Maximum Wiener index of unicyclic graphs with given bipartition

Jan Bok¹, Nikola Jedličková² and Jana Maxová³

¹ Computer Science Institute, Faculty of Mathematics and Physics, Charles University, Malostranské náměstí 25, 11800, Prague, Czech Republic. Email: bok@iuuk.mff.cuni.cz
² Department of Applied Mathematics, Faculty of Mathematics and Physics, Charles University, Malostranské náměstí 25, 11800, Prague, Czech Republic. Email: jedlickova@kam.mff.cuni.cz
³ Department of Mathematics, Faculty of Chemical Engineering, University of Chemistry and Technology, Technická 5, 166 28, Prague, Czech Republic. Email: maxovaj@vscht.cz

Abstract. The Wiener index is a widely studied topological index of graphs. One of the main problems in the area is to determine which graphs of given properties attain the extremal values of Wiener index.

In this paper we resolve an open problem posed by Du in [Wiener indices of trees and monocyclic graphs with given bipartition. International Journal of Quantum Chemistry, 112:1598–1605, 2012]. To this end we determine the unicyclic bipartite graphs with given size of parts having the maximum Wiener index. This completes the previous research in which the minimum case was solved.

2010 Mathematics Subject Classification: 05D99, 94C15

Keywords: Wiener index, topological indices, chemical graph theory, extremal graph theory, unicyclic graphs

1 Introduction

The Wiener index (also Wiener number) was introduced by Harry Wiener [14] as path number in 1947 to study the boiling points of paraffins. The Wiener index $W(G)$ of a connected graph $G = (V, E)$ is defined as

$$W(G) := \sum_{\{u,v\} \subseteq V} \operatorname{dist}_G(u,v).$$

In other words, it is the sum of the lengths of the shortest paths between all unordered pairs of vertices in the graph.

The Wiener index can be defined also in terms of transmission.
Definition 1. Let $G$ be a graph. The transmission of $v \in V(G)$ in $G$ (we denote it by $t_G(v)$) is the sum of distances between $v$ and all other vertices of $G$, i.e.

$$t_G(v) = \sum_{u \in V(G)} \text{dist}_G(u,v).$$

We can now write $W(G)$ alternatively as $W(G) := \frac{1}{2} \sum_{v \in V(G)} t_G(v)$.

Wiener index is one of the most studied topological indices in mathematical chemistry and it is still a very active research topic. As a purely mathematical concept, Wiener index was studied under different names: gross status [7], the transmission [13] and the distance of graphs [6], for example. Practical applications of this invariant are wide and apart from chemistry (summarized in [2]) there are applications in biology, communication theory, facility location, cryptography, just to name a few. We refer the reader to the numerous surveys, e.g. [3,9,10,15].

Extremal graph theory is a branch of mathematics dealing with finding the extremal graphs satisfying certain given set of properties (for more, see e.g. [1]). Many problems regarding Wiener index fall into this category of problems which is, by our opinion, nicely illustrated by the survey of Furtula et al. [15]. Also, as is seen in [10], there are many open problems in the area.

We recall that a graph is unicyclic (or monocyclic) if it is connected and contains exactly one cycle. There is a rich literature on extremal problems regarding Wiener index on unicyclic graphs, e.g. [4,8,11]. Section 4 of the aforementioned paper of Furtula et al. [15] is devoted to unicyclic graphs.

Regarding the unicyclic graphs with given bipartition $p,q$ and $p \leq q$, Du [5] showed that the minimum Wiener index is attained by the graph which is obtained by connecting $p - 2$ vertices to one vertex of a 4-cycle, and connecting $q - 2$ vertices to its neighbor on the 4-cycle. Moreover, if $p + q = 3$, then $C_6$ is also an extremal graph.

But the maximum case was left open.

Problem 1. [5] Find the graph(s) with the maximum Wiener index among unicyclic graphs on $n$ vertices with bipartition sizes $p$ and $q$, where $n = p + q$.

Our main result is the final resolution of this problem. We first need to define onion graphs.

Definition 2. The onion graph $On(k,l,m)$ is formed by a cycle of size four with antipodal vertices $u, v$, a set of $k$ pendant edges attached to the vertex $v$, path $P_l$ with one of the endpoints identified with the vertex $u$ and with $m$ pendant edges attached to the second endpoint of $P_l$. (For $l = 1$, the endpoints coincide.)

With this definition in hand we can now state our main theorem.
Theorem 1. The maximum Wiener index for \( n \)-vertex bipartite unicyclic graphs with given size of partitions \( p, q \) (\( 1 < p \leq q \)) is attained by exactly one graph:
\[
\text{On}([((q-p)/2], 2p - 3, [(q-p)/2])).
\]
Its Wiener index is equal to
\[
(2p - 5) \cdot [((q-p)/2)]((q-p)/2] + (p - 7)[(q-p)/2] + (13 - 7p)[(q-p)/2] + 2p^2q + (q-p)^2 + 2p^3 - 37p + 66.
\]

2 Lemmata

We will prove the main theorem with the help of the following lemmata. Each one yields some property of the extremal graph(s). Finally, we will collect these lemmata and conclude that there is a unique graph with the maximum Wiener index for given parameters. First we introduce a few preliminary definitions.

Throughout this paper, all graphs we consider are simple and connected.

For a graph \( G = (V, E) \) we write \( |G| \) for \( |V(G)| \). We also shorten \( \{u, v\} \) for an edge to \( uv \). The operation of vertex and edge insertion is written as \( G \cup v \) and \( G \cup uv \), respectively. For vertex and edge deletion we write analogously \( G - v \) and \( G - uv \), respectively.

We say that a graph on \( p + q \) vertices has a \((p, q)\)-partition if it is bipartite and the parts of the bipartition are of size \( p \) and \( q \). We often use \( P \) and \( Q \) for the set of vertices in part of size \( p \) and \( q \), respectively.

We denote by \( E_{p,q} \) (for \( 1 < p \leq q \) and \( p, q \in \mathbb{N} \)) the set of extremal graphs having the maximum possible Wiener index among all bipartite unicyclic graphs on \( p+q \) vertices with \((p,q)\)-partition. With this notation in hand, we can rephrase our aim as a search for characterizing the set \( E_{p,q} \) for every possible parameters \( p \) and \( q \).

Consider some unicyclic graph \( U \) having a unique cycle \( C \). We say that \( T \) is a rooted tree if it is a tree component of graph \( U' \) rooted in some vertex \( v \in V(C) \), where \( V(U') = V(U) \) and \( E(U') = E(U) - E(C) \).

Lemma 1. Every extremal graph \( G \in E_{p,q} \) contains 4-cycle.
Moreover, if \( x \) and \( y \) are arbitrary vertices in \( G \) such that \( \text{dist}_G(x, y) = \text{dist}_G(x, y') \), then necessarily one of the vertices \( x \) and \( y \) belongs to \( T_1 \). Without loss of generality we may suppose that \( x \in T_1 \).

Let us define \( I := \{4, \ldots, \frac{k}{2} + 1\} \). It is clear that for any \( x \in T_1 \) and any \( y \in V(G') \) holds \( \text{dist}_G(x, y) < \text{dist}_G(x, y') \) if and only if \( y \in T_i \) with \( i \in I \). Moreover, if \( x \in T_1 \) and \( y \in T_i, i \in I \) then
\[
\text{dist}_G(x, y) = \text{dist}_G(x, y) - 2.
\]

Our goal is to prove that \( W(G') > W(G) \). From the previous observations we get
\[
W(G') - W(G) \geq (k - 4) |T_1| \cdot |T_k| + (k - 4) |T_2| \cdot |T_k| - 2 \sum_{i \in I} |T_i| \cdot |T_i|.
\]

From the assumption \( |T_k| \geq |T_i| \) for every \( i = 1, \ldots, k \) and \( |I| = \frac{k}{2} - 2 = \frac{k-4}{2} \) follows that
\[
W(G') - W(G) \geq (k - 4) |T_1| \cdot |T_k| + (k - 4) |T_2| \cdot |T_k| - 2 \left( \frac{k-4}{2} \right) |T_1| \cdot |T_k|
\]
\[
= (k - 4) |T_2| \cdot |T_k|.
\]

As \( |T_i| \geq 1 \) for all \( i \) and \( k \geq 6 \) we get \( W(G') - W(G) > 0 \), a contradiction with the extremality of \( G \). \( \square \)

In the next proofs we use the following lemmata from the paper of Du [5] and from the paper of Polansky [12], respectively.
Lemma 2. Let \(G, H\) be two nontrivial connected graphs with \(u, v \in V(G)\) and \(w \in V(H)\). Let \(GuH\) (\(GvH\), respectively) be the graph obtained from \(G\) and \(H\) by identifying \(u\) (\(v\), respectively) with \(w\). If \(t_G(u) < t_G(v)\), then \(W(GuH) < W(GvH)\).

Lemma 3. Let \(G_u\) and \(G_v\) be two graphs with \(n_u\) and \(n_v\) vertices, respectively, and let \(u \in V(G_u)\) and \(v \in V(G_v)\). If \(G\) arises from \(G_u\) and \(G_v\) by identifying \(u\) and \(v\), then
\[
W(G) = W(G_u) + W(G_v) + (n_u - 1)t_{G_v}(v) + (n_v - 1)t_{G_u}(u).
\]

Lemma 4. Every extremal graph \(G \in E_{p,q}\) has at least one vertex of degree two on its cycle.

Proof. Assume that \(G \in E_{p,q}\) and denote by \(v_1, \ldots, v_4\) vertices on its cycle. We assume for a contradiction that there is a rooted tree \(T_i\) for each \(v_i\), \(i \in \{1, \ldots, 4\}\) such that \(|T_i| \geq 2\).

Let us define graphs \(G' := G \setminus (T_1 - v_1)\) and \(H := T_1\). Without loss of generality we may assume that \(v_1\) is in part \(P\) and \(|T_2| \leq |T_4|\). Our aim is to prove that \(t_{G'}(v_1) < t_{G'}(x)\) and then use Lemma 2.

We first observe that the transmission of \(v_1\) in \(G'\) can be written as
\[
t_{G'}(v_1) = t_{T_2}(v_2) + t_{T_3}(v_3) + t_{T_4}(v_4) + |T_2| + 2|T_3| + |T_4|.
\]

Let \(x \in V(T_2)\) be any vertex of \(T_2\) such that \(v_2x \in E(G)\). Such vertex must exist because \(|T_2| \geq 2\). Denote by \(T_x\) the tree component of \(G - v_2x\), see Figure 2.

Note that both \(x\) and \(v_1\) are in part \(P\). The transmission of \(x\) in \(G'\) is equal to
\[
t_{G'}(x) = t_{T_x}(x) + t_{T_2 \setminus T_x}(v_2) + |T_2 \setminus T_x| + t_{T_3}(v_3) + t_{T_4}(v_4) + 2|T_3| + 3|T_4| + 2.
\]
It is easy to see that \( t_{T_2}(v_2) = t_{T_2}(x) + t_{T_2 \setminus T_1}(v_2) + |T_2| \) and hence it follows
\[
\begin{align*}
t_{G'}(x) &= t_{T_2}(v_2) + t_{T_3}(v_3) + t_{T_4}(v_4) + |T_2| + 2|T_3| + 3|T_4| - 2|T_2| + 2.
\end{align*}
\]

By observing that \( T_x \subset T_2 \) and combining this with the assumption \( |T_2| \leq |T_4| \) we get
\[
\begin{align*}
t_{G'}(x) - t_{G'}(v_1) &= 2|T_4| - 2|T_2| + 2 > 0,
\end{align*}
\]
from which we conclude that \( t_{G'}(v_1) < t_{G'}(x) \).

Let \( G'v_1H \) be a graph obtained from \( G' \) and \( H \) by identifying \( v_1 \) in \( G' \) and \( v_1 \) in \( H \) and let \( G'xH \) be a graph obtained from \( G' \) and \( H \) by identifying \( x \) in \( G' \) with \( v_1 \) in \( H \). It is clear that \( G'v_1H \cong G \). By Lemma 2 we get \( W(G) = W(G'v_1H) < W(G'xH) \), a contradiction with \( G \) being extremal.

\[\blacksquare\]

**Lemma 5.** Every extremal graph \( G \in E_{p,q} \) has two antipodal vertices of degree 2 on its cycle.

**Proof.** We assume for a contradiction that \( G \in E_{p,q} \) and that it does not have two antipodal vertices on its cycle with degree 2. We distinguish two cases.

**Case 1.** Graph \( G \) has only one vertex of degree two on its cycle. Denote the vertices of cycle by \( v_1, \ldots, v_4 \) consecutively such that the vertex of degree two is denoted by \( v_3 \). We can proceed in the same way as in the proof of the previous lemma to get a contradiction.

**Case 2.** Graph \( G \) has exactly two vertices of degree two on its cycle and they are adjacent. We denote the vertices on the cycle \( v_1, \ldots, v_4 \) consecutively such that \( v_3 \) and \( v_4 \) have degree two. There is a tree \( T_1 \) rooted in \( v_1 \) such that \( |T_1| \geq 2 \) and a tree \( T_2 \) rooted in \( v_2 \) such that \( |T_2| \geq 2 \).

Again, we distinguish two cases.

**Case 2a.** We assume that at least one of \( v_1 \) and \( v_2 \) has degree at least 4. Without loss of generality suppose that \( v_2 \) is the vertex. Denote by \( x \) any of its neighbors in \( T_2 \) and by \( T_x \) the tree component of \( G - v_2x \).

We define graphs \( G' := G \setminus T_x \) and \( H := T_x \cup v_2x \). Note that \( v_2 \) is included in both of \( G' \) and \( H \) but the edge \( v_2x \) is only in \( E(H) \). See Figure 3. We will proceed in a similar way as in the proof of the previous lemma. We define \( T_2' := T_2 \setminus T_x \).

It holds
\[
\begin{align*}
t_{G'}(v_2) &= t_{T_2}(v_2) + t_{T_1}(v_1) + |T_1| + 3, \quad \text{and} \\
t_{G'}(v_4) &= t_{T_2}(v_2) + 2|T_2'| + t_{T_1}(v_1) + |T_1| + 1.
\end{align*}
\]

We assume that \( v_2 \) has degree at least 4 and thus \( |T_2'| \geq 2 \). It follows
\[
\begin{align*}
t_{G'}(v_4) - t_{G'}(v_2) &= 2|T_2'| - 2 > 0,
\end{align*}
\]
thus $t_{G'}(v_2) < t_{G'}(v_4)$.

Let $G'v_2H$ be a graph obtained from $G'$ and $H$ by identifying $v_2 \in V(G')$ and $v_2 \in V(H)$ and let $G'v_4H$ be a graph obtained from $G'$ and $H$ by identifying $v_4 \in V(G')$ with $v_2 \in V(H)$. Observe that $G'v_2H \cong G$. It follows from Lemma 2 that $W(G'v_2H) < W(G'v_4H)$, a contradiction because $G$ was extremal.

Case 2b. We assume that both $v_1$ and $v_2$ have degree 3. Without loss of generality we assume $|T_1| \leq |T_2|$. Let us denote by $x$ the vertex adjacent to $v_1$ that is not on the cycle and denote by $T_x$ the tree component of $G - v_1x$. Similarly, let us denote by $y$ the vertex adjacent to $v_2$ that is not on the cycle and by $T_y$ the tree component of $G - v_2y$. As $|T_1| \leq |T_2|$ also $|T_x| \leq |T_y|$. Let $G'$ be a graph obtained from $G$ by deleting $T_x$ and $T_2$. Further let $G''$ be the graph obtained from $G$ by deleting edge $v_2y$, adding edge $xy$ and edges from $v_2$ to all neighbors of $x$ in $T_x$, and, finally, by deleting edges between $x$ and its neighbors in $T_x$. Note that $G''$ has the same bipartition as $G$. See Figure 4. We calculate the Wiener indices of $G$ and $G''$.
\[ W(G) = \sum_{u \in T_x, v \in T_y} \text{dist}_G(u, v) + 4t_{T_x}(x) + |T_x|(1 + 4 + 3) + 4t_{T_y}(y) + |T_y|(1 + 4 + 3) + 8, \]

\[ W(G'') = \sum_{u \in T_x, v \in T_y} \text{dist}_{G''}(u, v) + 4t_{T_x}(x) + |T_x|(2 + 4) + 4t_{T_y}(y) + |T_y|(1 + 2 + 3 + 4) + 10. \]

Note that for any \( u \in T_x \) and any \( v \in T_y \) the distances in \( G \) and \( G'' \) are the same, i.e. \( \text{dist}_G(u, v) = \text{dist}_{G''}(u, v) \). We conclude that
\[ W(G'') - W(G) = 2|T_y| - 2|T_x| + 2 > 0, \]
a contradiction with the extremality of \( G \). \( \square \)

So far, it follows from the previous lemmata that for arbitrary \( p, q \geq 2 \) every graph in \( E_{p,q} \) contains a cycle \( C_4 \) with two antipodal vertices on \( C_4 \) of degree 2. We denote the vertices of \( C_4 \) by \( v_1, \ldots, v_4 \) consecutively such that \( v_2 \) and \( v_4 \) have degree two.

For the rest of our paper we need a definition of \textit{broom} graph.

**Definition 3.** For any \( a \geq 1 \) and \( b \geq 0 \) we say that a tree \( T \) is a \textit{broom} if \( T \) arises from a path \( P = x_1, \ldots, x_a \) on \( a \) vertices by adding \( b \) pendant vertices to \( x_a \). We say that \( x_1 \) is the root of the broom.

**Lemma 6.** If \( G \in E_{p,q} \) is a graph with a tree \( T_1 \) attached to \( v_1 \) and a \( T_2 \) attached to \( v_3 \) then both trees \( T_1 \) and \( T_2 \) are isomorphic to brooms with roots in \( v_1, v_3 \), respectively.

**Proof.** Let \( P = u_1, \ldots, u_t \) be a longest path in \( G \). We say that a vertex \( v \in V(G) \) is bad if
\[ \bullet \ \text{deg}_G(v) > 2 \text{ for } v \in V(G) \setminus \{u_2, u_{t-1}, v_1, v_3\}, \text{ or} \]
\[ \bullet \ \text{deg}_G(v) > 3 \text{ for } v \in \{v_1, v_3\} \setminus \{u_2, u_{t-1}\}. \]

Suppose for a contradiction that \( G \in E_{p,q} \) and trees attached to \( C_4 \) in \( G \) are not isomorphic to brooms. Thus there exits a bad vertex in path \( P \), different from \( v_2 \) and \( v_4 \) since these arc of degree two. Without loss of generality we may suppose that the bad vertex is in \( V(T_1) \). If there is more than one bad vertex in \( V(T_1) \), we will choose the one such that its distance \( u_2 \) is minimal possible and we denote such bad vertex as \( u_i \). Therefore, the subgraph of \( G \) induced by \( \{u_2, \ldots, u_i\} \) is a path and \( i \geq 3 \).

We set \( A := N(u_i) \setminus \{u_{i-1}, u_{i+1}, v_2, v_4\} \). Let \( H_1 \) be the component of \( G \setminus A \) containing the vertex \( u_i \) and let \( H_2 \) be the component of \( G \setminus \{u_{i-1}, u_{i+1}, v_2, v_4\} \)
containing the vertex \( u_i \). Note that \( G \) arises from \( H_1 \) and \( H_2 \) by identifying \( u_i \in V(H_1) \) with \( u_i \in V(H_2) \), or shortly \( G = H_1 u_i H_2 \). Let \( K \) be the component of \( G \setminus u_i \) that contains \( u_{i+1} \). Let \( k := \vert V(K) \vert \) and \( d = \deg_{H_1}(u_2) \). We distinguish three cases.

**Case 1.** \( k < d \)

We set \( G_1 := H_1 u_{i+2} H_2 \). In order to prove that \( W(G_1) > W(G) \) we compute the difference \( t_{H_1}(u_{i+2}) - t_{H_1}(u_i) \) and apply Lemma 2.

Note that there are at least \( i + d - 2 > d \) vertices \( v \) in \( V(H_1) \) such that their distance to \( u_{i+2} \) is bigger than their distance to \( u_i \), namely \( \dist_{H_1}(v, u_{i+2}) = \dist_{H_1}(v, u_i) + 2 \). Further note that \( \dist_{H_1}(u_{i+1}, u_i) = \dist_{H_1}(u_{i+1}, u_{i+2}) = 1 \) and that for at most \( k - 1 \) vertices \( v \) in \( V(H_1) \) \( (v \in V(K) \setminus u_{i+1}) \) the distance \( \dist_{H_1}(v, u_{i+2}) \geq \dist_{H_1}(v, u_i) - 2 \).

Thus we obtain that

\[
t_{H_1}(u_{i+2}) - t_{H_1}(u_i) \geq 2d - 2(k - 1) = 2(d - k) + 2 > 0,
\]

from which we conclude \( t_{H_1}(u_{i+2}) > t_{H_1}(u_i) \).

Observe that \( u_i \) and \( u_{i+2} \) are in the same part of \( G \). Hence, \( G_1 \) also has a \((p, q)\)-bipartition. Again, we conclude that \( W(G_1) > W(G) \), a contradiction.

**Case 2.** \( k \geq d \) and \( \dist_G(u_2, u_i) \) is even.

In this case we set \( G_2 := H_1 u_2 H_2 \). We aim to prove that \( W(G_2) > W(G) \) by computing the difference \( t_{H_1}(u_2) - t_{H_1}(u_i) \) and using Lemma 2.

Note that there are exactly \( d - 1 \) vertices \( v \) (the neighbors of \( u_2 \)) in \( V(H_1) \setminus \{u_2, \ldots, u_i\} \) such that \( \dist_{H_1}(v, u_i) = \dist_{H_1}(v, u_2) + (i - 2) \). Further note that for any \( v \in V(K) \) the distance \( \dist_{H_1}(v, u_i) = \dist_{H_1}(v, u_2) - (i - 2) \). Thus

\[
t_{H_1}(u_2) - t_{H_1}(u_i) = \sum_{v \in V(H_1) \setminus \{u_2, \ldots, u_i\}} \left( \dist_{H_1}(v, u_2) - \dist_{H_1}(v, u_i) \right) = k(i - 2) - (d - 1)(i - 2) = (i - 2)(k - d + 1) > 0
\]

as \( i \geq 3 \) and \( k \geq d \). It follows that \( t_{H_1}(u_2) > t_{H_1}(u_i) \). Note that again \( u_i \) and \( u_2 \) are in the same partition of \( G \) and thus \( G_2 \) also has a \((p, q)\)-bipartition. By Lemma 2 we obtain that \( W(G_2) > W(G) \), a contradiction.

**Case 3.** \( k \geq d \) and \( \dist_G(u_2, u_i) \) is odd.

We set \( G_3 := H_1 u_1 H_2 \). As \( u_i \) and \( u_1 \) are in the same partition of \( G \) and the graph \( G_3 \) also has a \((p, q)\)-bipartition. Observe that \( t_{H_1}(u_1) = t_{H_1}(u_2) + \vert V(H_1) \vert - 2 \) This implies that \( t_{H_1}(u_1) > t_{H_1}(u_2) > t_{H_1}(u_i) \) and again by Lemma 2 we obtain that \( W(G_3) > W(G) \), a contradiction.

\[\Box\]

**Lemma 7.** Let \( G \in E_{p,q} \). If \( |P| < |Q| \) then all pendant vertices belong to part \( Q \).
**Proof.** Suppose for a contradiction that there are two pendant vertices \( x \) and \( y \) such that \( x \in P \) and \( y \in Q \) (or vice versa). Clearly, \( x \) and \( y \) belong to distinct brooms of \( G \). Let \( u \) be the only neighbor of \( x \) and \( v \) be the only neighbor of \( y \) in \( G \). Without loss of generality we may assume that \( t_G(u) \leq t_G(v) \). Clearly \( t_G(y) = t_G(v) + n - 2 \). We define a graph \( G' = G - x \). It holds
\[
\begin{align*}
t_{G'}(u) &= t_G(u) - 1, \\
t_{G'}(y) &\geq t_G(y) - n + 2.
\end{align*}
\]
Therefore, we have
\[
t_{G'}(u) < t_{G'}(v) = t_G(v) = t_G(y) - n + 2 \leq t_{G'}(y).
\]
Clearly, \( G \cong G'uK_2 \). By Lemma 2 we have \( W(G) = W(G'uK_2) < W(G'vK_2) \), a contradiction. \( \square \)

We define the *height* of a rooted tree as the number of edges in the longest path between the root and a leaf of the tree.

**Lemma 8.** Let \( G \in E_{p,q} \) be an extremal graph. At least one of the trees (brooms) attached to \( C_4 \) in \( G \) has the height at most two.

**Proof.** From the previous lemmata it follows that \( G \) consists from \( C_4 \) with two brooms attached to antipodal vertices of the cycle (we denote these vertices \( v_0 \) and \( u_0 \)). We denote by \( w \) one of the vertices incident with \( v_0 \) and \( u_0 \) on the cycle and by \( w' \) the other one. Let \( v_0, \ldots, v_i \) be the vertices of the path in the broom attached to \( v_0 \) and \( a \) be the number of pendant vertices attached to \( v_i \). Similarly, we denote by \( u_0, \ldots, u_j \) the vertices on the path in the broom attached to \( u_0 \) and by \( b \) the number of pendant vertices adjacent to \( u_j \). See Figure 5 for an illustration.

![Fig. 5. A possible scenario in Lemma 8](image)

We assume for a contradiction that \( i, j \geq 2 \). Without loss of generality \( a \leq b \). We define a graph \( G' := G \setminus w \). We divide the rest of the proof into two cases, based on the parity of \( i \).

**Case 1.** We assume that \( i \) is even. Let \( G_1 \) be a graph obtained from \( G' \) by joining a vertex \( w \) to \( v_i \) and \( v_{i-2} \). Note that \( G_1 \) has the same partition as \( G \) and
$G_1$ has one of the brooms of height one. Observe that for Wiener indices of $G$ and $G_1$ holds

$$W(G) = W(G') + t_G(w),$$
$$W(G_1) = W(G') + t_{G_1}(w),$$

because the distances in $G'$ do not change when we add the vertex $w$. Now we calculate the transmission of $w$ in $G$ and $G_1$.

$$t_G(w) = 2 + \binom{i+2}{2} + a(i+2) + \binom{j+2}{2} + b(j+2),$$
$$t_{G_1}(w) = 3 + 2a + \binom{i+j+2}{2} + b(i+j+2).$$

Since we assume $a \leq b$ and $i, j \geq 2$, we get

$$t_{G_1}(w) - t_G(w) \geq 1 + i(b-a) > 0$$

and hence $W(G_1) > W(G)$, a contradiction.

Case 2. We assume that $i$ is odd. We will proceed in a similar way as in the first case. Let $G_2$ be a graph obtained from $G'$ by joining a vertex $w$ to $v_{i-1}$ and to vertex $v_{i-3}$. Note that in this case we may assume that $i \geq 3$ as for $i = 1$ we are done. Thus, $v_{i-3}$ exists.

$W(G)$ and $t_G(w)$ are the same as in the previous case and by a similar argument we get

$$W(G_2) = W(G') + t_{G_2}(w)$$
$$t_{G_2}(w) = 5 + 3a + \binom{i+j+1}{2} + b(i+j+1).$$

By an easy calculation we get $t_{G_2}(w) - t_G(w) > 0$ which implies $W(G_2) > W(G)$, a contradiction.

Lemma 9. Let $G$ be an extremal graph. At least one of the trees (brooms) attached to $C_4$ in $G$ has the height at most one. In other words, $G$ is an onion graph.

Proof. We denote two antipodal vertices of degree bigger than two on $C_4$ by $u$ and $v$. We also denote the broom attached to $u$ by $B_u$ and the broom attached to $v$ by $B_v$. It follows from Lemma 8 that at least one broom has the height at most 2, without loss of generality it is $B_u$. If the height of $B_u$ is equal to one we are done. We assume that height of $B_v$ is two (see Figure ??). Let $a$ be the number of pendant vertices in $B_u$. We distinguish two cases.

Case 1. We assume that $a = 1$. We define two graphs $G_1 := G \setminus (B_u - v)$ and $H_1 := B_v$. We denote by $y$ the only vertex of degree one in $G_1$. Note that $G$ can
be obtained from $G_1$ and $H_1$ by identifying $v \in V(G_1)$ with $v \in V(H_1)$. Let $G'$
be a graph obtained from $G_1$ and $H_1$ by identifying $y \in V(G_1)$ with $v \in V(H_1)$. See Figure 6
for an illustration of this transformation. Observe that $t_{G_1}(v) = 11$ and $t_{G_1}(y) = 13$. By Lemma 2
we have $W(G') > W(G)$, a contradiction.

**Fig. 6.** The transformation in the first case of Lemma 9.

*Case 2.* We assume that $a \geq 2$. Let $G_1$ and $H_1$ be defined as in the previous case. We create a graph $G_2$ in the following way. Denote by $s$ and $t$ the two antipodal vertices of degree two in the cycle in $G_1$. Attach to the vertex $s$ exactly $a - 2$ pendant vertices and attach to $t$ a path on four vertices $p_1, p_2, p_3, p_4$ with endpoints $p_1$ and $p_4$ by identifying $p_1$ with $t$. We denote the resulting graph by $G_2$. Note that $G_2$ has the same number of edges, the same number of vertices and the same partition as $G_1$.

Let $G'$ be a graph obtained from $G_2$ and $H_1$ by identifying $p_4 \in V(G_2)$ with $v \in V(H_1)$. See Figure 7 for a visualization. By Lemma 3 we get that for Wiener indices of $G$ and $G'$ holds

$$W(G) = W(G_1) + W(H_1) + (|V(H_1)| - 1)t_{G_1}(v) + (|V(G_1)| - 1)t_{H_1}(v),$$

$$W(G') = W(G_2) + W(H_1) + (|V(H_1)| - 1)t_{G_2}(v) + (|V(G_1)| - 1)t_{H_1}(v).$$

We need to prove that

$$W(G_2) - W(G_1) + (|V(H_1)| - 1) \cdot t_{G_2}(v) - t_{G_1}(v) > 0.$$ 

Firstly, we observe that for transmissions of $v$ holds

$$t_{G_1}(v) = 4a + 7,$$

$$t_{G_2}(v) = 6a + 7,$$
and it follows that \( (t_{G_2}(v) - t_{G_1}(v)) \geq 2a \). Secondly, we determine Wiener indices of \( G_1 \) and \( G_2 \). Note that there are exactly 5 + \( a \) edges in \( G_1 \), exactly \( a + 4 + \binom{a}{2} \) pairs of vertices in distance two, exactly \( 2a + 1 \) vertices in distance 3 in \( G_1 \), \( a \) vertices in distance 4 and there is no pair of vertices in distance bigger than 4 in \( G \). Hence we have

\[
W(G_1) = (5 + a) + 2\left[(a + 4) + \binom{a}{2}\right] + 3(2a + 1) + 4a \\
= 2\binom{a}{2} + 13a + 16.
\]

Similarly, we get

\[
W(G_2) = 5 + a + 2(2a - 1) + 2\binom{a - 2}{2} \\
+ 3(a + 2) + 4(a + 1) + 5(a - 1) + 6(a - 2) \\
= 2\binom{a - 2}{2} + 23a - 4.
\]

Then

\[
W(G_2) - W(G_1) = 23a - 4 - 13a - 16 - 4a + 6 = 6a - 14
\]

and finally for \( a \geq 2 \) we get

\[
(W(G_2) - W(G_1)) + (|V(H_1)| - 1) \cdot (t_{G_2}(v) - t_{G_1}(v)) \\
\geq 6a - 14 + (|V(H_1)| - 1)2a \geq 8a - 14 > 0.
\]

Which completes the proof. \( \square \)
**Lemma 10.** The Wiener index of the onion graph On\((k, l, m)\) is equal to
\[
k^2 + 7k + 8 + \frac{l^3 - l}{6} + m^2 + m \frac{l^2 + l - 2}{2} + (k + 3)\left(\frac{l^2 - l}{2} + ml\right) + (l + m - 1)(3k + 4).
\]

**Proof.** We will compute the Wiener index of particular subgraphs and then we repeatedly use Lemma 3.

Let \(u\) and \(v\) be two antipodal vertices in \(C_4\) and let \(v'\) be the vertex of degree \(k\) in \(K_{1,k}\). We denote by \(G_1\) a graph obtained from \(K_{1,k}\) and \(C_4\) by identifying \(v'\) in \(K_{1,k}\) with \(v\) in \(C_4\). Note that \(W(K_{1,k}) = k^2\). By Lemma 3 we get
\[
W(G_1) = k^2 + 8 + (k + 1 - 1)4 + 3k = k^2 + 7k + 8.
\]

Let \(G_2\) be a broom with path of length \(l\) and \(m\) pendant vertices. We denote by \(u_1\) and \(u_l\) endpoints of \(P_l\) in such way that pendant vertices are attached to \(u_l\). Observe that \(W(P_l) = \binom{l+1}{3}\) and \(W(K_{1,m}) = m^2\). For Wiener index of \(G_2\) holds by Lemma 3
\[
W(G_2) = \frac{l^3 - l}{6} + m^2 + (l - 1)m + m \frac{l^2 - l}{2}.
\]

Note that we can get \(G\) from \(G_1\) and \(G_2\) by identifying \(u \in G_1\) with \(u_1 \in G_2\). Note that \(|V(G_1)| = k + 4\) and \(|V(G_2)| = l + m\). For transmissions of \(u\) and \(u_1\) we have
\[
t_{G_1}(u) = 3k + 4,
\]
\[
t_{G_2}(u_1) = \frac{l^2 - l}{2} + ml.
\]

Again by Lemma 3 we get that Wiener index of \(G\) is equal to
\[
k^2 + 7k + 8 + \frac{l^3 - l}{6} + m^2 + m \frac{l^2 + l - 2}{2} + (k + 3)\left(\frac{l^2 - l}{2} + ml\right) + (l + m - 1)(3k + 4).
\]

\[\Box\]

The following lemma can be proved by an easy computation, so we skip the details.

**Lemma 11.** Let \(G\) be an onion graph \(On(k, l, m)\). Let \(v\) vertex on the cycle with \(k\) pendant vertices and \(u_l\) be the last vertex on the path of length \(l\) with \(m\) pendant vertices. Then
\[
t_G(v) = k + 1 + \left(\frac{l + 2}{2}\right) + m(l + 2),
\]
\[
t_G(u_l) = m + \left(\frac{l + 2}{2}\right) + l + k(l + 2).
\]
3 Proof of the main theorem

We are now ready to prove Theorem 1.

Proof (of Theorem 1). Let $G \in E_{p,q}$. From the previous series of lemmata we get that $G$ is an onion graph with all pendant vertices are in part $Q$. Now we determine parameters of the onion for $G$.

Let $G$ be isomorphic to $\text{On}(a, l, b)$ where $q - p = a + b$. Let $v$ be the vertex on the cycle with $a$ pendant vertices and $u_l$ be the last vertex on the path of length $l$ with $b$ pendant vertices. Since $q - p = a + b$ we get that $a = \lfloor \frac{q - p}{2} \rfloor$ implies $b = \lceil \frac{q - p}{2} \rceil$. Further note that $\text{On}(a, 1, b) \cong \text{On}(b, 1, a)$ and thus for $l = 1$ it might happen that $a = b + 1$.

Suppose for a contradiction that $a \neq \lfloor \frac{q - p}{2} \rfloor$. By the above reasoning there are only two cases to distinguish:

- $a \geq b + 1$ and $l \geq 2$, or
- $b \geq a + 2$.

Case 1. We assume that $a \geq b + 1$ and $l \geq 2$. We define two graphs $G_1 := \text{On}(a - 1, l, b)$ and $H_1 := K_2$. Clearly, $G$ can be obtained from $G_1$ and $H_1$ by identifying $v \in G_1$ with one of the vertices of $H_1$. Let us denote by $G'$ a graph obtained from $G_1$ and $H_1$ by identifying $u_l \in G_1$ with one of the vertices of $H_1$.

We use Lemma 11 for $k = a - 1, l$ and $m = b$ and we get

$$t_{G_1}(v) = a + \left( \frac{l + 2}{2} \right) + b(l + 2),$$

$$t_{G_1}(u_l) = b + \left( \frac{l + 2}{2} \right) + l + (a - 1)(l + 2),$$

$$t_{G_1}(u_l) - t_{G_1}(v) = l(a - b) + (a - b) - 2 > 0.$$

It follows from Lemma 2 that $W(G') > W(G)$, a contradiction.

Case 2. We assume that $b \geq a + 2$. Analogously to the previous case we define $G_2 := \text{On}(a, l, b - 1)$ and $H_2 := K_2$. Observe that $G$ can be obtained from $G_2$ and $H_2$ by identifying $u_l \in G_2$ with one of the vertices of $H_2$. We define $G''$ as a graph obtained from $G_2$ and $H_2$ by identifying $v \in G_2$ with one of the vertices of $H_2$. Again we use Lemma 11 for $k = a, l$ and $m = b - 1$ to compute the transmissions

$$t_{G_2}(v) = a + 1 + \left( \frac{l + 2}{2} \right) + (b - 1)(l + 2),$$

$$t_{G_2}(u_l) = b - 1 + \left( \frac{l + 2}{2} \right) + l + a(l + 2),$$

$$t_{G_2}(v) - t_{G_2}(u_l) = l(b - a - 2) + b - a > 0.$$
and by Lemma 2 we get $W(G') > W(G)$, a contradiction.

Therefore, $a = \lfloor (q - p)/2 \rfloor$, $b = \lceil (q - p)/2 \rceil$ and

$$l = p + q - a - b - 3 = p + q - (q - p) - 3 = 2p - 3.$$ 

From this we conclude that

$$G \cong \text{On}(\lfloor (q - p)/2 \rfloor, 2p - 3, \lceil (q - p)/2 \rceil).$$

Using Lemma 10 we get the exact value of its Wiener index which is equal to

$$(2p - 5) \cdot \lfloor (q - p)/2 \rfloor \lceil (q - p)/2 \rceil + (p - 7) \lfloor (q - p)/2 \rfloor + (13 - 7p) \lceil (q - p)/2 \rceil + 2p^2q + (q - p)^2 + 2p^3 - 37p + 66.$$ 

This finishes the proof. \qed

4 Conclusion and future work

We obtained the extremal graphs and values for the maximum Wiener index on unicyclic graphs with given bipartition. A natural next question is to consider the class of cacti. A cactus graph is a graph where every edge belongs to at most one cycle. Unicyclic graphs are precisely the cacti with one cycle.

Problem 2. What is the maximum Wiener index and the extremal graphs attaining such index for bipartite cacti graphs with given size of parts and number of cycles?

Acknowledgments

The first and the second author would like to acknowledge the support of the grant SVV-2017-260452. The first author was supported by the Charles University Grant Agency, project GA UK 1158216. The second author was supported by Student Faculty Grant of Faculty of Mathematics and Physics, Charles University.

References

1. B. Bollobás. Extremal graph theory. Courier Corporation, 2004.
2. D. Bonchev. The Wiener number—some applications and new developments. In Topology in Chemistry, pages 58–88. Elsevier, 2002.
3. A. Dobrynin, R. Entringer, and I. Gutman. Wiener index of trees: theory and applications. Acta Applicandae Mathematica, 66(3):211–249, 2001.
4. H. Dong and B. Zhou. Maximum Wiener index of unicyclic graphs with fixed maximum degree. *Ars Combinatorica*, 103:407–416, 2012.
5. Z. Du. Wiener indices of trees and monocyclic graphs with given bipartition. *International Journal of Quantum Chemistry*, 112:1598–1605, 2012.
6. R. C. Entringer, D. E. Jackson, and D. A. Snyder. Distance in graphs. *Czechoslovak Mathematical Journal*, 26(2):283–296, 1976.
7. F. Harary. Status and contrastatus. *Sociometry*, 22(1):23–43, 1959.
8. H. Hou, B. Liu, and Y. Huang. The maximum Wiener polarity index of unicyclic graphs. *Applied Mathematics and Computation*, 218(20):10149–10157, 2012.
9. M. Knor and R. Škrekovski. Wiener index of line graphs. *Quantitative Graph Theory: Mathematical Foundations and Applications*, pages 279–301, 2014.
10. M. Knor, R. Škrekovski, and A. Tepeh. Mathematical aspects of Wiener index. *Ars Mathematica Contemporanea*, 11:327–352, 2016.
11. M. Liu and B. Liu. On the Wiener polarity index. *MATCH Commun. Math. Comput. Chem*, 66(1):293–304, 2011.
12. O. E. Polansky and D. Bonchev. The Wiener number of graphs. i. general theory and changes due to some graph operations. *MATCH Commun. Math. Comput. Chem*, 21(133-186):72, 1986.
13. L. Šoltés. Transmission in graphs: a bound and vertex removing. *Mathematica Slovaca*, 41(1):11–16, 1991.
14. H. Wiener. Structural determination of paraffin boiling points. *Journal of the American Chemical Society*, 69(1):17–20, 1947.
15. K. Xu, M. Liu, K. Ch. Das, I. Gutman, and B. Furtula. A survey on graphs extremal with respect to distance-based topological indices. *MATCH Commun. Math. Comput. Chem*, 71(3):461–508, 2014.