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Calculating the edge Wiener and edge Szeged indices of graphs

H. Yousefi-Azari [a], M.H. Khalifeh [a], A.R. Ashrafi [b,*]

[a] School of Mathematics, Statistics and Computer Science, University of Tehran, Tehran, Islamic Republic of Iran
[b] Department of Mathematics, Faculty of Science, University of Kashan, Kashan 87317-51167, Islamic Republic of Iran

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ABSTRACT

The edge Szeged and edge Wiener indices of graphs are new topological indices presented very recently. It is not difficult to apply a modification of the well-known cut method to compute the edge Szeged and edge Wiener indices of hexagonal systems. The aim of this paper is to propose a method for computing these indices for general graphs under some additional assumptions.

1. Introduction

A graph invariant is any function on a graph that does not depend on a labeling of its vertices. There are many examples of graph invariants, especially those based on distances, which are applicable in chemistry. The Wiener index [1], defined as the sum of all distances between pairs of vertices in a graph, is probably the first and most studied such graph invariant, from both a theoretical and a practical point of view; see [2,3] for details.

Besides the Wiener index, we will consider several related indices; to define them, we first introduce some notation. Throughout the paper, we only consider simple connected graphs. For a graph G, $V(G)$ and $E(G)$ denote the vertex and edge set, respectively. The line graph $L(G)$ is a graph with $V(L(G)) = E(G)$ and two vertices of $L(G)$ are adjacent if and only if they have a common vertex in G. If H is another graph such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$ then we say that H is a subgraph of G, $H \leq G$. For two vertices $u, v \in V(G)$, the distance $d_G(u, v)$ ($d(u, v)$ for short) is defined as the length of a shortest path connecting them. Suppose $f = ab$ and $g = uv$ are arbitrary edges of G. Define $d_e(u, ab) = \mathrm{Min}\{d_G(u, a), d_G(u, b)\}$ and $D_G(f, g) = \mathrm{Min}\{d_e(u, f), d_e(v, f)\} = \mathrm{Min}\{d_e(b, g), d_e(a, g)\}$. A path P of length l is called an e-shortest path connecting edges f and g if $l = D(f, g)$ and pendants of P are end vertices of f and g. It is easily seen that $D_G(e, f) = d_{L(G)}(e, f) - 1$, where $L(G)$ denotes the line graph of G.

Set $M_u(v) = \{f \in E(G) \mid d_e(u, f) > d_e(v, f)\}$, $N_u(v) = \{x\hat{I}V(G) \mid d(u, x) < d(v, x)\}$, $m_u(v) = |M_u(v)|$ and $n_u(v) = |N_u(v)|$, where $u, v \in V(G)$. The edge $f = ab$ is said to be parallel with $g = uv$ and we write $f \parallel g$ if $d_e(u, f) = d_e(v, f)$. It is clear that the parallelism is not generally symmetric or transitive. Define

$$W_e(G) = \sum_{\{f,g\}\subseteq E_{(G)}} D_G(f, g) \quad (1)$$

$$Sz_e(G) = \sum_{f=uv\in E(G)} m_u(v)m_v(u) \quad (2)$$

$$Pl_e(G) = \sum_{f=uv\in E(G)} [m_u(v) + m_v(u)] \quad (3)$$

* Corresponding author. Tel.: +98 2166909240; fax: +98 3615552930.
E-mail address: alir.ashrafi@gmail.com (A.R. Ashrafi).

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$$Sz_{ev}(G) = 1/2 \sum_{e=uv\in E(G)} [n_u(v)m_v(u) + n_v(u) + m_u(v)]. \tag{4}$$

Eqs. (1) and (2) are recently defined graph invariants, named the edge Wiener [4,5] and the edge Szeged index [6,7], respectively. Eq. (3) defines the Padmakar–Ivan (PI) index of a graph G. The PI index is a more interesting graph invariant studied by very many researchers and we refer the readers to the papers [8–16] related to the PI index and its vertex version.

Throughout this paper our notation is standard and mainly taken from the standard book on graph theory. For the graph notation applicable in chemistry we refer the readers to the famous book of Trinajstic [17].

2. Results and discussion

Suppose G is a graph and $H \leq G$. The subgraph H is called convex if it contains all shortest paths for pairs of vertices in G already in H and H is said to be isometric, $H \ll G$, if for each pair of vertices $u; v \in V(H)$, $d_G(u; v) = d_H(u; v)$. For a subset X of $V(G)$, $\langle X\rangle_G$ denotes the subgraph of G induced by X, namely $V(\langle X\rangle_G) = X$ and $E(\langle X\rangle_G) = \{uv \in E(G) \mid u, v \in X\}$. The neighborhood of a vertex $v \in V(G)$, $N_G(v)$, is the set of vertices of G at distance 1 from v. A vertex v in a subgraph H of G is called a boundary vertex of H if $|N_G(v)| - |N_H(v)| > 0$. The set of all boundary vertices of H is denoted by ∂H.

The aim of this section is to present a new method for the calculation of edge Wiener and edge Szeged indices of graphs. We encourage interested readers to consult the papers [18–22] for background material as well as basic computational techniques. For the sake of completeness we state the following results which are crucial throughout the paper.

Theorem 1 *([18]). Suppose $H = \langle V(H)\rangle_G$ and there exists a convex subgraph I of G such that $\partial H \subseteq V(I) \subseteq V(H)$. Then H is a convex subgraph of G.*

Lemma 1 *([18]). Suppose $\{F_i\}_{i=1}^r$ is a partition of $E(G)$ such that $G \setminus F_i$ is a two-component graph with convex components G_i^1 and G_i^2. Then there exists a set R of shortest paths of G such that for each pair u, v of vertices of G, the following conditions hold:*

(a) *If $P_G(u, v) \in R$ and $\{u, v\}$ is contained in exactly one of $V(G_i^1)$ and $V(G_i^2)$ then $|E(P_G(u, v)) \cap F_i| = 0$.*
(b) *If $u \in V(G_i^1)$, $v \in V(G_i^1)$ and $P_G(u, v) \in R$ then $|E(P_G(u, v)) \cap F_i| = 1$.*

Theorem 2 *([23]). Suppose $\{F_i\}_{i=1}^r$ is a partition of the edges such that $G \setminus F_i$ is a two-component graph with convex components. Then G is bipartite.*

Theorem 3. *Suppose $\{F_i\}_{i=1}^r$ is a partition of $E(G)$ such that $G \setminus F_i$ is a two-component graph with convex components G_1^i and G_2^i. Then $W_e(G) = \sum_{i=1}^n |E(G_1^i)||E(G_2^i)|$.*

Proof. Let R be a multi-set of e-shortest paths of G such that for each edge $f, g \in E(G)$, there exists exactly one e-shortest path in R. Notice that it is possible for a path P to be an e-shortest path for different pairs of edges of G. Also, all vertices of degree > 1 are elements of R of length 0. For an edge $f \in E(G)$, $n_R(f)$ denotes the number of elements of R containing f. Therefore,

$$W_e(G) = \sum_{\{f,g\}\subseteq E(G)} D(f, g) = \sum_{f\in E(G)} n_R(f). \tag{5}$$

We claim that if G satisfies the conditions of our theorem, $e, f \in E(G)$ and $P_G(e, f) \in R$, then the following equality holds:

$$|P_G(e, f) \cap F_i| = \begin{cases} 0 & e, f \in G_1^i \text{ or } e, f \in G_2^i \quad \text{(i)} \\ 0 & e, f \in F_i \quad \text{(ii)} \\ 0 & e \in F_i \;\&\; (f \in G_1^i \text{ or } f \in G_1^i) \quad \text{(iii)} \\ 1 & e \in G_2^i \;\&\; f \in G_1^i. \quad \text{(iv)} \end{cases} \tag{6}$$

The cases Eq. (6)(i) and (iv) are immediate consequences of Lemma 1. We prove Eq. (6)(ii). To do this, we assume that $e_1 = a_1b_1$ and $e_2 = a_2b_2$ are edges of F_i. Since components of $G - F_i$ are convex, a_1 and b_1, as well as a_2 and b_2 do not belong to one component of $G - F_i$. Suppose that a shortest path in R connecting e_1 and e_2 trails from F_i, and a_1, a_2 are in a component of $G-F_i$ and b_1, b_2 are in another component of $G-F_i$. We now prove that $D(e_1, e_2) = \min\{d(a_1, a_2), d(b_1, b_2)\} < \min\{d(a_1, b_2), d(a_2, b_1)\}$. To do this, we assume that $\min\{d(a_1, a_2), d(b_1, b_2)\} = d(a_1, a_2) = \min\{d(a_1, b_2), d(a_2, b_1)\} = d(a_1, b_2)$. This shows that G has an add cycle, which is impossible by Theorem 2. If $d(a_1, a_2) > d(b_1, b_2)$ then we can find a shortest path of length $\leq d(a_1, a_2)$ connecting a_1 and a_2 which is not totally contained in a component containing a_1 and a_2, contradicting the convexity of the components of $G - F_i$.

Finally, to prove Eq. (6)(iii), we assume that $e_1 = a_1b_1 \in F_i$, $e_2 = a_2b_2 \in G_1^i$ and $a_1 \in V(G_1^i)$. If $D(e_1, e_2) = d_G^e(e_2, b_1)$ then G is not bipartite and if $D(e_1, e_2) > d_G^e(e_2, b_1)$ then G_1^i cannot be convex; these are impossible. This implies that $D(e_1, e_2) < d_G^e(e_2, b_1)$. Since $\{F_i\}_{i=1}^k$ is a partition of $E(G)$ and $G - F_i$ is disconnected, $\sum_{e\in F_i} n_R(e) = |E(G_1^i)||E(G_1^i)|$, which completes the proof. □

Corollary 1. *Suppose $\{F_i\}_{i=1}^k$ is a partition of $E(G)$ such that $G - F_i$ is a graph with convex components G_1^i and G_2^i. Then $W(L(G)) = \sum_{i=1}^k |E(G_1^i)||E(G_2^i)| + \binom{|E(G)|}{2}$.*

Proof. Since $D_G(e, f) = d_{L(G)}(e, f) - 1$, $W(L(G)) = W_e(G) + \binom{|E(G)|}{2}$, proving the result. □

Theorem 4. *Suppose $\{F_i\}_{i=1}^r$ is a partition of $E(G)$ such that $G \setminus F_i$ is a two-component graph with convex components G_1^i and G_2^i. Then $Sz_e(G) = \sum_{i=1}^n |F_i||E(G_1^i)||E(G_2^i)|$.*

Proof. Suppose $ab \in F_i$. Clearly, vertices a and b are in different components of $G - F_i$. If $a \in G_1^i$ then we show that for each $v \in G_1^i$, $d(a, v) < d(b, v)$. If not, $d(a, v) = d(b, v)$ or $d(a, v) > d(b, v)$. In the first case, there exists an odd cycle in G, which contradicts Theorem 2. In the second case, one can find a shortest path $P(a, v)$ in G such that G_1^i does not contain $P(a, v)$, which is impossible. So, for every $v \in G_1^i$ and ab $\in F_i$, $d(a, v) < d(b, v)$, where $a \in G_1^i$. Thus for each $e \in G_1^i$, $d_G^e(a, e) < d_G^e(b, e)$. By a similar argument, for each $e \in G_2^i$, $d_G^e(b, e) < d_G^e(a, e)$. We now assume that $uv \in F_i$ and $d(a, u) = d(b, u) + k$. If $k = 0$ then G is not bipartite, which contradicts Theorem 2. If $k < 0$ or $k > 2$ then G_1^i or G_2^i is not convex, respectively. Therefore, $d(b, v) = d(a, v) + 1$, $ab \parallel uv$ and $uv \parallel bv$.

On the other hand, $\{F_i, E(G_1^i), E(G_2^i)\}$ constitutes a partition for $E(G)$ and so if $uv \in F_i$ and $u \in G_1^i$ then $M_u(v) = E(G_2^i)$ and $M_v(u) = E(G_1^i)$. Thus $m_u(v)m_v(u) = |E(G_1^i)||E(G_2^i)|$ and we have

$$\begin{aligned} Sz_e(G) &= \sum_{uv\in E(G)} m_u(v)m_v(u) \\ &= \sum_{i=1}^{k}\sum_{uv\in F_i} |E(G_1^i)||E(G_2^i)| \\ &= \sum_{i=1}^{k} |F_i||E(G_1^i)||E(G_2^i)|, \end{aligned}$$

which completes our proof. □

Corollary 2. *With the conditions of Theorem 4, $PI_e(G) = |E(G)|^2 - \sum_{i=1}^k |F_i|^2$.*

Proof. In the proof of Theorem 4, we show that if $uv \in F_i$, $u \in G_1^i$, then $m_u(v) = |E(G_2^i)|$ and $m_v(u) = |E(G_1^i)|$. Since $E(G) = F_i \cup E(G_1^i) \cup E(G_2^i)$,

$$\begin{aligned} PI_e(G) &= \sum_{uv\in E(G)} [m_u(v) + m_v(u)] = \sum_{i=1}^{k}\sum_{e\in F_i}(|E(G)| - |F_i|) \\ &= \sum_{i=1}^{k} |F_i||E(G)| - \sum_{i=1}^{k} |F_i|^2 = |E(G)|^2 - \sum_{i=1}^{k} |F_i|^2, \end{aligned}$$

proving the result. □

Corollary 3. *If T is an n-vertex tree then $W_e(T) = Sz_e(T)$.*

Proof. By removing an edge of T, we obtain a two-component graph and both of the components are convex. To prove the result, it is enough to apply Theorems 3 and 4. □

Corollary 4. *Suppose $\{F_i\}_{i=1}^r$ is a partition of $E(G)$ such that $G \setminus F_i$ is a two-component graph with convex components G_1^i and G_2^i. Then*

$$Sz_{ev}(G) = \sum_{i=1}^{k}(|V(G_1^i)||E(G_2^i)| + |E(G_1^i)||V(G_2^i)|).$$

Proof. Apply the proof of Theorem 4. □

In what follows, we apply our results to compute the Wiener and edge Wiener index of the graph Y_n depicted in Fig. 1.

We now consider the coronene/circumcoronene homologous series X_k, $k \geq 0$. The first terms of this series are $X_0 =$ benzene, $X_1 =$ coronene, $X_2 =$ circumcoronene and $X_3 =$ circumcircumcoronene; see Fig. 2 where X_4 is shown.

It is clear that Y_n is isomorphic to the line graph of X_n. The edges seem to be geometrically parallel, constituting the partition $\{F_i\}$ of $E(G)$. By removing F_i from X_n, a graph is obtained in which one of the components, say $M(n, k)$, is depicted as in Fig. 3.

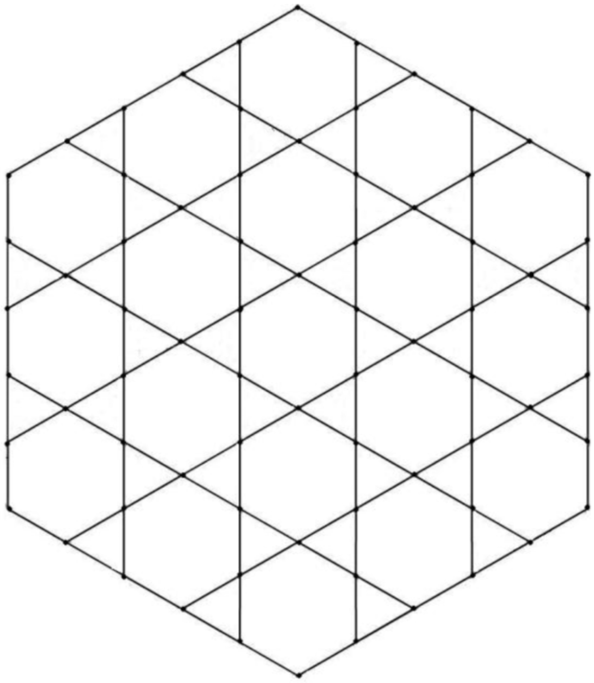

Fig. 1. The graph Y_2.

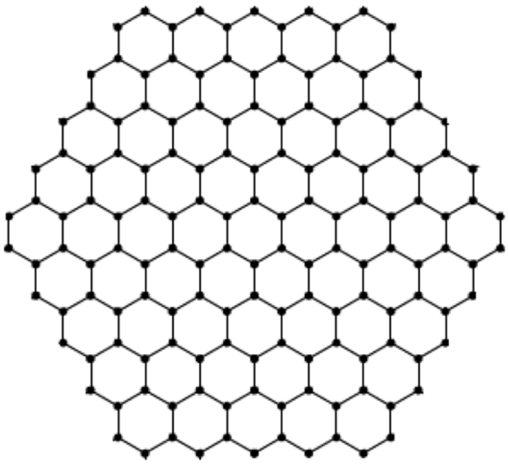

Fig. 2. The graph X_4.

Apply Theorem 3 and Corollary 1 to deduce that

$$\begin{aligned} W(y_n) &= W(L(X_n)) = W_e(X_n) + \binom{|E(X_n)|}{2} \\ &= 6\sum_{i=1}^{n}(|E(M(2n-i, n-i))|)(|E(X_n)| - |F_i| - |E(M(2n-i, n-i))|) \\ &\quad + 3|E(M(2n, n))|^2 + \binom{|E(X_n)|}{2}. \end{aligned} \tag{7}$$

On the other hand, $|E(M(n, k))| = 3nk + 2n + 5/2k - 3/2k^2 + 2$, $|E(X_n)| = 9n^2 + 15n + 6$ and $|F_i| = 2(n + i) - i$, $0 \le i \le n$. By substituting these values in Eq. (7), we obtain

$$W(L(X_n)) = 27 + 831/5n + 825/2n^2 + 507n^3 + 615/2n^4 + 369/5n^5.$$

The quantities PI_e, Sz_e and Sz_{ev} can also be calculated from the above calculations.

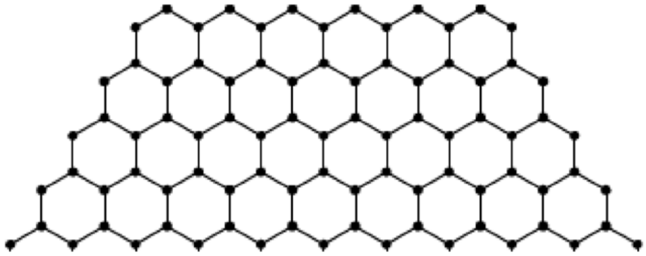

Fig. 3. The graph $M(9, 4)$.

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