On the second maximal and minimal Wiener index of unicyclic graphs with given girth *

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Abstract

Let G be a connected graph. The Wiener index of G is defined as $W(G) = \sum_{u,v \in V(G)} d_G(u,v)$, where $d_G(u,v)$ is the distance between u and v in G and the summation goes over all the unordered pairs of vertices. In this paper, we investigate the Wiener index of unicyclic graphs with given girth and characterize the extremal graphs with the second maximal and second minimal Wiener index.

1 Introduction

Let G be a connected graph. The Wiener index of a graph G is defined in [14] as: $W(G) = \sum_{u,v \in V(G)} d_G(u,v)$, where $d_G(u,v)$ is the distance between u and v in G and the summation goes over all the unordered pairs of vertices. The Wiener index is one of the most studied topological indices, both from a theoretical point of view and applications [1, 2, 8]. Other topological indices of various classes of graphs can be seen in [5, 11, 12, 15, 16].

An important direction in chemical graph theory is to determine the extremal (maximal or minimal) graphs with respect to some topological index in a certain classes of graphs. Du and Zhou in [3] characterized trees and unicyclic graphs with given matching number and minimal Wiener index. Using the connection between the Wiener index and the Laplacian coefficients, the authors in [9] determined the minimum Wiener index of trees

*Supported by The Postdoctoral Science Foundation of Central South University, China Postdoctoral Science Foundation(20110491275), NNSFC (11101245), NSFSD (BS2010SF017, ZR2011AQ005), BMNSF(4112052) and Research Grant 144007 of Serbian Ministry of Science.

with fixed diameter or radius. Fischermann et al. [4] determined the extremal trees with maximum and minimum Wiener index among trees with given maximum vertex degree. Xu and Xu [15] determined all the unicyclic graphs of order n with given maximum degree and maximal Hosoya index and minimal Merrifield-Simmons index.

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For two distinct vertices x and y in $V(G)$, the distance between x and y is the number of edges in a shortest path joining x and y. Let $D_G(u)$ be the sum of all distances from the vertex $u \in V(G)$ to all other vertices from $V(G)$. For $E' \subset E$, we use $G - E'$ to denote the graph obtained from G by deleting the edges in E'. If $e = uv \in E(G)$, we write $G - uv$ instead of $G - \{e\}$. Let C_n and P_n denote the cycle and path with n vertices, respectively. By $L_{n,k}$ we denote the graph obtained from C_k and P_{n-k+1} by identifying a vertex of C_k with one endvertex of P_{n-k+1}. We denote by $F_{n,k}$ the graph obtained from C_k by adding $n - k$ pendent vertices to a vertex of C_k.

A unicyclic graph is a connected graph with equal vertex number and edge number. Let $\mathcal{U}_{n,k}$ be the set of all unicyclic graphs of order $n \geq 3$ and girth $k \geq 3$. For $U_{n,k} \in \mathcal{U}_{n,k}$, if $k = n$, then $U_{n,k} \cong C_n$; if $k = n - 1$, then $U_{n,k} \cong L_{n,n-1}$. So in the following we assume that $3 \leq k \leq n - 2$.

The Wiener indices of C_n and $L_{n,n-1}$ are: $W(C_n) = \frac{n}{2}\lfloor\frac{n^2}{4}\rfloor$; $W(L_{n,n-1}) = \frac{n^3-n^2+6n-8}{8}$, if n is even; $W(L_{n,n-1}) = \frac{n^3-n^2+7n-7}{8}$, if n is odd.

The authors in [17] determined the extremal graphs with the maximal and minimal Wiener index among unicyclic graphs with n vertices and girth k.

Theorem 1.1 *Let $U_{n,k} \in \mathcal{U}_{n,k}$ $(3 \leq k \leq n-2)$ be a unicyclic graph with girth k.*

If k is even, then $\frac{k^3}{8} + (n-k)(\frac{k^2}{4} + n - 1) \leq W(U_{n,k}) \leq \frac{k^3}{8} + (n-k)(\frac{n^2+nk+3k-1}{6} - \frac{k^2}{12})$. The left equality holds if and only if $U_{n,k} \cong F_{n,k}$, and the right equality holds if and only if $U_{n,k} \cong L_{n,k}$.

If k is odd, then $\frac{k^3-k}{8} + (n-k)(\frac{k^2-1}{4} + n - 1) \leq W(U_{n,k}) \leq \frac{k^3-k}{8} + (n-k)(\frac{n^2+nk+3k-1}{6} - \frac{k^2}{12} - \frac{1}{4})$. The left equality holds if and only if $U_{n,k} \cong F_{n,k}$, and the right equality holds if and only if $U_{n,k} \cong L_{n,k}$.

Corollary 1.2 *Let G be a unicyclic graph of order $n \geq 4$. Then $n^2 - 2n \leq W(G) \leq \frac{1}{6}(n^3 - 7n + 12)$. The left equality holds if and only if $U \cong F_{n,3}$ for $n \geq 6$, and the right equality holds if and only if $G \cong L_{n,3}$. For $n = 4$, there are exactly two unicyclic graphs C_4 and $L_{4,3}$, with equal Wiener index 8. For $n = 5$, the left equality holds if and only if G is C_5 or $F_{5,3}$, with Wiener index 15.*

In this paper we continue the research and obtain the extremal graphs with the second maximal and second minimal Wiener index among unicyclic graphs with n vertices and girth k.

We implemented a linear $O(|V|)$ algorithm for calculating the Wiener index of unicyclic graphs. In Table 1, we present the computational results for the second-minimal and the second-maximal value of Wiener index of unicyclic graphs on $n = 5$ to $n = 14$ vertices for every girth $3 \leq k \leq n-2$, with the number of extremal graphs in the parenthesis. The extremal graphs $L^3_{n,k}$ are labeled with asterisk, while the other extremal graphs are $L^1_{n,k}$, where $L^3_{n,k}$ and $L^1_{n,k}$ are defined in Section 4.

	3	4	5	6	7	8	9	10	11	12
5	16 (1)									
5	16 (1)									
6	26 (1)	27 (1)								
6	29 (1)	28 (1)								
7	38 (1)	40 (1)	40 (1)							
7	48 (1)	46 (1)	41 (1)							
8	52 (1)	55 (1)	56 (1)	60 (1)						
8	74 (1)	71 (1)	63 (1)	62 (1)						
9	68 (1)	72 (1)	74 (1)	80 (1)	83 (1)					
9	108 (1)	104 (1)	93* (2)	90 (1)	85 (1)					
10	86 (1)	91 (1)	94 (1)	102 (1)	107 (1)	115 (1)				
10	151 (1)	146 (1)	133* (1)	127 (1)	118 (1)	118 (1)				
11	106 (1)	112 (1)	116 (1)	126 (1)	133 (1)	144 (1)	151 (1)			
11	204 (1)	198 (1)	183* (1)	174* (2)	162* (1)	158 (1)	154 (1)			
12	128 (1)	135 (1)	140 (1)	152 (1)	161 (1)	175 (1)	185 (1)			
12	268 (1)	261 (1)	244* (1)	233* (1)	218* (1)	209* (2)	200 (1)	202 (1)		
13	152 (1)	160 (1)	166 (1)	180 (1)	191 (1)	208 (1)	221 (1)	238 (1)	250 (1)	
13	344 (1)	336 (1)	317* (1)	304* (1)	286* (1)	274* (1)	260* (1)	256 (1)	254 (1)	
14	178 (1)	187 (1)	194 (1)	210 (1)	223 (1)	243 (1)	259 (1)	280 (1)	296 (1)	315 (1)
14	433 (1)	424 (1)	403* (1)	388* (1)	367* (1)	352* (1)	334* (1)	324* (1)	315 (1)	320 (1)

Table 1: Wiener index of unicyclic graphs with small order.

2 Preliminaries

Lemma 2.1 *[17] Let G_0 be a connected graph of order $n_0 > 1$ and $u \in V(G_0)$. Let T be a tree of order $n_1 > 1$ and $v \in V(T)$, $N_T(v) = \{v_1, v_2, \ldots, v_s\}$. Let G_1 be the graph obtained from G_0 and T by adding edge uv, $G_2 = G_1 - vv_1 - vv_2 - \ldots - vv_s + uv_1 + uv_2 + \ldots + uv_s$. Then $W(G_1) > W(G_2)$.*

Lemma 2.2 *[10] Let G be a connected graph and $v \in V(G)$. Graph $G^*_{s,m}$ is obtained from G by attaching two paths $P = vv_1 \ldots v_s$ and $Q = vu_1 \ldots u_m$ of lengths s and m $(s \geq m \geq 1)$ at v. Then $W(G^*_{s,m}) < W(G^*_{s+1,m-1})$.*

Lemma 2.3 *[17] Let G_0 be a connected graph of order $n_0 > 1$ and $u_0, v_0 \in V(G_0)$ be two distinct vertices in G_0. $P_s = u_1u_2 \ldots u_s$ and $P_t = v_1v_2 \ldots v_t$ are two paths of order s and t, respectively. Let G be the graph obtained from G_0, P_s and P_t by adding edges u_0u_1, v_0v_1. Suppose that $G_1 = G - u_0u_1 + v_tu_1$ and $G_2 = G - v_0v_1 + u_sv_1$. Then either $W(G) < W(G_1)$ or $W(G) < W(G_2)$ holds.*

Lemma 2.4 *[10] Let H,X,Y be three connected graphs disjoint in pairs. Suppose that u, v are two vertices of H, $v' \in V(X)$ and $u' \in V(Y)$. Let G be the graph obtained from H, X, Y by identifying v with v' and u with u', respectively. Let G' be the graph obtained from H, X, Y by identifying the vertices v, v', u', and G'' be the graph obtained from H, X, Y by identifying the vertices u, v', u'. Then $W(G') < W(G)$ or $W(G'') < W(G)$.*

3 The second minimal Wiener index

Let $F^1_{n,k}$ and $F^2_{n,k}$ be the unicyclic graphs depicted in Fig. 1. The graph $F^1_{n,k}$ is obtained from a cycle C_k by attaching $n-k-1$ pendent vertices to a vertex u_0 of C_k, and one pendent vertex to a vertex $v_0 \neq u_0$ of C_k. The graph $F^2_{n,k}$ is obtained from C_k by attaching $n-k-2$ pendent vertices and a path P_2 to a vertex u_0 of C_k.

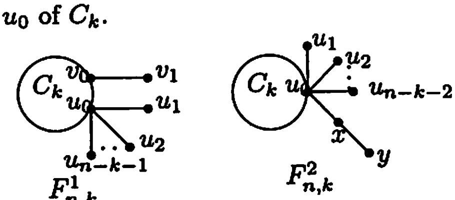


Figure 1. Two extremal unicyclic graphs

Lemma 3.1 *Let $U_{n,k} \in \mathcal{U}_{n,k}$ be a unicyclic graph with the second minimal Wiener index and girth k $(3 \leq k \leq n-2)$. Then $U_{n,k}$ must be of the form $F^i_{n,k}$ $(i = 1, 2)$.*

Proof. Let C_k be the unique cycle in $U_{n,k}$. Note that there is at least one vertex u on C_k of degree greater than two.

If there are at least three vertices on C_k of degree greater than 2, then by Lemma 2.1 and Lemma 2.4, there exists a graph of the form $F^1_{n,k}$ such that $W(U_{n,k}) > W(F^1_{n,k}) > W(F_{n,k})$, which contradicts to the fact that $U_{n,k}$ has the second minimal Wiener index. Hence, there are at most two vertices in C_k of degree at least 3.

If there are exactly two vertices of C_k with degree at least 3, then by Lemma 2.1 and Lemma 2.4, we conclude that $U_{n,k}$ must be of the form $F^1_{n,k}$.

If there is exactly one vertex of C_k with degree at least 3, then by Lemma 2.1, we conclude that $U_{n,k}$ must be of the form $F^2_{n,k}$. ■

Now we can present the proof of the main result of this section.

Theorem 3.2 *Let $U_{n,k} \in \mathcal{U}_{n,k}$ be a unicyclic graph with the second minimal Wiener index and girth k ($3 \leq k \leq n-2$). Then $U_{n,k} \cong F^1_{n,k}$ (as shown in Fig. 1).*

Proof. By Lemma 3.1, we need to compare $W(F^1_{n,k})$ and $W(F^2_{n,k})$.

We can calculate the Wiener index of $W(F^1_{n,k})$ by summing the Wiener index of $F_{n-1,k}$ and $D_{F^1_{n,k}}(v_1)$. Let l be the distance between u_0 and v_0.

$W(F^1_{n,k}) = \frac{k^3}{8} + (n-k-1)(\frac{k^2}{4} + n - 2) + \frac{k^2}{4} + (n-k-1)(l+1) + n - 1$, if k is even;

$W(F^1_{n,k}) = \frac{k^3-k}{8} + (n-k-1)(\frac{k^2-1}{4} + n - 2) + \frac{k^2-1}{4} + (n-k-1)(l+1) + n - 1$, if k is odd.

It follows that $W(F^1_{n,k})$ attains the minimum for $l = 1$.

Similarly, we have

$W(F^2_{n,k}) = \frac{k^3}{8} + (n-k-1)(\frac{k^2}{4} + n - 2) + \frac{k^2}{4} + 3n - k - 5$, if k is even;

$W(F^2_{n,k}) = \frac{k^3-k}{8} + (n-k-1)(\frac{k^2-1}{4} + n - 2) + \frac{k^2-1}{4} + 3n - k - 5$, if k is odd.

From the above computations, it follows $W(F^1_{n,k}) - W(F^2_{n,k}) = (3n - 2k - 3) - (3n - k - 5) = -k + 2 < 0$, and $F^1_{n,k}$ has the second minimal Wiener index in $\mathcal{U}_{n,k}$. ∎

For $n = 5$ the second minimum Wiener index is 16, which is achieved only for $F_{5,4}$ and $F^1_{5,3}$. For $n = 6$, the second minimum Wiener index is 26 which is achieved only for $F_{6,4}$, $F_{6,5}$ and $F^1_{6,3}$.

Corollary 3.3 *Among unicyclic graphs on $n \geq 7$ vertices, the second minimum Wiener index is $n^2 - n - 4$ which is achieved only at $F_{n,4}$ or $F^1_{n,3}$.*

Proof. According to Theorem 1.1 and Theorem 3.2, the second minimum value of the Wiener index is achieved at $F_{n,k}$ ($k \neq 3$) or $F^1_{n,k}$.

Case 1. The graphs $F_{n,k}$ with $k > 3$.

If k is odd, from Theorem 1.1, we have $W(F_{n,5}) = n^2 - 10$ and $W(F_{n,k}) - W(F_{n,5}) = \frac{1}{4}(k^2 - 4k - 5)n - \frac{k^3}{8} + \frac{9k}{8} + 10 \geq \frac{1}{4}(k^2 - 4k - 5)(k+1) - \frac{k^3}{8} + \frac{9k}{8} + 10 = \frac{1}{8}(k-5)(k^2 - k - 14) \geq 0$, with equality if and only if $k = 5$ and $n = 6$.

If k is even, we have $W(F_{n,4}) = n^2 - n - 4$ and $W(F_{n,k}) - W(F_{n,4}) = \frac{1}{4}(k^2 - 4k)n - \frac{k^3}{8} + k + 4 \geq \frac{1}{4}(k^2 - 4k)(k+1) - \frac{k^3}{8} + k + 4 = \frac{1}{8}(k-4)^2(k+2) \geq 0$, with equality if and only if $k = 4$.

It is easy to see that $W(F_{n,5}) > W(F_{n,4})$ for $n > 6$ and $W(F_{6,5}) = W(F_{6,4})$.

Case 2. The graphs $F^1_{n,k}$.

If $k > 3$ is odd, we have $W(F^1_{n,3}) = n^2 - n - 4$ and $W(F^1_{n,k}) - W(F^1_{n,3}) = \frac{k-3}{8}(2n(k-1) - k^2 - 3k - 8) \geq \frac{k-3}{8}(2(k+1)(k-1) - k^2 - 3k - 8) = \frac{k-3}{8}(k-5)(k+2) \geq 0$, with equality if and only if $k = 5$ and $n = k + 1$.

If $k > 4$ is even, we have $W(F^1_{n,4}) = n^2 - 9$ and $W(F^1_{n,k}) - W(F^1_{n,4}) = \frac{k-4}{8}(2nk - k^2 - 4k - 16) \geq \frac{k-4}{8}(2(k+1)k - k^2 - 4k - 16) = \frac{k-4}{8}(k^2 - 2k - 16) \geq 0$.

It is easy to see that $W(F^1_{n,3}) < W(F^1_{n,4})$ for $n > 5$.

Combining the above two cases, we get that the second minimum Wiener index is achieved for $F_{n,4}$ and $F^1_{n,3}$. ■

4 The second maximal Wiener index

Let $H_1 = L^1_{n,k}(s,t)$, $H_2 = L^2_{n,k}(s,t)$ and $H_3 = L^3_{n,k}(s,t;l)$ be the graphs described below, where $s + t = n - k$ and $1 \leq l \leq t - 1$.

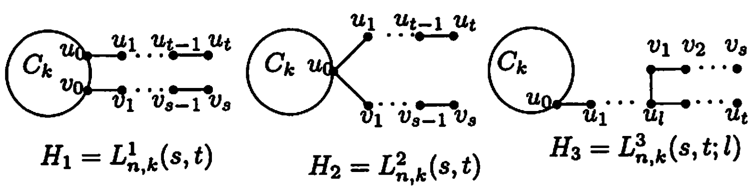


Figure 2. Three classes of unicyclic graphs

Lemma 4.1 *Let $U_{n,k} \in \mathcal{U}_{n,k}$ be a unicyclic graph with the second maximal Wiener index and girth k $(3 \leq k \leq n-2)$. Then $U_{n,k}$ is of the form H_i $(i = 1,2,3)$, where $s + t + k = n$ (as shown in Fig. 2).*

Proof. Let C_k be the unique cycle in $U_{n,k}$. By Theorem 1.1, there exist at least two vertices of degree greater than two in $U_{n,k}$. Note that there is at least one vertex u on C_k of degree greater than two.

If there are at least three vertices on C_k of degree greater than 2, then by Lemma 2.2 and Lemma 2.3, there exists a graph of the form H_1 such that $W(U_{n,k}) < W(H_1) < W(L_{n,k})$, which contradicts to the fact that $U_{n,k}$ has the second maximal Wiener index. Hence, there are at most two vertices in C_k of degree at least 3.

Case 1. $3 \leq k \leq n-4$.

If $deg(u) \geq 5$, by Lemma 2.2 and Lemma 2.3, there exists a graph of the form H_2 such that $W(U_{n,k}) < W(H_2) < W(L_{n,k})$, which is a contradiction. Hence, $3 \leq deg(u) \leq 4$. Let v be a vertex of degree greater than 2, different from u. We consider the following two subcases.

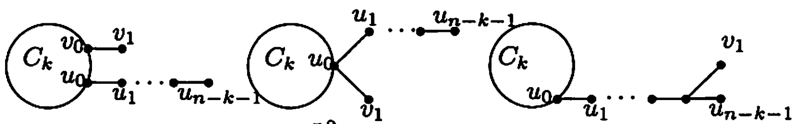
Subcase 1.1. $v \in V(C_k)$. Similarly we have $3 \leq deg(v) \leq 4$. If at least one of the vertices u and v has degree 4, then by Lemma 2.2, there exists a graph of the form H_1 such that $W(U_{n,k}) < W(H_1) < W(L_{n,k})$, which is a contradiction. Therefore, it follows $deg(u) = deg(v) = 3$ and all other vertices of $U_{n,k}$ have degree 1 or 2.

Subcase 1.2 $v \notin V(C_k)$. If there are other vertices not from C_k with degree greater than 2, then by Lemma 2.3, there exists a graph of the form

H_3 such that $W(U_{n,k}) < W(H_3) < W(L_{n,k})$, which is impossible. Hence, we can assume that u and v are the only vertices of degree greater than 2 in $U_{n,k}$. Similarly as above, we conclude that $deg(u) = 3$ and $deg(v) = 3$.

Case 2. $k = n-3$, $k = n-2$. Using a similar reasoning as in Case 1, we can get that G must be of the form H_1, which implies the result. ■

Let $\mathcal{L}^i_{n,k}$ be the set of all unicyclic graphs of the form like H_i $(i = 1, 2, 3)$, respectively.



$L^1_{n,k}$ $L^2_{n,k}$ $L^3_{n,k}$

Figure 3. The extremal unicyclic graphs

Lemma 4.2 *For* $3 \le k \le n-4$, $L^i_{n,k}$ $(i = 1, 2, 3)$ *(see Fig. 3) is the only graph with the second maximal Wiener index in* $\mathcal{L}^i_{n,k}$ $(i = 1, 2, 3)$, *respectively.*

Proof. We will consider three cases.

Case 1. For graphs in $\mathcal{L}^1_{n,k}$. Let $L^1_{n,k}(s,t) \setminus \{u_2, \ldots, u_t, v_2, \ldots, v_s\}$ be the graph G_0 from Lemma 2.3. Then, we get $W(L^1_{n,k}(s,t)) \le W(L^1_{n,k}(1, n-k-1))$, which implies the result.

Case 2. For graphs in $\mathcal{L}^2_{n,k}$. By repetitive application of Lemma 2.2, we get the result.

Case 3. For graphs in $\mathcal{L}^3_{n,k}$. By Lemma 2.2, we have $W(L^3_{n,k}(s,t;l)) \le W(L^3_{n,k}(1, n-k-1; l))$. This means that the pendent vertex v_1 is attached at u_l, $1 \le l \le n-k-2$. Color the vertices in $L^3_{n,k}(1, n-k-1; l) \setminus \{u_{l-1}, u_l, u_{l+1}, \ldots, u_{n-k-1}, v_1\}$ red, and $u_{l-1}, u_l, u_{l+1}, \ldots, u_{n-k-1}$ blue. It follows that $W(L^3_{n,k}(1, n-k-1; l)) \le W(L^3_{n,k}(1, n-k-1; n-k-2))$, because the distance between a red vertex and a blue vertex remains unchanged, the sum of distances between v_1 and blue vertices remains unchanged, while the distance between a red vertex and v_1 increases. The equality holds if and only if $l = n-k-2$. ■

Now we can present the proof of the main result of this section. The cases $5 \le n \le 12$ are presented in Table 1.

Theorem 4.3 *Let* $U_{n,k} \in \mathcal{U}_{n,k}$ *be a unicyclic graph with the second maximal Wiener index and girth* k $(3 \le k \le n-2)$ *and* $n \ge 13$.
(i) If $k = 3$, $k = 4$, $k = n-3$ *or* $k = n-2$, *then* $U_{n,k} \cong L^1_{n,k}$ *(as shown in Fig. 3), with* $d(u_0, v_0) = \lfloor \frac{k}{2} \rfloor$;
(ii) If $5 \le k \le n-4$, *then* $U_{n,k} \cong L^3_{n,k}$ *(as shown in Fig. 3).*

Proof. By Lemma 4.1 and Lemma 4.2, we need only to consider the values $W(L^1_{n,k})$, $W(L^2_{n,k})$ and $W(L^3_{n,k})$. From Lemma 2.4, we have $W(L^1_{n,k}) > W(L^2_{n,k})$. Therefore, we need to compare $W(L^1_{n,k})$ and $W(L^3_{n,k})$.

It is well known that (see [6]) $D_{C_k}(u) = \lfloor \frac{k^2}{4} \rfloor$.

We can calculate the Wiener index of $W(L^1_{n,k})$ by summing the Wiener index of $L_{n-1,k}$ and $D_{L^1_{n,k}}(v_1)$. Let l be the distance between u_0 and v_0.

$W(L^1_{n,k}) = \frac{k^3}{8} + (n-k-1)(\frac{(n-1)^2+(n-1)k+3k-1}{6} - \frac{k^2}{12}) + \frac{k^2}{4} + \frac{(n-k)(n-k-1)}{2} + (n-k-1)l + n - 1$, if k is even;

$W(L^1_{n,k}) = \frac{k(k^2-1)}{8} + (n-k-1)(\frac{(n-1)^2+(n-1)k+3k-1}{6} - \frac{k^2}{12} - \frac{1}{4}) + \frac{k^2-1}{4} + \frac{(n-k)(n-k-1)}{2} + (n-k-1)l + n - 1$, if k is odd.

We get that $W(L^1_{n,k})$ attains the maximum value for $l = \lfloor \frac{k}{2} \rfloor$.

Similarly, we have

$W(L^3_{n,k}) = \frac{k^3}{8} + (n-k-1)(\frac{(n-1)^2+(n-1)k+3k-1}{6} - \frac{k^2}{12}) + \frac{k^2}{4} + \frac{(n-k-2)(n-k-1)}{2} + (n-k-1)k + 2$, if k is even;

$W(L^3_{n,k}) = \frac{k(k^2-1)}{8} + (n-k-1)(\frac{(n-1)^2+(n-1)k+3k-1}{6} - \frac{k^2}{12} - \frac{1}{4}) + \frac{k^2-1}{4} + \frac{(n-k-2)(n-k-1)}{2} + (n-k-1)k + 2$, if k is odd.

From the above computations, for $3 \le k \le n-3$ it follows $W(L^1_{n,k}) - W(L^3_{n,k}) = \left(\frac{(n-k)(n-k-1)}{2} + (n-k-1)\lfloor \frac{k}{2} \rfloor + n - 1\right) = -\left(\frac{(n-k-2)(n-k-1)}{2} + (n-k-1)k + 2\right) = -(n-k-1)\left(\lceil \frac{k}{2} \rceil - 1\right) + n - 3$.

Consider the quadratic function $f(k) = -(n-k-1)\left(\lceil \frac{k}{2} \rceil - 1\right) + n - 3$. We have $f(4) = 2 > 0$ and $f(5) = 9 - n < 0$; while on the other side, $f(n-4) = n + 6 - 3\lceil \frac{n}{2} \rceil < 0$ and $f(n-3) = n - 1 - 2\lceil \frac{n-3}{2} \rceil > 0$. For $5 \le k \le n-4$, we conclude that $f(k) < 0$ and $L^3_{n,k}$ has the second maximum Wiener index, while for $k = 3, 4, n-3, n-2$ the graph $L^1_{n,k}$ has the second maximum Wiener index. ■

From the above proof and the values $f(5)$, $f(n-4)$ and $f(n-3)$, it follows that for $(n,k) \in \{(9,5),(11,6),(12,8)\}$, there are two extremal unicyclic graphs (as shown in Table 1).

Corollary 4.4 *Among unicyclic graphs on $n \ge 5$ vertices, the second maximum Wiener index is $\frac{1}{6}(n^3 - 13n + 36)$ which is achieved only at $L_{n,4}$ or $L^1_{n,3}$.*

Proof. According to Theorem 1.1 and Theorem 4.3, the second maximal value of the Wiener index is achieved at $L_{n,k}$ $(k \ne 3)$, $L^1_{n,k}$ or $L^3_{n,k}$.

Case 1. The graphs $L_{n,k}$ with $k > 3$.

If k is odd, we have $W(L_{n,5}) = \frac{1}{6}(n^3 - 25n + 90)$ and $W(L_{n,5}) - W(L_{n,k}) = \frac{1}{4}(k^2 - 2k - 15)n - \frac{5}{24}k^3 + \frac{1}{2}k^2 - \frac{7k}{24} + 15 \ge \frac{1}{4}(k^2 - 2k + 15)(k+1) - \frac{5}{24}k^3 + \frac{1}{2}k^2 - \frac{7k}{24} + 15 = \frac{1}{24}(k-5)(k^2 + 11k - 54) \ge 0$, with equality if and only if $k = 5$ and $n = 6$.

If k is even, we have $W(L_{n,4}) = \frac{1}{6}(n^3 - 13n + 36)$ and $W(L_{n,4}) - W(L_{n,k}) = \frac{1}{4}(k^2 - 2k - 8)n - \frac{5}{24}k^3 + \frac{1}{2}k^2 - \frac{k}{6} + 6 \geq \frac{1}{4}(k^2 - 2k - 8)(k + 1) - \frac{5}{24}k^3 + \frac{1}{2}k^2 - \frac{k}{6} + 6 = \frac{1}{24}(k - 4)(k + 12)(k - 2) \geq 0$, with equality if and only if $k = 4$.

It is easy to see that $W(L_{n,5}) < W(L_{n,4})$ for $n \geq 5$.

Case 2. The graphs $L^1_{n,k}$.

If $k > 3$ is odd, we have $W(L^1_{n,3}) = \frac{1}{6}(n^3 - 13n + 36)$ and $W(L^1_{n,3}) - W(L^1_{n,k}) = \frac{1}{4}(k^2-9)n-\frac{5}{24}k^3-\frac{7}{24}k+\frac{13}{2} \geq \frac{1}{4}(k^2-9)(k+1)-\frac{5}{24}k^3-\frac{7}{24}k+\frac{13}{2} = \frac{k-3}{24}(k^2 + 9k - 34) \geq 0$, with equality if and only if $k = 3$.

If $k > 4$ is even, we have $W(L^1_{n,4}) = \frac{1}{6}(n^3 - 19n + 66)$ and $W(L^1_{n,4}) - W(L^1_{n,k}) = \frac{1}{4}(k^2-16)n-\frac{5}{24}k^3+\frac{1}{3}k+12 \geq \frac{1}{4}(k^2-16)(k+1)-\frac{5}{24}k^3+\frac{1}{3}k+12 = \frac{k-4}{24}(k^2 + 10k - 48) \geq 0$, with equality if and only if $k = 4$.

It is easy to see that $W(L^1_{n,3}) > W(L^1_{n,4})$ for $n \geq 5$.

Case 3. The graphs $L^3_{n,k}$.

If $k > 3$ is odd, we have $W(L^3_{n,3}) = \frac{1}{6}(n^3 - 13n + 30)$ and $W(L^3_{n,3}) - W(L^3_{n,k}) = \frac{1}{4}(k^2 - 2k - 3)n - \frac{5}{24}k^3 + \frac{1}{2}k^2 - \frac{7}{24}k + 2 \geq \frac{1}{4}(k^2 - 2k - 3)(k + 1) - \frac{5}{24}k^3 + \frac{1}{2}k^2 - \frac{7}{24}k + 2 = \frac{k-3}{24}(k + 10)(k - 1) \geq 0$, with equality if and only if $k = 3$.

If $k > 4$ is even, we have $W(L^3_{n,4}) = \frac{1}{6}(n^3 - 19n + 54)$ and $W(L^3_{n,4}) - W(L^3_{n,k}) = \frac{1}{4}(k^2 - 2k - 8)n - \frac{5}{24}k^3 + \frac{1}{2}k^2 - \frac{1}{6}k + 6 \geq \frac{1}{4}(k^2 - 2k - 8)(k + 1) - \frac{5}{24}k^3 + \frac{1}{2}k^2 - \frac{1}{6}k + 6 = \frac{k-4}{24}(k + 12)(k - 2) \geq 0$, with equality if and only if $k = 4$.

It is easy to see that $W(L^3_{n,3}) > W(L^3_{n,4})$ for $n \geq 5$.

Combining the above three cases, and comparing $\frac{1}{6}(n^3 - 13n + 36)$ with $W(L^3_{n,3})$, we get that the second maximum Wiener index is achieved for $L_{n,4}$ and $L^1_{n,3}$. ■

Acknowledgement: The authors are grateful to the referee for his many helpful comments to an earlier version of this paper.

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