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Largest Wiener Index of Unicyclic Graphs with Given Bipartition

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Abstract

The Wiener index of a connected graph is the sum of distances between all unordered pairs of its vertices. In this paper, we first identify the graphs whose Wiener index is second largest among trees with given bipartition. Based on this result, the largest Wiener index of unicyclic graphs with given bipartition is determined and the corresponding extremal graphs are characterized.

1 Introduction

All graphs considered in this paper are simple, finite, and undirected. We follow the terminology and notation of Bondy and Murty in [1] for those not defined here. For a connected graph G, we use $V(G), E(G), n$ and m to denote the vertex set, edge set, order and size of G, respectively. The *cyclomatic number* μ of a connected graph G is the minimum number of edges that must be removed from G in order to transform it to an acyclic graph. It is known that $\mu = m - n + 1$, see [15]. A *unicyclic* graph is a graph with $\mu = 1$. Throughout this paper, let P_n, S_n and C_n denote a path, a star and a cycle on n vertices, respectively.

Let G be a connected graph. For a subset S of the edge (vertex, respectively) set of G, we use $G - S$ to denote the graph obtained by deleting the edges (vertices and incident

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edges, respectively) in S. If $S = \{uv\}$ ($\{v\}$, respectively), we write $G - uv$ ($G - v$, respectively) for short. Let $G + uv$ denote the graph obtained from G by adding the edge $uv \notin E(G)$. For a subgraph H of G, denote by $|H|$ the number of vertices in $V(H)$ and simply write $G - H$ for the graph $G - V(H)$. Let $d_G(v)$ be the degree of the vertex v in G. For $u, v \in V(G)$, we use P_{uv} to denote the path connecting u and v. Let $d_G(u, v)$ denote the distance between the vertices u and v in G, and let $D_G(u)$ denote the sum of distances between u and all the other vertices of G, that is, $D_G(u) = \sum_{v \in V(G)} d_G(u, v)$.

The *Wiener index* of a connected graph G, denoted by $W(G)$, is defined as the sum of distances between all unordered pairs of its vertices, i.e.,

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

This graph invariant was proposed by Wiener in 1947, while its equivalent definition as above was first given by Hosoya [9] in 1971. The Wiener index has found many applications in chemistry and has been extensively studied, see surveys [10, 11, 16] and the references therein. For P_n and C_n, we can easily get their Wiener indices.

Lemma 1. *[3]* $W(P_n) = \binom{n+1}{3}$.

Lemma 2. *[14]*

$$W(C_n) = \begin{cases} \frac{1}{8}n^3 & \textit{if } n \textit{ is even;} \\ \frac{1}{8}n(n^2 - 1) & \textit{otherwise.} \end{cases}$$

One of the fundamental problems for a graph invariant is to determine its extremal (maximum and minimum) values among certain classes of graphs. Entringer et al. [7] proved that among all connected graphs on n vertices, the Wiener index is maximized by the path P_n, while minimized by the complete graph K_n. For trees of order n, the maximum Wiener index is obtained by the path P_n, and the minimum for the star S_n in [3]. Tang et al. [14] characterized the graphs with the first three maximum and minimum Wiener indices among all the unicyclic graphs of order n. Besides, the extremal graphs that maximize or minimize the Wiener index among trees or unicyclic graphs with prescribed maximum degree, diameter, matching and independence numbers, etc., have been studied (see [2, 6, 8, 12, 13]).

Du [4] considered the Wiener indices of trees and unicyclic graphs with given bipartition. He determined the smallest Wiener indices and characterized the corresponding extremal graphs. For two nonnegative integers p, q, we say a graph G has a (p, q)-*bipartition*, if G is a bipartite-graph with bipartition sizes p and q. Let $H(r; x, y)$ be the tree obtained by attaching x and y vertices, respectively, to the two end vertices of the path on r vertices, where $r \geq 1, x \geq y \geq 0$. We simply write $T(p, q)$ for the graph $H(2q-1; \lceil \frac{p-q+1}{2} \rceil, \lfloor \frac{p-q+1}{2} \rfloor)$, as shown in Figure 1. For the largest Wiener index of trees, Du [4] got the following.

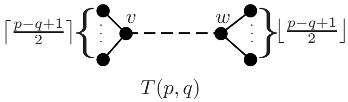

Figure 1. The graph $T(p, q)$.

Theorem 1. *[4] Let G be a tree with a (p, q)-bipartition, where $p \geq q \geq 1$. Then*

$$W(G) \leq pq(2q-3) + p(p+1) + (q-1)\left[\left\lfloor \frac{(p-q+1)^2}{2} \right\rfloor - \frac{2}{3}q(q-2)\right]$$

with equality if and only if $G \cong T(p, q)$.

However, the largest Wiener index of unicyclic graphs with given bipartition remains open. Knor et al. [10] proposed the following problem.

Problem 1. *[10] Find the largest Wiener index among unicyclic graphs on n vertices with bipartition sizes p and q, where $n = p + q$.*

In this paper, we first identify the graphs whose Wiener index is second largest among trees with given bipartition. Based on this result, the largest Wiener index of unicyclic graphs with given bipartition is determined and the corresponding extremal graphs are characterized, which completely solves Problem 1.

2 Second largest Wiener index of trees

Let G_1, G_2 be two nontrivial connected graphs with $x \in V(G_1)$ and $y \in V(G_2)$, to *identify* x and y is to replace these vertices by a single vertex incident to all the edges which were incident to either x in G_1 or y in G_2. The authors [4, 5] stated the following three fundamental lemmas, which are very useful throughout this paper.

Lemma 3. *[4] Let G, H be two nontrivial connected graphs with $u, v \in V(G)$, $w \in V(H)$. Let GuH (GvH, respectively) be the graph obtained from G and H by identifying u(v, respectively) with w. If $D_G(u) < D_G(v)$, then $W(GuH) < W(GvH)$.*

Lemma 4. *[5] Let Q_1 and Q_2 be two vertex-disjoint connected graphs such that $u \in V(Q_1)$ and $v \in V(Q_2)$. For integer $j \geq 1$, let $G_u (G_v$, respectively) be the graph obtained by joining u and v by a path of length j and attaching z pendant vertices to u (v, respectively). Then*

$$W(G_v) - W(G_u) = jz(|V(Q_1)| - |V(Q_2)|).$$

Lemma 5. *[4] Let t, a, b, p, q be positive integers. Let $t \geq 4$ and $q \geq 2$.*

(1) If $a \geq b \geq 2$, then $W(H(t; a-1, b-1)) > W(H(t-2; a, b))$.

(2) If $p \geq q+1$, then $W(H(2q-1; p-q, 1)) > W(H(2q-2; p-q+1, 1))$.

(3) If $a \geq b+2$, then $W(H(2q-1; a-1, b+1)) > W(H(2q-1; a, b))$.

Let $T'(p,q)$ be the graph $H(2q-1; \lceil \frac{p-q+1}{2} \rceil + 1, \lfloor \frac{p-q+1}{2} \rfloor - 1)$, and $T''(p,q)$ the graph obtained from $H(2q-1; \lceil \frac{p-q+1}{2} \rceil - 1, \lfloor \frac{p-q+1}{2} \rfloor)$ by adding some new pendent vertex as shown in Figure 2. Obviously, $T'(p,q)$ and $T''(p,q)$ are bipartite-graphs with a (p,q)-bipartition. Inspired by the proof of Theorem 1 [4], we determine the second largest Wiener index of trees with given bipartition.

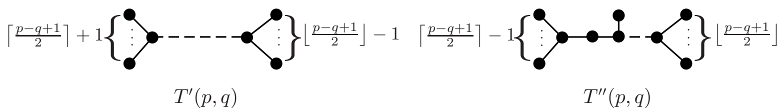

Figure 2. The graphs $T'(p,q)$ and $T''(p,q)$.

Theorem 2. *Let G be a tree with a (p,q)-bipartition, where $p \geq q \geq 3$. Moreover, $G \ncong T(p,q)$. Then*

(1) for $p-q$ odd,

$$W(G) \leq pq(2q-3) + p(p+1) + (q-1)\left[\left\lfloor \frac{(p-q+1)^2}{2} \right\rfloor - \frac{2}{3}q(q-2) - 2\right]$$

with equality if and only if $G \cong T'(p,q)$;

(2) for $p-q$ even,

$$W(G) \leq pq(2q-3) + p(p+1) + (q-1)\left[\left\lfloor \frac{(p-q+1)^2}{2} \right\rfloor - \frac{2}{3}q(q-2) - 4\right] + 4$$

with equality if and only if $G \cong T''(p,q)$.

To prove Theorem 2, we need the lemma below.

Lemma 6. *Let $p \geq q \geq 3$. Then*

(1) for $p-q$ odd, $W(T(p,q)) - W(T'(p,q)) = 2q-2$;

(2) for $p-q$ even, $W(T(p,q)) - W(T''(p,q)) = 4q-8$.

Proof. (1) Let $p-q$ be odd. Set $Q_1 = S_{1+\lceil \frac{p-q+1}{2} \rceil}$ and $Q_2 = S_{\lfloor \frac{p-q+1}{2} \rfloor}$. Let u and v be the centers of Q_1 and Q_2, respectively. Then the graph obtained by joining u and v by a path of length $j = 2q-2$ and attaching $z = 1$ pendant vertex to u (v, respectively) coincides with $T'(p,q)$ ($T(p,q)$, respectively). Then by Lemma 4,

$$W(T(p,q)) - W(T'(p,q)) = (2q-2) \cdot 1 \cdot \left(1 + \left\lceil \frac{p-q+1}{2} \right\rceil - \left\lfloor \frac{p-q+1}{2} \right\rfloor \right) = 2q-2.$$

(2) Let $p-q$ be even. Set $Q_1 = H(2q-3; \lfloor \frac{p-q+1}{2} \rfloor, 0)$ and $Q_2 = S_{\lceil \frac{p-q+1}{2} \rceil}$. Let u be the leaf of Q_1 such that its neighbor is of degree 2, and v be the center of Q_2. Then the graph obtained by joining u and v by a path of length $j = 2$ and attaching $z = 1$ pendant vertex to u (v, respectively) coincides with $T''(p,q)$ ($T(p,q)$, respectively). Then by Lemma 4,

$$W(T(p,q)) - W(T''(p,q)) = 2 \cdot 1 \cdot \left(2q-3 + \left\lfloor \frac{p-q+1}{2} \right\rfloor - \left\lceil \frac{p-q+1}{2} \right\rceil \right) = 4q-8.$$

■

Proof of Theorem 2: Let G be a tree with a (p,q)-bipartition with the second largest Wiener index. We may partition $V(G)$ into two disjoint subsets $V_1(G)$ and $V_2(G)$, where $|V_1(G)| = p$ and $|V_2(G)| = q$. Let $P = u_1 u_2 \ldots u_{t-1} u_t$ be a diametrical path of G. Note that G is not a star (i.e. $t \geq 4$). Assume that $d_G(u_2) \leq d_G(u_{t-1})$.

(1) Let $p-q$ be odd.

If $G \cong T'(p,q)$, by Theorem 1 and Lemma 6, we have that

$$\begin{aligned} W(G) &= W(T(p,q)) - 2q + 2 \\ &= pq(2q-3) + p(p+1) + (q-1)\left[\left\lfloor \frac{(p-q+1)^2}{2} \right\rfloor - \frac{2}{3}q(q-2) - 2\right]. \end{aligned}$$

Next we suppose that $G \ncong T'(p,q)$. In the following, under the assumption that $p-q$ is odd, the proof falls into three cases based on the number of vertices on P different from u_2, u_{t-1} with degree at least three.

Case 1.1 Suppose that there does not exist a vertex on P different from u_2, u_{t-1} with degree at least three, which means $G \cong H(t-2; a, b)$ ($a \geq b \geq 1$, $a + b = p + q - t + 2$).

If $d_G(u_2, u_{t-1})$ is odd (i.e. t even), then $u_2 \in V_1(G)$ and $u_{t-1} \in V_2(G)$. Furthermore, G has a $(\frac{t-2}{2} + a, \frac{t-2}{2} + b)$-bipartition, that is, $p = \frac{t-2}{2} + a$, $q = \frac{t-2}{2} + b$ ($a > b$). Suppose that

$b \geq 2$. Clearly, $H(t; a-1, b-1) \ncong T(p,q)$ and $H(t; a-1, b-1)$ has a (p,q)-bipartition. By Lemma 5 and Theorem 1, $W(G) = W(H(t-2; a, b)) < W(H(t; a-1, b-1)) < W(T(p,q))$, a contradiction. Now assume that $b = 1$, implying that $t - 2 = 2q - 2$ and $a = p - q + 1$, that is, $G \cong H(2q-2; p-q+1, 1)$. Since $G \ncong T'(p,q)$ and $p-q$ is odd, we have $p-q \geq 3$. Then $H(2q-1; p-q, 1) \ncong T(p,q)$ and it has a (p,q)-bipartition. By Lemma 5 and Theorem 1, $W(G) = W(H(2q-2; p-q+1, 1)) < W(H(2q-1; p-q, 1)) < W(T(p,q))$, a contradiction.

If $d_G(u_2, u_{t-1})$ is even (i.e. t odd), then $u_2, u_{t-1} \in V_2(G)$. What's more, we have $t - 2 = 2q - 1$ and $a + b = p - q + 1$ since G has a (p,q)-bipartition. Let $a = \lceil \frac{p-q+1}{2} \rceil + s$ and $b = \lfloor \frac{p-q+1}{2} \rfloor - s$, where $s \geq 2$. Then by a similar way of the proof in Lemma 6(1), we have

$$\begin{aligned} W(T(p,q)) - W(G) &= (2q-2) \cdot s \cdot \left[\left(1 + \left\lceil \frac{p-q+1}{2} \right\rceil \right) - \left(\left\lfloor \frac{p-q+1}{2} \right\rfloor - s + 1 \right) \right] \\ &= (2q-2)s^2 \end{aligned}$$

However, we have $W(T(p,q)) - W(T'(p,q)) = 2q - 2$ by Lemma 6. Hence, $W(G) < W(T'(p,q)) < W(T(p,q))$, a contradiction.

Case 1.2 Suppose that there exists exactly one vertex u_i $(3 \leq i \leq t-2)$ on P different from u_2, u_{t-1} with degree at least three.

Let $A = \{v_1, v_2, \ldots, v_k\}$ be the neighbors of u_i in G different from u_{i-1}, u_{i+1}, where $k = d_G(u_i) - 2 \geq 1$. Let H_1 (H_2, respectively) be the component of $G - A$ ($G - \{u_{i-1}u_i, u_iu_{i+1}\}$, respectively) containing u_i. Then G can be obtained from H_1 and H_2 by identifying $u_i \in V(H_1)$ with $u_i \in V(H_2)$. Next, we further divide our discussion into two subcases based on whether H_2 is a star.

Subcase 1.2.1 H_2 is not a star.

(a) Suppose that $d_G(u_2, u_i)$ is even.

Let G_1 be the tree obtained from H_1 and H_2 by identifying $u_2 \in V(H_1)$ with $u_i \in V(H_2)$. Obviously, $G_1 \ncong T(p,q)$ and G_1 has a (p,q)-bipartition. Let n_1 be the number of vertices of the component of $H_1 - u_iu_{i+1}$ containing u_{i+1}. We have

$$\begin{aligned} D_{H_1}(u_2) - D_{H_1}(u_i) &= \sum_{x \in V(H_1)\backslash\{u_2,u_3,\ldots,u_{i-1},u_i\}} [d_{H_1}(x,u_2) - d_{H_1}(x,u_i)] \\ &= (i-2)[n_1 - (d_{H_1}(u_2) - 1)] \\ &\geq (i-2)[d_{H_1}(u_{t-1}) - (d_{H_1}(u_2) - 1)] \\ &= (i-2)(d_G(u_{t-1}) - d_G(u_2) + 1) > 0, \end{aligned}$$

and thus, $D_{H_1}(u_2) > D_{H_1}(u_i)$. Now by Lemma 3 and Theorem 1, $W(G) < W(G_1) < W(T(p,q))$, a contradiction.

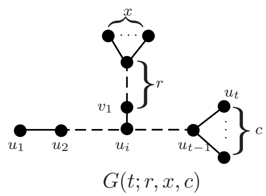

Figure 3. The graph $G(t;r,x,c)$.

(b) Suppose that $d_G(u_2,u_i)$ is odd.

$(b1)$ If $H_2 \cong H(r;x,1)$ $(r \geq 2, x \geq 1)$, set $d_G(u_{t-1}) = c+1(\geq 2)$, then $t+r+x+c = p+q+1$ and $G \cong G(t;r,x,c)$ as shown in Figure 3. Let G_2 be the tree obtained from $H_3 = H_1 + u_iv_1$ and $H_4 = H_2 - u_iv_1$ by identifying $u_2 \in V(H_3)$ with $v_1 \in V(H_4)$. Clearly, $G_2 \ncong T(p,q)$ and G_2 has a (p,q)-bipartition. Note that $i \geq r+2 \geq 4$ and $t-i \geq r+1 \geq 3$, since P is a diametrical path of G. Furthermore, $i-2$ is odd, which means $i \geq 5$. Then

$$\begin{aligned} D_{H_3}(u_2) - D_{H_3}(v_1) &= \sum_{x \in V(H_3)\backslash\{u_2,u_3,\ldots,u_i,v_1\}} [d_{H_3}(x,u_2) - d_{H_3}(x,v_1)] \\ &= d_{H_3}(u_1,u_2) - d_{H_3}(u_1,v_1) + \\ &\qquad \sum_{x \in V(H_3)\backslash\{u_1,u_2,\ldots,u_i,v_1\}} [d_{H_3}(x,u_2) - d_{H_3}(x,v_1)] \\ &= 1 - i + (i-3)(t-i+c-1) \geq 2(i-4) > 0. \end{aligned}$$

Then by Lemma 3 and Theorem 1, $W(G) < W(G_2) < W(T(p,q))$, a contradiction.

$(b2)$ Otherwise, let G_3 be the tree obtained from H_1 and H_2 by identifying $u_1 \in V(H_1)$ with $u_i \in V(H_2)$. Obviously, $G_3 \ncong T(p,q)$ and G_3 has a (p,q)-bipartition. Note that $D_{H_1}(u_1) - D_{H_1}(u_2) = |V(H_1)| - 2 > 0$. Together with the fact $D_{H_1}(u_2) > D_{H_1}(u_i)$ in

Subcase 1.2.1(a), we get that $D_{H_1}(u_1) > D_{H_1}(u_i)$. Now by Lemma 3 and Theorem 1, $W(T(p,q)) > W(G_3) > W(G)$, a contradiction.

Subcase 1.2.2 H_2 is a star.

(a) Suppose that $d_G(u_2, u_i)$ is even. Hence $i \geq 4$. If u_i is the center of H_2, $d_G(u_2) = \lfloor \frac{p-q+1}{2} \rfloor - k + 1$ and $t = 2q+1$, then $d_G(u_{t-1}) = \lceil \frac{p-q+1}{2} \rceil + 1$. Assume that $k = 1$. Note that $T'(p,q)$ (G, respectively) can be obtained from $G - v_1$ by attaching $z = 1$ pendant vertex to u_{t-1} (u_i, respectively). Then it follows from Lemma 4 that

$$W(G) - W(T'(p,q)) = (t-1-i) \cdot 1 \cdot \left[\left(\left\lceil \frac{p-q+1}{2} \right\rceil + 1 \right) - \left(\left\lfloor \frac{p-q+1}{2} \right\rfloor - 1 + i - 1 \right) \right] = (t-1-i)(3-i) < 0.$$

So we have $W(G) < W(T'(p,q)) < W(T(p,q))$, a contradiction.

Now assume that $k \geq 2$. Then G can be obtained from $H_5 = H_1 + u_i v_k$ and $H_6 = H_2 - u_i v_k$ by identifying $u_i \in V(H_5)$ with $u_i \in V(H_6)$. Let G_4 be the graph obtained from H_5 and H_6 by identifying $u_2 \in V(H_5)$ with $u_i \in V(H_6)$. Clearly, $G_4 \ncong T(p,q)$ and G_4 has a (p,q)-bipartition. By directly calculating, $D_{H_5}(u_2) - D_{H_5}(u_i) = (i-2)(t-i+k) > 0$. Then by Lemma 3 and Theorem 1, we have $W(G) < W(G_4) < W(T(p,q))$, a contradiction.

For the other cases, we can get a contradiction by a similar discussion to Subcase 1.2.1(a).

(b) Suppose that $d_G(u_2, u_i)$ is odd. If u_i is a leaf of H_2, $d_G(u_2) = 2$, $d_G(u_{t-1}) = \lceil \frac{p-q+1}{2} \rceil + 1$ and $t = 2q-1$, then $G \cong G(2q-1; 1, \lfloor \frac{p-q+1}{2} \rfloor, \lceil \frac{p-q+1}{2} \rceil)$. In a similar discussion to Subcase 1.2.1($b1$), we can obtain a contradiction.

If u_i is the center of H_2, $d_G(u_2) = 2$, $d_G(u_{t-1}) = \lceil \frac{p-q+1}{2} \rceil + 1$ and $t = 2q$, then $k = \lfloor \frac{p-q+1}{2} \rfloor$. We can deduce a contradiction whether $k = 1$ or $k \geq 2$ in a similar discussion to Subcase 1.2.2(a).

For the other cases, similarly to Subcase 1.2.1($b2$), we can reach a contradiction.

Case 1.3 Suppose that there exist at least two vertices on P different from u_2, u_{t-1} with degree at least three. Let u_i $(3 \leq i \leq t-2)$ be such a vertex satisfying $d_G(u_2, u_i)$ is as small as possible. We may deduce a contradiction whether $d_G(u_2, u_i)$ is even or odd in a similar discussion of Subcase 1.2.1.

(2) Let $p - q$ be even.

If $G \cong T''(p,q)$, by Theorem 1 and Lemma 6,

$$\begin{aligned} W(G) &= W(T(p,q)) - 4q + 8 \\ &= pq(2q-3) + p(p+1) + (q-1)\left[\left\lfloor \frac{(p-q+1)^2}{2} \right\rfloor - \frac{2}{3}q(q-2) - 4\right] + 4. \end{aligned}$$

Next we suppose that $G \ncong T''(p,q)$. Similarly, we can divide our proof into three cases.

Case 2.1 Suppose that there does not exist a vertex on P different from u_2, u_{t-1} with degree at least three, which means $G \cong H(t-2; a, b)$ $(a \geq b \geq 1, a+b = p+q-t+2)$.

(a) If $d_G(u_2, u_{t-1})$ is odd (i.e. t even), then $u_2 \in V_1(G)$ and $u_{t-1} \in V_2(G)$. Furthermore, G has a $(\frac{t-2}{2}+a, \frac{t-2}{2}+b)$-bipartition, that is, $p = \frac{t-2}{2}+a$, $q = \frac{t-2}{2}+b$. Suppose that $b \geq 2$. If $a = b = 2$, then $W(T(p,q)) - W(G) = 2(2q-3) > W(T(p,q)) - W(T''(p,q))$. Hence $W(G) < W(T''(p,q)) < W(T(p,q))$, a contradiction. If $a > b \geq 2$ or $a = b \geq 3$, then $H(t; a-1, b-1) \ncong T(p,q)$ and $H(t; a-1, b-1)$ has a (p,q)-bipartition. By Lemma 5 and Theorem 1, $W(G) = W(H(t-2; a, b)) < W(H(t; a-1, b-1)) < W(T(p,q))$, a contradiction.

Now assume that $b = 1$, implying that $t-2 = 2q-2$ and $a = p-q+1$, that is, $G \cong H(2q-2; p-q+1, 1)$. Since $G \ncong T(p,q)$, we have $p-q \geq 2$. If $p-q = 2$, $W(T(p,q)) - W(G) = 2(2q-2)$ and $W(T(p,q)) - W(T''(p,q)) = 2(2q-4)$, which means $W(G) < W(T''(p,q)) < W(T(p,q))$, a contradiction. Suppose $p-q \geq 3$, then $H(2q-1; p-q, 1) \ncong T(p,q)$ and it has a (p,q)-bipartition. By Lemma 5 and Theorem 1, $W(G) = W(H(2q-2; p-q+1, 1)) < W(H(2q-1; p-q, 1)) < W(T(p,q))$, a contradiction.

(b) If $d_G(u_2, u_{t-1})$ is even, then $u_2, u_{t-1} \in V_2(G)$ and $t-2 = 2q-1$. Let $a = \lceil \frac{p-q+1}{2} \rceil + s$ and $b = \lfloor \frac{p-q+1}{2} \rfloor - s$, where $s \geq 1$. Then with a proof similar to Lemma 6(1), we have that

$$W(T(p,q)) - W(G) = (2q-2) \cdot s \cdot (s+1) > W(T(p,q)) - W(T''(p,q)) = 2(2q-4).$$

Thus, $W(G) < W(T''(p,q)) < W(T(p,q))$, a contradiction.

Case 2.2 Suppose that there exists exactly one vertex u_i $(3 \leq i \leq t-2)$ on P different from u_2, u_{t-1} with degree at least three.

Let $A = \{v_1, v_2, \ldots, v_k\}$ be the neighbors of u_i in G different from u_{i-1}, u_{i+1}, where $k = d_G(u_i) - 2 \geq 1$. Let H_1 (H_2, respectively) be the component of $G - A$ ($G - \{u_{i-1}u_i, u_iu_{i+1}\}$, respectively) containing u_i. If H_2 is not a star, we can get a contradiction similar to Subcase 1.2.1. Assume that H_2 is a star.

(a) Suppose that $d_G(u_2, u_i)$ is even.

Observe that $i \geq 4$. If u_i is the center of H_2, $d_G(u_2) = \lfloor \frac{p-q+1}{2} \rfloor - k + 1$ and $t = 2q + 1$, then $d_G(u_{t-1}) = \lceil \frac{p-q+1}{2} \rceil + 1$. Suppose that $k = 1$. Then, G can be obtained from $H_7 = G - u_{t-1}u_t$ and $H_8 = u_{t-1}u_t$ by identifying $u_{t-1} \in V(H_7)$ with $u_{t-1} \in V(H_8)$. Let G_5 be the graph obtained from H_7 and H_8 by identifying $u_2 \in V(H_7)$ with $u_{t-1} \in V(H_8)$. Clearly, $G_5 \ncong T(p, q)$ and G_5 has a (p, q)-bipartition. Moreover, $D_{H_7}(u_2) - D_{H_7}(u_{t-1}) = (i - 1 + t - 2) - (t - i + 1) = 2i - 4 > 0$. By Lemma 3 and and Theorem 1, we have $W(G) < W(G_5) < W(T(p, q))$, a contradiction. For the case that $k \geq 2$, we can obtain a contradiction in a similar discussion to Subcase 1.2.2(a).

If u_i is the center of H_2, $d_G(u_2) = \lceil \frac{p-q+1}{2} \rceil - k + 1$ and $t = 2q + 1$, then $d_G(u_{t-1}) = \lfloor \frac{p-q+1}{2} \rfloor + 1$. Suppose that $k = 1$. Note that $T''(p, q)$ (G, respectively) can be obtained from $G - v_1$ by attaching $z = 1$ pendant vertex to u_4 (u_i, respectively). Then

$$\begin{aligned} W(T''(p,q)) - W(G) &= (i-4)\left[\left\lfloor \frac{p-q+1}{2} \right\rfloor + t - i - \left(\left\lceil \frac{p-q+1}{2} \right\rceil - 1 + 3\right)\right] \\ &= (i-4)(t-i-3). \end{aligned}$$

Since $G \ncong T''(p, q)$, we get that $i > 4$ and $t + 1 - i > 4$. Now we have $W(G) < W(T''(p, q)) < W(T(p, q))$, a contradiction. Suppose $k \geq 2$. We can deduce a contradiction in a similar discussion to Subcase 1.2.2(a).

For the other cases, we can get a contradiction similar to Subcase 1.2.2(a).

(b) Suppose that $d_G(u_2, u_i)$ is odd.

We can always find a graph G' such that G' has a (p, q)-bipartition and $W(G) < W(G') < W(T(p, q))$ by a similar way to Subcase 1.2.2(b), which is impossible.

Case 2.3. Suppose that there exist at least two vertices on P different from u_2, u_{t-1} with degree at least three. We can deduce a contradiction in a similar way of Case 1.3.

Therefore, the proof is complete. ■

Theorem 3. *Let G be a tree with a (p, q)-bipartition, where $p \geq q = 2$. Moreover, $G \ncong T(p, 2)$. Then $W(G) \leq p^2 + 3p + \lfloor \frac{(p-1)^2}{2} \rfloor - 2$ with equality if and only if $G \cong T'(p, 2)$.*

Proof. If $G \cong T'(p, 2)$, then $W(G) = W(T'(p, 2)) = p^2 + 3p + \lfloor \frac{(p-1)^2}{2} \rfloor - 2$.

Let $G \ncong T'(p, 2)$ and let $P = u_1u_2 \ldots u_{t-1}u_t$ $(4 \leq t \leq 5)$ be a diametrical path of G. Suppose that $d_G(u_2) \leq d_G(u_{t-1})$. Note that there does not exist a vertex on P different from u_2, u_{t-1} of degree at least three. If u_2 and u_{t-1} are in the same vertex class, it follows that $W(G) < W(T'(p,2))$ in a discussion similar to Case 1.1 in Theorem 2. Otherwise, $t = 4$ and $d_G(u_2) = 2$. Since $G \ncong T(p,2)$ and $G \ncong T'(p,2)$, we have $p \geq 5$. Then $W(T'(p,2)) - W(G) = 2 \cdot (p - \lfloor \frac{p-1}{2} \rfloor) \cdot (\lfloor \frac{p-1}{2} \rfloor - 1) > 0$. Therefore, $W(G) < W(T'(p,2))$. ■

3 Largest Wiener index of unicyclic graphs

Let G be a unicyclic graph of order n with its unique cycle $C_\gamma = u_1u_2\ldots u_\gamma u_1$. For $1 \leq i \leq \gamma$, we use T_i to denote the component containing u_i in the subgraph $G - E(C_\gamma)$. Such a unicyclic graph is denoted by $C_\gamma(T_1, T_2, \ldots, T_\gamma)$. Let $\ell_i = |T_i| - 1, i = 1, 2, \ldots, \gamma$. Then $\sum_{i=1}^{\gamma} \ell_i = n - \gamma$.

With a proof similar to [14], we give the following formula for calculating the Wiener index of unicyclic graphs.

Theorem 4. *Let $G = C_\gamma(T_1, T_2, \ldots, T_\gamma)$ be a unicyclic graph. Then*

$$\begin{aligned} W(G) =& W(C_\gamma) + \sum_{i=1}^{\gamma} \ell_i D_{C_\gamma}(u_i) + \sum_{i=1}^{\gamma} W(T_i) \\ &+ \sum_{i=1}^{\gamma-1} \sum_{j=i+1}^{\gamma} (\ell_i\omega_j + \ell_i\ell_j d_{C_\gamma}(u_i, u_j) + \ell_j\omega_i), \end{aligned} \tag{1}$$

where $\omega_i = D_{T_i}(u_i)$.

We use $U(p,q)$ to denote the unicyclic graph obtained from $T(p,q)$ by adding some edge, that is, the first graph as shown in Figure 4. Now, we determine the largest Wiener index of unicyclic graphs with given bipartition.

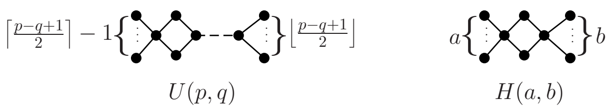

Figure 4. The graphs $U(p,q)$ and $H(a,b)$.

Theorem 5. *Let G be a bipartite unicyclic graph with a (p,q)-bipartition, where $p \geq q \geq 2$. Then*

$$\begin{aligned} W(G) \leq& pq(2q-1) + p(p-3) + (q-1)\left[\left\lfloor \frac{(p-q+1)^2}{2} \right\rfloor - \frac{2}{3}q(q+1)\right] \\ &- 2(2q-3)\left\lfloor \frac{p-q+1}{2} \right\rfloor + 2 \end{aligned}$$

with equality if and only if $G \cong U(p,q)$.

Proof. Note that when $q = 2$, $G \cong H(a, b)$, where $H(a, b)$ is the graph in Figure 4 with $a \geq b \geq 0$ and $a + b = p - 2$. By direct calculation, we have $W(G) = W(H(a, b)) = p^2 + 3p - 2 + 2ab$. Under the condition that $a + b = p - 2$, $W(H(a, b))$ attains the maximum value if $a = \left\lceil \frac{p-2}{2} \right\rceil = \left\lfloor \frac{p-1}{2} \right\rfloor$ and $b = \left\lfloor \frac{p-2}{2} \right\rfloor = \left\lceil \frac{p-1}{2} \right\rceil - 1$, which means $G \cong H(\left\lceil \frac{p-2}{2} \right\rceil, \left\lfloor \frac{p-2}{2} \right\rfloor) \cong U(p, 2)$. In the following, we assume that $q \geq 3$.

Let $G = C_\gamma(T_1, T_2, \ldots, T_\gamma)$ be a unicyclic graph with a (p, q)-bipartition and $\ell_1 \geq \ell_i$ for each $2 \leq i \leq \gamma$. Then $\sum_{i=1}^{\gamma} \ell_i = p + q - \gamma$, $\ell_1 \geq \left\lceil \frac{p+q-\gamma}{\gamma} \right\rceil$, $4 \leq \gamma \leq 2q$ and γ is even.

We calculate the Wiener index of the graph $G - u_1u_\gamma$ with a similar formula to the equality (1) as follows:

$$W(G - u_1u_\gamma) = W(P_\gamma) + \sum_{i=1}^{\gamma} \ell_i D_{P_\gamma}(u_i) + \sum_{i=1}^{\gamma} W(T_i) + \sum_{i=1}^{\gamma-1} \sum_{j=i+1}^{\gamma} (\ell_i \omega_j + \ell_i \ell_j d_{P_\gamma}(u_i, u_j) + \ell_j \omega_i), \tag{2}$$

where $\omega_i = D_{T_i}(u_i)$.

(1) − (2), one gets

$$W(G - u_1u_\gamma) - W(G) = W(P_\gamma) - W(C_\gamma) + \sum_{i=1}^{\gamma} \ell_i (D_{P_\gamma}(u_i) - D_{C_\gamma}(u_i)) + \sum_{i=1}^{\gamma-1} \sum_{j=i+1}^{\gamma} \ell_i \ell_j (d_{P_\gamma}(u_i, u_j) - d_{C_\gamma}(u_i, u_j)). \tag{3}$$

By direct calculation, for $1 \leq i \leq \frac{\gamma}{2}$,

$$D_{P_\gamma}(u_i) - D_{C_\gamma}(u_i) = D_{P_\gamma}(u_{\gamma+1-i}) - D_{C_\gamma}(u_{\gamma+1-i}) = \left(\frac{\gamma}{2} + 1 - i\right)\left(\frac{\gamma}{2} - i\right). \tag{4}$$

We should point out that $W(U(p, q)) = W_1 - (2 + 2\ell_1^1)$, where $W_1 = W(T(p, q))$ and $\ell_1^1 = 2q - 4 + \left\lfloor \frac{p-q+1}{2} \right\rfloor$. Note that $2 + 2\ell_1^1 \leq p + 3q - 5$. We use W_2 to denote the value of the second largest Wiener index of trees with a given (p, q)-bipartition. Since $q \geq 3$, it follows from Lemma 6, Theorem 1 and Theorem 2 that

$$W_1 - W_2 \geq 2q - 2. \tag{5}$$

We proceed to show $W(G) < W(U(p, q) = W_1 - (2 + 2\ell_1^1)$ if $G \ncong U(p, q)$.

Case 1. $6 \leq \gamma \leq 2q$ and γ is even.

(i) If $G - u_1u_\gamma \cong T(p, q)$, we have $W(G - u_1u_\gamma) = W_1$. Let v, w denote the two vertices in $T(p, q)$ as shown in Figure 1. Then there are at most two ways to get G

from $T(p,q)$: (I) both u_1 and u_γ are on the path P_{vw}, in which case by (3) and (4) we have $W(G-u_1u_\gamma)-W(G)=W(P_\gamma)-W(C_\gamma)+\ell_1(D_{P_\gamma}(u_1)-D_{C_\gamma}(u_1))+\ell_\gamma(D_{P_\gamma}(u_\gamma)-D_{C_\gamma}(u_\gamma))+\ell_1\ell_\gamma(d_{P_\gamma}(u_1,u_\gamma)-d_{C_\gamma}(u_1,u_\gamma))=\binom{\gamma+1}{3}-\frac{\gamma^3}{8}+\frac{\gamma}{2}(\frac{\gamma}{2}-1)(p+q-\gamma)+(\gamma-2)\ell_1\ell_\gamma$; (II) only one of u_1 and u_γ is on the path P_{vw}, in which case by (3) and (4) we similarly have $W(G-u_1u_\gamma)-W(G)=\binom{\gamma+1}{3}-\frac{\gamma^3}{8}+(\frac{\gamma}{2}-1)(\frac{\gamma}{2}-2)(p+q-\gamma)+2(\frac{\gamma}{2}-1)\ell_1+(\gamma-4)\ell_1\ell_{\gamma-1}$. No matter which case happens, we always have

$$\begin{aligned}W(G-u_1u_\gamma)-W(G)&>\binom{\gamma+1}{3}-\frac{\gamma^3}{8}+(\frac{\gamma}{2}-1)(\frac{\gamma}{2}-2)(p+q-\gamma)\\&=-\frac{5}{24}\gamma^3+(\frac{3}{2}+\frac{p+q}{4})\gamma^2-\left[\frac{13}{6}+\frac{3(p+q)}{2}\right]\gamma+2(p+q).\quad(6)\end{aligned}$$

Set $g(\gamma)=-\frac{5}{24}\gamma^3+(\frac{3}{2}+\frac{p+q}{4})\gamma^2-\left[\frac{13}{6}+\frac{3(p+q)}{2}\right]\gamma+2(p+q)$. Then we have $g'(\gamma)\geq min\{g'(6),g'(2q)\}$ since $g''(6)=\frac{p+q+1}{2}>0$. And $g(\gamma)\geq min\{g(6),g(2q)\}$ because $g'(6)>0$ $(p\geq q\geq 3)$. Since $g(2q)-g(6)=p(q^2-3q)-\frac{2}{3}q^3+3q^2-\frac{13}{3}q+4\geq\frac{1}{3}q(q^2-13)+4\geq\frac{1}{3}\times 3\times(3^2-13)+4=0$, we get $g(\gamma)\geq g(6)$. We continue the inequality (6) and obtain

$$\begin{aligned}W(G-u_1u_\gamma)-W(G)&>g(6)=2(p+q)-4\\&\geq p-q+1+(2+2\ell_1^1)\\&>2+2\ell_1^1.\end{aligned}$$

Thus, we have $W(G)<W_1-(2+2\ell_1^1)=W(U(p,q))$ in this case.

(ii) If $G-u_1u_\gamma\ncong T(p,q)$, we have $W(G-u_1u_\gamma)\leq W_2$. Recall that $\ell_1\geq\left\lceil\frac{p+q-\gamma}{\gamma}\right\rceil$. By (3) and (4), we get

$$\begin{aligned}W(G-u_1u_\gamma)-W(G)&=W(P_\gamma)-W(C_\gamma)+\sum_{i=1}^{\gamma}\ell_i(D_{P_\gamma}(u_i)-D_{C_\gamma}(u_i))+\\&\quad+\sum_{i=1}^{\gamma-1}\sum_{j=i+1}^{\gamma}\ell_i\ell_j(d_{P_\gamma}(u_i,u_j)-d_{C_\gamma}(u_i,u_j))\\&\geq\binom{\gamma+1}{3}-\frac{\gamma^3}{8}+\frac{\gamma}{2}(\frac{\gamma}{2}-1)\ell_1\\&\geq\binom{\gamma+1}{3}-\frac{\gamma^3}{8}+\frac{\gamma}{2}(\frac{\gamma}{2}-1)\left\lceil\frac{p+q-\gamma}{\gamma}\right\rceil\\&\geq\frac{\gamma^3}{24}-\frac{\gamma^2}{4}+(\frac{1}{3}+\frac{p+q}{4})\gamma-\frac{p+q}{2}\\&\geq\frac{6^3}{24}-\frac{6^2}{4}+(\frac{1}{3}+\frac{p+q}{4})\cdot 6-\frac{p+q}{2}\\&=p+q+2.\quad(7)\end{aligned}$$

From (5) and (7), we obtain

$$\begin{aligned} W(G) &\leq W(G - u_1u_\gamma) - (p + q + 2) \\ &\leq W_2 - (p + q + 2) \\ &\leq W_1 - (p + 3q) \\ &< W_1 - (2 + 2\ell_1^1). \end{aligned}$$

Thus, we have $W(G) < W(U(p, q))$ in this case.

Case 2. $\gamma = 4$ and $\ell_4 \neq 0$.

By (3) and (4), we have $W(G - u_1u_4) - W(G) = 2 + 2(\ell_1 + \ell_4) + 2\ell_1\ell_4$.

(i) If $G - u_1u_4 \cong T(p, q)$, we have $W(G - u_1u_4) = W_1$ and $\ell_1 + \ell_4 = p + q - 4$. Then $W(G - u_1u_4) - W(G) = 2 + 2(\ell_1 + \ell_4) + 2\ell_1\ell_4 \geq 2 + 2(p + q - 4) + 2 = 2(p + q) - 4 \geq p - q + 1 + (2 + 2\ell_1^1)$. Thus, we have $W(G) < W_1 - (2 + 2\ell_1^1) = W(U(p, q))$ in this case.

(ii) If $G - u_1u_4 \ncong T(p, q)$, we have $W(G - u_1u_4) \leq W_2$. Recall that $\ell_1 \geq \lceil \frac{p+q-4}{4} \rceil$. So we have $W(G - u_1u_4) - W(G) = 2 + 2(\ell_1 + \ell_4) + 2\ell_1\ell_4 \geq 4\ell_1 + 4 \geq p + q$. Then with (5), we get

$$\begin{aligned} W(G) &\leq W(G - u_1u_4) - (p + q) \\ &\leq W_2 - (p + q) \\ &\leq W_1 - (p + 3q - 2) \\ &< W_1 - (2 + 2\ell_1^1). \end{aligned}$$

Thus, we have $W(G) < W(U(p, q))$ in this case.

Case 3. $\gamma = 4$ and $\ell_4 = 0$.

By (3) and (4), we have $W(G - u_1u_4) - W(G) = 2 + 2\ell_1$.

(i) If $G - u_1u_4 \cong T(p, q)$ and $G \ncong U(p, q)$, then we have $p - q$ is even and $p - q > 0$. And in this case, we have $\ell_1 = 2q - 4 + \lceil \frac{p-q+1}{2} \rceil, \ell_2 = \ell_4 = 0, \ell_3 = \lfloor \frac{p-q+1}{2} \rfloor - 1$, which means $W(G - u_1u_4) = W_1$ and $\ell_1 > \ell_1^1$. Thus, we get $W(G) < W(U(p, q))$ in this case.

(ii) If $G - u_1u_4 \ncong T(p, q)$, we have $W(G - u_1u_4) \leq W_2$.

First, we suppose one of ℓ_2 and ℓ_3 equals 0, say $\ell_2 = 0$. Then we have $\ell_1 \geq \lceil \frac{p+q-4}{2} \rceil$, otherwise $\sum_{i=1}^{4} \ell_i < p+q-4$, a contradiction. Then together with (5), we obtain

$$\begin{aligned} W(G) &= W(G-u_1u_4)-(2+2\ell_1) \\ &\leq W_2-(p+q-2) \\ &\leq W_1-(p+3q-4) \\ &< W_1-(2+2\ell_1^1). \end{aligned}$$

Thus, we have $W(G) < W(U(p,q))$ in this case.

Now, we consider the subcase that $\ell_2 \geq 1$ and $\ell_3 \geq 1$. Set $G_1 = G-u_1u_4$. Let H_1 denote the graph $G-(V(T_2)\setminus\{u_2\})$. Then G_1 can be obtained from H_1 and T_2 by identifying $u_2 \in V(H_1)$ and $u_2 \in V(T_2)$. Let G_2 be the tree obtained from H_1 and T_2 by identifying $u_4 \in V(H_1)$ and $u_2 \in V(T_2)$. Clearly, $G \cong G_1+u_1u_4 \cong G_2+u_1u_4$. So $W(G) = W(G_1)-(2+2\ell_1) = W(G_2)-[2+2(\ell_1+\ell_2)+2\ell_1\ell_2]$ by (3) and (4). Moreover, $W(G_2) \leq W_2$ and $\ell_1+\ell_2 \geq \lceil \frac{p+q-4}{2} \rceil$ (otherwise, $\sum_{i=1}^{4} \ell_i < p+q-4$, a contradiction). Hence, with (5), we have

$$\begin{aligned} W(G) &= W(G_2)-[2+2(\ell_1+\ell_2)+2\ell_1\ell_2] \\ &\leq W_2-[4+2(\ell_1+\ell_2)] \\ &\leq W_2-(p+q) \\ &\leq W_1-(p+3q-2) \\ &< W_1-(2+2\ell_1^1). \end{aligned}$$

Thus, we have $W(G) < W(U(p,q))$ in this case.

Our proof is thus complete. ■

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