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A Relation between the Edge Szeged Index and the Ordinary Szeged Index*

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Abstract. A relation is established between the edge Szeged index and the ordinary Szeged index for unicyclic graphs.

1 Introduction

Topological indices are numerical quantities associated with chemical structures via their hydrogen–depleted graphs, which are used in theoretical chemistry for the design of chemical compounds with given physicochemical properties or given pharmacologic and biological activities. The Wiener index is one of the oldest and the most thoroughly studied topological indices [1–3].

We consider simple graphs. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, let $d_G(u,v)$ be the distance between u and v in G, i.e., the number of edges in a shortest path connecting u and v in G. The Wiener index of G is defined as [3]

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v) \ .$$

For $e \in E(G)$ incident with vertices u and v, we write $e = uv$ or $e = vu$. For $e = uv \in E(G)$, let $n_1(e|G)$ and $n_2(e|G)$ be respectively the number of vertices of G lying

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closer to vertex u than to vertex v and the number of vertices of G lying closer to vertex v than to vertex u. If G is a tree, then $W(G) = \sum_{e \in E(G)} n_1(e|G) n_2(e|G)$ [3].

As a generalization of the above property of the Wiener index for trees, the (ordinary) Szeged index of a connected graph G is defined as [4]

$$Sz(G) = \sum_{e \in E(G)} n_1(e|G) \cdot n_2(e|G) \ .$$

It has been studied extensively both for its mathematical properties and for its chemical applications, see [5] and references cited therein.

For $e = uv \in E(G)$ and $w \in V(G)$, the distance between e and w in G is defined as $d_G(e, w) = \min\{d_G(u, w), d_G(v, w)\}$. Let $m_1(e|G)$ be the number of edges of G lying closer to vertex u than vertex v and $m_2(e|G)$ the number of edges of G lying closer to vertex v than vertex u. The edge Szeged index of G is defined as [6]

$$Sz_e(G) = \sum_{e \in E(G)} m_1(e|G) \cdot m_2(e|G) \ .$$

Some properties for this index have been established in [6, 7].

If G is a n-vertex tree, then $Sz_e(G) = Sz(G) - (n-1)^2$, see [6]. Now we establish a relation between the edge Szeged index and the ordinary Szeged index for unicyclic graphs.

2 Result

Recall that a unicyclic graph is a connected graph with a unique cycle. Let G be an n-vertex unicyclic graph for which the vertices of its unique cycle C_r are labelled consecutively by $v_1, v_2, \ldots, v_r$. The deletion of all edges of the cycle C_r of G results in r vertex-disjoint trees $T_1, T_2, \ldots, T_r$ such that T_i and the cycle C_r have exactly one vertex, say v_i in common, for $1 \leq i \leq r$. Such a unicyclic graph is denoted by $C_r(T_1, T_2, \ldots, T_r)$. Let $|H| = |V(H)|$ for a graph H. Obviously, any n-vertex unicyclic graph G with cycle length r is of the form $C_r(T_1, T_2, \ldots, T_r)$, where $\sum_{i=1}^{r} |T_i| = n$.

Lemma 1 *Let $G = C_r(T_1, T_2, \ldots, T_r)$ with $|G| = n$. Then*

$$Sz_e(G) = \begin{cases} \sum_{i=1}^{r} W(T_i) + \sum_{i=1}^{r}(|G| - |T_i| + 1)D(v_i|T_i) \\ + \sum_{i=1}^{r}\sum_{j=1}^{r} |T_i||T_j|d_{C_r}(v_i, v_j) - \sum_{i<j} |T_i||T_j| - n^2 + nr & \text{if } r \text{ is odd}, \\ \\ \sum_{i=1}^{r} W(T_i) + \sum_{i=1}^{r}(|G| - |T_i| + 1)D(v_i|T_i) \\ + \sum_{i=1}^{r}\sum_{j=1}^{r} |T_i||T_j|d_{C_r}(v_i, v_j) - n^2 + r & \text{if } r \text{ is even}. \end{cases}$$

Proof. For $i = 1, 2, \ldots, r$ and $e \in E(T_i)$ incident with vertices u and v, we write $e = uv$ such that $d_{T_i}(u, v_i) > d_{T_i}(v, v_i)$.

Obviously, $w \in V(T_i)$ is counted $d_{T_i}(w, v_i)$ times in the sum $\sum_{e\in E(T_i)} n_1(e|T_i)$, and thus $\sum_{e\in E(T_i)} n_1(e|T_i) = D(v_i|T_i)$ for $i = 1, 2, \ldots, r$ (see [8]). Note that $m_k(e|T_i) = n_k(e|T_i) - 1$ for $k = 1, 2$. Thus the contribution to $Sz_e(G)$ of the edges outside the unique cycle of G is equal to

$$\begin{aligned} A &= \sum_{i=1}^{r} \sum_{e\in E(T_i)} m_1(e|G) \cdot m_2(e|G) \\ &= \sum_{i=1}^{r} \sum_{e\in E(T_i)} m_1(e|T_i) \cdot (m_2(e|T_i) + |E(G)| - |E(T_i)|) \\ &= \sum_{i=1}^{r} \sum_{e\in E(T_i)} m_1(e|T_i)m_2(e|T_i) + \sum_{i=1}^{r} (|E(G)| - |E(T_i)|) \sum_{e\in E(T_i)} m_1(e|T_i) \\ &= \sum_{i=1}^{r} Sz_e(T_i) + \sum_{i=1}^{r} (|E(G)| - |E(T_i)|) \sum_{e\in E(T_i)} (n_1(e|T_i) - 1) \\ &= \sum_{i=1}^{r} W(T_i) - \sum\_i = 1^r(|T_i| - 1)^2 + \sum_{i=1}^{r} (|G| - |T_i| + 1) \sum_{e\in E(T_i)} (n_1(e|T_i) - 1) \\ &= \sum_{i=1}^{r} W(T_i) + \sum_{i=1}^{r}(|G| - |T_i|) \sum_{e\in E(T_i)} n_1(e|T_i) \\ &+ \sum_{i=1}^{r} \sum_{e\in E(T_i)} n_1(e|T_i) - |G| \sum_{i=1}^{r} |E(T_i)| \end{aligned}$$

$$= \sum_{i=1}^{r} W(T_i) + \sum_{i=1}^{r} (|G| - |T_i| + 1) D(v_i|T_i) - n(n-r) \ .$$

If r is even and $e \in E(C_r)$, then $m_1(e|G) = n_1(e|G) - 1$, $m_2(e|G) = n_2(e|G) - 1$, and thus the contribution to $Sz_e(G)$ of the edges in the unique cycle of G is equal to

$$\begin{aligned} B &= \sum_{e \in E(C_r)} m_1(e|G) m_2(e|G) \\ &= \sum_{e \in E(C_r)} (n_1(e|G) - 1)(n_2(e|G) - 1) \\ &= \sum_{e \in E(C_r)} n_1(e|G) n_2(e|G) - \sum_{e \in E(C_r)} (n_1(e|G) + n_2(e|G)) + r \\ &= \sum_{e \in E(C_r)} n_1(e|G) n_2(e|G) - nr + r \\ &= \sum_{i=1}^{r} \sum_{j=1}^{r} |T_i||T_j| d_{C_r}(v_i, v_j) - nr + r \end{aligned}$$

If r is odd and $e \in E(C_r)$, then $m_1(e|G) = n_1(e|G)$, $m_2(e|G) = n_2(e|G)$, and thus the contribution to $Sz_e(G)$ of the edges in the unique cycle of G is equal to

$$\begin{aligned} B &= \sum_{e \in E(C_r)} m_1(e|G) m_2(e|G) \\ &= \sum_{e \in E(C_r)} n_1(e|G) n_2(e|G) \\ &= \sum_{i=1}^{r} \sum_{j=1}^{r} |T_i||T_j| d_{C_r}(v_i, v_j) - \sum_{i<j} |T_i||T_j|. \end{aligned}$$

Now the result follows easily as $Sz_e(G) = A + B$. □

Let $\delta(n) = 0$ if n is even and $\delta(n) = 1$ if n is odd. Gutman et al. [8] showed that

$$\begin{aligned} Sz(G) &= \sum_{i=1}^{r} W(T_i) + \sum_{i=1}^{r} (|G| - |T_i|) D(v_i|T_i) \\ &\quad + \sum_{i=1}^{r} \sum_{j=1}^{r} |T_i||T_j| d_{C_r}(v_i, v_j) - \delta(r) \sum_{i<j} |T_i||T_j|. \end{aligned}$$

By Lemma 1 and the above formula for $Sz(G)$, we have the following relation between the edge Szeged index and the ordinary Szeged index for unicyclic graphs.

Theorem 1 *Let $G = C_r(T_1, T_2, \ldots, T_r)$ with $|G| = n$. Then*

$$Sz_e(G) = Sz(G) + \sum_{i=1}^{r} D(v_i|T_i) - n^2 + \begin{cases} nr & \text{if } r \text{ is odd,} \\ r & \text{if } r \text{ is even.} \end{cases}$$

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