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Extremal Wiener Index of Graphs with Given Number of Vertices of Odd Degree

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Abstract

The Wiener index of a connected graph is the sum of distances between all pairs of vertices. Let $\mathbb{G}(n, 2k)$ be the set of all graphs on n vertices with exactly $2k$ vertices of odd degree. $\mathbb{G}(n, 0)$ is just the set of all Eulerian graphs on n vertices. In Gutman et al. (2014) and Dankelmann (2021), the authors characterized the graphs $\mathbb{G}(n, 0)$ with the first four minimum Wiener index and the first two maximum Wiener index. In the paper, we characterize the graph in $\mathbb{G}(n, 2k)$ with the minimum Wiener index for all $0 \le k \le \frac{n}{2}$, and the graph in $\mathbb{G}(n, 2)$ with the first-maximum and second-maximum Wiener index.

1 Introduction

All graphs considered in this article are finite, undirected, connected, without loops and multiple edges. Let $G = (V, E)$ be a graph. The *distance* between vertices u and v of G, denoted by $d_G(u, v)$, is the number of edges on a shortest path connecting these vertices in G. The distance of a vertex

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$v \in V(G)$, $\sigma_G(v)$, is the sum of distances between v and all other vertices of G. The *Wiener index* of G is a graph invariant based on distances in a graph. It is denoted by $W(G)$ and defined as the sum of distances between all pairs of vertices in G:

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

The Wiener index is the oldest and one among the most investigated topological indices in mathematical chemistry and in related disciplines. It has been investigated extensively in many literature. From the middle of the 1970s, the Wiener index gained much popularity and new results related to it are constantly being reported. For a review, historical details and further bibliography on the chemical applications of the Wiener index see [2, 3, 6, 9, 11].

An Euler tour is a closed walk in a graph that traverses every edge exactly once. A graph is Eulerian if it admits an Euler tour, and a graph is Eulerian if and only if it is connected and all its vertices have even degrees. Recently, the Wiener index of an Eulerian graph was considered in [1, 5]. Gutman, Cruz and Rada [5] characterized the Eulerian graphs with the first four minimal Wiener indices, and proved that the cycle is the unique graph maximising the Wiener index among all Eulerian graphs of given order. They also conjectured that for Eulerian graphs of order $n \geq 26$ the graph consisting of a cycle on $n-2$ vertices and a triangle that share a vertex is the unique Eulerian graph with second largest Wiener index. This conjecture was proved by Dankelmann [1].

Note that an Eulerian graph has no vertex of odd degree. This leads naturally to determine the extremal Wiener indices and characterize the extremal graphs among all graphs with given number of vertices of odd degree. It is well known that every nontrivial tree has at least two vertices of degree one. Among all trees of given order that have only vertices of odd degrees, Lin [7] characterized the trees which maximize and minimize the Wiener index, then trees with second, third, ..., seventeenth maximal Wiener index were characterized in [4]. Also, Lin [8] characterized the trees which minimize and maximize the Wiener index among all trees with given number of vertices of even degree, respectively.

In this paper, we continue to study the extremal Wiener index of graphs with $2k$ vertices of odd degree. Specially, they are Eulerian for $k = 0$.

Let $\mathbb{G}_{n,2k}$ be the set of all n-vertex graphs with exactly $2k$ vertices of odd degree, where $0 \leq k \leq \frac{n}{2}$. We will characterize the graphs among $\mathbb{G}_{n,2k}$ with the smallest, the first and the second greatest Wiener indices.

Some terminologies and notations we use are as follows. Let $G = (V, E)$ be a graph, a path $P = v_1v_2 \cdots v_t$ is a pendant path of G if $d_G(v_t) = 1$, $d_G(v_1) \geq 3$ and $d_G(v_2) = \cdots = d_G(v_{t-1}) = 2$. An edge $e \in E$ of a connected graph G is called a cut edge if the graph $G - e$ obtained by deleting the edge e is disconnected. A vertex $u \in V$ of a simple and connected graph G is called a cut vertex if the graph $G - u$ obtained by deleting the vertex u is disconnected. If v is a cut vertex of G and H a component of $G - v$, then we say that the subgraph $G[V(H) \cup \{u\}]$, induced by $V(H) \cup \{u\}$, is a branch of G at u. If u is a vertex of G, then the number of vertices of G adjacent to u is called the degree of u in G, denoted by $d_G(v)$.

2 The graph with the minimal Wiener index

Denote by K_n the complete graph on n vertices. If n is odd, then K_n has no vertex of odd degree. If n is even, then all vertices in K_n are of odd degree. Let M_t be a set of t independent edges from K_n. Then $K_n \setminus M_t \in \mathbb{G}_{n,2k}$, where $t = k$ for odd n and $t = \frac{n}{2} - k$ for even n.

Theorem 1. *(i) If n is odd, then the unique graph among $\mathbb{G}_{n,2k}$ with the minimal Wiener index is $K_n \setminus M_k$;*
(ii) If n is even, then the unique graph among $\mathbb{G}_{n,2k}$ with the minimal Wiener index is $K_n \setminus M_{\frac{n}{2}-k}$.

Proof. Let $G \in \mathbb{G}_{n,2k}$, $V(G) = \{v_1, v_2, \cdots, v_n\}$ and $v_1, v_2, \cdots, v_{2k}$ all vertices of odd degree in G.

If n is odd, then $d_G(v_i) \leq n - 2$ and at least one vertex in G is not adjacent to v_i, $\sigma_G(v_i) \geq 2 + 1 + \cdots + 1 = n$ for $1 \leq i \leq 2k$. Moreover,

$\sigma_G(v_j) \geq 1 + 1 + \cdots + 1 = n - 1$ for $2k + 1 \leq j \leq n$. So, we have

$$\begin{aligned} W(G) &= \frac{1}{2} \sum_{v \in V(G)} \sigma_G(v) \geq \frac{1}{2}(2kn + (n - 2k)(n - 1)) \\ &= \frac{1}{2}(n^2 - n) + k = \binom{n}{2} + k \end{aligned}$$

with equality if and only if $d_G(v_i) = n - 2$ $(1 \leq i \leq 2k)$ and $d_G(v_j) = n - 1$ $(2k + 1 \leq j \leq n)$, i.e., $G \cong K_n \setminus M_k$.

If n is even, then $d_G(v_j) \leq n - 2$ and at least one vertex in G is not adjacent to v_j, $\sigma_G(v_j) \geq 2 + 1 + \cdots + 1 = n$ for $2k + 1 \leq j \leq n$. Moreover, $\sigma_G(v_i) \geq 1 + 1 + \cdots + 1 = n - 1$ for $1 \leq i \leq 2k$. So, we have

$$\begin{aligned} W(G) &= \frac{1}{2} \sum_{v \in V(G)} \sigma_G(v) \geq \frac{1}{2}(2k(n - 1) + (n - 2k)n) \\ &= \frac{1}{2}n^2 - k = \binom{n}{2} + \left(\frac{n}{2} - k\right) \end{aligned}$$

with equality if and only if $d_G(v_i) = n - 1$ $(1 \leq i \leq 2k)$ and $d_G(v_j) = n - 2$ $(2k + 1 \leq j \leq n)$, i.e., $G \cong K_n \setminus M_{\frac{n}{2} - k}$. ■

Corollary. *(Gutman, Cruz and Rada [5])*
(i) If n is odd, then the unique Eulerian graph of order n with minimal Wiener index is K_n.
(ii) If n is even, then the unique Eulerian graph of order n with minimal Wiener index is $K_n \setminus M_{\frac{n}{2} - k}$ (the cocktail-party graph).

3 Graphs with the maximal Wiener indices

In this section, we consider the elements with the maximal Wiener index among $\mathbb{G}_{n,2k}$. For $k = 0$, it was shown in [5] that the cycle C_n on n vertices is the unique graph with the maximal Wiener index among $\mathbb{G}_{n,0}$ (all Eulerian graphs on n vertices). Now, for $k = 1$, we will determine the graphs with the first and the second maximal Wiener indices among $\mathbb{G}_{n,2}$.

Note that $P_n \in \mathbb{G}_{n,2}$, and it is well-known that for any graph G on n

vertices,

$$W(G) \leq \frac{n(n+1)(n-1)}{6}$$

with equality if and only if G is the path P_n on n vertices. Therefore, we have

Theorem 2. *P_n is the unique graph with the maximal Wiener index among $\mathbb{G}_{n,2}$.*

We see that all vertices of the extremal graph P_n have the smallest possible degree (the odd degree is 1 and the even degree is 2). So, it is plausible to expect that the element of $\mathbb{G}_{n,2}$ with the second maximal Wiener index be a graph with $n-2$ vertices of degree 2, a vertex of degree 1 and a vertex of degree 3, i.e., a graph on n vertices obtained by coalescing one vertex of the cycle C_a with a pendant vertex of the path P_{n-a+1}, denoted by $H_{n,a}$. The graph $H_{6,4}$ is displayed as in Figure 1.

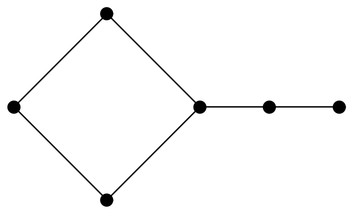

Figure 1. The graph $H_{6,4}$.

Lemma 1. *If $3 \leq a \leq n-1$, then*

$$W(H_{n,a}) = \frac{(2n-a)}{2}\left\lfloor\left(\frac{a}{2}\right)^2\right\rfloor + \frac{(n+2a-1)(n-a+1)(n-a)}{6}.$$

Moreover, $W(H_{n,a}) \leq W(H_{n,3}) = \frac{n^3-7n+12}{6}$ with equality holds if and only if $a=3$.

Proof. Let v be the coalescing vertex of C_a and P_{n-a+1}, $b=n-a+1$. Then v is a cut vertex of $H_{n,a}$, and

$$W(H_{n,a}) = \sum_{\{x,y\}\subseteq V(C_a)} d_{C_a}(x,y) + \sum_{\{x,y\}\subseteq V(P_b)} d_{P_b}(x,y)$$

$$+\sum_{x\in V(C_a)\setminus\{v\}}\sum_{y\in V(P_b)\setminus\{v\}}(d_{C_a}(x,v)+d_{P_b}(v,y))$$
$$=W(C_a)+W(P_b)+(a-1)\sigma_{P_b}(v)+(b-1)\sigma_{C_a}(v).$$

It is easy to see that $W(C_a)=\frac{a}{2}\lfloor(\frac{a}{2})^2\rfloor$, $\sigma_{C_a}(v)=\lfloor(\frac{a}{2})^2\rfloor$, and $W(P_b)=\frac{b(b+1)(b-1)}{6}$, $\sigma_{P_b}(v)=\frac{b(b-1)}{2}$. So, we can obtain that

$$W(H_{n,a})=\frac{a}{2}\left\lfloor\left(\frac{a}{2}\right)^2\right\rfloor+\frac{b(b+1)(b-1)}{6}+(a-1)\frac{b(b-1)}{2}+(b-1)\left\lfloor\left(\frac{a}{2}\right)^2\right\rfloor$$
$$=\frac{(2n-a)}{2}\left\lfloor\left(\frac{a}{2}\right)^2\right\rfloor+\frac{(n+2a-1)(n-a+1)(n-a)}{6}.$$

Specially, $W(H_{n,3})=\frac{n^3-7n+12}{6}$.

Now, we show that $W(H_{n,a})<W(H_{n,3})$ for $4\le a\le n-1$.

Since $\lfloor(\frac{a}{2})^2\rfloor\le\frac{a^2}{4}$, we have

$$W(H_{n,a})\le\frac{4n^3-6a^2n+5a^3+12an-12a^2-4n+4a}{24}$$

and

$$W(H_{n,3})-W(H_{n,a})\ge\frac{-5a^3+6a^2n+12a^2-12an-4a-24n+48}{24}.$$

Let $f(a)=-5a^3+6a^2n+12a^2-12an-4a-24n+48$, where $4\le a\le n-1$. Then f is a polynomial of degree 3 with its leading coefficient $-5<0$, the derivative $f'(a)=-15a^2+12na+24a-12n-4$. Since $f'(4)=36n-148>0$, $f(4)=24n-96>0$ and $f(n-1)=n^3+3n^2-49n+69>0$ for $n\ge5$, we have $f(a)>0$ for $4\le a\le n-1$. This implies that $W(H_{n,3})>W(H_{n,a})$ for $4\le a\le n-1$. ∎

Some bounds on the Wiener index and on the total distance of vertices in 2-connected and 2-edge-connected graphs are given in [10].

Lemma 2. *[10] (a) Let G be a 2-edge connected graph of order n. Then*

$$W(G)\le\frac{n}{2}\left\lfloor(\frac{n}{2})^2\right\rfloor$$

with equality if and only if G is a cycle.

(b) Let G be a 2-connected graph of order n and v a vertex of G. Then

$$\sigma_G(v) \leq \left\lfloor (\frac{n}{2})^2 \right\rfloor$$

with equality if G is a cycle.
(c) Let G be a 2-edge connected graph of order n and v a vertex of G. Then

$$\sigma_G(v) \leq \frac{n(n-1)}{3}.$$

Lemma 3. *Let G be a connected graph of order n and v a vertex with $d_G(v) = s$. Then*

$$\sigma_G(v) \leq \frac{(n-s)(n-s+1)}{2} + s - 1$$

and $\sigma_G(v) \leq \frac{(n-3)(n-2)}{2} + 2$ for $3 \leq s \leq n-1$.

Proof. From $d_G(v) = s$, we have

$$\sigma_G(v) \leq s + 2 + 3 + \cdots + (n-s) = \frac{(n-s)(n-s+1)}{2} + s - 1.$$

It is easy to show that $\frac{(n-s)(n-s+1)}{2} + s - 1 \leq \frac{(n-3)(n-2)}{2} + 2$ for $3 \leq s \leq n-1$. ■

Now, we characterize the elements of $\mathbb{G}(n, 2)$ with the second greatest Wiener index. Let $G \in \mathbb{G}(n, 2)$. If the degrees of the only two vertices of odd degree in G are 1 and at least 3, respectively, then we have the following result.

Lemma 4. *Let $G \in \mathbb{G}(n, 2)$. If one of its only two vertices of odd degree has degree 1 and the other one has degree at least 3, then*

$$W(G) \leq W(H_{n,3})$$

with equality if and only if $G = H_{n,3}$.

Proof. Suppose to the contrary that the lemma is not valid, and let n be the minimum value of G for which the lemma fails. Since G has a vertex of degree 1, G must have a pendant path $P_b = v_1v_2\cdots v_b$, where v_1 is a cut vertex with $d_G(v_1) \geq 3$. Let K be the union of the branches at v_1 distinct from P_b, and $a = |V(K)|$. Then $a + b = n + 1$, and

$$W(G) = W(K) + W(P_b) + (a-1)\sigma_{P_b}(v_1) + (b-1)\sigma_K(v_1).$$

If $a = 3$ or $a = 4$, then K is 2-connected. From Lemma 2, $W(K) \leq W(C_a) = \frac{a}{2}\lfloor(\frac{a}{2})^2\rfloor$, $\sigma_K(v_1) \leq \sigma_{C_a}(v_1) = \lfloor(\frac{a}{2})^2\rfloor$. We have

$$\begin{aligned} W(G) &\leq W(C_a) + W(P_b) + (a-1)\sigma_{P_b}(v_1) + (b-1)\sigma_{C_a}(v_1) \\ &= W(H_{n,a}) \leq W(H_{n,3}) \end{aligned}$$

with equality if and only if $a = 3$, i.e., $G = H_{n,3}$.

If $a \geq 5$, K may or may not be 2-edge connected.

Case 1. There is no cut edge in K, or K is 2-edge connected.

It follows from Lemma 2 that $W(K) \leq \frac{a}{2}\lfloor(\frac{a}{2})^2\rfloor$ and $\sigma_K(v_1) \leq \frac{a(a-1)}{3}$. On the other hand, $W(P_b) = \frac{b(b+1)(b-1)}{6}$ and $\sigma_{P_b}(v_1) = \frac{b(b-1)}{2}$. We have

$$\begin{aligned} W(G) &\leq \frac{a}{2}\left\lfloor(\frac{a}{2})^2\right\rfloor + \frac{b(b+1)(b-1)}{6} + (a-1)\frac{b(b-1)}{2} + (b-1)\frac{a(a-1)}{3} \\ &= \frac{n^3 - a^2n + an - n - a^2 + a}{6} + \frac{a}{2}\left\lfloor(\frac{a}{2})^2\right\rfloor. \end{aligned}$$

Note that $W(H_{n,3}) = \frac{n^3-7n+12}{6}$,

$$W(H_{n,3}) - W(G) \geq \frac{a^2n - (a+6)n + a^2 - a + 12}{6} - \frac{a}{2}\left\lfloor(\frac{a}{2})^2\right\rfloor.$$

If $a = 5$, we have $W(H_{n,3}) - W(G) = \frac{14n-58}{6} > 0$ for $n \geq a + 1 = 6$, i.e., $W(G) < W(H_{n,3})$.

If $a \geq 6$, from $\frac{a}{2}\lfloor(\frac{a}{2})^2\rfloor \leq \frac{a^3}{8}$, we have

$$W(H_{n,3}) - W(G) \geq \frac{4a^2n - 3a^3 + 4a^2 - 4an - 4a - 24n + 48}{24}.$$

Let $f(a) = 4a^2n - 3a^3 + 4a^2 - 4an - 4a - 24n + 48$, where $6 \leq a \leq n - 1$. Then f is a polynomial of degree 3 with its leading coefficient $-3 < 0$, the derivative $f'(a) = -9a^2 + 8na + 8a - 4n - 4$. Since $f'(6) = 44n - 280 > 0$, $f(6) = 96n - 480 > 0$ and $f(n-1) = n^3 + n^2 - 37n + 59 > 0$ for $n \geq 7$, we have $f(a) > 0$ for $6 \leq a \leq n-1$. Therefore, $W(H_{n,3}) > W(H_{n,a})$.

Case 2. There is a cut edge in K. Then v_1 is not a vertex of odd degree in G, otherwise, K is Eulerian and no cut edge in K.

Let uw be a cut edge farthest from v_1, see Figure 2, x the vertex of odd degree with degree at least 3 in G. Then x must belong to H, where H is the branch of $G - uw$ containing u, H is 2-edge connected. Let F be the union of the branches at u different from H, we have

$$W(G) = W(H) + W(F) + (p-1)\sigma_F(u) + (q-1)\sigma_H(u),$$

where $p = |V(H)|$, $q = |V(F)|$ and $p + q = n + 1$.

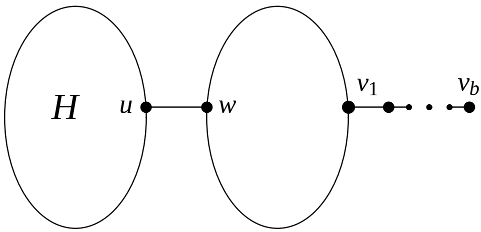

Figure 2. The graph G of Case 2 in Lemma 4.

Note that F is a connected graph with exactly two vertices v_b, u of odd degree and containing two pendant paths $v_1v_2\cdots v_b$ and $uw\cdots$. Then $F = F_1 \bigcup F_2$, where $F_2 = v_1v_2\cdots v_b$ and F_1 is the union of the branches at v_1 in F different from F_2, and F_1 is a connected graph with exactly two vertices of odd degree, their degrees in F_1 are 1 and at least 3, respectively. And

$$W(F) = W(F_1) + W(F_2) + (r-1)\sigma_{F_2}(v_1) + (b-1)\sigma_{F_1}(v_1),$$

where $r = |V(F_1)|$, $r + b = q + 1$.

Since G is a smallest counterexample that does not satisfy this lemma, we have $W(F_1) \leq W(H_{r,3}) = \frac{r^3-7r+12}{6}$. Also, $W(F_2) = W(P_b) = \frac{b(b+1)(b-1)}{6}$, $\sigma_{F_2}(v_1) = \frac{b(b-1)}{2}$, and $\sigma_{F_1}(v_1) \leq \frac{(r-3)(r-2)}{2} + 2$ from Lemma

3, we have

$$W(F) \le \frac{r^3-7r+12}{6} + \frac{b(b+1)(b-1)}{6}$$

$$+ (r-1)\frac{b(b-1)}{2} + (b-1)(\frac{(r-3)(r-2)}{2} + 2)$$

$$= \frac{q^3-12qr+29q+12r^2-36r+12}{6}.$$

And

$$W(H_{q,3}) - W(F) \ge \frac{q^3-7q+12}{6} - \frac{q^3-12qr+29q+12r^2-36r+12}{6}$$

$$= 2(q-r)(r-3) > 0 \ (4 \le r < q).$$

So, we have $W(F) < W(H_{q,3}) = \frac{q^3-7q+12}{6}$.

Since H is 2-edge connected, $W(H) \le \frac{p}{2}\lfloor(\frac{p}{2})^2\rfloor$ and $\sigma_H(u) \le \frac{p(p-1)}{3}$ by Lemma 2. Clearly, $W(F) < \frac{q^3-7q+12}{6}$ and $\sigma_F(u) \le 1+2+\cdots+(q-1) = \frac{q(q-1)}{2}$. Now,

$$W(G) = W(H) + W(F) + (p-1)\sigma_F(u) + (q-1)\sigma_H(u)$$

$$< \frac{p}{2}\left\lfloor(\frac{p}{2})^2\right\rfloor + \frac{q^3-7q+12}{6} + (p-1)\frac{q(q-1)}{2} + (q-1)\frac{p(p-1)}{3}.$$

From $p+q = n+1$, $q = n-p+1$, by simple calculation, it can be obtained that

$$\begin{aligned}
&\left[\frac{n^3-p^2n+pn-n-p^2+p}{6}\right] \\
&-\left[\frac{q^3-7q+12}{6} + (p-1)\frac{q(q-1)}{2} + (q-1)\frac{p(p-1)}{3}\right] \\
=&\left[\frac{n^3-p^2n+pn-n-p^2+p}{6}\right] - \left[\frac{n^3-p^2n+pn-7n-p^2+7p+6}{6}\right] \\
=&n-p-1 > 0
\end{aligned}$$

and

$$W(G) < \frac{p}{2}\left\lfloor(\frac{p}{2})^2\right\rfloor + \frac{n^3-p^2n+pn-n-p^2+p}{6}.$$

So, we have $W(G) < W(H_{n,3})$ by the same calculation as Case 1. ■

Finally, we show that $H_{n,3}$ is the unique graph with the second Wiener index among $\mathbb{G}(n,2)$.

Theorem 3. *Let G be the graph of order n and exactly two vertices of odd degree that is not a path. Then*

$$W(G) \le W(H_{n,3})$$

with equality if and only if $G = H_{n,3}$.

Proof. Let x, y be the unique two vertices of odd degree in G. We consider three cases according to the degrees of x, y in G, where $d_G(x) \le d_G(y)$.

Case 1. $d_G(x) = 1$ and $d_G(y) \ge 3$.

From Lemma 4, we have $W(G) \le W(H_{n,3})$ with equality if and only if $G = H_{n,3}$.

Case 2. $d_G(x) = d_G(y) = 1$.

Let $P_b = v_1 v_2 \cdots v_b$ be a pendant path of G, where $v_b = y$ and $d_G(v_1) \ge 3$. Then $G = P_b \bigcup K$, where K is the union of branches at v_1 different from P_b. Let $|V(K)| = a = n - b + 1$, we have

$$W(G) = W(K) + W(P_b) + (a-1)\sigma_{P_b}(v_1) + (b-1)\sigma_K(v_1).$$

Note that K is a connected graph with exactly two vertices x, v_1 of odd degree, and $d_K(x) = 1$, $d_K(v_1) > 1$, we have $W(K) \le W(H_{a,3}) = \frac{a^3-7a+12}{6}$ from Case 1. Since the odd number $d_K(v_1) = d_G(v_1) - 1 \ge 3$, $\sigma_K(v_1) \le \frac{(a-3)(a-2)}{2} + 2$ by Lemma 3. Clearly, $W(P_b) = \frac{b(b+1)(b-1)}{6}$ and $\sigma_{P_b}(v_1) = \frac{b(b-1)}{2}$, $b = n - a + 1$, $4 \le a \le n-1$. So,

$$\begin{aligned} W(G) \le & \frac{a^3-7a+12}{6} + \frac{b(b+1)(b-1)}{6} + (a-1)\frac{b(b-1)}{2} \\ & + (b-1)\frac{(a-3)(a-2)}{2} + 2 \\ = & \frac{n^3 - 12na + 29n + 12a^2 - 36a + 12}{6} \\ < & \frac{n^3 - 7n + 12}{6} = W(H_{n,3}) \end{aligned}$$

and $W(G) < W(H_{n,3})$.

Case 3. $d_G(x) \geq 3$ and $d_G(y) \geq 3$.

Subcase 3.1. G has no cut edge. Then G is 2-edge connected and different from C_n. By Lemma 2, we have $W(G) < W(C_n) = \frac{n}{2}\lfloor(\frac{n}{2})^2\rfloor$. And

$$W(H_{n,3}) - W(G) > \frac{n^3 - 7n + 12}{6} - \frac{n}{2}\left\lfloor(\frac{n}{2})^2\right\rfloor = \frac{n(n^2 - 28) + 48}{24} \geq 0,$$

i.e., $W(G) < W(H_{n,3})$.

Subcase 3.2. There is a cut edge in G.

Let uw be an end-cut edge in G, and H be the block without cut edge of $G - uw$. With loss of generality, we assume that H contains the cut vertex u of G contained in H. Let K be the union of the branches at u distinct from H, and $a = |V(H)|$ and $b = |V(K)|$. Then $b = n - a + 1$, and

$$W(G) = W(H) + W(K) + (a - 1)\sigma_K(u) + (b - 1)\sigma_H(u).$$

For $a = 3$ or $a = 4$, then H is 2-connected, have $W(H) \leq W(C_a)$ and $\sigma_H(u) \leq \sigma_{C_a}(u)$. Clearly, $W(K) \leq \frac{b^3-7b+12}{6} < W(P_b)$ and $\sigma_K(u) \leq \sigma_{P_b}(u)$. Thus, have

$$W(G) < W(H_{n,a}) \leq W(H_{n,3}).$$

For $a \geq 5$, we note that H is 2-edge connected, $W(H) \leq \frac{a}{2}\lfloor(\frac{a}{2})^2\rfloor$ and $\sigma_H(u) \leq \frac{a(a-1)}{3}$ by Lemma 2. K contains exactly two vertices of odd degree, one is the vertex u with $d_K(u) = 1$ and the other is x or y with degree at least 3. From Lemma 4, $W(K) \leq \frac{b^3-7b+12}{6}$. Clearly, $\sigma_K(u) \leq 1 + 2 + \cdots + (b - 1) = \frac{b(b-1)}{2}$, and

$$\begin{aligned} W(G) &\leq \frac{a}{2}\left\lfloor(\frac{a}{2})^2\right\rfloor + \frac{b^3 - 7b + 12}{6} + (a - 1)\frac{b(b - 1)}{2} + (b - 1)\frac{a(a - 1)}{3} \\ &< \frac{n^3 - a^2n + an - n - a^2 + a}{6} + \frac{a}{2}\left\lfloor(\frac{a}{2})^2\right\rfloor. \end{aligned}$$

We have $W(G) < W(H_{n,3})$ by the same calculation as in Case 1 of Lemma 4. ■

From [1,5], if n is odd, then the graphs with the first-minimal, second-minimal, third-minimal, and fourth-minimal Wiener index among $\mathbb{G}(n,0)$ are K_n, the graphs obtained from K_n by deleting the edges of a triangle, of a quadrangle, and of a pentagon, respectively; if n is even, then the graphs with the first-minimal, second-minimal, third-minimal, and fourth-minimal Wiener index among $\mathbb{G}(n,0)$ are the cocktail-party graph CP_n, the graphs obtained from CP_n by deleting the edges of a triangle, of a quadrangle, and of a pentagon, respectively. The graphs with the first-maximal and second-maximal Wiener index among $\mathbb{G}(n,0)$ are C_n and $C_{n,3}$ obtained from the disjoint union of two cycles on $n-2$ vertices and 3 vertices for all n with exception of six values. Based on our results, the graph with the minimal Wiener index among $\mathbb{G}(n,2k)$ for $0 \leq k \leq \frac{n}{2}$ is characterized, and the graphs with the first-maximal and second-maximal Wiener index among $\mathbb{G}(n,2k)$ for $k = 0, 1$ are characterized.

These results lead to a natural question which we pose as a problem.

Problem. What is the maximum Wiener index and the extremal graph among $\mathbb{G}(n,2k)$, where $2 \leq k \leq \frac{n}{2}$?

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References

[1] P. Dankelmann, Proof of a conjecture on the Wiener index of Eulerian graphs, *Discr. Appl. Math.* **301** (2021) 99–108.

[2] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[3] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247–294.

[4] B. Furtula, Odd-vertex-degree trees maximizing Wiener index, *Kragujevac J. Math.* **37** (2013) 129–134.

[5] I. Gutman, R. Cruz, J. Rada, Wiener index of Eulerian graphs, *Discr. Appl. Math.* **162** (2014) 247–250.

[6] I. Gutman, J. H. Potgieter, Wiener index and intermolecular forces, *J. Serb. Chem. Soc.* **62** (1997) 185–192.

[7] H. Lin, Extremal Wiener index of trees with all degrees odd, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 287–292.

[8] H. Lin, Extremal Wiener index of trees with given number of vertices of even degree, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 311–320.

[9] S. Nikolić, N. Trinajstić, Z. Mihalić, The Wiener index: developments and applications, *Croat. Chem. Acta* **68** (1995) 105–129.

[10] J. Plesnik, On the sum of all distances in a graph or digraph, *J. Graph Theory* **8** (1984) 1–21.

[11] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.