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ON THE WIENER INDEX OF UNICYCLIC GRAPHS

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Abstract

The Wiener index of a graph G is defined as $W(G) = \sum_{u,v} d_G(u, v)$, where $d_G(u, v)$ is the distance between u and v in G, and the sum goes over all pairs of vertices. In this paper, we characterize the connected unicyclic graph with minimum Wiener indices among all connected unicyclic graphs of order n and girth g with k pendent vertices.

Keywords: Wiener index, Unicyclic graph, Girth, Pendent vertex.

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1. Introduction

All graphs considered here are finite and simple. For undefined terminology and notation refer to [3]. For $x \in V(G)$, we denote the neighborhood and the degree of x by $N_G(x)$ and $d_G(x)$, respectively. A *pendent vertex* is a vertex of degree 1. For two vertices x and y $(x \neq y)$, the *distance between x and y* is the number of edges in a shortest path joining x and y. The *distance of a vertex* $x \in V(G)$, denoted by $D_G(v)$, is the sum of distances between x and all other vertices of G. The *girth* of a graph G is the length of a shortest cycle in G, with the girth of an acyclic graph being infinite. We will use $G - x$ or $G - xy$ to denote the graph that arises from G by deleting the vertex $x \in V(G)$ or the edge $xy \in E(G)$. Similarly, $G + xy$ is a graph that arises from G by adding an edge $xy \notin E(G)$, where $x,\ y \in V(G)$.

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The *Wiener index* is a well-known distance-based topological index introduced as a structural descriptor for acyclic organic molecules [12]. It is defined as the sum of distances between all pairs of vertices of a simple graph G:

$$W(G) = \sum_{u,v} d_G(u,v).$$

The graphical invariant $W(G)$ has been studied by many researchers (see, for example, [1]-[2], [4]-[11]) under different names such as *distance*, *transmission*, *total status* and *sum of all distances.* Apparently, the chemist Harry Wiener was the first to point out in 1947 that $W(G)$ is well correlated with certain physico-chemical properties of the organic compound from which G is derived. In 1976, Entringer, Jackson and Snyder published a paper [8] which is historically the first mathematics paper on $W(G)$. For the results and further references the reader may refer to a recent survey [5].

A quantity closely related to $W(G)$ is the mean distance, or the average distance between the vertices. When G represents a network (e.g., an interconnection network connecting many processors), the average distance of G between the nodes of the network is a measure of the average delay of messages for traversing from one node to another.

A unicyclic graph is a connected graph with n vertices and n edges. Let G be a unicyclic graph of order n and girth g with k pendent vertices. If $g = n$ or $k = 0$, then $G \cong C_n$, a cycle of order n. Therefore, in the following, we assume that $3 \le g \le n-1$ and $1 \le k \le n-3$. Let $\mathcal{U}_{n,g,k} = \{G : G$ is a connected unicyclic graph of order n and girth g with k pendent vertices, $3 \le g \le n-1$, $1 \le k \le n-3\}$.

In this paper, the minimum Wiener indices of unicyclic graphs in the set $\mathcal{U}_{n,g,k}$ are characterized.

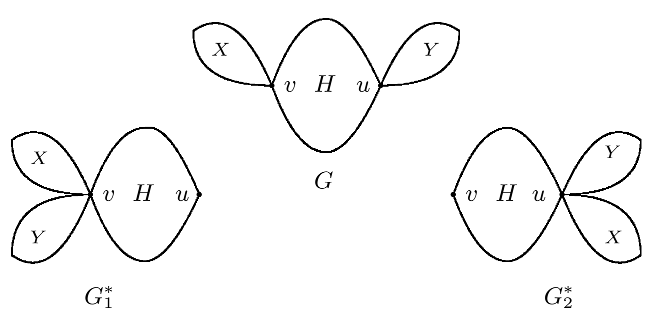
2. Lemmas

First we give some lemmas which are used in the proof of our results.

2.1. Lemma. *Let H, X, Y be three connected pairwise vertex-set disjoint graphs. Suppose that u, v are two vertices of H, v' is a vertex of X, u' is a vertex of Y. Let G be the graph obtained from H, X, Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices v, v', u', and let G_2^* be the graph obtained from H, X, Y by identifying vertices u, v', u' (see Figure 1). Then*

$$W(G_1^*) < W(G) \text{ or } W(G_2^*) < W(G). \qquad \square$$

Figure 1



2.2. Lemma. [10] *Let G be a non-trivial connected graph, and $P = v_0v_1v_2\cdots v_k$, $Q = u_0u_1u_2\cdots u_m$ two paths of lengths k, m ($k \ge m \ge 1$), respectively, where $v_i \notin V(G)$, $0 \le$*

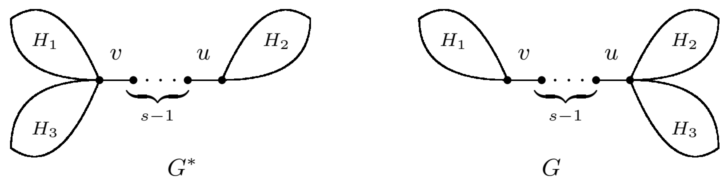
$i \le k$ and $u_j \notin V(G)$, $0 \le j \le m$. Suppose that $v \in V(G)$. Let $G^*_{k,m}$ be the graph obtained from G, P, Q by identifying v, v_0, u_0 as a single vertex v. Then

$$W(G^*_{k,m}) < W(G^*_{k+1,m-1}).$$

2.3. Lemma. *Let H_1, H_2, H_3 be three connected pairwise vertex-set disjoint graphs. Suppose that v is a vertex of H_1, u is a vertex of H_2, and w is a vertex of H_3. Let G be the graph obtained from H_1, H_2, H_3 by adding a path P of length $s \ge 1$ joining u with v and identifying vertices u with w, respectively. Let G^* be the graph obtained from H_1, H_2, H_3 by adding a path P of length $s \ge 1$ joining u with v and identifying v with w, respectively (see Figure 2). If $|V(H_1)| > |V(H_2)|$, then*

$$W(G^*) < W(G). \qquad \square$$

Figure 2



Proof. We have

$$\begin{aligned} W(G) - W(G^*) &= \sum_{x \in V(H_1), y \in V(H_3)} [d_G(x,y) - d_{G^*}(x,y)] \\ &\qquad + \sum_{x \in V(H_2), y \in V(H_3)} [d_G(x,y) - d_{G^*}(x,y)] \\ &= s|V(H_3)|(|V(H_1)| - |V(H_2)|) \\ &> 0. \end{aligned} \qquad \square$$

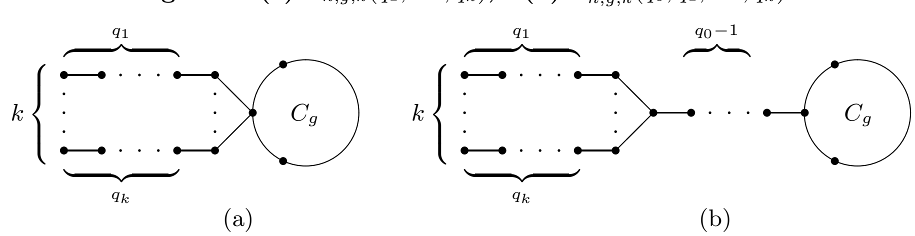
3. Conclusions

In this section, we will give the minimum Wiener index in the set $\mathcal{U}_{n,g,k}$. In order to formulate our results, we need to define some unicyclic graphs (see Figure 3) as follows.

Let $U_{n,g,k}(q_1, \ldots, q_k)$ (see Figure 3(a)) be a unicyclic graph of order n created from a cycle C_g of order g by attaching k ($k \ge 1$) paths of length p_i to one vertex of C_g, respectively, where $n = g + \sum_{i=1}^{k} q_i$, $q_i \ge 1$, $i = 1, \ldots, k$.

Let $U^*_{n,g,k}(q_0, q_1, \ldots, q_k)$ (see Figure 3(b)) be a unicyclic graph of order n created from a unicyclic graph $U_{g+q_0,g,1}(q_0)$ of order g by attaching k ($k \ge 2$) paths of length p_i to one pendent vertex of $U_{g+q_0,g,1}(q_0)$, respectively, where $n = g + \sum_{i=0}^{k} q_i$, $q_i \ge 1$, $i = 0, 1, \ldots, k$.

Figure 3. (a) $U_{n,g,k}(q_1, \ldots, q_k)$, **(b)** $U^*_{n,g,k}(q_0, q_1, \ldots, q_k)$



Denote $U_{n,g,k}(q_1,\dots,q_k)$ with $|q_i-q_j|\le 1,\ 1\le i,j\le n$ by $U_{n,g,k}$, and $U^*_{n,g,k}(q_0,q_1,\dots,q_k)$ with $|q_i-q_j|\le 1,\ 1\le i,j\le n$ and $q_i-g-q_0\le 1$ for $1\le i\le k$ by $U^*_{n,g,k}$. Then we have the following results.

3.1. Proposition.

(i) $W(U_{n,g,k+1})<W(U_{n,g,k})$ *for* $g>\lfloor\frac{n-g}{k}\rfloor$;
(ii) $W(U^*_{n,g,k})<W(U^*_{n,g,k-1})$ *for* $g\le\lfloor\frac{n-g}{k}\rfloor$ *and* $n-g\not\equiv 0(mod\ k)$;
(iii) $W(U_{n,g,k})=W(U^*_{n,g,k})$ *for* $n=(k+1)g$.

Proof. Using Lemma 2.2 repeatedly, (i) and (ii) hold. From the proof of Lemma 2.3, (iii) holds. □

Now we present two propositions that will be used in the proof of our main results. In the following two propositions, we always assume that $G\in\mathcal{U}_{n,g,k}$, and let C be the unique cycle of order g in G.

3.2. Proposition. *Suppose that G be chosen such that $W(G)$ is as small as possible. Then there is a unique vertex $w\in V(C)$ such that $d_G(w)\ge 3$.*

Proof. Assume that $d_G(w_i)\ge 3$ for $w_i\in V(C),\ i=1,2$. Let $N_G(w_1)=\{x_1,\dots,x_s,u_1,u_2\}$ and $N_G(w_2)=\{y_1,\dots,y_t,v_1,v_2\}$, where $u_1,u_2,v_1,v_2\in V(C)$ and $s,t\ge 1$. Set $G_1^*=G-\{w_2y_1,\dots,w_2y_t\}+\{w_1y_1,\dots,w_1y_t\}$ and $G_2^*=G-\{w_1x_1,\dots,w_1x_s\}+\{w_2x_1,\dots,w_2x_s\}$. Then $G_1^*,G_2^*\in\mathcal{U}_{n,g,k}$.

By Lemma 2.1, we have $W(G_1^*)<W(G)$ or $W(G_2^*)<W(G)$, a contradiction. Thus there is a unique vertex $w\in V(C)$ such that $d_G(w)\ge 3$. □

3.3. Proposition. *Suppose that G be chosen such that $W(G)$ is as small as possible. Then $G\cong U_{n,g,k}(q_1,\dots,q_k)$ or $G\cong U^*_{n,g,k}(q_0,q_1,\dots,q_k)$.*

Proof. By Proposition 3.2, we may let $w\in V(C)$ be the unique vertex with $d_G(w)\ge 3$. Then G is a graph obtained from C by attaching a tree T with k pendent vertices at w.

Suppose that $G\not\cong U_{n,g,k}(q_1,\dots,q_k)$. We will first show that there is a unique vertex $u\in V(G)\setminus V(C)$ satisfying $d_G(u)\ge 3$. Otherwise, we let $u,v\in V(G)\setminus V(C)$ with $d_G(u)\ge 3$, $d_G(v)\ge 3$. Set $N_G(u)=\{u_1,\dots,u_a\}$ and $N_G(v)=\{v_1,\dots,v_b\}$. Then $a,b\ge 3$. Since $u,v\notin V(C)$, there is a unique (u,v)-path P_{uv} in G. Similarly, there is a unique (w,v)-path P_{wv} and a unique (w,u)-path P_{wu} in G. Without loss of generality, we may assume that $u_1,v_1\in V(P_{uv})$ (possibly $u_1=v_1$ or $u_1=v,\ v_1=u$), and that $u_2\in V(P_{wu})$ (or $v_2\in V(P_{wv})$, resp.) if $u\in V(P_{wv})$ (or $v\in V(P_{wu})$, resp.). Set $G_1^*=G-\{uu_3,\dots,uu_a\}+\{vu_3,\dots,vu_a\}$ and $G_2^*=G-\{vv_3,\dots,vv_b\}+\{uv_3,\dots,uv_b\}$. Then $G_1^*,G_2^*\in\mathcal{U}_{n,g,k}$. By Lemma 2.1, we have $W(G_1^*)<W(G)$ or $W(G_2^*)<W(G)$, a contradiction.

Therefore, in the following, we may let v be the unique vertex of $V(G)\setminus V(C)$ with $d_G(v)\ge 3$. Put $N_G(v)=\{v_1,\dots,v_b\}$, $b\ge 3$ and $N_G(w)=\{w',w'',w_1,\dots,w_m\}$, $m\ge 1$, where $w',w''\in V(C)$ and w_1,v_1 are the two vertices that belong to the unique (w,v)-path (possibly $w_1=v_1$). Let $P^0_{q_i}$ be a (v,u_i)-path of length q_i, where u_i are the pendent vertices of G, $2\le i\le b$.

Next we will show that $G\cong U^*_{n,g,k}(q_1,\dots,q_k)$. Otherwise, we have $d_G(w)\ge 4$ and $m\ge 2$. Set $X=C$ and $Y=\bigcup_{3\le l\le b}P^0_{q_l}$. Let $G_1^*=G-\{ww',ww''\}+\{vw',vw''\}$ and $G_2^*=G-\{vv_3,\dots,vv_b\}+\{wv_3,\dots,wv_b\}$. Then $G_1^*,G_2^*\in\mathcal{U}_{n,g,k}$. By Lemma 2.1, we have $W(G_1^*)<W(G)$ or $W(G_2^*)<W(G)$, a contradiction. Thus $G\cong U^*_{n,g,k}(q_1,\dots,q_k)$.

Therefore the proof of the proposition is complete. □

3.4. Theorem. *Suppose that* $G \in \mathfrak{U}_{n,g,k}$, $1 \le k \le n-3$, $3 \le g \le n-1$. *If* $g > \lfloor \frac{n-g}{k} \rfloor$, *then* $W(G) \ge W(U_{n,g,k})$ *and equality holds if and only if* $G \cong U_{n,g,k}$.

Proof. We have to prove that if $G \in \mathfrak{U}_{n,g,k}$, then $W(G) \ge W(U_{n,g,k})$ with equality only if $G \cong U_{n,g,k}$. If $k = 1$, then $G \cong U_{n,g,1}$, and hence the result holds. Therefore in the following, we assume that $k \ge 2$. Let C be the unique cycle of order g in G. Choose G such that $W(G)$ is as small as possible. Then by Proposition 3.2, we may let w be the unique vertex of C with $d_G(w) \ge 3$.

If $G \ncong U_{n,g,k}(q_1, \dots, q_k)$, then by Proposition 3.3, $G \cong U^*_{n,g,k}(q_0, q_1, \dots, q_k)$. Let w_0 be the unique vertex of $V(G) \setminus \{w\}$ with $d_G(w_0) = k+1 \ge 3$, and let $P^0_{q_i}$ be a (w_0, v_i)-path of length q_i, where the v_i denote the pendent vertices of G, $1 \le i \le k$. Let $N_G(w_0) = \{w'_0, w'_1, \dots, w'_k\}$, where w'_0 belongs to the unique (w, w_0)-path (possibly $w'_0 = w$). Assume, without loss of generality, that $q_1 = \min\{q_j : 1 \le j \le k\}$. Then $g > q_1 + 1$ as $g > \lfloor \frac{n-g}{k} \rfloor$. Set $H_1 = C$, $H_2 = P^0_{q_1}$, $H_3 = \bigcup_{2 \le l \le k} P^0_{q_l}$. Let $G^* = G - \{w_0w'_2, \dots, w_0w'_k\} + \{ww'_2, \dots, ww'_k\}$. Then $G^* \in \mathfrak{U}_{n,g,k}$. By Lemma 2.3, we have $W(G) > W(G^*)$, a contradiction with our choice. Therefore $G \cong U_{n,g,k}(q_1, \dots, q_k)$, and hence, by Lemma 2.2, $G \cong U_{n,g,k}$.

Therefore the proof of the theorem is complete. □

3.5. Theorem. *Suppose that* $G \in \mathfrak{U}_{n,g,k}$, $2 \le k \le n-3$, $3 \le g \le n-1$. *If* $g \le \lfloor \frac{n-g}{k} \rfloor$ *and* $n - g \not\equiv 0(\mathrm{mod}\ k)$, *then* $W(G) \ge W(U^*_{n,g,k})$, *and equality holds if and only if* $G \cong U^*_{n,g,k}$.

Proof. We have to prove that if $G \in \mathfrak{U}_{n,g,k}$, then $W(G) \ge W(U^*_{n,g,k})$, with equality only if $G \cong U^*_{n,g,k}$. Let C be the unique cycle of order g in G. Choose G such that $W(G)$ is as small as possible. Then by Proposition 3.2, we may let w be the unique vertex of C with $d_G(w) \ge 3$. Set $N_G(w) = \{w', w'', w_1, \dots, w_m\}$, where $w', w'' \in V(C)$ and $m \ge 1$.

If $G \cong U_{n,g,k}(q_1, \dots, q_k)$, then we let P_{q_i} be a (w, v_i)-path of length q_i with $w_i \in V(P_{q_i})$ for $1 \le i \le k$, where v_i denote the pendent vertices of G. Assume, without loss of generality, that $q_1 = \max\{q_j : 1 \le j \le k\}$. Then $q_1 > g$ as $g \le \lfloor \frac{n-g}{k} \rfloor$ and $n - g \not\equiv 0(\mathrm{mod}\ k)$. Set $H_1 = C$, $H_2 = P_{q_1}$, $H_3 = \bigcup_{2 \le l \le m} P_{q_l}$. Let $G^* = G - \{ww_2, \dots, ww_k\} + \{w_1w_2, \dots, w_1w_k\}$. Then $G^* \in \mathfrak{U}_{n,g,k}$. By Lemma 2.3, we have $W(G) > W(G^*)$, a contradiction with our choice. Hence $G \ncong U_{n,g,k}(q_1, \dots, q_k)$, and thus by Proposition 3.3, $G \cong U^*_{n,g,k}(q_0, q_1, \dots, q_k)$. By Lemma 2.2, $G \cong U^*_{n,g,k}$.

Therefore the proof of the theorem is complete. □

3.6. Theorem. *Suppose that* $G \in \mathfrak{U}_{n,g,k}$, $2 \le k \le n-3$, $3 \le g \le n-1$. *If* $n = (k+1)g$, *then* $W(G) \ge W(U_{n,g,k}) = W(U^*_{n,g,k})$, *and equality holds if and only if* $G \cong U_{n,g,k}$ *or* $G \cong U^*_{n,g,k}$.

Proof. We have to prove that if $G \in \mathfrak{U}_{n,g,k}$, then $W(G) \ge W(U_{n,g,k}) = W(U^*_{n,g,k})$, with equality only if $G \cong U_{n,g,k}$ or $G \cong U^*_{n,g,k}$. Choose G such that $W(G)$ is as small as possible. By an argument similar to the proofs of Theorems 3.4 and 3.5, $G \cong U_{n,g,k}$ or $G \cong U^*_{n,g,k}$.

Therefore the proof of the theorem is complete. □

By Lemma 3.1 and Theorems 3.4–3.6, we have the following result.

3.7. Corollary. [11] *Let* G *be a unicyclic graph of order* n *and girth* g. *Then*

$$W(U_{n,g,n-g}) \le W(G) \le W(U_{n,g,1}),$$

and equality on the left holds if and only if $G \cong U_{n,g,n-g}$, *and equality on the right holds if and only if* $G \cong U_{n,g,1}$. □

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