The Second-minimum Gutman Index of The Unicyclic Graphs With Given Girth *

Yahui Hu †, Yaoping Hou, Zhangdong Ouyang
Department of Mathematics, Hunan First Normal University, Changsha 410205, P.R.China,

Abstract

Let G be a simple connected graph with the vertex set $V(G)$. The Gutman index $Gut(G)$ of G is defined as $\sum\limits_{\{x,y\}\subseteq V(G)} d_G(x)\, d_G(y)\, d_G(x,y)$, where $d_G(v)$ is the degree of the vertex v in G and $d_G(x,y)$ the distance between the vertices x and y in G. In this paper, the second-minimum Gutman index of the unicyclic graphs on n vertices and girth m is characterized.

AMS Classification: 05C20; 05C35
Keywords: Gutman Index; Girth; Unicyclic Graph

1 Introduction

All graphs considered in this paper are simple and connected. Let G be a graph, we denote by $d_G(v)$ and $d_G(u,v)$ the degree of a vertex v in G and the usual distance between the vertices u and v in G, respectively.

The Wiener index $W(G) = \sum\limits_{\{u,v\}\subseteq V(G)} d_G(u,v)$ of a connected graph G is a graph invariant much studied in both mathematical and chemical literature, for details see the references [2, 5, 7, 10, 11, 12]. In this paper we are concerned with a variant of the Wiener index called the Schultz index of the second kind [10], but for which the name Gutman index has also been used [16]. Throughout this paper, the latter name is used.

*Research Supported by NNSF of China (11171102, 11301169) and Aid Program for Science and Technology Innovative Research Team in High Educational Institutions of Hunan Province.

†E-mail: huyahuifn@yeah.net

The Gutman index of a connected graph G is defined as

$$Gut(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u) d_G(v) d_G(u,v).$$

The Gutman index of graphs attracts attention just recently. Dankelmann et al. [6] presented an asymptotic upper bound for the Gutman index. Dankelmann, Knor et al. [6, 14] established the relation between the edge-Wiener index and Gutman index of graphs. Gutman [10] gave the following relation between the Gutman and the Wiener index for a tree T on n vertices,

$$Gut(T) = 4W(T) - (2n-1)(n-1).$$

Andova et al. [1] proved that among all connected graphs on n vertices the star, S_n, is the unique graph with minimal Gutman index, and the path, P_n, is the unique graph with maximal Gutman index.

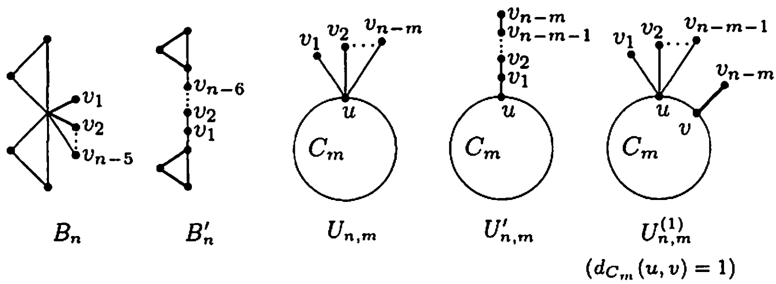

Fig. 1. Graphs with extremal Gutman indices.

We denote by C_m the cycle of length m. Among all connected bicyclic graphs on n vertices, Chen et al. [3] determined that B_n is the unique graph having minimal Gutman index, and Feng et al. [9] determined that B'_n is the unique graph having maximal Gutman index. Chen et al. [4] proved that $U_{n,3}$ is the unique unicyclic graph on n vertices having minimal Gutman index, and $U'_{n,m}$ is the unique unicyclic graph on n vertices and girth m having maximal Gutman index. Feng et al. [8] proved that $U_{n,m}$ is the unique unicyclic graph on n vertices and girth m having minimal Gutman index.

In this paper, we study the Gutman index of unicyclic graphs with given girth m. By introducing some graph transformations, we prove that $U^{(1)}_{n,m}$ (see Fig. 1) is the unique graph with the second-minimum Gutman index among all the unicyclic graphs with n vertices and girth m.

2 Some Graph Transformations

Let G be a simple connected graph. For a subset M of the edge set of G, $G - M$ denotes the graph obtained from G by deleting the edges in M, for a subset W of the edge set of the complement of G, $G + W$ denotes the graph obtained from G by adding the edges in W, and for $H \subseteq V(G)$, $G - H$ denotes the graph obtained from G by deleting the vertices of H and the edges incident with them. For a vertex u in G, $G + uv$ denotes the graph obtained from G by attaching pendant vertex v to u.

Lemma 2.1 *[8] Let v be a vertex of degree $p+1$ in the graph G, which is not a star, such that $vv_1, vv_2, \ldots, vv_p$ are pendant edges incident with v, and u is the neighborhood of v distinct from $v_1, v_2, \ldots, v_p$. Let G' be the graph obtained from G by removing edges $vv_1, vv_2, \ldots, vv_p$ and adding new edges $uv_1, uv_2, \ldots, uv_p$ (shown in Fig. 2). Then $Gut(G') < Gut(G)$.*

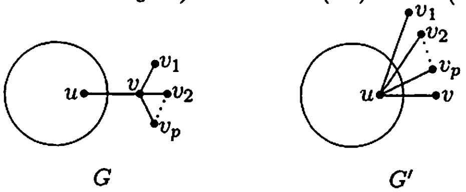

Fig. 2. Graphs G and G' in Lemma 2.1.

Lemma 2.2 *[3] Let u and v be two vertices in G, $u_1, u_2, \ldots, u_s (s \geq 1)$ the pendant vertices adjacent to u, $v_1, v_2, \ldots, v_t (t \geq 1)$ the pendant vertices adjacent to v. Let $G' = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}$, $G'' = G - \{uu_1, uu_2, \ldots, uu_s\} + \{vu_1, vu_2, \ldots, vu_s\}$, and $|V(G - \{u_1, u_2, \ldots, u_s, v_1, v_2, \ldots, v_t\})| \geq 3$ (shown in Fig. 3). Then $Gut(G) > \min\{Gut(G'), Gut(G'')\}$.*

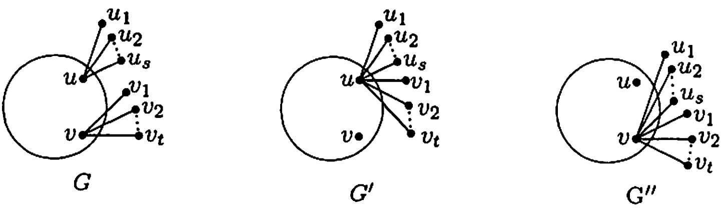

Fig. 3. Graphs G, G' and G'' in Lemma 2.2.

From Lemma 2.2, we have

Lemma 2.3 *Let C_m be a cycle of length m and $u, v \in V(C_m)$. Let $G = C_m + uu_1 + uu_2 + \cdots + uu_s + vv_1 + vv_2 + \cdots + vv_t$, $G' = G - \{vv_1, vv_2, \ldots, vv_{t-1}\} + \{uv_1, uv_2, \ldots, uv_{t-1}\}$, where $s, t \geq 2$ (shown in Fig. 4). Then $Gut(G) > Gut(G')$.*

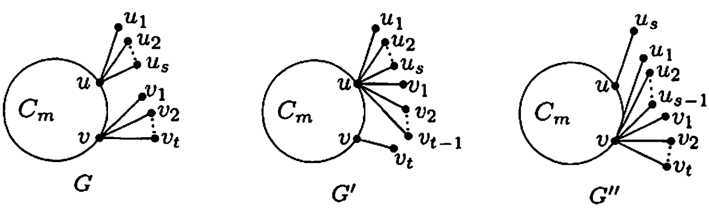

Fig. 4. Graphs G, G' and G'' in Lemma 2.3.

Proof. Let

$$G'' = G - \{uu_1, uu_2, \dots, uu_{s-1}\} + \{vu_1, vu_2, \dots, vu_{s-1}\}.$$

Clearly

$$G' \cong G'' \text{ and } |V(G - \{u_1, u_2, \dots, u_{s-1}, v_1, v_2, \dots, v_{t-1}\})| = m + 2 > 3.$$

It follows that $Gut(G) > \min\{Gut(G'), Gut(G'')\} = Gut(G')$ from Lemma 2.2. □

For convenience, we denote $d_G(x)d_G(y)d_G(x,y)$ by $D_G(x,y)$. Let T_u be a rooted tree with the root u. The level $l(v)$ of the vertex v in T_u is the distance from the root u to the vertex v. $h(T_u) = \max\limits_{v \in V(T_u)} \{l(v)\}$ is called the height of the rooted tree T_u.

A rooted tree T_u is called a $(2,1)$-rooted tree if it satisfies the following two conditions,

(i) $h(T_u) = 2$;

(ii) All vertices on the level 2 are adjacent to a common vertex on the level 1.

We write $G = G_1 u G_2$ if G_1 and G_2 are two induced subgraphs of G with $V(G_1) \cap V(G_2) = \{u\}$ and $V(G_1) \cup V(G_2) = V(G)$.

Lemma 2.4 *Let $G = C_m u T_u$, where T_u is a $(2,1)$-rooted tree, let $G' = C_m u T'_u$, where T'_u be a $(2,1)$-rooted tree and exactly one vertex on the level 2, and $|V(T_u)| = |V(T'_u)|$. Then $Gut(G) \geq Gut(G')$, and the equality holds if and only if $G \cong G'$, where the graphs G and G' are shown in Fig. 5.*

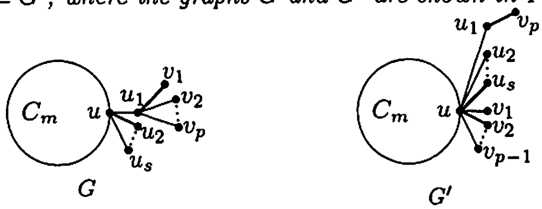

Fig. 5. Graphs G and G' in Lemma 2.4.

Proof. Let $G = C_m + uu_1 + uu_2 + \cdots + uu_s + u_1v_1 + u_1v_2 + \cdots + u_1v_p$,

$$G' = G - \{u_1v_1, u_1v_2, \dots, u_1v_{p-1}\} + \{uv_1, uv_2, \dots, uv_{p-1}\}.$$

Clearly, $G = G'$ and $Gut(G) = Gut(G')$ for $p = 1$. Now we show that $Gut(G) > Gut(G')$ for $p > 1$.

Let $A_1 = V(C_m) - \{u\}$, $\quad A_2 = \{u_2, u_3, \dots, u_s\} \cup \{v_p\}$,

$A_3 = \{v_1, v_2, \dots, v_{p-1}\}$, $\quad A_4 = \{u, u_1\}$.

Clearly $V(G)(= V(G'))$ is a disjoint union of the sets A_1, A_2, A_3 and A_4. We have

$$\begin{aligned} &Gut(G) - Gut(G') \\ &= \Big(\sum_{\{x,y\} \subseteq A_1} + \sum_{\{x,y\} \subseteq A_2} + \sum_{\{x,y\} \subseteq A_3} + \sum_{\{x,y\} \subseteq A_4} + \sum_{x \in A_1, y \in A_2} + \sum_{x \in A_1, y \in A_3} \\ &+ \sum_{x \in A_1, y \in A_4} + \sum_{x \in A_2, y \in A_3} + \sum_{x \in A_2, y \in A_4} + \sum_{x \in A_3, y \in A_4} \Big)(D_G(x,y) - D_{G'}(x,y)). \end{aligned}$$

Since

$$\Big(\sum_{\{x,y\}\subseteq A_1}+\sum_{\{x,y\}\subseteq A_2}+\sum_{\{x,y\}\subseteq A_3}+\sum_{x\in A_1,y\in A_2}\Big)(D_G(x,y)-D_{G'}(x,y))=0,$$

$$\begin{aligned}&\sum_{\{x,y\}\subseteq A_4}(D_G(x,y)-D_{G'}(x,y))\\&=D_G(u,u_1)-D_{G'}(u,u_1)=(s+2)(p+1)-2(s+p+1)=s(p-1),\end{aligned}$$

$$\begin{aligned}&\sum_{x\in A_1,y\in A_3}(D_G(x,y)-D_{G'}(x,y))=|A_3|\sum_{x\in A_1}(D_G(x,v_1)-D_{G'}(x,v_1))\\&=(p-1)\sum_{x\in A_1}[2(d_{C_m}(x,u)+2)-2(d_{C_m}(x,u)+1)]=2(m-1)(p-1),\end{aligned}$$

$$\begin{aligned}&\sum_{x\in A_1,y\in A_4}(D_G(x,y)-D_{G'}(x,y))\\&=\sum_{x\in A_1}(D_G(x,u)-D_{G'}(x,u))+\sum_{x\in A_1}(D_G(x,u_1)-D_{G'}(x,u_1))\\&=\sum_{x\in A_1}(2(s+2)d_{C_m}(x,u)-2(s+p+1)d_{C_m}(x,u))\\&+\sum_{x\in A_1}(2(p+1)(d_{C_m}(x,u)+1)-2\cdot 2(d_{C_m}(x,u)+1))=2(m-1)(p-1),\end{aligned}$$

$$\begin{aligned}&\sum_{x\in A_2,y\in A_3}(D_G(x,y)-D_{G'}(x,y))=|A_3|\sum_{x\in A_2}(D_G(x,v_1)-D_{G'}(x,v_1))\\&=(p-1)\Big(\sum_{x\in\{u_2,u_3,\ldots,u_s\}}(D_G(x,v_1)-D_{G'}(x,v_1))+(D_G(v_p,v_1)-D_{G'}(v_p,v_1))\Big)\\&=(p-1)((s-1)(D_G(u_2,v_1)-D_{G'}(u_2,v_1))+(2-3))\\&=(p-1)((s-1)(3-2)-1)=(s-2)(p-1),\end{aligned}$$

$$\begin{aligned}&\sum_{x\in A_2,y\in A_4}(D_G(x,y)-D_{G'}(x,y))\\&=\sum_{x\in A_2}(D_G(x,u)-D_{G'}(x,u))+\sum_{x\in A_2}(D_G(x,u_1)-D_{G'}(x,u_1))\\&=\sum_{x\in\{u_2,u_3,\ldots,u_s\}}(D_G(x,u)-D_{G'}(x,u))+(D_G(v_p,u)-D_{G'}(v_p,u))\\&\quad+\sum_{x\in\{u_2,u_3,\ldots,u_s\}}(D_G(x,u_1)-D_{G'}(x,u_1))+(D_G(v_p,u_1)-D_{G'}(v_p,u_1))\\&=(s-1)((s+2)-(s+p+1))+((s+2)\cdot 2-(s+p+1)\cdot 2)\\&\quad+(s-1)((p+1)\cdot 2-2\cdot 2)+((p+1)-2)=(s-2)(p-1),\end{aligned}$$

and $\sum_{x\in A_3,y\in A_4}(D_G(x,y)-D_{G'}(x,y))=|A_3|\sum_{y\in A_4}(D_G(v_1,y)-D_{G'}(v_1,y))$

$$\begin{aligned}&=(p-1)(D_G(v_1,u)-D_{G'}(v_1,u)+D_G(v_1,u_1)-D_{G'}(v_1,u_1))\\&=(p-1)(2\cdot(s+2)-(s+p+1)+(p+1)-2\cdot 2)=s(p-1).\end{aligned}$$

Hence

$$\begin{aligned}&Gut(G)-Gut(G')\\&=s(p-1)+2(m-1)(p-1)+2(m-1)(p-1)\\&\quad+(s-2)(p-1)+(s-2)(p-1)+s(p-1)\\&=4(p-1)(m+s-2)>0\text{ for }p>1,\ m\ge 3\text{ and }s\ge 1.\end{aligned}$$

Thus

$Gut(G)\ge Gut(G')$, and the equality holds if and only if $G\cong G'$. □

Lemma 2.5 *Let* $u,v\in V(C_m)$ *and* $d_{C_m}(u,v)=1$. *Let* $G'=C_m+uv_1+uv_2+\cdots+uv_{n-m-1}+v_1v_{n-m}$, $U_{n,m}^{(1)}=G'-\{v_1v_{n-m}\}+\{vv_{n-m}\}$. *Then*

$Gut(G') > Gut(U_{n,m}^{(1)})$, *where the graphs* G' *and* $U_{n,m}^{(1)}$ *are shown in Fig. 6.*

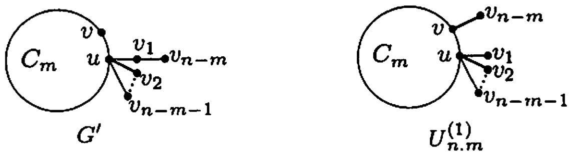

Fig. 6. Graphs G' and $U_{n,m}^{(1)}$ in Lemma 2.5.

Proof. Let $A_1 = V(C_m) - \{u, v\}$, $A_2 = \{v_2, v_3, \ldots, v_{n-m-1}\}$ and $A_3 = \{u, v, v_1, v_{n-m}\}$. Then $V(G')(= V(U_{n,m}^{(1)}))$ is a disjoint union of the sets A_1, A_2 and A_3. We have

$$Gut(G') - Gut(U_{n,m}^{(1)}) = \Big(\sum_{\{x,y\}\subseteq A_1} + \sum_{\{x,y\}\subseteq A_2} + \sum_{\{x,y\}\subseteq A_3} + \sum_{x\in A_1, y\in A_2} + \sum_{x\in A_1, y\in A_3} + \sum_{x\in A_2, y\in A_3}\Big)(D_{G'}(x,y) - D_{U_{n,m}^{(1)}}(x,y)).$$

Since

$$\Big(\sum_{\{x,y\}\subseteq A_1} + \sum_{\{x,y\}\subseteq A_2} + \sum_{x\in A_1, y\in A_2}\Big)(D_{G'}(x,y) - D_{U_{n,m}^{(1)}}(x,y)) = 0,$$

$$\begin{aligned}
&\sum_{\{x,y\}\subseteq A_3} (D_{G'}(x,y) - D_{U_{n,m}^{(1)}}(x,y))\\
&= (D_{G'}(u,v) - D_{U_{n,m}^{(1)}}(u,v)) + (D_{G'}(u,v_1) - D_{U_{n,m}^{(1)}}(u,v_1))\\
&\quad + (D_{G'}(u,v_{n-m}) - D_{U_{n,m}^{(1)}}(u,v_{n-m})) + (D_{G'}(v,v_1) - D_{U_{n,m}^{(1)}}(v,v_1))\\
&\quad + (D_{G'}(v,v_{n-m}) - D_{U_{n,m}^{(1)}}(v,v_{n-m})) + (D_{G'}(v_1,v_{n-m}) - D_{U_{n,m}^{(1)}}(v_1,v_{n-m}))\\
&= (2(n-m+1) - 3(n-m+1)) + (2(n-m+1) - (n-m+1)) + (2(n-m+\\
&\quad 1) - 2(n-m+1)) + (2\cdot 2\cdot 2 - 3\cdot 1\cdot 2) + (2\cdot 3 - 3\cdot 1) + (2\cdot 1 - 3) = 4,
\end{aligned}$$

$$\begin{aligned}
&\sum_{x\in A_1, y\in A_3} (D_{G'}(x,y) - D_{U_{n,m}^{(1)}}(x,y))\\
&= \sum_{x\in A_1} ((D_{G'}(x,u) - D_{U_{n,m}^{(1)}}(x,u)) + (D_{G'}(x,v) - D_{U_{n,m}^{(1)}}(x,v))\\
&\quad + (D_{G'}(x,v_1) - D_{U_{n,m}^{(1)}}(x,v_1)) + (D_{G'}(x,v_{n-m}) - D_{U_{n,m}^{(1)}}(x,v_{n-m})))\\
&= \sum_{x\in A_1} (0 + (2\cdot 2d_{C_m}(x,v) - 2\cdot 3d_{C_m}(x,v)) + (2\cdot 2(d_{C_m}(x,u)+1)\\
&\quad - 2\cdot 1(d_{C_m}(x,u)+1)) + (2(d_{C_m}(x,u)+2) - 2(d_{C_m}(x,v)+1)))\\
&= \sum_{x\in A_1} 4(d_{C_m}(x,u) - d_{C_m}(x,v) + 1) = \sum_{x\in A_1} 4 = 4(m-2),
\end{aligned}$$

$$\begin{aligned}
&\sum_{x\in A_2, y\in A_3} (D_{G'}(x,y) - D_{U_{n,m}^{(1)}}(x,y))\\
&= |A_2| \sum_{y\in A_3} (D_{G'}(v_{n-m-1},y) - D_{U_{n.m}^{(1)}}(v_{n-m-1},y))\\
&= (n-m-2)((D_{G'}(v_{n-m-1},u) - D_{U_{n,m}^{(1)}}(v_{n-m-1},u))\\
&\quad + (D_{G'}(v_{n-m-1},v) - D_{U_{n,m}^{(1)}}(v_{n-m-1},v))\\
&\quad + (D_{G'}(v_{n-m-1},v_1) - D_{U_{n,m}^{(1)}}(v_{n-m-1},v_1))
\end{aligned}$$

$+ (D_{G'}(v_{n-m-1}, v_{n-m}) - D_{U^{(1)}_{n,m}}(v_{n-m-1}, v_{n-m})))$
$= (n-m-2)(0 + (2 \cdot 2 - 3 \cdot 2) + (2 \cdot 2 - 2) + (3-3)) = 0.$

Hence

$$Gut(G') - Gut(U^{(1)}_{n,m}) = 4 + 4(m-2) + 0 = 4(m-1) > 0 \text{ for } m \geq 3.$$

Therefore $Gut(G') > Gut(U^{(1)}_{n,m})$. □

3 The Second-minimum Gutman Index of Unicyclic Graphs with Girth m

Lemma 3.1 *[3, 11]*

$$Gut(C_m) = 4W(C_m) = \begin{cases} \frac{m^3-m}{2}, & if \quad m \text{ is odd}, \\ \frac{m^3}{2}, & if \quad m \text{ is even}. \end{cases}$$

Lemma 3.2 *Let C_m be a cycle of length m and u be any vertex on C_m. Then*

$$\sum_{v \in V(C_m)} d_{C_m}(u,v) = \begin{cases} \frac{m^2-1}{4}, & if \quad m \text{ is odd}, \\ \frac{m^2}{4}, & if \quad m \text{ is even}. \end{cases}$$

Proof. Since

$$W(C_m) = \sum_{\{u,v\} \subseteq V(C_m)} d_{C_m}(u,v) = \frac{1}{2} \sum_{u \in V(C_m)} \sum_{v \in V(C_m)} d_{C_m}(u,v),$$

note that $\sum_{v \in V(C_m)} d_{C_m}(u,v) = \sum_{v \in V(C_m)} d_{C_m}(w,v)$ for any $u, w \in V(C_m)$, hence $W(C_m) = \frac{1}{2} m \sum_{v \in V(C_m)} d_{C_m}(u,v)$. Thus, it follows from Lemma 3.1 that

$$\frac{1}{2} m \sum_{v \in V(C_m)} d_{C_m}(u,v) = \begin{cases} \frac{m^3-m}{8}, & if \quad m \text{ is odd}, \\ \frac{m^3}{8}, & if \quad m \text{ is even}. \end{cases}$$

This implies that

$$\sum_{v \in V(C_m)} d_{C_m}(u,v) = \begin{cases} \frac{m^2-1}{4}, & if \quad m \text{ is odd}, \\ \frac{m^2}{4}, & if \quad m \text{ is even}. \end{cases}$$

The proof is completed. □

Let $\mathcal{U}_n$ and $\mathcal{U}_{n,m}$ be the set of all unicyclic graphs of order n and all unicyclic graphs on n vertices and girth m, respectively.

Let u, v be two distinct vertices on the cycle C_m with $d_{C_m}(u,v) = k (1 \leq k \leq \lfloor \frac{m}{2} \rfloor)$. Let $U_{n,m} = C_m + uv_1 + uv_2 + \cdots + uv_{n-m}$, $U^{(k)}_{n,m} = C_m + uv_1 + uv_2 + \cdots + uv_{n-m-1} + vv_{n-m}$.

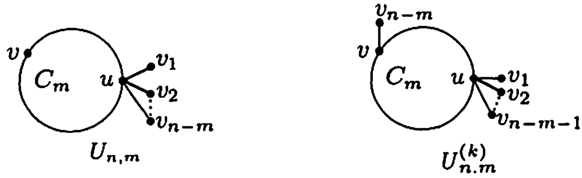

Fig. 7. Graphs $U_{n,m}$ and $U_{n,m}^{(k)}$.

Lemma 3.3 *[4]*

$$Gut(U_{n,m}) = \begin{cases} 2n^2 + (m^2 - 2m - 2)n - \frac{1}{2}m^3 + \frac{3}{2}m, & if \quad m \text{ is odd}, \\ 2n^2 + (m^2 - 2m - 1)n - \frac{1}{2}m^3 + m, & if \quad m \text{ is even}. \end{cases}$$

Lemma 3.4 *[4] For any $U \in \mathcal{U}_{n,m}$, we have $Gut(U_{n,m}) \le Gut(U)$, and the equality holds if and only if $U \cong U_{n,m}$.*

Theorem 3.5 *For $1 \le k \le \lfloor \frac{m}{2} \rfloor$, we have $Gut(U_{n,m}^{(k)}) = Gut(U_{n,m}) + 4k(n - m - 1)$.*

Proof. Let $A_1 = V(C_m) - \{u, v\}$, $A_2 = \{u, v\}$, $A_3 = \{v_1, v_2, \dots, v_{n-m-1}\}$ and $A_4 = \{v_{n-m}\}$. Then $V(U_{n,m}^{(k)})(= V(U_{n,m}))$ is a disjoint union of the sets A_1, A_2, A_3 and A_4. We have

$$\begin{aligned} & Gut(U_{n,m}^{(k)}) - Gut(U_{n,m}) \\ = & \Big(\sum_{\{x,y\} \subseteq A_1} + \sum_{\{x,y\} \subseteq A_2} + \sum_{\{x,y\} \subseteq A_3} + \sum_{x \in A_1, y \in A_2} + \sum_{x \in A_1, y \in A_3} + \sum_{x \in A_1, y \in A_4} \\ & + \sum_{x \in A_2, y \in A_3} + \sum_{x \in A_2, y \in A_4} + \sum_{x \in A_3, y \in A_4} \Big) (D_{U_{n,m}^{(k)}}(x,y) - D_{U_{n,m}}(x,y)). \end{aligned}$$

Since

$$\Big(\sum_{\{x,y\} \subseteq A_1} + \sum_{\{x,y\} \subseteq A_3} + \sum_{x \in A_1, y \in A_3} \Big) (D_{U_{n,m}^{(k)}}(x,y) - D_{U_{n,m}}(x,y)) = 0,$$

$$\begin{aligned} & \sum_{\{x,y\} \subseteq A_2} (D_{U_{n,m}^{(k)}}(x,y) - D_{U_{n,m}}(x,y)) = D_{U_{n,m}^{(k)}}(u,v) - D_{U_{n,m}}(u,v) \\ = & \ 3(n - m + 1)k - 2(n - m + 2)k = k(n - m - 1), \end{aligned}$$

$$\begin{aligned} & \sum_{x \in A_1, y \in A_2} (D_{U_{n,m}^{(k)}}(x,y) - D_{U_{n,m}}(x,y)) \\ = & \sum_{x \in A_1} (D_{U_{n,m}^{(k)}}(x,u) - D_{U_{n,m}}(x,u)) + \sum_{x \in A_1} (D_{U_{n,m}^{(k)}}(x,v) - D_{U_{n,m}}(x,v)) \\ = & \sum_{x \in A_1} (2(n - m + 1)d_{C_m}(x,u) - 2(n - m + 2)d_{C_m}(x,u)) \\ & + \sum_{x \in A_1} (2 \cdot 3d_{C_m}(x,v) - 2 \cdot 2d_{C_m}(x,v)) \\ = & -2 \sum_{x \in A_1} d_{C_m}(x,u) + 2 \sum_{x \in A_1} d_{C_m}(x,v) \\ = & -2\Big(\sum_{x \in V(C_m)} d_{C_m}(x,u) - d_{C_m}(v,u) \Big) + 2\Big(\sum_{x \in V(C_m)} d_{C_m}(x,v) - d_{C_m}(u,v) \Big) \end{aligned}$$

$$= -2 \sum_{x \in V(C_m)} d_{C_m}(x,u) + 2 \sum_{x \in V(C_m)} d_{C_m}(x,v) = 0,$$

$$\sum_{x \in A_1, y \in A_4} (D_{U_{n,m}^{(k)}}(x,y) - D_{U_{n,m}}(x,y))$$
$$= \sum_{x \in A_1} (D_{U_{n,m}^{(k)}}(x, v_{n-m}) - D_{U_{n,m}}(x, v_{n-m}))$$
$$= \sum_{x \in A_1} (2(d_{C_m}(x,v) + 1) - 2(d_{C_m}(x,u) + 1))$$
$$= 2 \sum_{x \in A_1} (d_{C_m}(x,v) - d_{C_m}(x,u)) = 0,$$

$$\sum_{x \in A_2, y \in A_3} (D_{U_{n,m}^{(k)}}(x,y) - D_{U_{n,m}}(x,y))$$
$$= \sum_{y \in A_3} (D_{U_{n,m}^{(k)}}(u,y) - D_{U_{n,m}}(u,y)) + \sum_{y \in A_3} (D_{U_{n,m}^{(k)}}(v,y) - D_{U_{n,m}}(v,y))$$
$$= |A_3|(D_{U_{n,m}^{(k)}}(u,v_1) - D_{U_{n,m}}(u,v_1)) + |A_3|(D_{U_{n,m}^{(k)}}(v,v_1) - D_{U_{n,m}}(v,v_1))$$
$$= (n-m-1)((n-m+1) - (n-m+2))$$
$$+ (n-m-1)(3(k+1) - 2(k+1)) = k(n-m-1),$$

$$\sum_{x \in A_2, y \in A_4} (D_{U_{n,m}^{(k)}}(x,y) - D_{U_{n,m}}(x,y))$$
$$= D_{U_{n,m}^{(k)}}(u, v_{n-m}) - D_{U_{n,m}}(u, v_{n-m}) + D_{U_{n,m}^{(k)}}(v, v_{n-m}) - D_{U_{n,m}}(v, v_{n-m})$$
$$= (n-m+1)(k+1) - (n-m+2) + 3 - 2(k+1) = k(n-m-1),$$

and

$$\sum_{x \in A_3, y \in A_4} (D_{U_{n,m}^{(k)}}(x,y) - D_{U_{n,m}}(x,y))$$
$$= \sum_{x \in A_3} (D_{U_{n,m}^{(k)}}(x, v_{n-m}) - D_{U_{n,m}}(x, v_{n-m})) = |A_3|(D_{U_{n,m}^{(k)}}(v_1, v_{n-m}) - D_{U_{n,m}}(v_1, v_{n-m})) = (n-m-1)((k+2) - 2) = k(n-m-1).$$

It follows that

$$Gut(U_{n,m}^{(k)}) - Gut(U_{n,m})$$
$$= k(n-m-1) + 0 + 0 + k(n-m-1) + k(n-m-1) + k(n-m-1)$$
$$= 4k(n-m-1).$$

This implies that $Gut(U_{n,m}^{(k)}) = Gut(U_{n,m}) + 4k(n-m-1)$, where $1 \le k \le \lfloor \frac{m}{2} \rfloor$. □

From Theorem 3.5, we have

Theorem 3.6 *$Gut(U_{n,m}^{(k)}) \le Gut(U_{n,m}^{(k+1)})$, where $1 \le k \le \lfloor \frac{m}{2} \rfloor - 1$.*

Combining Lemma 3.3 and Theorem 3.5, we have

Theorem 3.7 $Gut(U_{n,m}^{(k)}) =$

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

where $1 \le k \le \lfloor \frac{m}{2} \rfloor$.

Let $C_m = u_1u_2\cdots u_mu_1$, we denote by $C_m(T_{u_1}, T_{u_2}, \ldots, T_{u_m})$ the unicyclic graph with the cycle C_m such that the deletion of all edges on C_m results in m vertex-disjoint trees $T_{u_1}, T_{u_2}, \ldots, T_{u_m}$ with $u_i \in V(T_{u_i})$ for $i = 1, 2, \ldots, m$.

Theorem 3.8 *Let $U \in \mathcal{U}_{n,m}$ and $U \ncong U_{n,m}$. Then $Gut(U) \geq (U_{n,m}^{(1)})$, and the equality holds if and only if $U \cong U_{n,m}^{(1)}$.*

Proof. For any unicyclic graph $U \in \mathcal{U}_{n,m}$ and $U \ncong U_{n,m}$, it is clear that $n > m$. Let the unique cycle in U be C_m, then there exists at least one vertex on C_m, say u, whose degree $d_U(u) > 2$.

Case 1. u is the unique vertex on C_m with $d_U(u) > 2$.

Let $U = C_m uT_u$, where T_u is a rooted tree with the root u and $h(T_u) \geq 2$. By using Lemma 2.1 repeatedly, we can find a unicyclic graph $U' = C_m uT'_u \in \mathcal{U}_{n,m}$ such that T'_u is a $(2,1)$-rooted tree, and $Gut(U) \geq Gut(U')$ (we take $U' = U$ when T_u is a $(2,1)$-rooted tree).

By Lemma 2.4, there exists a unicyclic graph $U'' = C_m uT''_u \in \mathcal{U}_{n,m}$ such that T''_u is a $(2,1)$-rooted tree with the unique vertex on level 2 and $Gut(U') \geq Gut(U'')$ (we take $U'' = U'$ when T'_u is a $(2,1)$-rooted tree with the unique vertex on level 2). By Lemma 2.5, $Gut(U'') > Gut(U_{n,m}^{(1)})$.

Therefore $Gut(U) > Gut(U_{n,m}^{(1)})$.

Case 2. There exist at least two vertices in C_m whose degrees (in U) are greater than 2. We show that $Gut(U) \geq Gut(U_{n,m}^{(1)})$, and the equality holds if and only if $U \cong U_{n,m}^{(1)}$.

Let $C_m = u_1u_2\cdots u_mu_1$ and $U = C_m(T_{u_1}, T_{u_2}, \ldots, T_{u_m})$, where T_{u_i} is a rooted tree of order r_i at the root u_i for $i = 1, 2, \ldots, m$ (Note that T_{u_i} is trivial when $r_i = 1$). Using Lemma 2.1 more than once, there exists the unicyclic graph $U_1 = C_m(S_{u_1}, S_{u_2}, \ldots, S_{u_m}) \in \mathcal{U}_{n,m}$, where S_{u_i} is a star of order r_i at the center u_i for $i = 1, 2, \ldots, m$, such that $Gut(U) \geq Gut(U_1)$, and the quality holds if and only if $U \cong U_1$. Using Lemma 2.2 more than once, there exists a unicyclic graph $U_2 = C_m + u_{t_1}v_1 + u_{t_1}v_2 + \cdots + u_{t_1}v_a + u_{t_2}v_{a+1} + u_{t_2}v_{a+2} + \cdots + u_{t_2}v_{n-m} \in \mathcal{U}_{n,m}$, where $1 \leq a \leq n-m-1$, $1 \leq t_1 < t_2 \leq m$, and $Gut(U_1) \geq Gut(U_2)$ (with the equality when $U_1 \cong U_2$). Let $d_{C_m}(u_{t_1}, u_{t_2}) = k$, then $1 \leq k \leq \lfloor \frac{m}{2} \rfloor$. By Lemma 2.3, we have $Gut(U_2) \geq Gut(U_{n,m}^{(k)})$ with the equality if and only if $a = 1, n-m-1$. By Theorem 3.1, we have $Gut(U_{n,m}^{(k)}) \geq Gut(U_{n,m}^{(1)})$, and the equality holds if and only if $k = 1$.

Therefore $Gut(U) \geq Gut(U_{n,m}^{(1)})$, and the equality holds if and only if $U \cong U_{n,m}^{(1)}$. □

Acknowledgements

The authors are grateful to the referee for his/her helpful comments and useful suggestions on the earlier version of this paper.

References

[1] V. Andova, D. Dimitrov, J. Fink and R. Skrekovski, Bounds on Gutman index, MATCH Commun. Math. Comput. Chem. 67 (2012) 515–524.

[2] D. Bonchev, The Wiener number C Some applications and new developments, in: D. H. Rouvray, R. B. King (Eds.), Topology in Chemistry - Discrete Mathematics of Molecules, Horwood, Chichester, 2002, 58–88.

[3] S. Chen and W. Liu, Extremal modified Schultz index of bicyclic graphs, MATCH Commun. Math. Comput. Chem. 64 (2010) 767–782.

[4] S. Chen and W. Liu, Extremal unicyclic graphs with respect to modified Schultz index, Util. Math. 86 (2011) 87–94.

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

[6] P. Dankelmann, I. Gutman, S. Mukwembi and H. C. Swart, The edge-wiener index of a graph, Discrete Math. 309 (2009) 3452–3457.

[7] R. C. Entringer, Distance in graphs: trees, J. Combin. Math. Combin. Comput. 24 (1997) 65–84.

[8] L. Feng, The Gutman index of unicyclic graphs, Discrete Mathematics, Algorithms and Applications, Vol. 4, No. 03 (2012) 1250031 (8 pages).

[9] L. Feng and W. Liu, The maximal gutman index of bicyclic graphs, MATCH Commun. Math. Comput. Chem. 66 (2011) 699–708.

[10] I. Gutman, Selected properties of the Schultz molecular topological index. J. Chem. inf. Comput. Sci. 34 (1994) 1087–1089.

[11] I. Gutman and O. E. Polansky, Mathematical Concepts in Organic Chemistry (Springer, Berlin, 1986)

[12] I. Gutman, Y. Yeh, S. Lee and Y. Luo, Some recent results in the theory of the Wiener number, Indian J. Chem. 32 A (1993) 651–661.

[13] D. J. Klein, Z. Mihalic, D. Plavsic and N. Trinajstic, Molecular topological index: A relation with the Wiener index. J. Chem. Inf. Comput. Sci. 32 (1992) 304–305.

[14] M. Knor, P. Potocnik and R. Skrekovski, Relationship between the edge-Wiener index and the Gutman index of a graph, Discr. Appl. Math. 167 (2014) 197–201.

[15] H. P. Schultz, Topological organic chemistry. 1. Graph theory and topological indices of alkanes. J. Chem. Inf. Comput. Sci. 29 (1989) 227–228.

[16] R. Todeschini and V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.

[17] H. Wiener, Structual determination of paraffin boiling points. J. Amer. Chem. Soc. 69 (1947) 17–20.