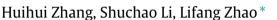
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On the further relation between the (revised) Szeged index and the Wiener index of graphs^{\star}



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1. Introduction

ABSTRACT

In 2010, Hansen et al. proposed three conjectures on the differences between the (revised) Szeged index and the Wiener index for a connected graph *G*. Recently, the above conjectures were solved by Chen et al. (2014). In this paper, as a continuance of it, we study some further relation between the (revised) Szeged index and Wiener index of connected graphs. Some sharp bounds on the difference between the (revised) Szeged index and Wiener index are established and the corresponding extremal graphs are characterized. © 2016 Elsevier B.V. All rights reserved.

Throughout this paper, we only consider finite, simple and connected graph $G = (V_G, E_G)$, where V_G is the vertex set and E_G is the edge set. Let \mathscr{G}_n be the set of all *n*-vertex connected graphs. We follow the notation and terminologies in [3] except if otherwise stated.

For $u, v \in V_G$, $d_G(u, v)$ denotes the *distance* between u and v in G. Throughout the text we denote by C_n and K_n the cycle and complete graph on n vertices, respectively. For a vertex subset S of G, let G[S] denote the subgraph induced by S. The *Wiener index* (or *transmission*) of G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V_G} d_G(u,v).$$
(1.1)

This graph invariant has been extensively studied; see, e.g., [11,12,20]. Let e = uv be an edge of *G*, and define three sets as follows:

 $N_u(e) = \{ w \in V_G : d_G(u, w) < d_G(v, w) \}, \qquad N_v(e) = \{ w \in V_G : d_G(v, w) < d_G(u, w) \}, \\ N_0(e) = \{ w \in V_G : d_G(u, w) = d_G(v, w) \}.$

Thus, $N_u(e) \cup N_v(e) \cup N_0(e)$ is a partition of V_G with respect to e. The number of vertices of $N_u(e)$, $N_v(e)$ and $N_0(e)$ is denoted by $n_u(e)$, $n_v(e)$ and $n_0(e)$, respectively. Evidently, $n_u(e) + n_v(e) + n_0(e) = |V_G|$. In particular, if G is bipartite, then the equality $n_0(e) = 0$ holds for all $e \in E_G$. Therefore, $n_u(e) + n_v(e) = |V_G|$ for any edge e of a bipartite graph G.

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Given a tree *T*, its Wiener index can be defined alternatively as [12,28]:

$$W(T) = \sum_{e=uv \in E_T} n_u(e)n_v(e).$$
(1.2)

Motivated by (1.2), Gutman [10] proposed a graph invariant, named as the Szeged index, defined by

$$Sz(G) = \sum_{e=uv \in E_G} n_u(e)n_v(e),$$

where G is any graph, not necessarily connected. Evidently, the Szeged index is defined as a proper extension of (1.2) with respect to the transmission of trees.

Randić [26] observed that the Szeged index does not take into account the contributions of the vertices at equal distances from the endpoints of an edge, and so he put forward a modified version of the Szeged index which is named as the *revised Szeged index*. The revised Szeged index of a connected graph *G* is defined as

$$Sz^*(G) = \sum_{e=uv \in E_G} \left(n_u(e) + \frac{n_0(e)}{2} \right) \left(n_v(e) + \frac{n_0(e)}{2} \right).$$

For some properties and applications of the Szeged index and the revised Szeged index one may be referred to those in [2,6,14,19,24,25,29].

It is known that for a connected graph G, $Sz^*(G) \ge Sz(G) \ge W(G)$, and it is easy to see that $Sz^*(G) = Sz(G) = W(G)$ if G is a tree. Dobrynin and Gutman [7] investigated the structure of a connected graph G with the property of $Sz(G) - W(G) \ge 0$ and conjectured that Sz(G) = W(G) holds if and only if every block of G is a complete graph. This conjecture was proved by the same authors in [8]. Further more, Khodashenas, Nadjafi-Arani, Ashrafi and Gutman [15] give a much simpler proof for this result. It is interesting to see that Nadjafi-Arani, Khodashenas and Ashrafi [22] investigated the structure of a graph G with Sz(G) - W(G) = n, here n is not the order of G. Also in [23], they discussed graphs whose Szeged and Wiener numbers differ by 4 and 5, and mentioned the conjecture that $Sz(G) - W(G) \ge 2n - 5$ for graphs in which at least one block is not a complete graph. Then Klavžar and Nadjafi-Arani [16] studied Sz(G) - W(G) in network. For more recent results on the difference between the (revised) Szeged index and Wiener index, one may be referred to [17,18].

AutoGraphiX has been used to study the relations involving invariants by several graph theorists. One may be referred to [1,4,9] for more details. Three conjectures were made by Hansen et al. in 2010 [13] by using the computer program AutoGraphiX, and proved by Chen et al. in [5,6], which are described as in the following theorems.

Theorem 1.1 ([5,6]). Let *G* be a connected bipartite graph with $n \ge 4$ vertices and $|E_G| \ge n$ edges. Then $Sz(G) - W(G) \ge 4n - 8$. Moreover, the bound is best possible when the graph is composed of a cycle C_4 on 4 vertices and a tree *T* on n - 3 vertices sharing a single vertex.

Theorem 1.2 ([5]). Let G be a connected graph with $n \ge 5$ vertices with an odd cycle and girth $g \ge 5$. Then $Sz(G) - W(G) \ge 2n - 5$. The equality holds if and only if G is composed of a cycle C_5 on 5 vertices, and one tree rooted at a vertex of the C_5 or two trees, respectively, rooted at two adjacent vertices of the C_5 .

Theorem 1.3 ([5]). Let G be a connected graph with $n \ge 4$ vertices and $|E_G| \ge n$ edges and with an odd cycle. Then

$$Sz^*(G) - W(G) \ge \frac{n^2 + 4n - 6}{4}.$$

Moreover, the bound is best possible when the graph is composed of a cycle C_3 on 3 vertices and a tree T on n - 2 vertices sharing a single vertex.

For convenience, let \mathcal{U}_n be the set of all *n*-vertex graphs each of which is obtained from a cycle C_5 on 5 vertices and one tree rooted at a vertex of C_5 or two trees, respectively, rooted at two adjacent vertices of the C_5 . Let $\mathcal{U}'_n = \{G | G \in \mathcal{G}_n \text{ and each block of } G \text{ is a complete graph}\}$, \mathcal{U}''_n be the set of all *n*-vertex graphs each of which is obtained from a cycle C_3 on 3 vertices and a tree T on n - 2 vertices by sharing a single vertex. Combining with Theorems 1.1 and 1.2, we may know that sharp lower bound on the difference Sz(G) - W(G) of connected graph G is determined and the corresponding extremal graphs are also characterized. In view of Theorem 1.3, sharp lower bound on the difference $Sz^*(G) - W(G)$ of connected graph G is determined and the corresponding extremal graphs are identified as well.

Motivated directly from the results obtained in [5,6], it is natural and interesting for us to study some further relationship between Sz(G) and W(G) (resp. between $Sz^*(G)$ and W(G)) of graphs along this line. In this paper some sharp bounds on Sz(G) - W(G) (resp. $Sz^*(G) - W(G)$) are established and the structure of the corresponding extremal graphs is characterized respectively.

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