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RELATIONSHIP BETWEEN EDGE SZEGED AND EDGE WIENER INDICES OF GRAPHS

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Abstract. Let G be a connected graph and $\xi(G) = Sz_e(G) - W_e(G)$, where $W_e(G)$ denotes the edge Wiener index and $Sz_e(G)$ denotes the edge Szeged index of G. In an earlier paper, it is proved that if T is a tree then $Sz_e(T) = W_e(T)$. In this paper, we continue our work to prove that for every connected graph G, $Sz_e(G) \geq W_e(G)$ with equality if and only if G is a tree. We also classify all graphs with $\xi(G) \leq 5$. Finally, for each non-negative integer $n \neq 1$ there exists a graph G such that $\xi(G) = n$.

1. Introduction

Throughout this paper we consider only simple connected graphs. For a graph G, $V(G)$ and $E(G)$ denote the set of all vertices and edges, respectively. As usual, the distance between the vertices u and v of G is denoted by $d_G(u,v)(d(u,v)$ for short) and it is defined as the number of edges in a minimal path connecting them. The Wiener index $W(G)$ is defined as the sum of all distances between vertices of G ([21]). The Wiener index has noteworthy applications in chemistry and interested readers can be referred to papers [4, 5] and references therein for details. We denote by K_n, $K_{m,n}$, P_n and C_n the complete $n-$vertex graph, $(m,n)-$complete bipartite graph, path and cycle on n vertices, respectively.

We now describe some notations which will be kept throughout. A biconnected graph is a connected graph in which two vertices must be removed to disconnect the graph. A maximal biconnected subgraph is called a block. Suppose G is a graph, $w \in V(G)$ and $e = uv, f = ab \in E(G)$. Then $N_u(e)$ denotes the set of all vertices closer to u than v and $M_u(e)$ is the set of all

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edges closer to u than v. The sets $N_v(e)$ and $M_v(e)$ are defined analogously. Set $n_u(e) = |N_u(e)|$, $m_u(e) = |M_u(e)|$ and define:

$$d'(w,e) = \min\{d(w,u), d(w,v)\},$$
$$D(e,f) = \min\{d'(u,f), d'(v,f)\},$$

see [8, 9] for details. The edge Wiener index ([3, 11]) and the edge Szeged index ([8]) of G are defined as follows:

$$W_e(G) = \sum_{\{e,f\}\subseteq E(G)} D(e,f),$$
$$Sz_e(G) = \sum_{e=uv\in E(G)} m_u(e)m_v(e).$$

Notice that in computing edge Szeged index of G, edges equidistant from both ends of the edge $e = uv$ are not counted.

The line graph $L(G)$ of a graph G is a graph such that each vertex of $L(G)$ represents an edge of G and any two vertices of $L(G)$ are adjacent if and only if their corresponding edges share a common endpoint in G. Therefore,

$$d_{L(G)}(e,f) = D_G(e,f) + 1 \tag{1.1}$$

$$W(L(G)) - W_e(G) = \binom{|E(G)|}{2}. \tag{1.2}$$

Lukovits ([16]) introduced an all-path version of the Wiener index. To explain, we assume that G is a connected graph with $V(G) = \{1, 2, ..., n\}$. Then $P(G) = \sum_{i<j}\sum_{P\in\pi_{i,j}} |P|$ is called the "all-path" version of the Wiener index. Here, $\pi_{i,j}$ denotes the set of all path connecting vertices i, j and the summations have to be performed between all pairs of vertices i and j and for all paths between i and j. In the mentioned paper some mathematical properties of $P(G)$ together with its extremal values are investigated.

In the next section, we consider a graph G and present a "path-vertex" matrix in the line graph of G to study the relationship between edge Wiener and edge Szeged indices of G. This matrix is defined in a similar way as "all-path" index of Lukovits.

By [19] a Krausz decomposition of a simple graph H is a partition of $E(H)$ into cliques such that each vertex of H appears in at most two of the cliques. The following two results are important in our main results:

PROPOSITION 1.1 (See [19, 7.1.39] and [20]). *There is not a graph except from K_3 containing two distinct Krausz decompositions. In particular, ($K_{1,3}$, K_3) is the only pair of non isomorphic connected graphs with isomorphic line graphs.*

PROPOSITION 1.2 (See [19, Theorem 7.1.16] and [10, 14]). *For a simple graph G, there is a solution to $L(H) = G$ if and only if G decomposes into complete subgraphs, with each vertex of G appearing in at most two in the list.*

A triangle T in a graph G is said to be odd if $|N(v) \bigcap V(T)|$ is odd for some $v \in V(G)$, where $N(v)$ denotes the neighborhood of the vertex v. It is called even if $|N(v) \bigcap V(T)|$ is even for every $v \in V(G)$.

PROPOSITION 1.3 (See [19, Theorem 7.1.17]). *For a simple graph G, there is a solution to $L(H) = G$ if and only if G does not have an induced subgraph isomorphic to $K_{1,3}$ or an induced subgraph isomorphic to $K_4 - e$ such that its triangles are not simultaneously odd.*

The following lemma is crucial throughout the paper:

LEMMA 1.4. *Let G be a connected graph. Then the following are holds:*

a) *The blocks of $L(G)$ are complete if and only if G is isomorphic to the complete graph K_3 or a tree.*
b) *If G has an incomplete block then G has an induced subgraph isomorphic to $K_4 - e$ or a cycle $C_n, n \geq 4$.*

PROOF. See [19, Theorem 7.1.16] and [2, Proposition 1] for details. ◻

Throughout this paper our notation is standard and taken mainly from [17–19]. The set of all shortest paths connecting vertices a and b of G is denoted by $P_G(a, b)$ and for a shortest path P, $l(P)$ denotes the length of P.

Suppose G is a graph and H is a subgraph of G. H is called an isometric subgraph of G, written $H \ll G$, if for each pair x, y of vertices in H, $d_H(x, y) = d_G(x, y)$. We encourage the reader to consult [1, 22] for computational techniques and [13, 15] for the algebraic point of view of the Wiener and Szeged indices of graphs.

2. MAIN RESULTS

In [6], Dobrynin and Gutman conjectured that $Sz(G) = W(G)$ if and only if every block of G is complete. They proved in [7] their conjecture. In [12] a new simpler proof of this conjecture is presented. In this section, we extend this result to the case of edge version. In an exact phrase, we prove that $Sz_e(G) = W_e(G)$ if and only if G is a tree.

Suppose $Y = \{P_1, P_2, \cdots, P_{\binom{m}{2}}\}$ is a set of shortest paths in $L(G)$ such that for every edges $\alpha, \beta \in E(G)$, $\alpha \neq \beta$, there exists a unique path $P \in Y$ connecting vertices α and β in $L(G)$. The set Y is called a complete set of shortest paths of $L(G)$ (CSSP for short) and CSSP($L(G)$) denotes the set of all CSSP of $L(G)$. Define the matrix $B_Y = [b_{ij}]$ as follows:

$$b_{ij} = \begin{cases} 1 & e_j \in V(P_i - \{p_{i1}, p_{i(l(P_i)+1)}\}) \\ 0 & \text{otherwise} \end{cases},$$

where $V(P_i) = \{p_{i1}, \cdots, p_{i(l(P_i)+1)}\}$. To clarify our definition we compute below this matrix for a graph G isomorphic to a triangle with a pendant. Clearly, $L(G)$ is isomorphic to $K_4 - e$ and we have:

$$B_Y = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

where Y is the set of shortest paths e_1e_2, $e_1e_2e_3$, e_1e_4, e_2e_3, e_2e_4, e_3e_4 in $L(G)$.

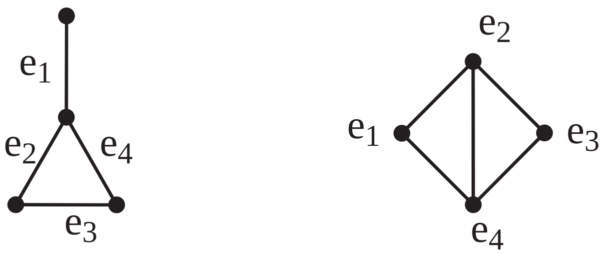

FIGURE 1. The graphs G and $L(G)$.

Obviously, if P_i is a path connecting vertices α and β in $L(G)$ then $d_{L(G)}(\alpha, \beta) - 1$ is the number of non-zero entries in the i^{th} row of B_Y. Thus by Eq. (1), the summation of all entries in B_Y is equal to the edge Wiener index of G.

LEMMA 2.1. *Let $P = u_1, u_2, \cdots, u_n$ be a shortest path of a graph G where $e_i = u_iu_{i+1}$, $i = 1, 2, \cdots, n-1$. Then for all $i = 2, \cdots, n-2$*

$$e_1 \in M_{u_i}(e_i) \qquad \textit{and} \qquad e_n \in M_{u_{i+1}}(e_i).$$

PROOF. To traverse the path P from the source vertex u_1 to the destination vertex u_n, we traverse the vertex u_i before u_{i+1} and so

$$d'(e_1, u_{i+1}) = d'(e_1, u_i) + d(u_i, u_{i+1}).$$

This implies that $e_1 \in M_{u_i}(e_i)$ and $e_n \in M_{u_{i+1}}(e_i)$. □

Suppose G is an $m-$edge graph and Y is a $CSSP$ of $L(G)$. It is clear that $|Y| = \binom{m}{2}$. If $e_j = uv$ is an edge of G then we define $\xi_Y(e_j) = m_u(e_j)m_v(e_j) - \sum_i b_{ij}$ and $\xi_Y(G) = \sum_{e \in G} \xi_Y(e)$. It is easy to see that $\xi_Y(G) = Sz_e(G) - W_e(G)$ and so the value of $\xi_Y(G)$ is independent from Y. From now on for simplifying our notation we write $\xi(G)$ instead of $\xi_Y(G)$. If H is an isometric subgraph of G then we define $\xi_Y(H) = \sum_{e\in E(H)} \xi_Y(e)$. Notice that $\xi_Y(H)$ is not independent from Y. Moreover, it is easily seen that $\xi_Y(H) \leq \xi(G)$.

THEOREM 2.2. *Let G be a connected graph. Then $W_e(G) \geq Sz_e(G)$ with equality if and only if G is a tree. Moreover,*

a) *If $L(G)$ contains an induced subgraph $H \cong K_4 - e$, then $\xi(G) \geq 3$.*
b) *Suppose $C_n, n \geq 4$ is a minimal induced cycle of $L(G)$. Then $\xi(G) \geq n$, for every $n \geq 5$. If $n = 4$, then $\xi(G) \geq 2$.*

PROOF. Suppose G is an arbitrary connected graph,

$$E(G) = \{e_1 = \alpha_1\beta_1, \cdots, e_m = \alpha_m\beta_m\},$$

$Y \in CSSP(L(G))$, $B_Y = [b_{ij}]$ and for each $P_i \in Y$,

$$V(P_i) = \{e_{i_1} = \alpha_{i_1}\alpha_{i_2}, \cdots, e_{i_{l(P_i)+1}} = \alpha_{i_{l(P_i)+1}}\alpha_{i_{l(P_i)+2}}\}.$$

By Lemma 2.1, $b_{ii_r} = 1$ if and only if $e_{i_1} \in M_{\alpha_{i_r}}(e_{i_r})$ and $e_{i_{l(P_i)+1}} \in M_{\alpha_{i_{r+1}}(e_{i_r})}$, where $2 \leq r \leq l(P_i)$. Therefore, the summation of entries of the j^{th} column of B_Y is at most $m_{\alpha_j}(e_j)m_{\beta_j}(e_j)$ with equality if and only if for every $e_i \in M_{\alpha_r}(e_r)$ and $e_j \in M_{\beta_r}(e_r)$ the shortest path connecting e_i and e_j containing e_r is an element of Y. In other words, for each vertex e_i, e_j in $L(G)$ there exists a unique shortest path P connecting them through e_r, where $e_i \in M_{\alpha_r}(e_r)$, $e_j \in M_{\beta_r}(e_r)$ and $1 \leq r \leq m$. Then the summation of all entries in a given column is $m_{\alpha_r}(e_r)m_{\beta_r}(e_r)$ and the summation of numbers in these column is equal to the edge Szeged index of G. Therefore, $Sz_e(G) \geq W_e(G)$. If G is a tree then each block of $L(G)$ is complete and so between every two vertices $e_i, e_j \in V(L(G))$ there exists a unique shortest path through vertex e_k, $e_i \in M_{\alpha_k}(e_k)$ and $e_j \in M_{\beta_k}(e_k)$. So, $Sz_e(G) = W_e(G)$, as desired.

Suppose $W_e(G) = Sz_e(G)$. Then for every edge $e_k = \alpha_k\beta_k \in E(G)$, the summation of all entries in the column corresponding to the edge e_k is equal to $m_{\alpha_k}(e_k)m_{\beta_k}(e_k)$. In other words, if e_k is chosen, $e_i \in M_{\alpha_k}(e_k)$ and $e_j \in M_{\beta_k}(e_k)$ then every shortest path in $L(G)$ connecting e_i and e_j has to contain the edge e_k. Therefore, $L(G)$ cannot have an induced cycle of length $n \geq 4$ or a subgraph isomorphic to $K_4 - e$. To prove, suppose $L(G)$ has an induced subgraph H isomorphic to $K_4 - e$. Apply Krausz decomposition to prove that G has a cycle T of length three. Choose an edge $e = uv$ of T. Then the edge f_1 adjacent to u in T is belong to $M_u(e)$ and the edge f_2 adjacent to v in T is belong to $M_v(e)$. But, the shortest path connecting f_1 and f_2 in $L(G)$ doesn't pass the vertex e of $L(G)$ and so $\xi(e) \geq 1$. By considering each edge of T and a similar argument, one can prove $\xi(G) \geq 3$. Now, suppose that $L(G)$ has at least an induced cycle of length $n \geq 4$. Let $C_n \geq 4$, be a minimal induced cycle of $L(G)$. We first assume that n is even. Clearly, for every antipodal vertices x and y of C_n, there are two shortest paths in $L(G)$ connecting x and y. Thus $\xi(G) \geq (\frac{n}{2})(\frac{n-2}{2})$.

Next suppose that n is odd. We use C_n to construct an $n-$cycle D in G. By Krausz decomposition and Proposition 1.2, edges of C_n are in distinct cliques of Krausz decomposition. We prove that D is an isometric cycle in G. Put $D = v_1v_2...v_nv_1$. If D is not isometric then without lose of generality we can choose vertices v_i and v_j from D such that there exists a shortest path $P : (v_i =)u_1u_2 \cdots u_k(= v_j)$ in G such that $V(P) \cap V(D) = \{v_i, v_j\}$. Consider the cycles $C_1 : u_1u_2 \cdots u_kv_{j+1} \cdots v_i$ and $C_2 : u_1u_2 \cdots u_kv_{j-1} \cdots v_i$. Then these cycles induce two cycles C'_1 and C'_2 in $L(G)$, see Figure 2. Obviously, $u_t \neq v_s$, $2 \leq t \leq k-1$ and $1 \leq s \leq n$. So, C'_1 and C'_2 are induced cycles in $L(G)$. Since C_n, $n \geq 4$, is the minimal induced cycle of $L(G)$, C'_1 and C'_2 have length three. Thus, $n = 4$ which is impossible. Therefore, if $n \geq 5$ then D is isometric.

For every edge $e_i = v_iv_{i+1}$, there are edges $e_r = e_{\frac{n+1}{2}+i} = v_{\frac{n+1}{2}+i}v_{\frac{n+1}{2}+i+1}$ and $e_s = e_{\frac{n-1}{2}+i} = v_{\frac{n-1}{2}+i}v_{\frac{n+1}{2}+i}$ such that $e_r \in M_{v_i}(e_i)$ and $e_s \in M_{v_{i+1}}(e_i)$. On the other hand, there is no a shortest path in $L(G)$ connecting e_r and e_s through the vertex e_i of C_n. Therefore, for each vertex e_i of C_n, $\xi(e_i) \geq 1$ and so $\xi(G) \geq n$. Thus, by Lemma 1.4(b) and the fact that $W_e(K_3) = 0 = Sz_e(K_3) - 3$, the blocks of $L(G)$ are complete. Finally, by Lemma 1.4(a), G is a tree which completes the proof. ∎

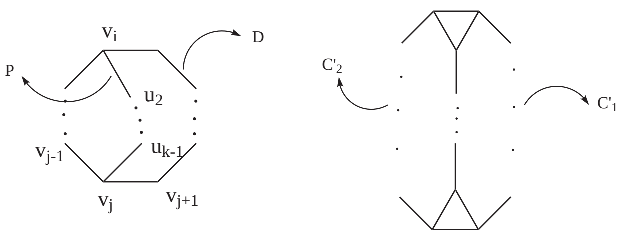

FIGURE 2. An isometric subgraph of G and its image in $L(G)$.

COROLLARY 2.3. *Let G be a connected graph containing k isometric cycles isomorphic to C_4 and r isometric cycles $C_{n_1}, \cdots, C_{n_r}$ such that $n_i \neq 5$, $1 \leq i \leq r$. Then $\xi(G) \geq n_1 + n_2 + \cdots n_r + 2k$.*

THEOREM 2.4. *Let G be a connected graph. Then $\xi(G) \neq 1$.*

PROOF. Suppose $\xi(G) = 1$. So, by Theorem 2.2 and Lemma 1.4(a), $L(G)$ has an incomplete block B. By Lemma 1.4(b), B has an induced $n-$cycle $C_n, n \geq 4$, or an induced subgraph H isomorphic to $K_4 - e$. Apply the second part of Theorem 2.2 to complete the proof. ∎

THEOREM 2.5. *The following statements hold:*

a) $\xi(G) = 2$ *if and only if* G *is a cycle of length four.*
b) $\xi(G) = 3$ *if and only if* G *is a cycle of length three.*
c) $\xi(G) = 4$ *if and only if* G *is isomorphic to a triangle with a pendant or a square with a pendant.*
d) $\xi(G) = 5$ *if and only if* G *is isomorphic to a graph* G *constructed from a triangle and two pendants.*

PROOF. a) Suppose $\xi(G) = 2$. By second part of Theorem 2.2 and Lemma 1.4, one can see that there exists an isometric induced cycle C of length 4 in $L(G)$. We claim that $|V(L(G))| = 4$. To do this, we assume that there is a vertex y, $y \notin V(C)$ and y is adjacent to some vertices of C. If y is adjacent to one vertex of C, three vertices of C or two non-adjacent vertices of C then Proposition 1.3 leads to a contradiction. If y is adjacent to all vertices of C then by Krausz decomposition we must have at least two triangles in the graph G and by the Corollary 2.3, $\xi(G) \geq 6$. This leads to another contradiction. Finally, if y and two adjacent vertices of C constitute a triangle then by Krausz decomposition and Proposition 1.2, G has an induced subgraph H isomorphic to a square with a pendant. Notice that the subgraph H is isometric. Otherwise, G is containing a square and a triangle or two squares with a common edge. In each case by Corollary 2.3, $\xi(G) \geq 6$ which contradicts our assumption. Since $H \ll G$, it can easily see that $\xi(G) > 3$ which is our final contradiction. Therefore, G is a cycle of length 4. The converse is trivial.

b) It is clear that if G is isomorphic to a cycle of length 3 then $\xi(G) = 3$. Suppose $\xi(G) = 3$ and $G \ncong K_3$. Thus, by Lemma 1.4(b) and Theorem 2.2, there exists an induced subgraph H which is isomorphic to $K_4 - e$ or an $n-$cycle C_n, $n \geq 4$ in $L(G)$. If H is a shortest induced cycle of length n, $n \geq 4$, then by the second part of Theorem 2.2, $n = 4$. In this case, by the proof of part (a), $\xi(G) = 2$ or $\xi(G) \geq 4$, which is impossible. We now assume that the subgraph H is isomorphic to $K_4 - e$. By Krausz decomposition, H makes a triangle in G. Since for each edge f of this triangle $\xi(f) \geq 1$, $\xi(G) \geq 3$. On the other hand, consider two vertices of degree 2 in H. Then there are two shortest paths connecting these vertices in $L(G)$. Therefore, for at least one vertex e of degree three in H, $\xi(e)$ is exceed at least one. This implies that $\xi(G) \geq 4$, leads to a contradiction.

c) It is obvious that if G is isomorphic to a triangle with a pendant edge or a square with a pendant then $\xi(G) = 4$. Suppose $\xi(G) = 4$. A similar argument as part (b) show that $L(G)$ has an induced subgraph H isomorphic to $K_4 - e$ or an $n-$cycle C_n, $n \geq 4$. If H is an minimal $n-$cycle with $n \geq 4$ then by the second part of Theorem 2.2, $n = 4$. Apply the argument of part (a) to prove that $\xi(G) \geq 5$ or y and two adjacent vertices of C constitutes a triangle in $L(G)$. Therefore, G is containing a subgraph H isomorphic to a square with a pendant. We claim that $H \ll G$. Otherwise, G contains at least two isometric cycles and by Corollary 2.3, $\xi(G) \geq 5$, a contradiction. If there exists another vertex of G adjacent to a vertex of H then G contains an isometric subgraph L such that one of the following hold:

1) L is isomorphic to a square with two pendants,
2) L is constructed from a square and a path of length 3 by identifying a vertex of square and a pendant of path,
3) L has at least two isometric cycles.

In each case $\xi(G) \geq 5$ leads to a contradiction. Therefore, the graph G is isomorphic to a square with a pendant. If H is isomorphic to $K_4 - e$ then a case by case argument as above show that $L(G) = H = K_4 - e$. Therefore, G is a triangle with a pendant edge.

d) The proof is similar to those given for the cases that $\xi(G) = 2, 3$ or 4. □

In the end of this paper, we prove that for each non-negative integer $n \neq 1$ there exists a graph G such that $\xi(G) = n$. To do this, we notice that for a tree T, $\xi(T) = 0$ and $\xi(C_4) = 2$. Consider a triangle T with a fixed vertex v. Define a graph H by considering T and add n new vertices to T by connecting them to the vertex v. Then $\xi(H) = n + 3$. Therefore, for each non-negative integer $n \neq 1$, there exists a graph G such that $\xi(G) = n$.

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