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NOTE ON THE UNICYCLIC GRAPHS WITH THE FIRST THREE LARGEST WIENER INDICES

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Abstract. Let $G = (V, E)$ be a simple connected graph with vertex set V and edge set E. Wiener index $W(G)$ of a graph G is the sum of distances between all pairs of vertices in G, i.e., $W(G) = \sum_{\{u,v\} \subseteq G} d_G(u, v)$, where $d_G(u, v)$ is the distance between vertices u and v. In this note we give more precisely the unicyclic graphs with the first tree largest Wiener indices, that is, we found another class of graphs with the second largest Wiener index.

1. Introduction

Let us denote by $V(G)$ and $E(G)$ the set of vertices and edges, respectively, of a simple connected graph G. The order of G we will denote by $n(G)$ and it is n. We deal with unicyclic graphs, that is, the number of the edges is also n. If e is an edge of G, $G - \{e\}$ represents graph obtained from G by deleting edge e. The distance $d_G(u, v)$ between vertices u and v in G is the number of edges on a shortest path connecting these vertices. The distance of a vertex $v \in V(G)$, denoted by $d_G(v)$, is the sum of distances between v and all other vertices of G, $d_G(v) = \sum_{x \in V(G)} d_G(v, x)$. The Wiener index $W(G)$ of G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq G} d_G(u, v) = \frac{1}{2} \sum_{v \in V(G)} d_G(v). \tag{1.1}$$

This topological index was introduced by Wiener 1947 in [11]. This index found application in chemistry [3, 6]. At the begining, it was conceived only for trees.

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Wiener showed that for tree T on n vertices

$$W(T) = \sum_e n_1(e)n_2(e), \tag{1.2}$$

where summation goes over all edges of tree, $n_1(e)$ and $n_2(e)$ are the number of vertices which lie in the components of $T - \{e\}$. The definition of the Wiener index in terms of distances between vertices of a graph, such as equation (1.1) was first given by Hosoya [4]. This index attracted attention chemists and mathematicians. We will mentioned some important results. Between the trees the smallest Wiener index has the star S_n and the largest has the path P_n, while among connected graphs the smallest Wiener index has the complete graph K_n and the largest the path P_n [1, 2]. Operations on graphs which augment or reduce the Wiener index was studied in [5, 7–9]. The recent results on the distance based topological indices one can find in [12].

In this paper we improve theorem given in [10] about the unicyclic graphs with the first three largest Wiener indices, i.e., we found new class of graph with the second largest Wiener index.

2. Improvement

We use terminology from [10]. Let $G = (V, E)$ be an unicyclic graph with its unique circuit $C_m = v_1v_2 \dots v_mv_1$ of length m, $T_1, T_2, \dots, T_k$, $0 \le k \le m$, are all nontrivial components (they are all nontrivial trees) of $G - E(C_m)$, u_i is the common vertex of T_i and C_m, $i = 1, 2, \dots, k$. Such graph is denoted by $C_m^{u_1,u_2,\dots,u_k}(T_1, T_2, \dots, T_k)$. Specially, $G = C_n$ for $k = 0$. And if $k = 1$, we write $C_m(T_1)$ instead of $C_m^{u_1}(T_1)$. Let $n(T_i) = l_i + 1$, $i = 1, 2, \dots, k$, then $l = l_1 + l_2 + \cdots + l_k = n - m$. P_n is a path of order n.

Theorem 2.1. [10] *Let $G = C_m^{u_1,u_2,\dots,u_k}(T_1, T_2, \dots, T_k)$ be an (n, n)-graph of order $n \ge 6$. If $G \ncong C_3(P_{n-2}), C_4(P_{n-3})$, then*

$$W(G) \le W(C_3^{u_1}(T(n-5, 1, 1))) < W(C_4(P_{n-3})) < W(C_3(P_{n-2})),$$

with the equality if and only if $G \cong C_3^{u_1}(T(n-5, 1, 1))$, where $C_3^{u_1}(T(n-5, 1, 1))$ is showed in Figure 1.

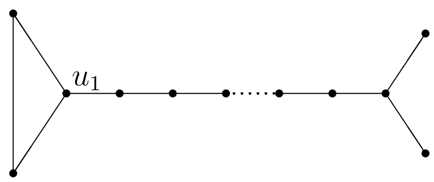

Figure 1. Graph $C_3^{u_1}(T(n-5, 1, 1))$

We discovered another class of graph $C_3^{u_1,u_2}(P_2, P_{n-3})$ with the second largest Wiener index. Graph from this class is showed in Figure 2.

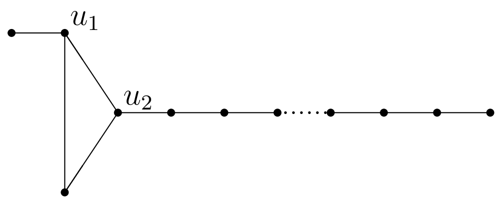

Figure 2. Graph $C_3^{u_1,u_2}(P_2, P_{n-3})$

Our improved theorem is the following theorem.

Theorem 2.2. *Let $G = C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)$ be an (n,n)-graph of order $n \geq 6$. If $G \ncong C_3(P_{n-2}), C_4(P_{n-3}), C_3^{u_1,u_2}(P_2, P_{n-3})$, then*

$$\begin{aligned} W(G) &\leq W(C_3^{u_1}(T(n-5,1,1))) < W(C_3^{u_1,u_2}(P_2, P_{n-3})) = W(C_4(P_{n-3})) \\ &< W(C_3(P_{n-2})), \end{aligned}$$

with the equality if and only if $G \cong C_3^{u_1}(T(n-5,1,1))$, and for $n = 7$ equality holds for $G \cong C_3^{u_1,u_2}(P_3, P_3)$.

In order to prove this theorem we use next theorem from [10].

Theorem 2.3. [10] *Let $G = C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)$ be an (n,n)-graph. Then*

$$\begin{aligned} W(G) =& W(C_m) + (n-m)\omega + (m-1)\sum_{i=1}^{k}\omega_i + \sum_{i=1}^{k} W(T_i) \\ &+ \sum_{i=1}^{k-1}\sum_{j=i+1}^{k}(l_i\omega_j + l_i l_j d_{C_m}(u_i,u_j) + l_j\omega_i), \end{aligned}$$

where $l_i = n(T_i) - 1$, $\omega_i = d_{T_i}(u_i)$, $i = 1, 2, \ldots, k$, $\omega = d_{C_m}(u)$, $u \in V(C_m)$.

Proof of Theorem 2.1. Using Theorem 2.3, we calculate the Wiener index of $C_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})$, i.e.,

$$\begin{aligned} W(C_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})) =& W(C_3) + (n-3)d_{C_3}(u) + 2(d_{P_{l_1+1}}(u_1) + d_{P_{l_2+1}}(u_2)) \\ &+ W(P_{l_1+1}) + W(P_{l_2+1}) + l_1 d_{P_{l_2+1}}(u_2) + l_1 l_2 d_{C_3}(u_1,u_2) \\ &+ l_2 d_{P_{l_1+1}}(u_1) \\ =& 3 + 2(n-3) + 2\left(\binom{l_1+1}{2} + \binom{l_2+1}{2}\right) + \binom{l_1+2}{3} \\ &+ \binom{l_2+2}{3} + l_1\binom{l_2+1}{2} + l_1 l_2 + l_2\binom{l_1+1}{2} \\ =& \frac{1}{6}\left(12n - 18 + l_1^3 + 9l_1^2 + 8l_1 + l_2^3 + 9l_2^2 + 8l_2\right. \\ &\left.+ 3l_1 l_2(l_1 + l_2 + 4)\right). \end{aligned}$$

Since $l_1 + l_2 = n - 3$, we get

$$W(C_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})) = \frac{1}{6}\left(n^3 - 7n + 12 - 6l_1l_2\right).$$

Since $W(C_3^{u_1}(T(n-5,1,1))) = \frac{1}{6}(n^3 - 13n + 30)$, we have

$$W(C_3^{u_1,u_2}(P_{l_1+1}, P_{l_2+1})) - W(C_3^{u_1}(T(n-5,1,1))) = n - 3 - l_1l_2.$$

If $l_1 = 1$ and $l_2 = n - 4$, we have $n - 3 - l_1l_2 = 1 > 0$, which means that the graphs $C_3^{u_1,u_2}(P_2, P_{n-3})$ have greater Wiener-index than $C_3^{u_1}(T(n-5,1,1)$ and $W(C_3^{u_1,u_2}(P_2, P_{n-3})) = n^3 - 13n + 36 = W(C_4(P_{n-3}))$. If $l_1 = 2$ and $l_2 = n - 5$, we have $n - 3 - l_1l_2 = 7 - n$, which is equal to 0 for $n = 7$. $\square$

The Theorem 2.1 is symmetrical with Theorem 7 from [10] which characterize the graphs with three smallest Wiener indices.

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