On the Wiener index of unicyclic graphs with given girth *

Guihai Yu, Lihua Feng
School of Mathematics
Shandong Institute of Business and Technology
191 Binhaizhong Road, Yantai, Shandong, P.R. China, 264005.
Email: fenglh@163.com

Abstract

The Wiener index of a graph 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 sum goes over all the pairs of vertices. In this paper, we investigate the Wiener index of unicyclic graphs with given girth and characterize the extremal graphs with the minimal and maximal Wiener index.

Key words: Unicyclic graph; girth; Wiener index
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1 Introduction

In 1947, Harold Wiener introduced the first chemical index, now called the Wiener index, and published a series of papers to show that there are excellent correlations between the Wiener index of the molecular graph of an organic compound and a variety of physical and chemical indices. The Wiener index of a graph G, defined as [9]:

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

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where $d_G(u,v)$ is the distance between u and v in G and the sum goes over all the pairs of vertices. An important direction is to determine the graphs with maximal, or minimal Wiener index in a given class of graphs. Up to now, many researchers have investigate the Wiener index ([3]-[4], [6]-[14]).

Next we introduce some graph notations. 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. The distance of a vertex $x \in V(G)$, denoted by $D_G(x)$, is the sum of distance between x and all other vertices of G. Let G' be the subgraph of G, $D_G(x, G')$ denotes the sum of distances between x and all other vertices of G'. Let $E' \subset E$, 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 $H_{n,k}$ the graph obtained from C_k by adding $n-k$ pendant vertices to a vertex of C_k. For other notations in graph theory, we can refer to [2].

A unicyclic graph is a connected graph which has equal vertex number and edge number. Let $\mathcal{U}_{n,k}$ be the set of unicyclic graphs of order $n \geq 3$ with girth $k \geq 3$. For $U_{n,k} \in \mathcal{U}_{n,k}$, if $k = n$, then $U_{n,k} \cong C_k$; if $k = n-1$, then $U_{n,k} \cong L_{n,n-1}$. So in the following, we assume that $3 \leq k \leq n-2$. In this paper, we study the Wiener index of unicyclic graphs with given girth and characterize the extremal graphs. In fact, we get the following results.

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 $U_{n,k} \cong H_{n,k}$, 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 $U_{n,k} \cong H_{n,k}$, and the right equality holds if and only if $U_{n,k} \cong L_{n,k}$.

Corollary 1.2 *Let U be a unicyclic graph of order $n \geq 4$. Then*

$$n^2 - n \leq W(U) \leq \frac{1}{6}(n^3 - 7n + 12).$$

The left equality holds if and only if $U \cong H_{n,3}$, and the right equality holds if and only if $U \cong L_{n,3}$.

2 Lemmas and Results

Lemma 2.1 *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 $v \in V(T)$, $N_T(v) = \{v_1, v_2, \cdots, v_s\}$. Let G_1 be the graph obtained from G_0 and T by adding edge uv, $G_2 = G_1 - vv_1 - vv_2 - \cdots - vv_s + uv_1 + uv_2 + \cdots + uv_s$. Then*

$$W(G_1) > W(G_2).$$

Proof. By definition of Wiener index, we have $W(G_1) = \sum_{x,y \in V(G_0)} d_{G_1}(x,y) + \sum_{x \in V(G_0), y \in V(T-v)} d_{G_1}(x,y) + \sum_{x,y \in V(T-v)} d_{G_1}(x,y) + \sum_{x \in V(G_0)} d_{G_1}(x,v) + \sum_{x \in V(T-v)} d_{G_1}(x,v)$.

It is easy to see that

$$\begin{aligned}
\sum_{x,y \in V(G_0)} d_{G_1}(x,y) &= \sum_{x,y \in V(G_0)} d_{G_2}(x,y), \\
\sum_{x \in V(G_0), y \in V(T-v)} d_{G_1}(x,y) &= \sum_{x \in V(G_0), y \in V(T')} (d_{G_2}(x,y) + 1), \\
\sum_{x,y \in V(T-v)} d_{G_1}(x,y) &= \sum_{x,u \in V(T')} d_{G_2}(x,y), \\
\sum_{x \in V(G_0)} d_{G_1}(x,v) &= \sum_{x \in V(G_0)} d_{G_2}(x,v), \\
\sum_{x \in V(T-v)} d_{G_1}(x,v) &= \sum_{x \in V(T')} (d_{G_2}(x,v) - 1),
\end{aligned}$$

where $T' = G_2 - G_0 - v$ is the subgraph of G_2.

So we have

$$\begin{aligned}
& W(G_1) - W(G_2) \\
= & \sum_{x \in V(G_0), y \in V(T-v)} d_{G_1}(x,y) + \sum_{x \in V(T-v)} d_{G_1}(x,v)
\end{aligned}$$

$$
\begin{aligned}
& - \sum_{x\in V(G_0),y\in V(T')} d_{G_2}(x,y) - \sum_{x\in V(T')} d_{G_2}(x,v) \\
= & \sum_{x\in V(G_0),y\in V(T-v)} d_{G_1}(x,y) - \sum_{x\in V(G_0),y\in V(T')} d_{G_2}(x,y) \\
& + \sum_{x\in V(T-v)} d_{G_1}(x,v) - \sum_{x\in V(T')} d_{G_2}(x,v)) \\
= & n_0(n_1-1)\cdot 1 + (n_1-1)\cdot(-1) \\
= & (n_0-1)(n_1-1) \\
> & 0.
\end{aligned}
$$

This implies the result. ■

Lemma 2.2 *[8] Let G_0 be a connected graph and $u_1, u_2 \in V(G_0)$. Let G be the graph obtained from G_0 by attaching k_1, k_2 pendant edges to u_1, u_2, respectively. Let G_i be the graph obtained by attaching $k_1 + k_2$ pendant edges to u_i ($i = 1, 2$). Then $W(G_1) < W(G)$, or $W(G_2) < W(G)$.*

Lemma 2.3 *[7] Let G be a connected graph and $v \in V(G)$. Suppose $G^*_{s,m}$ be the graphs obtained by attaching two paths $P = vv_1 \cdots v_s$, $Q = vu_1 \cdots u_m$ of lengths s, m ($s \geq m \geq 1$) to G at v. Then $W(G^*_{s,m}) < W(G^*_{s+1,m-1})$.*

By Lemma 2.3, we have the following lemma.

Lemma 2.4 *Let G_0 be a connected graph and $u \in V(G_0)$. Assume that G_1 is the graph obtained from G_0 by attaching a tree T of order n_1 to u and G_2 is the graph obtained from G_0 by attaching a path P_{n_1} by its endvertex at u. Then $W(G_1) < W(G_2)$.*

Lemma 2.5 *[1] Let $uv \in E(G)$ be a cut edge in G, and let G_1 and G_2 be two components of $G - uv$ with $n_1 = |V(G_1)|$ and $n_2 = |V(G_2)|$. Suppose that $u \in V(G_1)$ and $v \in V(G_2)$, then*

$$W(G) = W(G_1) + W(G_2) + n_1 D_G(v, G_2) + n_2 D_G(u, G_1) + n_1 n_2.$$

Lemma 2.6 *Let G_0 be a unicyclic graph of order $n_0 > 1$ and $u_0, v_0 \in V(G_0)$ be two distinct vertices in G_0. $P_s = u_1u_2 \cdots u_s$ and $P_t =$*

$v_1 v_2 \cdots v_t$ *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.*

Proof. Let G', G'' be the component containing u_0 and v_0 of $G - u_0u_1, G - v_0v_1$, respectively. For the cut edges $u_0u_1, v_0v_1 \in E(G)$, by Lemma 2.5, we have

$W(G) = W(G_0)+W(P_s)+W(P_t)+(n_0+t)D_G(u_1, P_s)+sD_G(u_0, G')+ n_0D_G(v_1, P_t) + tD_G(v_0, G_0) + s(n_0 + t) + n_0 \cdot t.$

For cut edges $v_0v_1, u_0u_1 \in E(G)$, we have

$W(G) = W(G_0)+W(P_s)+W(P_t)+(n_0+s)D_G(v_1, P_t)+tD_G(v_0, G'')+ n_0D_G(u_1, P_s) + sD_G(u_0, G_0) + t(n_0 + s) + n_0 \cdot s.$

Similarly, by Lemma 2.5, we can get

$W(G_1) = W(G_0)+W(P_s)+W(P_t)+(n+t)D_{G_1}(u_1, P_s)+sD_{G_1}(v_t, G')+ n_0D_{G_1}(v_1, P_t) + tD_{G_1}(v_0, G_0) + s(n_0 + t) + n_0 \cdot t,$

$W(G_2) = W(G_0) + W(P_s) + W(P_t) + (n_0 + s)D_{G_2}(v_1, P_t) + tD_{G_2}(u_s, G'') + n_0D_{G_2}(u_1, P_s) + sD_{G_2}(u_0, G_0) + t(n_0 + s) + n_0 \cdot s.$

It is not difficult to find that

$$\begin{aligned}
D_G(u_0, G') &= D_G(u_0, G_0) + D_G(u_0, P_t), \\
D_{G_1}(v_t, G') &= D_{G_1}(v_t, G_0) + D_{G_1}(v_t, P_t) \\
&= D_G(v_0, G_0) + n_0 t + \sum_{i=1}^{t-1} i, \\
D_G(v_0, G'') &= D_G(v_0, G_0) + D_G(v_0, P_s), \\
D_{G_2}(u_s, G'') &= D_{G_2}(u_s, G_0) + D_{G_2}(u_s, P_s) \\
&= D_G(u_0, G_0) + n_0 s + \sum_{i=1}^{s-1} i.
\end{aligned}$$

So we have

$W(G) - W(G_1) = s\Big(D_G(u_0, G_0) + D_G(u_0, P_t) - D_G(v_0, G_0) - n_0 t - \sum_{i=1}^{t-1} i\Big),$

$W(G) - W(G_2) = t\Big(D_G(v_0, G_0) + D_G(v_0, P_s) - D_G(u_0, G_0) - n_0 s - \sum_{i=1}^{s-1} i\Big).$

If $W(G) - W(G_1) \geq 0$, then

$$\begin{aligned}
& W(G) - W(G_2) \\
= \;& t\Big(D_G(v_0, G_0) + D_G(v_0, P_s) - D_G(u_0, G_0) - n_0 s - \sum_{i=1}^{s-1} i\Big) \\
\leq \;& t\Big(D_G(u_0, P_t) - n_0 t - \sum_{i=1}^{t-1} i + D_G(v_0, P_s) - n_0 s - \sum_{i=1}^{s-1} i\Big) \\
= \;& t\Big(D_G(u_0, P_t) + D_G(v_0, P_s) - n_0(t+s) - (\sum_{i=1}^{t-1} i + \sum_{i=1}^{s-1} i)\Big) \\
= \;& t\Big(D_G(v_0, P_t) + tD + D_G(u_0, P_s) + sD - n_0(t+s) \\
& -(\sum_{i=1}^{t-1} i + \sum_{i=1}^{s-1} i)\Big) \\
= \;& t\Big(\sum_{i=1}^{t} i + \sum_{i=1}^{s} i + (s+t)D - n_0(t+s) - (\sum_{i=1}^{t-1} i + \sum_{i=1}^{s-1} i)\Big) \\
= \;& t(t+s)(1 + D - n_0),
\end{aligned}$$

where D is the distance between u_0 and v_0 in G_0.

Since $D \leq \frac{n_0-1}{2}$, hence

$$\begin{aligned}
& W(G) - W(G_2) \\
< \;& t(t+s)(1 + \frac{n_0 - 1}{2} - n_0) \\
= \;& t(t+s)\frac{1 - n_0}{2} \\
< \;& 0.
\end{aligned}$$

So we complete the proof. ■

Now we can present the proof of Theorem 1.1.

Proof. **(Theorem 1.1)** By Lemmas 2.1, 2.2, we can get the left inequalities. By Lemmas 2.3, 2.4 and 2.6, we can get the right inequalities. The computation of $W(H_{n,k})$,$W(C_k)$ and $W(L_{n,k})$ can be found in [5].

$$W(C_k) = \begin{cases} \frac{k^3}{8}, & if\ k\ is\ even; \\ \frac{k(k^2-1)}{8}, & if\ k\ is\ odd. \end{cases}$$

$$W(H_{n,k}) = \begin{cases} \frac{k^3}{8} + (n-k)(\frac{k^2}{4} + n - 1), & if\ k\ is\ even; \\ \frac{k(k^2-1)}{8} + (n-k)(\frac{k^2-1}{4} + n - 1), & if\ k\ is\ odd. \end{cases}$$

$$W(L_{n,k}) = \begin{cases} \frac{k^3}{8} + (n-k)(\frac{n^2+nk+3k-1}{6} - \frac{k^2}{12}), & if\ k\ is\ even; \\ \frac{k(k^2-1)}{8} + (n-k)(\frac{n^2+nk+3k-1}{6} - \frac{k^2}{12} - \frac{1}{4}), & if\ k\ is\ odd. \end{cases}$$

■

Proof. **(Corollary 1.2)** If k is odd, from the proof of Theorem 1.1, we have

$$W(H_{n,k}) = n^2 + \frac{1}{4}(k^2 - 4k - 5)n - \frac{k^3}{8} + \frac{9k}{8},$$

$$W(H_{n,3}) = n^2 - 2n.$$

So we have

$$\begin{aligned} & W(H_{n,k}) - W(H_{n,3}) \\ = & \frac{1}{4}(k^2 - 4k + 3)n - \frac{k^2}{8} + \frac{9k}{8} \\ \geq & \frac{1}{4}(k^2 - 4k + 3)k - \frac{k^2}{8} + \frac{9k}{8} \\ = & \frac{1}{8}k(k^2 - 8k + 15) \\ \geq & 0, \end{aligned}$$

since $k^2 - 4k + 3 \geq 0$, $k^2 - 8k + 15 \geq 0$ if $k \geq 3$ and k is odd.

Similarly, if k is even, we can get $W(H_{n,k}) \geq W(H_{n,4})$. Note that $W(H_{n,4}) = n^2 - n - 4$, it is easy to see that $W(H_{n,4}) \geq W(H_{n,3})$ for $n \geq 4$. So we have the left inequality.

As above, if k is odd, from the proof of Theorem 1.1, we have

$$W(L_{n,k}) = \frac{1}{6}\left[n^3 + (-\frac{3}{2}k^2 + 3k - \frac{5}{2})n + \frac{5}{4}k^3 - 3k^2 + \frac{7k}{24}\right],$$

$$W(L_{n,3}) = \frac{1}{6}(n^3 - 7n + 12).$$

So we get

$$\begin{aligned} & W(L_{n,3}) - W(L_{n,k}) \\ = \ & \frac{1}{4}(k^2 - 2k - 3)n - \frac{5}{24}k^3 + \frac{1}{2}k^2 - \frac{7k}{24} + 2 \\ \geq \ & \frac{1}{4}(k^2 - 2k - 3)k - \frac{5}{24}k^3 + \frac{1}{2}k^2 - \frac{7k}{24} + 2 \\ = \ & \frac{1}{24}(k^3 - 25k + 48) \\ \geq \ & 0, \end{aligned}$$

the last inequality holds since $k^2 - 2k - 3 \geq 0$, $k^3 - 25k + 48 \geq 0$ if $k \geq 3$ and k is odd.

Similarly, if k is even, we can get $W(L_{n,k}) \leq W(L_{n,4})$. Note that $W(L_{n,4}) = \frac{1}{6}(n^3 - 13n + 36)$, it is easy to see that $W(L_{n,4}) \leq W(L_{n,3})$ for $n \geq 4$. So we get the right inequality. ■

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