < as it is in $N_1(e \mid G)$ and changing < into $\leq$ in $N_2(e \mid G)$).

Observations 3.2:

a) For the path P_n $(n \geq 2)$, $Sz^* P_n = Sz P_n$.

b) For any star $K_{1,n}$ $(n \geq 1)$, $Sz(K_{1,n}) = Sz^* (K_{1,n})$.

c) For the complete graph $K_{m,n}$ $(m,n \geq 1)$, $Sz^*(K_{m,n}) = Sz(K_{m,n})$.

d) For any interger $n \geq 2$, $Sz^*(C_{2n}) = Sz(C_{2n})$.

Theorem 3.3: For $n \geq 2$, $Sz^*(K_n) = \dfrac{n(n-1)^2}{2}$.

Proof: With the same notation as in Th.2.3,

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$N_1^*(e = uv \mid K_n) = \{w \in V(G): d(w, u) \le d(w, v)\} = \{V(G) \backslash \{v_2\}$ and $N_2^*(e = uv \mid K_n) = \{w \in V(G): d(w, v) \le d(w,u)\} = \{v_2\}$.

So $n_1^*(e \mid K_n) = (n-1)$ and $n_2^*(e \mid K_n) = 1$.

This is true for all the edges e of K_n. Hence

$$Sz^*(K_n) = \sum_{e \in E(Kn)} (n-1).1 = \frac{n(n-1)^2}{2}.$$

Theorem 3.4: For $n \ge 2$, $Sz^*(C_{2n-1}) = n(n-1)(2n-1)$.

Proof: With the same notation as in Th.2.6, for any edge v_iv_{i+1} (i = 1, 2,..., 2n-1) (with the convention $v_{2n} = v_1$), we get that

$n_1^*(v_iv_{i+1} \mid C_{2n-1}) = (n-1) + 1 = n$ and $n_2^*(v_iv_{i+1} \mid C_{2n-1}) = n-1$

(the excluded single vertex, in each case, enters into the set $N_1^*(\ )$ under consideration).

$$\text{So, } Sz^*(C_{2n-1}) = \sum_{i=1}^{2n-1} n(n-1) = n(n-1)(2n-1).$$

Observation 3.5: In the other way of defining the modified index, we get the same $Sz^*(K_n)$, $Sz^*(C_{2n-1})$, since in these cases we get the sums $\sum_{e \in E(Kn)} 1.(n-1)$ and $\sum_{i=1}^{2n-1} (n-1).n$ respectively.

Theorem 3.6: For the wheel $K_1 v\, C_n$ ($n \ge 3$), $Sz(K_1 \vee C_n) = \begin{cases} \dfrac{n^2(n+6)}{4} & (if \quad n \quad is \quad even), \\ \dfrac{n}{4}(n^2+6n-3) & (if \quad n \quad is \quad odd). \end{cases}$

With the same notation as in Th.(2.7),

$N_1^*(e_i \mid (K_1 v\, C_n)) = V(K_1 v\, C_n) \backslash \{v_i\}$ and $N_2^*(e_i \mid (K_1 v\, C_n)) = \{v_i\}$.

So, $n_1^*(e_i \mid (K_1 v\, C_n)) \,.\, n_2^*(e_i \mid (K_1 v\, C_n)) = (n+1-1)(1) = n$ (3.6.1)

Case (i): Suppose n is even $\Rightarrow n \ge 4$.

As in Th.2.6 (case (i)), for each edge f_i (i = 1,...n) with the convention $v_{n+1} = v_1$, we get

$(n_1(f_i) \mid C_n) + 1 = n/2 + 1$ (3.6.2)

(Since u_0 is added in $N_1^*(\ )$)

and
$n_2^*(f_i \mid (K_1 v\, C_n)) = n_2(f_i \mid C_n) = n/2$ (3.6.3)

By (3.6.1), (3.6.2) and (3.6.3)

$$Sz^*(K_1 \text{ v } C_n) = n.n\left(\frac{n}{2} + 1\right)\left(\frac{n}{2}\right) = n^2\,\frac{(n+6)}{4}.$$

Case (ii): Suppose n is odd.

As in Th.2.6 case (i), for each edge f_i we get that

$$n_1^*(f_i \mid (K_1 \text{ v } C_n)) = \frac{(n-1)}{2} + 1 + 1 = \frac{(n+3)}{2} \qquad (3.6.4)$$

and

$n_2^*(f_i \mid (K_1 v\ C_n)) = \dfrac{(n-1)}{2}$ ... (3.6.5)

By (3.6.1), (3.6.4) and (3.6.5), we get

$$Sz^* (K_1 v\ C_n) = n.n + n\frac{(n+3)}{2}\ \frac{(n-1)}{2} = \frac{n}{4}\ (n^2 + 6n - 3).$$

Observation 3.7: In the other way of defining the modified index, we get that $n_1^*(e_i \mid (K_1 v\ C_n) = (n-2)$ and $n_2^*(e_i \mid (K_1 v\ C_n) = 3$ and the other relations remain the same. So, the corresponding index is

$3n\ (n-2) + n(\frac{n}{2} + 1)(\frac{n}{2})$ when n is even and

$3n\ (n-2) + n\dfrac{(n+3)}{2}\ \dfrac{(n-1)}{2}$ when n is odd.

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