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Research Article

Elliptic Sombor index of trees and unicyclic graphs

Zikai Tang, Yunping Li, Hanyuan Deng*

School of Mathematics and Statistics, Hunan Normal University, Changsha, Hunan, China

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Abstract

Let $G = G(V, E)$ be a simple connected graph with vertex set V and edge set E. The elliptic Sombor index of G is defined as $ESO(G) = \sum_{uv\in E}(d(u) + d(v))\sqrt{d^2(u) + d^2(v)}$, where $d(u)$ denotes the degree of vertex u. In this paper, the maximal value of the elliptic Sombor index of trees with a given diameter or matching number or number of pendent vertices is determined. The extremal values of the elliptic Sombor index of unicyclic graphs are also found. Furthermore, those trees and unicyclic graphs that achieve the obtained extremal values are characterized.

Keywords: elliptic Sombor index; extremal value; tree (graph); unicyclic graph.

2020 Mathematics Subject Classification: 05C05, 05C07, 05C09, 05C35.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$ such that $n = |V(G)|$ and $m = |E(G)|$. The degree of a vertex v in G, denoted by $d_G(v)$ (or $d(v)$), is the number of its neighbors. A pendent vertex is a vertex of degree one. If the vertices u and v are adjacent, then the edge connecting them is labeled as $e = uv$. The cycle and path of order n are denoted by C_n and P_n, respectively. The distance between vertices u and v in G, denoted by $d_G(u, v)$ (or $d(u, v)$), is the length of a shortest path between u and v. The diameter of G is the number $\max_{u,v\in V(G)} d_G(u, v)$.

Numerous vertex-degree-based (VDB) graph invariants – also known as “topological indices” – have been put forward and thoroughly examined in the literature on mathematical chemistry [5–9, 13]. A general formula for such topological indices is given as follows:

$$TI(G) = \sum_{uv\in E(G)} F(d_G(u), d_G(v)),$$

where $F(x, y)$ is a function with the property $F(x, y) = F(y, x)$. In the standard formulation of the theory of VDB topological indices, $TI(G)$ depends on the vertices of G, so that the single parameter associated with each vertex is its vertex degree. An alternative interpretation of VDB indices has been offered in [6]. Based on a geometric interpretation, Gutman [6] introduced the following index, namely the Sombor index, and established its basic properties:

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d_G^2(u) + d_G^2(v)}\,.$$

Numerous studies have so far been conducted on the Sombor index, including those on its chemical applicability [10, 12], the extremal values of the Sombor index of trees with specified parameters [2], and the extremal values of the Sombor index of unicyclic and bicyclic graphs [3]. The existing bounds and extremal results related to the Sombor index and its variants were collected in [11].

Recently, a novel geometric method for constructing vertex-degree-based topological indices was proposed by Gutman, Furtula, and Oz [8]. This method is based on an ellipse whose focal points represent the degrees of a pair of adjacent vertices. The area of the ellipse induces the following vertex-degree-based topological index of remarkable simplicity, which was referred to as the elliptic Sombor index:

$$ESO(G) = \sum_{uv\in E(G)} (d_G(u) + d_G(v))\sqrt{d_G^2(u + d_G^2(v)}. \tag{1}$$

In [8], the main mathematical properties of the elliptic Sombor index, particularly its relations to some earlier known indices, were established and its potential applications were analyzed.

*Corresponding author (hydeng@hunnu.edu.cn).

For an edge subset $M \subseteq E(G)$, if every pair of edges in M has no common endpoint, then M is called a matching of G. A matching M is a maximum matching if there is no other matching M' of G such that $|M| > |M'|$. The number of edges in a maximum matching of G is called the matching number of G, denoted by $\beta(G)$. A maximum matching M with $|M| = \beta$ is also known as a β-matching. If M is a matching, the ends of every edge of M are called matched under M, and every vertex incident with an edge of M is known as an M-saturated.

In this paper, we give the maximal value of the elliptic Sombor index of trees with given (i) number of pendent vertices, (ii) diameter, and (iii) matching number. We also determine extremal values of the elliptic Sombor index of unicyclic graphs. Furthermore, we characterize those trees and unicyclic graphs that achieve the obtained extremal values.

2. Preliminaries

In this section, we give some lemmas that will be used in the subsequent sections.

Lemma 2.1. *Let $g(x,y) = (x+y)\sqrt{x^2+y^2}$ for $x > 0$ and $y > 0$. The function $g(x,y)$ is strictly increasing in x and in y.*

Proof. Since
$$\frac{\partial g}{\partial x} = \sqrt{x^2+y^2} + \frac{x(x+y)}{\sqrt{x^2+y^2}} > 0 \quad \text{and} \quad \frac{\partial g}{\partial y} = \sqrt{x^2+y^2} + \frac{y(x+y)}{\sqrt{x^2+y^2}} > 0$$
for $x > 0$ and $y > 0$, the lemma holds. □

Lemma 2.2. *Let $\rho(x,y) = \sqrt{x^2+y^2} + \frac{x(x+y)}{\sqrt{x^2+y^2}}$ with $x > 0$ and $y > 0$. The function $\rho(x,y)$ is strictly increasing in x and in y.*

Proof. Since
$$\rho_x(x,y) = \frac{x}{\sqrt{x^2+y^2}} + \frac{(2x+y)(x^2+y^2) - x^2(x+y)}{(x^2+y^2)^{\frac{3}{2}}} = \frac{2x^3+3xy^2+y^3}{(x^2+y^2)^{\frac{3}{2}}} > 0$$
and
$$\rho_y(x,y) = \frac{y}{\sqrt{x^2+y^2}} + \frac{x(x^2+y^2) - xy(x+y)}{(x^2+y^2)^{\frac{3}{2}}} = \frac{y^3+x^3}{(x^2+y^2)^{\frac{3}{2}}} > 0$$
for $x > 0$ and $y > 0$, the lemma holds. □

Lemma 2.3. *Let G be a graph and $P = v_1v_2, \ldots, v_k$ be an induced sub-path in G, where $d_G(v_1) \geq 2$ and $d_G(v_k) \geq 2$. Let $G' = G - \{v_kw : w \in N(v_k)\backslash\{v_{k-1}\}\} + \{v_1w : w \in N(v_k)\backslash\{v_{k-1}\}\}$. The process of transforming G into G' is called path-lifting transformation, see Figure 2.1. It holds that $ESO(G) < ESO(G')$.*

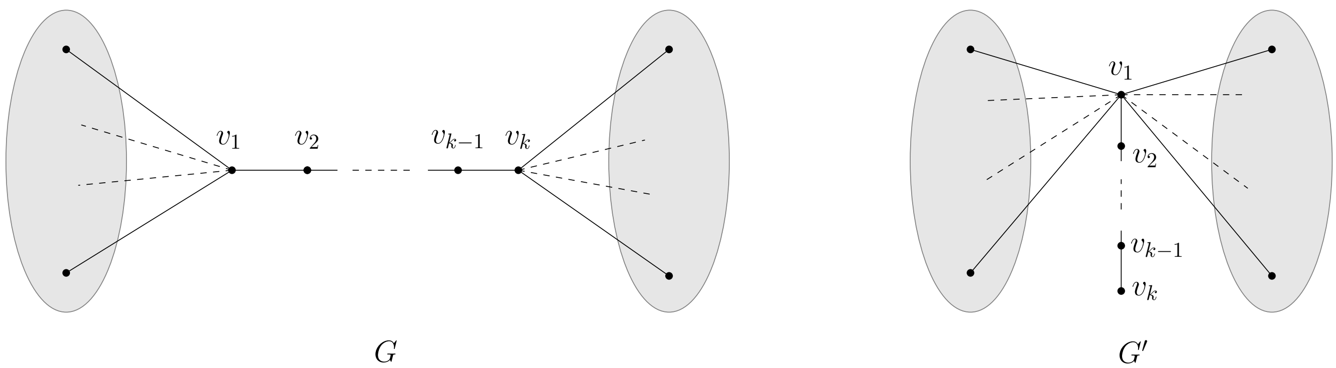

Figure 2.1: The path-lifting transformation.

Proof. Let $\phi(x,y) = (2+x)\sqrt{4+x^2} + (2+y)\sqrt{4+y^2} - (x+y+1)\sqrt{4+(x+y-1)^2} - 3\sqrt{5}$, where $x \geq 2$ and $y \geq 2$. If $x-1 > 0$ and $y-1 > 0$, then by Lemma 2.2 we have
$$\frac{\partial \phi(x,y)}{\partial x} = \sqrt{4+x^2} + \frac{x(2+x)}{\sqrt{4+x^2}} - \sqrt{4+(x+y-1)^2} - \frac{(x+y+1)(x+y-1)}{\sqrt{4+(x+y-1)^2}} = g(x,2) - g(x+y-1,2) < 0$$
$$\frac{\partial \phi(x,y)}{\partial y} = \sqrt{4+y^2} + \frac{y(2+y)}{\sqrt{4+y^2}} - \sqrt{4+(x+y-1)^2} - \frac{(x+y+1)(x+y-1)}{\sqrt{4+(x+y-1)^2}} < 0.$$
Hence, the function $\phi(x,y)$ is strictly decreasing in $x \geq 2$ and in $y \geq 2$. In the following discussion, for convenience, let $d_G(v_1) = x \geq 2$ and $d_G(v_k) = y \geq 2$.

Case 1. $k > 2$.
By Lemma 2.1, we have

$$\begin{aligned}
ESO(G) - ESO(G') &= (2+x)\sqrt{4+x^2} + \sum_{w\in N(v_1)\setminus\{v_2\}} (x+d_G(w))\sqrt{x^2+d_G^2(w)} \\
&\quad + (2+y)\sqrt{4+y^2} + \sum_{w\in N(v_k)\setminus\{v_{k-1}\}} (y+d_G(w))\sqrt{y^2+d_G^2(w)} \\
&\quad - \sum_{w\in N(v_1)\cup N(v_k)\setminus\{v_2,v_{k-1}\}} (x+y-1+d_G(w))\sqrt{(x+y-1)^2+d_G^2(w)} \\
&\quad - (x+y+1)\sqrt{4+(x+y-1)^2} - 3\sqrt{5} \\
&= (2+x)\sqrt{4+x^2} + (2+y)\sqrt{4+y^2} - (x+y+1)\sqrt{4+(x+y-1)^2} - 3\sqrt{5} \\
&\quad + \sum_{w\in N(v_1)\setminus\{v_2\}} \left((x+d_G(w))\sqrt{x^2+d_G^2(w)} - (x+y-1+d_G(w))\sqrt{(x+y-1)^2+d_G^2(w)} \right) \\
&\quad + \sum_{w\in N(v_k)\setminus\{v_{k-1}\}} \left((y+d_G(w))\sqrt{y^2+d_G^2(w)} - (x+y-1+d_G(w))\sqrt{(x+y-1)^2+d_G^2(w)} \right) \\
&< (2+x)\sqrt{4+x^2} + (2+y)\sqrt{4+y^2} - (x+y+1)\sqrt{4+(x+y-1)^2} - 3\sqrt{5} \quad \text{(by Lemma 2.1)} \\
&< \phi(2,2) < 0.
\end{aligned}$$

Case 2. $k = 2$.
Since $1 + (x+y-1)^2 - x^2 - y^2 = 2(xy - x - y) + 1 > 0$ for $x \geq 2$ and $y \geq 2$, by Lemma 2.1 we have

$$\begin{aligned}
ESO(G) - ESO(G') &= (x+y)\sqrt{x^2+y^2} + \sum_{w\in N(v_1)\setminus\{v_2\}} (x+d_G(w))\sqrt{x^2+d_G^2(w)} \\
&\quad + \sum_{w\in N(v_2)\setminus\{v_1\}} (y+d_G(w))\sqrt{y^2+d_G^2(w)} - (x+y)\sqrt{1+(x+y-1)^2} \\
&\quad - \sum_{w\in N(v_1)\cup N(v_2)\setminus\{v_1,v_2\}} (x+y-1+d_G(w))\sqrt{(x+y-1)^2+d_G^2(w)} \\
&< (x+y)\left(\sqrt{x^2+y^2} - \sqrt{1+(x+y-1)^2}\right) < 0.
\end{aligned}$$

In both cases, we have $ESO(G) < ESO(G')$. □

If G is a graph and $P = v_1v_2$ is an induced sub-path in G, then the path-lifting transformation in Lemma 2.3 is also known as the edge-lifting transformation. Any tree T with $n \geq 4$ vertices may be transformed into the star S_n (or the path P_n) by using the edge-lifting transformation (or its inverse, respectively). This observation provides the following result established in [8].

Theorem 2.1 (see [8]). *If T is a tree with $n \geq 2$ vertices, S_n is the n-vertex star, and P_n is the n-vertex path, then*

$$ESO(P_n) \leq ESO(T) \leq ESO(S_n),$$

where the left and right equalities hold if and only if $T \cong P_n$ and $T \cong S_n$, respectively.

3. Elliptic Sombor index of trees

In this section, we determine the maximal value of the elliptic Sombor index of trees with a given number of pendent vertices, diameter, or matching number. Let T_n^k be the set of trees with n vertices and k pendent vertices. Let $Spider(n_1, n_2, \ldots, n_k)$ be the starlike tree (that is, a tree having exactly one vertex of degree greater than 2) such that the length of its i-th branch is n_i, where $n_1 \geqslant n_2 \geqslant \cdots \geqslant n_k \geqslant 1$. It is obvious that $Spider(n_1, n_2, \ldots, n_k) \in T_n^k$ if and only if $\sum_{i=1}^k n_i = n - 1$. The tree $Spider(n_1, n_2, \ldots, n_k)$ is illustrated in Figure 3.1.

Lemma 3.1. *If $f(x,y) = (x+y-2+a)\sqrt{(x+y-2)^2+a^2} - (x+a)\sqrt{x^2+a^2} - (y+b)\sqrt{y^2+b^2}$ with $x, y \geqslant 3$ and $a \geqslant b \geqslant 1$, then the function $f(x,y)$ is strictly increasing in x and in y.*

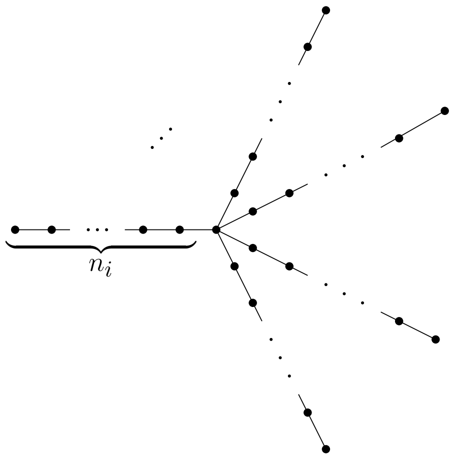

Figure 3.1: The tree $Spider(n_1, n_2, \dots, n_k)$.

Proof. Since $x + y - 2 > x \geqslant 3$ and $a \geqslant b \geqslant 1$, by Lemma 2.2 we have

$$\begin{aligned} f_x(x,y) &= \left(\sqrt{(x+y-2)^2+a^2} + \frac{(x+y-2)(x+y-2+a)}{\sqrt{(x+y-2)^2+a^2}}\right) - \left(\sqrt{x^2+a^2} + \frac{x(x+a)}{\sqrt{x^2+a^2}}\right) \\ &= \rho(x+y-2,a) - \rho(x,a) > 0, \\ f_y(x,y) &= \left(\sqrt{(x+y-2)^2+a^2} + \frac{(x+y-2)(x+y-2+a)}{\sqrt{(x+y-2)^2+a^2}}\right) - \left(\sqrt{y^2+b^2} + \frac{y(y+b)}{\sqrt{y^2+b^2}}\right) \\ &= \rho(x+y-2,a) - \rho(y,b) \geqslant \rho(x+y-2,b) - \rho(y,b) > 0. \end{aligned}$$

Thus, the lemma holds. □

Lemma 3.2. *If $h(x,y) = (x+1+y)\sqrt{(x+1)^2+y^2} - (x+y)\sqrt{x^2+y^2}$ with $x, y \geqslant 3$, then the function $h(x,y)$ is strictly increasing in x and in y.*

Proof. Since $x + 1 > x \geqslant 3$, by Lemma 2.2 we have

$$\begin{aligned} h_x(x,y) &= \sqrt{(x+1)^2+y^2} + \frac{(x+1+y)(x+1)}{\sqrt{(x+1)^2+y^2}} - \sqrt{x^2+y^2} - \frac{(x+y)x}{\sqrt{x^2+y^2}} \\ &= \rho(x+1,y) - \rho(x,y) > 0, \\ h_y(x,y) &= \sqrt{(x+1)^2+y^2} + \frac{(x+1+y)y}{\sqrt{(x+1)^2+y^2}} - \sqrt{x^2+y^2} - \frac{(x+y)y}{\sqrt{x^2+y^2}} \\ &= \rho(y,x+1) - \rho(y,x) > 0. \end{aligned}$$

Hence, the lemma holds. □

Lemma 3.3. *Let $k(x,y,z) = (x+z)\sqrt{x^2+z^2} - (y+z)\sqrt{y^2+z^2}$ with $x, y \geq 3$ and $1 \leq z \leq 2$. Then, the function $k(x,y,z)$ is strictly increasing in z if $x \geqslant y$ and strictly decreasing in z if $x \leqslant y$.*

Proof. Since

$$k_z(x,y,z) = \sqrt{x^2+z^2} + \frac{(x+z)z}{\sqrt{x^2+z^2}} - \sqrt{y^2+z^2} - \frac{(y+z)z}{\sqrt{y^2+z^2}} = \rho(z,x) - \rho(z,y),$$

the lemma holds. □

Lemma 3.4. *If $G \in T_n^k$ has the maximum elliptic Sombor index, then G contains at most one vertex with the degree greater than 2, where $k \geqslant 3$.*

Proof. Suppose to the contrary that there are at least two vertices u and v with the degree greater than 2 in G. Let $d(u) = x$ and $d(v) = y$, where $x \geqslant y \geqslant 3$.

Case 1. $d(u,v) = 1$.
Let $N(u) = \{u_1, u_2, \dots, u_{x-1}, v\}$, $N(v) = \{v_1, v_2, \dots, v_{y-1}, u\}$, $d(u_1) = a, d(v_1) = b$ and $a \geqslant b \geqslant 1$. In addition, we define

$G' = G - \{vv_k : v_k \in N(v)\backslash\{v_1\}\} + \{uv_k : v_k \in N(v)\backslash\{v_1\}\}$, see Figure 3.2. Then, $d_{G'}(u) = x + y - 2$ and $d_{G'}(v) = 2$. By Lemma 3.1 and Lemma 3.2, we have

$$\begin{aligned} ESO(G') - ESO(G) \geqslant & \Bigg((d_{G'}(u) + d_{G'}(v))\sqrt{d^2_{G'}(u) + d^2_{G'}(v)} + (d_{G'}(u) + d_{G'}(u_1))\sqrt{d^2_{G'}(u) + d^2_{G'}(u_1)} \\ & + (d_{G'}(v) + d_{G'}(v_1))\sqrt{d^2_{G'}(v) + d^2_{G'}(v_1)} \Bigg) - \Bigg((d(u) + d(v))\sqrt{d^2(u) + d^2(v)} \\ & + (d(u) + d(u_1))\sqrt{d^2(u) + d^2(u_1)} + (d(v) + d(v_1))\sqrt{d^2(v) + d^2(v_1)} \Bigg) \\ = & \Big((x + y - 2 + 2)\sqrt{(x + y - 2)^2 + 2^2} + (x + y - 2 + a)\sqrt{(x + y - 2)^2 + a^2} \\ & + (2 + b)\sqrt{2^2 + b^2} \Big) - \Big((x + y)\sqrt{x^2 + y^2} + (x + a)\sqrt{x^2 + a^2} + (y + b)\sqrt{y^2 + b^2} \Big) \\ \geqslant & \Big((x + y - 2 + a)\sqrt{(x + y - 2)^2 + a^2} - (x + a)\sqrt{x^2 + a^2} - (y + b)\sqrt{y^2 + b^2} \Big) \\ & + (2 + b)\sqrt{2^2 + b^2} \\ = & f(x, y) + (2 + b)\sqrt{2^2 + b^2} \geqslant f(3, 3) + (2 + b)\sqrt{2^2 + b^2} \\ = & \Big[(4 + a)\sqrt{16 + a^2} - (3 + a)\sqrt{9 + a^2} \Big] - \Big[(3 + b)\sqrt{9 + b^2} - (2 + b)\sqrt{2^2 + b^2} \Big] \\ = & h(3, a) - h(2, b) > h(2, a) - h(2, b) \geqslant 0, \end{aligned}$$

a contradiction to the choice of G.

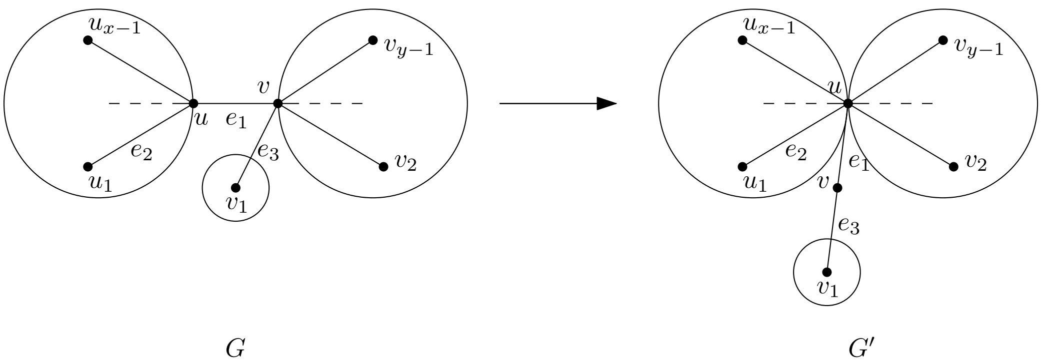

Figure 3.2: The transformation $G \to G' = G - \{vv_k : v_k \in N(v)\backslash\{v_1\}\} + \{uv_k : v_k \in N(v)\backslash\{v_1\}\}$.

Case 2. $d(u, v) \geqslant 2$.

By Case 1, $P = uu_x \ldots v_y v$ is an induced sub-path in G. Let $N(u) = \{u_1, u_2, \ldots, u_{x-1}, u_x\}$, $N(v) = \{v_1, v_2, \ldots, v_{y-1}, v_y\}$, $d(u_1) = a$, $d(v_1) = b$, and $d(v_2) = c$, then $1 \leqslant a, b, c \leqslant 2$. Let $G'' = G - \{vv_k : v_k \in N(v)\backslash\{v_1, v_y\}\} + \{uv_k : v_k \in N(v)\backslash\{v_1, v_y\}\}$, see Figure 3.3. Then, $d_{G''}(u) = x + y - 2$ and $d_{G''}(v) = 2$.

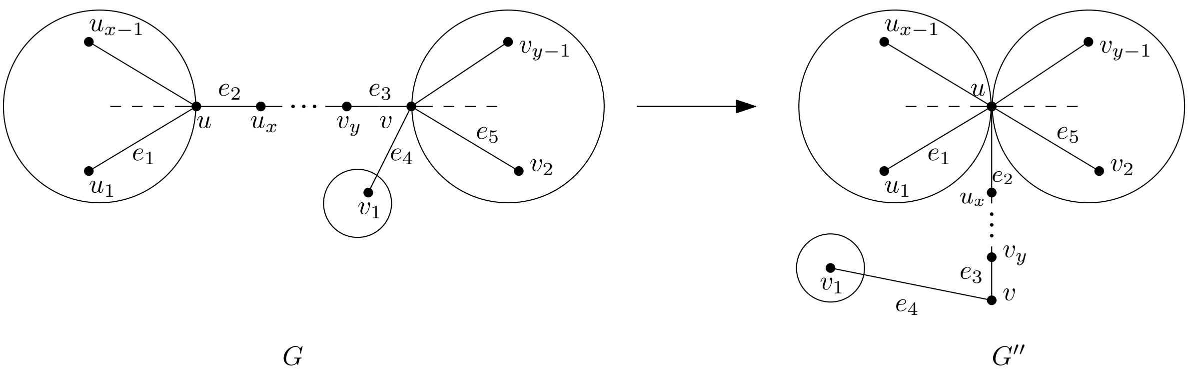

Figure 3.3: The transformation $G \to G'' = G - \{vv_k : v_k \in N(v)\backslash\{v_1, v_y\}\} + \{uv_k : v_k \in N(v)\backslash\{v_1, v_y\}\}$.

By Lemma 3.3, we have

$$
\begin{aligned}
ESO(G') - ESO(G) \geq & \Bigg((d_{G''}(u) + d_{G''}(u_1))\sqrt{d^2_{G''}(u) + d^2_{G''}(u_1)} + (d_{G''}(u) + d_{G''}(u_x))\sqrt{d^2_{G''}(u) + d^2_{G''}(u_x)} \\
& + (d_{G''}(v) + d_{G''}(v_y))\sqrt{d^2_{G''}(v) + d^2_{G''}(v_y)} + (d_{G''}(v) + d_{G''}(v_1))\sqrt{d^2_{G''}(v) + d^2_{G''}(v_1)} \\
& + (d_{G''}(u) + d_{G''}(v_2))\sqrt{d^2_{G''}(u) + d^2_{G''}(v_2)} \Bigg) \\
& - \Bigg((d(u) + d(u_1))\sqrt{d^2(u) + d^2(u_1)} + (d(u) + d(u_x))\sqrt{d^2(u) + d^2(u_x)} \\
& + (d(v) + d(v_y))\sqrt{d^2(v) + d^2(v_y)} + (d(v) + d(v_1))\sqrt{d^2(v) + d^2(v_1)} \\
& + (d(v) + d(v_2))\sqrt{d^2(v) + d^2(v_2)} \Bigg) \\
= & \Big((x+y-2+a)\sqrt{(x+y-2)^2 + a^2} + (x+y-2+2)\sqrt{(x+y-2)^2 + 2^2} \\
& + (2+2)\sqrt{2^2 + 2^2} + (2+b)\sqrt{2^2 + b^2} + (x+y-2+c)\sqrt{(x+y-2)^2 + c^2} \Big) \\
& - \Big((x+a)\sqrt{x^2 + a^2} + (x+2)\sqrt{x^2 + 2^2} + (y+2)\sqrt{y^2 + 2^2} + (y+b)\sqrt{y^2 + b^2} \\
& + (y+c)\sqrt{y^2 + c^2} \Big) \\
= & k(x+y-2, x, a) + k(2, y, b) + k(x+y-2, y, c) \\
& + (x+y)\sqrt{(x+y-2)^2 + 4} + 8\sqrt{2} - (x+2)\sqrt{x^2+4} - (y+2)\sqrt{y^2+4} \\
\geq & k(x+y-2, x, 1) + k(2, y, 2) + k(x+y-2, y, 1) \\
& + (x+y)\sqrt{(x+y-2)^2 + 4} + 8\sqrt{2} - (x+2)\sqrt{x^2+4} - (y+2)\sqrt{y^2+4} \\
= & \Big((x+y-1)\sqrt{(x+y-2)^2 + 1} - (x+1)\sqrt{x^2+1} \Big) + \Big(8\sqrt{2} - (y+2)\sqrt{y^2+4} \Big) \\
& + \Big((x+y-1)\sqrt{(x+y-2)^2 + 1} - (y+1)\sqrt{y^2+1} \Big) \\
& + (x+y)\sqrt{(x+y-2)^2 + 4} + 8\sqrt{2} - (x+2)\sqrt{x^2+4} - (y+2)\sqrt{y^2+4} \\
= & 2(x+y-1)\sqrt{(x+y-2)^2+1} + (x+y)\sqrt{(x+y-2)^2+4} - (x+1)\sqrt{x^2+1} \\
& - (x+2)\sqrt{x^2+4} - 2(y+2)\sqrt{y^2+4} - (y+1)\sqrt{y^2+1} + 16\sqrt{2}.
\end{aligned}
$$

It is easy to check that the function

$$2(x+y-1)\sqrt{(x+y-2)^2+1} + (x+y)\sqrt{(x+y-2)^2+4} - (x+1)\sqrt{x^2+1} - (x+2)\sqrt{x^2+4} - 2(y+2)\sqrt{y^2+4} - (y+1)\sqrt{y^2+1}$$

is strictly increasing in x and in y for $x, y \geqslant 3$. Hence, we have

$$ESO(G') - ESO(G) \geqslant 10\sqrt{17} + 12\sqrt{5} - 4\sqrt{10} - 15\sqrt{13} - 4\sqrt{10} + 16\sqrt{2} > 0,$$

a contradiction to the choice of G. □

Lemma 3.5. *Let $G = Spider(n_1, \ldots, n_i, \ldots, n_j, 1, \ldots, 1) \in T_n^k$ such that $n_i \geq 3$ and $n_j > 1$ $(1 \leq i \leq j)$, then*

$$ESO(Spider(n_1, \ldots, n_i, \ldots, n_j, 1, \ldots, 1)) < ESO(Spider(n_1, \ldots, n_i - 1, \ldots, n_j, 2, \ldots, 1)).$$

Proof. Let $v \in V(G)$ be the unique vertex with the maximum degree k. Let vu, uz and vw be three edges in G such that $d_G(u) = d_G(z) = 2$ and $d_G(w) = 1$. Take $N_0(v) = N(v) \backslash \{w, u\}$ and let $G' = G - \sum_{v_i \in N_0(v)} vv_i + \sum_{v_i \in N_0(v)} uv_i$, see Figure 3.4.

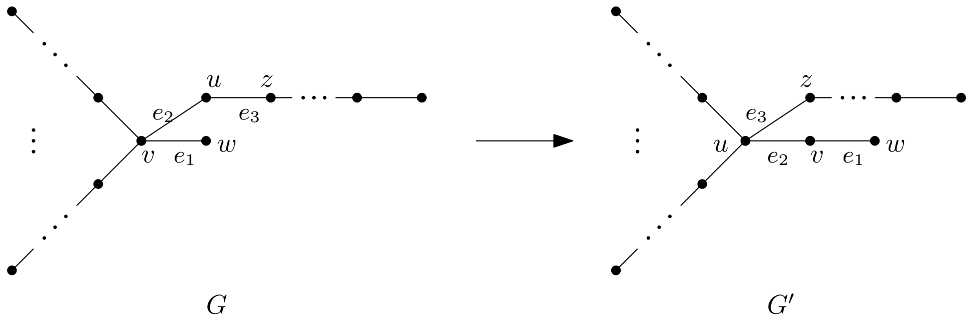

Figure 3.4: The transformation $G = Spider(n_1, \ldots, n_i, \ldots, n_j, 1, \ldots, 1) \to G' = Spider(n_1, \ldots, n_i - 1, \ldots, n_j, 2, \ldots, 1)$.

Note that $G' = Spider(n_1, \ldots, n_i - 1, \ldots, n_j, 2, \ldots, 1)$, $d_{G'}(v) = 2$ and $d_{G'}(u) = k$. By Lemma 3.2, we have

$$\begin{aligned} ESO(G') - ESO(G) &= (d_{G'}(v) + d_{G'}(w))\sqrt{d^2_{G'}(v) + d^2_{G'}(w)} + (d_{G'}(u) + d_{G'}(v))\sqrt{d^2_{G'}(u) + d^2_{G'}(v)} \\ &\quad - (d(v) + d(w))\sqrt{d^2(v) + d^2(w)} - (d(u) + d(z))\sqrt{d^2(u) + d^2(z)} \\ &= (k+2)\sqrt{k^2 + 2^2} - (k+1)\sqrt{k^2 + 1^2} + 3\sqrt{5} - 8\sqrt{2} \\ &= h(1,k) + 3\sqrt{5} - 8\sqrt{2} \\ &\geqslant 5\sqrt{13} - 4\sqrt{10} + 3\sqrt{5} - 8\sqrt{2} > 0, \end{aligned}$$

as desired $\square$

Lemma 3.6. *If $G = Spider(n_1, n_2, \ldots, n_k) \in T_n^k$ with $n_1 \geqslant n_2 \geqslant \cdots \geqslant n_k \geqslant 2$, and $G' = Spider(n'_1, n'_2, \ldots, n'_k) \in T_n^k$ with $n'_1 \geqslant n'_2 \geqslant \cdots \geqslant n'_k \geqslant 2$, then $ESO(G) = ESO(G')$.*

Proof. Note that

$$\begin{aligned} ESO(G) &= k(k+2)\sqrt{k^2 + 2^2} + k(1+2)\sqrt{1^2 + 2^2} + (n - 1 - 2k)(2+2)\sqrt{2^2 + 2^2} \\ &= k(k+2)\sqrt{k^2 + 4} + 3k\sqrt{6} + 8(n - 1 - 2k)\sqrt{2} = ESO(G'). \end{aligned}$$

$\square$

Theorem 3.1. *If $G \in T_n^k$ has the maximum elliptic Sombor index, then $G \cong Spider(n_1, n_2, \ldots, n_k)$, where $\sum_{i=1}^{k} n_i = n - 1$ and $n_1 \geqslant n_2 \geqslant \cdots \geqslant n_k \geqslant 1$. If $k \geqslant \lfloor n/2 \rfloor$ then $1 \leqslant n_i \leqslant 2$ and if $k < \lfloor n/2 \rfloor$ then $n_i \geqslant 2$.*

Proof. By Lemma 3.4, there is only one vertex with degree greater than 2 in G and hence $G \cong Spider(n_1, n_2, \ldots, n_k)$. If $k > \lfloor n/2 \rfloor$, then by Lemma 3.5 we have $1 \leqslant n_i \leqslant 2$ and hence there is only one graph with the maximum elliptic Sombor index. If $k < \lfloor n/2 \rfloor$, then by Lemma 3.5 we have $n_i \geqslant 2$ and hence by Lemma 3.6, the tree with the maximum elliptic Sombor index is not unique. If n is even and $k = n/2$, then by Lemma 3.5 the graph $Spider(2, 2, \ldots, 1, 1)$ is the tree with the maximum elliptic Sombor index and it satisfies $1 \leqslant n_i \leqslant 2$. Finally, if n is odd and $k = (n-1)/2$, then by Lemma 3.5 the graph $Spider(2, 2, \ldots, 2)$ is the unique tree with the maximum elliptic Sombor index. $\square$

Let C_n^d be the set of trees with n vertices and d diameter. Let $C(t_1, \ldots, t_{d-1})$ be the caterpillar illustrated in Figure 3.5. It is obvious that $C(t_1, \ldots, t_{d-1}) \in C_n^d$ if and only if $t_1 + t_2 + \cdots + t_{d-1} = n - d - 1$.

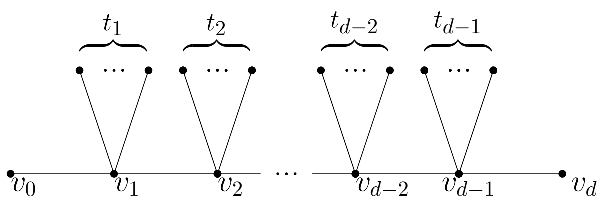

Figure 3.5: The caterpillar $C(t_1, \ldots, t_{d-1})$.

Lemma 3.7. *Let $d \geqslant 4$. If $G = C(t_1, \ldots, t_{d-1}) \in C_n^d$ has the maximum elliptic Sombor index, then $t_1 = 0$ and $t_{d-1} = 0$.*

Proof. Suppose to the contrary that $t_1 \neq 0$. Let i, $i \neq 1$, be the least integer such that $t_i \neq 0$ and the corresponding vertex is v_i.

Case 1. $d(v_1, v_i) = 1$.
In this case, we have $v_i = v_2$. For convenience, let $d(v_3) = y$. Certainly, $y \geqslant 2$. Define

$$G' = G - \{v_1 v_k : v_k \in N(v_1)\backslash\{v_0, v_2\}\} + \{v_2 v_k : v_k \in N(v_1)\backslash\{v_0, v_2\}\},$$

see Figure 3.6.

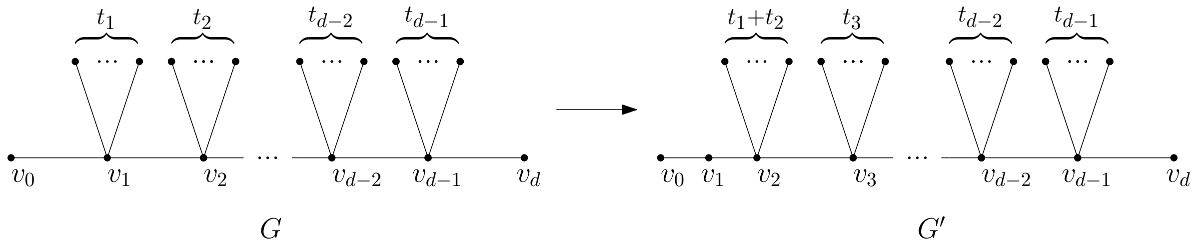

Figure 3.6: The transformation $G = C(t_1, t_2, \ldots, t_{d-1}) \to G' = C(0, t_2 + t_1, \ldots, t_{d-1})$.

Note that $G' = C(0, t_2 + t_1, \ldots, t_{d-1}) \in C_n^d$, $d_{G'}(v_1) = 2$, $d_{G'}(v_2) = t_2 + t_1 + 2$, and the degrees of other vertices remain the same. Thus, we have

$$\begin{aligned}
ESO(G') - ESO(G) &= \Bigg((d_{G'}(v_1) + d_{G'}(v_0))\sqrt{d^2_{G'}(v_1) + d^2_{G'}(v_0)} + (d_{G'}(v_2) + d_{G'}(v_1))\sqrt{d^2_{G'}(v_2) + d^2_{G'}(v_1)} \\
&\quad + (d_{G'}(v_2) + d_{G'}(v_3))\sqrt{d^2_{G'}(v_2) + d^2_{G'}(v_3)} + (t_2 + t_1)(d_{G'}(v_2) + 1)\sqrt{d^2_{G'}(v_2) + 1^2} \Bigg) \\
&\quad - \Bigg((d(v_1) + d(v_0))\sqrt{d^2(v_1) + d^2(v_0)} + (d(v_2) + d(v_1))\sqrt{d^2(v_2) + d^2(v_1)} \\
&\quad + (d(v_2) + d(v_3))\sqrt{d^2(v_2) + d^2(v_3)} + t_1(d(v_1) + 1)\sqrt{d^2(v_1) + 1^2} \\
&\quad + t_2(d(v_2) + 1)\sqrt{d^2(v_2) + 1^2} \Bigg) \\
&= \Bigg(3\sqrt{5} + (t_2 + t_1 + 4)\sqrt{(t_2 + t_1 + 2)^2 + 4} + (t_2 + t_1 + 2 + y)\sqrt{(t_2 + t_1 + 2)^2 + y^2} \\
&\quad + (t_2 + t_1)(t_2 + t_1 + 3)\sqrt{(t_2 + t_1 + 2)^2 + 1} \Bigg) - \Bigg((t_1 + 3)\sqrt{(t_1 + 2)^2 + 1} \\
&\quad + (t_1 + t_2 + 4)\sqrt{(t_1 + 2)^2 + (t_2 + 2)^2} + (t_2 + 2 + y)\sqrt{(t_2 + 2)^2 + y^2} \\
&\quad + t_1(t_1 + 3)\sqrt{(t_1 + 2)^2 + 1} + t_2(t_2 + 3)\sqrt{(t_2 + 2)^2 + 1} \Bigg) \\
&\geqslant 3\sqrt{5} + t_1\sqrt{(t_2 + t_1 + 2)^2 + y^2} + 2t_1 t_2\sqrt{(t_2 + t_1 + 2)^2 + 1} - (t_1 + 3)\sqrt{(t_1 + 2)^2 + 1} \\
&\geqslant 3\sqrt{5} + 2t_1 t_2\sqrt{(t_2 + t_1 + 2)^2 + 1} - 3\sqrt{(t_1 + 2)^2 + 1}.
\end{aligned}$$

It is easy to check that the function $2t_1 t_2\sqrt{(t_2 + t_1 + 2)^2 + 1} - 3\sqrt{(t_1 + 2)^2 + 1}$ is strictly increasing for $t_1, t_2 \geqslant 1$ in t_1 and in t_2. Hence, we have $ESO(G') - ESO(G) \geqslant 3\sqrt{5} + 2\sqrt{17} - 3\sqrt{10} > 0$, a contradiction to the choice of G.

Case 2. $d(v_1, v_i) \geqslant 2$.
In the present case, we have $d(v_j) = 2$ with $2 \leqslant j \leqslant i - 1$. For convenience, let $d(v_{i+1}) = y$. Evidently, $y \geqslant 2$. Now, we take $G' = G - \{v_1 v_k : v_k \in N(v_1)\backslash\{v_0, v_2\}\} + \{v_i v_k : v_k \in N(v_1)\backslash\{v_0, v_2\}\}$, see Figure 3.7.

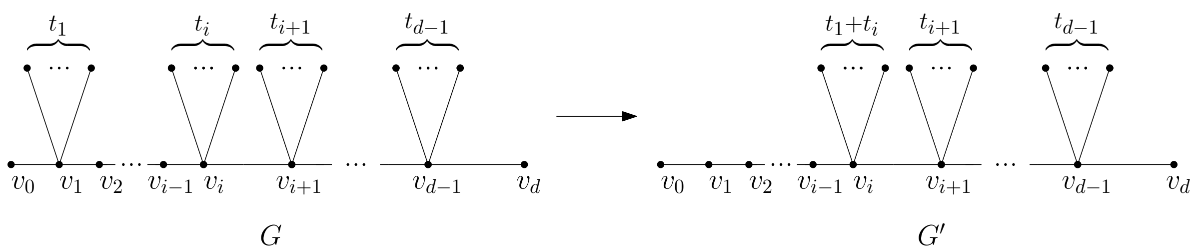

Figure 3.7: The transformation $G = C(t_1, 0, \ldots, 0, t_i, \ldots, t_{d-1}) \to G' = C(0, \ldots, 0, t_i + t_1, \ldots, t_{d-1})$.

Note that $G' = C(0,\dots,0,t_i+t_1,\dots,t_{d-1}) \in C_n^d$, $d_{G'}(v_1) = 2$, $d_{G'}(v_i) = t_i + t_1 + 2$, and degrees of other vertices remain the same. Hence, we have

$$
\begin{aligned}
ESO(G') - ESO(G) = \Big(& (d_{G'}(v_1)+d_{G'}(v_0))\sqrt{d_{G'}^2(v_1)+d_{G'}^2(v_0)} + (d_{G'}(v_2)+d_{G'}(v_1))\sqrt{d_{G'}^2(v_2)+d_{G'}^2(v_1)} \\
& + (d_{G'}(v_i)+d_{G'}(v_{i-1}))\sqrt{d_{G'}^2(v_i)+d_{G'}^2(v_{i-1})} + (d_{G'}(v_i)+d_{G'}(v_{i+1}))\sqrt{d_{G'}^2(v_i)+d_{G'}^2(v_{i+1})} \\
& + (t_i+t_1)(d_{G'}(v_i)+1)\sqrt{d_{G'}^2(v_i)+1^2} \Big) - \Big((d(v_1)+d(v_0))\sqrt{d^2(v_1)+d^2(v_0)} \\
& + (d(v_2)+d(v_1))\sqrt{d^2(v_2)+d^2(v_1)} + (d(v_i)+d(v_{i-1}))\sqrt{d^2(v_i)+d^2(v_{i-1})} \\
& + (d(v_i)+d(v_{i+1}))\sqrt{d^2(v_i)+d^2(v_{i+1})} + t_1(d(v_1)+1)\sqrt{d^2(v_1)+1^2} \\
& + t_i(d(v_i)+1)\sqrt{d^2(v_i)+1^2} \Big) \\
= \Big(& 3\sqrt{5} + 8\sqrt{2} + (t_i+t_1+4)\sqrt{(t_i+t_1+2)^2+4} + (t_i+t_1+2+y)\sqrt{(t_i+t_1+2)^2+y^2} \\
& + (t_i+t_1)(t_i+t_1+3)\sqrt{(t_i+t_1+2)^2+1} \Big) - \Big((t_1+3)\sqrt{(t_1+2)^2+1} \\
& + (t_1+4)\sqrt{(t_1+2)^2+4} + (t_i+4)\sqrt{(t_i+2)^2+4} + (t_i+2+y)\sqrt{(t_i+2)^2+y^2} \\
& + t_1(t_1+3)\sqrt{(t_1+2)^2+1} + t_i(t_i+3)\sqrt{(t_i+2)^2+1} \Big) \\
\geqslant & \, 3\sqrt{5} + 8\sqrt{2} + t_1\sqrt{(t_i+t_1+2)^2+y^2} + 2t_it_1\sqrt{(t_i+t_1+2)^2+1} - 2\sqrt{(t_1+2)^2+4} \\
& - 2\sqrt{(t_i+2)^2+4} - (t_1+3)\sqrt{(t_1+2)^2+1} \\
\geqslant & \, 3\sqrt{5} + 8\sqrt{2} + 2t_it_1\sqrt{(t_i+t_1+2)^2+1} - 2\sqrt{(t_1+2)^2+4} - 2\sqrt{(t_i+2)^2+4} - 3\sqrt{(t_1+2)^2+1}.
\end{aligned}
$$

It is easy to check that the function $2t_it_1\sqrt{(t_i+t_1+2)^2+1} - 2\sqrt{(t_1+2)^2+4} - 2\sqrt{(t_i+2)^2+4} - 3\sqrt{(t_1+2)^2+1}$ is strictly increasing for $t_1, t_i \geqslant 1$ and hence we have

$$ESO(G') - ESO(G) \geqslant 3\sqrt{5} + 8\sqrt{2} + 2\sqrt{17} - 2\sqrt{13} - 2\sqrt{13} - 3\sqrt{10} > 0,$$

a contradiction to the choice of G. □

Lemma 3.8. *Let $d \geqslant 4$. If $G = C(t_2,\dots,t_{d-2}) \in C_n^d$ has the maximum elliptic Sombor index, then there is only one $t_i \neq 0$.*

Proof. Suppose to the contrary that there are $t_i, t_j \neq 0$. Let i, $i \geqslant 2$, be the least integer such that $t_i \neq 0$ and suppose that the corresponding vertex is v_i. Then, we have $d(v_{i-1}) = 2$. Similarly, take j, $i+1 \leqslant j \leqslant d-2$, such that $t_j \neq 0$ and suppose that the corresponding vertex is v_j.

Case 1. $d(v_i, v_j) = 1$.
Here, we have $v_j = v_{i+1}$. For convenience, let $d(v_{i+2}) = y \geqslant 2$, and define

$$G' = G - \{v_iv_k : v_k \in N(v_i)\backslash\{v_{i-1}, v_{i+1}\}\} + \{v_{i+1}v_k : v_k \in N(v_i)\backslash\{v_{i-1}, v_{i+1}\}\},$$

see Figure 3.8.

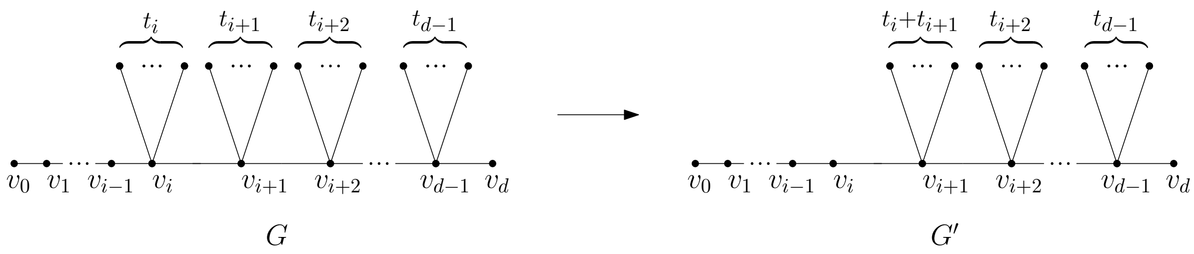

Figure 3.8: The transformation $G = C(0,\dots,0,t_i,t_{i+1},\dots,t_{d-1}) \to G' = C(0,\dots,0,t_{i+1}+t_i,\dots,t_{d-1})$.

Note that $G' = C(0, \ldots, 0, t_{i+1}+t_i, \ldots, t_{d-1}) \in C_n^d$, $d_{G'}(v_i) = 2$, $d_{G'}(v_{i+1}) = t_{i+1}+t_i+2$, and degrees of other vertices remain the same. Thus, we have

$$\begin{aligned}
ESO(G') - ESO(G) = &\Big((d_{G'}(v_i) + d_{G'}(v_{i-1}))\sqrt{d_{G'}^2(v_i) + d_{G'}^2(v_{i-1})} + (d_{G'}(v_i) + d_{G'}(v_{i+1}))\sqrt{d_{G'}^2(v_i) + d_{G'}^2(v_{i+1})} \\
&+ (d_{G'}(v_{i+1}) + d_{G'}(v_{i+2}))\sqrt{d_{G'}^2(v_{i+1}) + d_{G'}^2(v_{i+2})} \\
&+ (t_i + t_{i+1})(d_{G'}(v_{i+1}) + 1)\sqrt{d_{G'}^2(v_{i+1}) + 1^2} \Big) - \Big((d(v_i) + d(v_{i-1}))\sqrt{d^2(v_i) + d^2(v_{i-1})} \\
&+ (d(v_i) + d(v_{i+1}))\sqrt{d^2(v_i) + d^2(v_{i+1})} + (d(v_{i+1}) + d(v_{i+2})\sqrt{d^2(v_{i+1}) + d^2(v_{i+2})} \\
&+ t_i(d(v_i) + 1)\sqrt{d^2(v_i) + 1^2} + t_{i+1}(d(v_{i+1}) + 1)\sqrt{d^2(v_{i+1}) + 1^2} \Big) \\
= &\Big(8\sqrt{2} + (t_i + t_{i+1} + 4)\sqrt{(t_{i+1} + t_i + 2)^2 + 4} + (t_{i+1} + t_i + 2 + y)\sqrt{(t_{i+1} + t_i + 2)^2 + y^2} \\
&+ (t_{i+1} + t_i)(t_{i+1} + t_i + 3)\sqrt{(t_{i+1} + t_i + 2)^2 + 1} \Big) - \Big((t_i + 4)\sqrt{(t_i + 2)^2 + 4} \\
&+ (t_{i+1} + t_i + 4)\sqrt{(t_{i+1} + 2)^2 + (t_i + 2)^2} + (t_{i+1} + 2 + y)\sqrt{(t_{i+1} + 2)^2 + y^2} \\
&+ t_i(t_i + 3)\sqrt{(t_i + 2)^2 + 1} + t_{i+1}(t_{i+1} + 3)\sqrt{(t_{i+1} + 2)^2 + 1} \Big) \\
\geqslant &\, 8\sqrt{2} + t_i\sqrt{(t_{i+1} + t_i + 2)^2 + y^2} + 2t_{i+1}t_i\sqrt{(t_{i+1} + t_i + 2)^2 + 1} - (t_i + 4)\sqrt{(t_i + 2)^2 + 4} \\
\geqslant &\, 8\sqrt{2} + 2t_{i+1}t_i\sqrt{(t_{i+1} + t_i + 2)^2 + 1} - 4\sqrt{(t_i + 2)^2 + 4}.
\end{aligned}$$

It is easy to check that the function $2t_{i+1}t_i\sqrt{(t_{i+1} + t_i + 2)^2 + 1} - 4\sqrt{(t_i + 2)^2 + 4}$ is strictly increasing for $t_{i+1}, t_i \geqslant 1$ and hence we have $ESO(G') - ESO(G) \geqslant 8\sqrt{4} + 2\sqrt{17} - 4\sqrt{13} > 0$, a contradiction of the choice of G.

Case 2. $d(v_1, v_i) \geqslant 2$.
In this case, we have $d(v_k) = 2$ with $i + 1 \leqslant k \leqslant j - 1$. For convenience, let $d(v_{j+1}) = y$. Define

$$G' = G - \{v_iv_k : v_k \in N(v_i)\backslash\{v_{i-1}, v_{i+1}\}\} + \{v_jv_k : v_k \in N(v_i)\backslash\{v_{i-1}, v_{i+1}\}\},$$

see Figure 3.9.

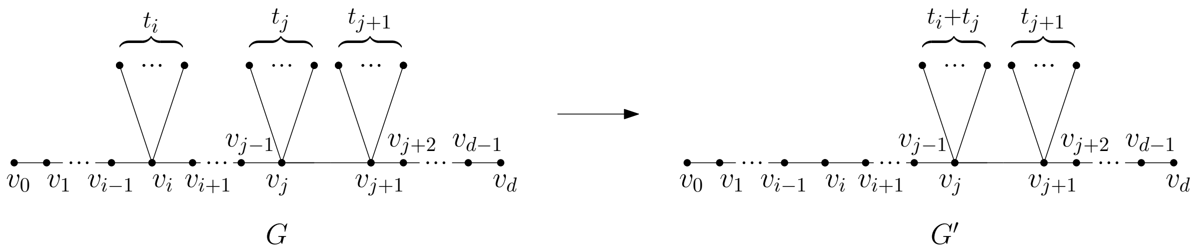

Figure 3.9: The transformation $G = C(0, \ldots, 0, t_i, 0, \ldots, 0, t_j, \ldots, t_{d-1}) \to G' = C(0, \ldots, 0, t_j + t_i, \ldots, t_{d-1})$.

Note that $G' = C(0, \ldots, 0, t_j + t_i, \ldots, t_{d-1}) \in C_n^d$, $d_{G'}(v_i) = 2$, $d_{G'}(v_j) = t_i + t_j + 2$, and degrees of other vertices remain the same. Thus, we have

$$\begin{aligned}
ESO(G') - ESO(G) = &\Big((d_{G'}(v_i) + d_{G'}(v_{i-1}))\sqrt{d_{G'}^2(v_i) + d_{G'}^2(v_{i-1})} + (d_{G'}(v_i) + d_{G'}(v_{i+1}))\sqrt{d_{G'}^2(v_i) + d_{G'}^2(v_{i+1})} \\
&+ (d_{G'}(v_j) + d_{G'}(v_{j-1}))\sqrt{d_{G'}^2(v_j) + d_{G'}^2(v_{j-1})} + (d_{G'}(v_j) + d_{G'}(v_{j+1}))\sqrt{d_{G'}^2(v_j) + d_{G'}^2(v_{j+1})} \\
&+ (t_i + t_j)(d_{G'}(v_j) + 1)\sqrt{d_{G'}^2(v_j) + 1^2} \Big) - \Big((d(v_i) + d(v_{i-1}))\sqrt{d^2(v_i) + d^2(v_{i-1})} \\
&+ (d(v_i) + d(v_{i+1}))\sqrt{d^2(v_i) + d^2(v_{i+1})} + (d(v_j) + d(v_{j-1}))\sqrt{d^2(v_j) + d^2(v_{j-1})} \\
&+ (d(v_j) + d(v_{j+1}))\sqrt{d^2(v_j) + d^2(v_{j+1})} + t_i(d(v_i) + 1)\sqrt{d^2(v_i) + 1^2} \\
&+ t_j(d(v_j) + 1)\sqrt{d^2(v_j) + 1^2} \Big).
\end{aligned}$$

Consequently, we have

$$\begin{aligned}ESO(G')-ESO(G)=&\Big(8\sqrt{2}+8\sqrt{2}+(t_i+t_j+4)\sqrt{(t_i+t_j+2)^2+4}+(t_i+t_j+2+y)\sqrt{(t_i+t_j+2)^2+y^2}\\&+(t_i+t_j)(t_i+t_j+3)\sqrt{(t_i+t_j+2)^2+1}\Big)-\Big((t_i+4)\sqrt{(t_i+2)^2+4}\\&+(t_i+4)\sqrt{(t_i+2)^2+4}+(t_j+4)\sqrt{(t_j+2)^2+4}+(t_j+2+y)\sqrt{(t_j+2)^2+y^2}\\&+t_i(t_i+3)\sqrt{(t_i+2)^2+1}+t_j(t_j+3)\sqrt{(t_j+2)^2+1}\Big)\\&\geqslant 16\sqrt{2}+t_i\sqrt{(t_i+t_j+2)^2+y^2}+2t_it_j\sqrt{(t_i+t_j+2)^2+1}-(t_i+8)\sqrt{(t_i+2)^2+4}\\&\geqslant 16\sqrt{2}+2t_it_j\sqrt{(t_i+t_j+2)^2+1}-8\sqrt{(t_i+2)^2+4}.\end{aligned}$$

Note that the function $2t_it_j\sqrt{(t_i+t_j+2)^2+1}-8\sqrt{(t_i+2)^2+4}$ is strictly increasing for $t_i,t_j\geqslant 1$ and hence

$$ESO(G')-ESO(G)\geqslant 16\sqrt{2}+2\sqrt{17}-8\sqrt{13}>0,$$

which is a contradiction of the choice of G. □

Consider the set C_n^d. If $d=2$ then the tree with the maximum elliptic Sombor index is S_n and if $d=3$ then by Theorem 3.1, the tree with the maximum elliptic Sombor index is $Spider(2,1,\ldots,1)$. In the following, we consider $d\geqslant 4$.

Theorem 3.2. *Let $d\geqslant 4$. If $G\in C_n^d$ has the maximum elliptic Sombor index then $G\cong C(0,..0,t_i,0,\ldots,0)$, $t_i=n-d-1$, $2\leqslant i\leqslant d-2$, and*

$$ESO(G)=(n-d-1)(n-d+2)\sqrt{(n-d+1)^2+1}+2(n-d+3)\sqrt{(n-d+1)^2+4}+8(d-4)\sqrt{2}+6\sqrt{5}.$$

Proof. Let $G\in C_n^d$ be the graph with the maximum elliptic Sombor index. By Lemma 2.3 (the edge-lifting transformation), we have $G\in C(t_1,t_2,\ldots,t_d)$. By Lemma 3.7 and Lemma 3.8, we have $G\cong C(0,..0,t_i,0,\ldots,0)$, where $t_i=n-d-1$ and $2\leqslant i\leqslant d-2$. □

Let $\mathfrak{T}_{n,\beta}$ be the set of trees with order n and matching number β. Let T_n^β be the tree obtained from the star $S_{n-\beta+1}$ by subdividing its $\beta-1$ pendent edges. It is obvious that $T_n^\beta\in\mathfrak{T}_n^\beta$ and it has a perfect matching for $n=2\beta$. The trees T_n^β and $T_{2\beta}^\beta$ are illustrated in Figure 3.10. Firstly we give some useful lemmas which will be used in next.

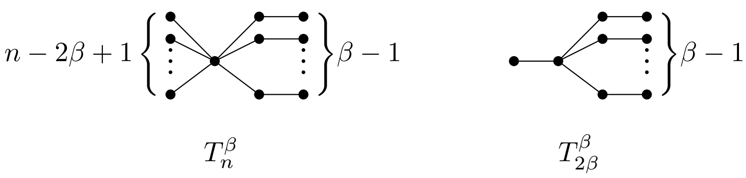

Figure 3.10: The trees T_n^β and $T_{2\beta}^\beta$ with order n and matching number β; in the second tree, $n=2\beta$.

In the following, we discuss extremal values of the elliptic Sombor index of trees with a given matching number.

Lemma 3.9 (see [1, 4]). *(i). If $T\in\mathfrak{T}_{2\beta,\beta}$ and $\beta\geq 2$, then T contains a pendent vertex whose unique neighbor has degree 2.*
(ii). If $T\in\mathfrak{T}_{n,\beta}$ and $n>2\beta$, then there is a β-matching M and a pendent vertex v such that M does not saturate v.

Lemma 3.10. *Let $T\in\mathfrak{T}_{n,\beta}$ be a tree with the maximum elliptic Sombor index and M be a β-matching of T.*
(i). If $e=uv\in M$, then e is a pendent edge of T.
(ii). If v is not a pendent vertex of T, then v is M-saturated.
(iii). The tree T contains at most one vertex of degree greater than 2.

Proof. (i). Suppose to the contrary that $e=uv\in M$ but it is not a pendent edge of T. Let

$$T'=T-\{uw:w\in N_T(u)\backslash\{v\}\}+\{vw:w\in N_T(u)\backslash\{v\}\}.$$

It is clear that $T'\in\mathfrak{T}_{n,\beta}$. By Lemma 2.3, we have $ESO(T')>ESO(T)$, a contradiction to the choice of T.

(ii). If $T \cong S_n$, then the result follows immediately. If $T \ncong S_n$ and if the vertex v is not a pendent vertex in T, then there is a vertex $u \in N_T(v)$ such that u is not a pendent vertex. Since v is not M-saturated, we have $uv \notin M$. Let $T'' = T - \{uw : w \in N_T(u)\backslash\{v\}\} + \{vw : w \in N_T(u)\backslash\{v\}\}$. Note that $T'' \in \mathfrak{T}_{n,\beta}$. By Lemma 2.3, we have $ESO(T'') > ESO(T)$, a contradiction to the choice of T.

(iii). Suppose to the contrary that there are at least two vertices of degree greater than 2 in T. By (i) and (ii), there must be an edge uv such that each of the two vertices u, v, has a degree greater than 2 and is adjacent to a pendent vertex in T (see Figure 3.11).

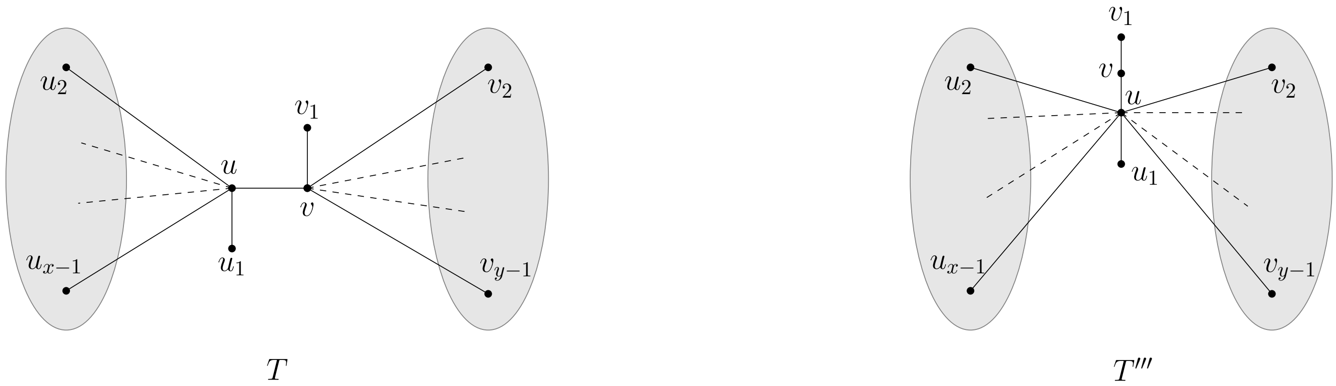

Figure 3.11: The transformation used in part (iii) of Lemma 3.10.

Let $N_T(u) = \{u_1, u_2, \ldots, u_{x-1}, v\}(x \geq 3)$, $N_T(v) = \{v_1, v_2, \ldots, v_{y-1}, u\}(y \geq 3)$ and $d_T(u_1) = d_T(v_1) = 1$. Let

$$T''' = T - \{vv_i \mid i = 2, \ldots, y-1\} + \{uv_i \mid i = 2, \ldots, y-1\},$$

see Figure 3.11. Note that $T''' \in \mathfrak{T}_{n,\beta}$. Also, we have $d_T(u) = x$, $d_T(v) = y$, $d_{T'''}(u) = x+y-2$, $d_{T'''}(v) = 2$, and degrees of other vertices are not changed.

Let $\psi(x,y) = (1+x)\sqrt{1+x^2} + (1+y)\sqrt{1+y^2} - (x+y-1)\sqrt{(x+y-2)^2+1} - 3\sqrt{5}$ for $x, y \geq 3$. Since $x+y-2 > x$, by Lemma 2.2 we have

$$\begin{aligned}\frac{\partial\psi(x,y)}{\partial x} &= \sqrt{1+x^2} + \frac{x(1+x)}{\sqrt{1+x^2}} - \sqrt{1+(x+y-2)^2} - \frac{(x+y-1)(x+y-2)}{\sqrt{1+(x+y-2)^2}} \\ &= \rho(x,1) - \rho(x+y-2,1) < 0\end{aligned}$$

and

$$\frac{\partial\psi(x,y)}{\partial y} = \sqrt{1+y^2} + \frac{y(1+y)}{\sqrt{1+x^2}} - \sqrt{1+(x+y-1)^2} - \frac{(x+y-1)(x+y-2)}{\sqrt{1+(x+y-2)^2}} < 0.$$

Hence, the function $\psi(x,y)$ is strictly decreasing in x and in y. Since $(x+y-2)^2 + 4 - (x^2 - y^2) = 2xy - 4(x+y) + 8 > 0$, we have

$$\begin{aligned}ESO(T) - ESO(T'') &< (x+y)\sqrt{x^2+y^2} + (1+x)\sqrt{1+x^2} + (1+y)\sqrt{1+y^2} - 3\sqrt{5} \\ &\quad - (x+y-1)\sqrt{(x+y-2)^2+1} - (x+y)\sqrt{(x+y-2)^2+4} \\ &< \psi(x,y) \leq \psi(3,3) < 0,\end{aligned}$$

a contradiction to the choice of T. □

Theorem 3.3. *If $T \in \mathfrak{T}_{2\beta,\beta}$, then*

$$6\sqrt{5} + 8(2\beta-3)\sqrt{2} \leq ESO(T) \leq (\beta+1)\sqrt{1+\beta^2} + (\beta-1)\Big((\beta+2)\sqrt{4+\beta^2} + 3\sqrt{5}\Big),$$

where the left equality holds if and only if $T \cong P_{2\beta}$, while the right equality holds if and only if $T \cong T_{2\beta}^{\beta}$ (see Figure 3.10).

Proof. Since $P_{2\beta} \in \mathfrak{T}_{2\beta,\beta}$, by Theorem 2.1 we have $ESO(T) \geq 6\sqrt{5} + 8(2\beta-3)\sqrt{2}$ with equality if and only if $T \cong P_{2\beta}$. If $T \in \mathfrak{T}_{2\beta,\beta}$ has the maximum elliptic Sombor index, then by Lemma 3.10 we have

$$ESO(T) \leq (\beta+1)\sqrt{1+\beta^2} + (\beta-1)\Big((\beta+2)\sqrt{4+\beta^2} + 3\sqrt{5}\Big)$$

with equality if and only if $T \cong T_{2\beta}^{\beta}$. □

By using Lemma 3.10, we also obtain the following result directly.

Theorem 3.4. *Let* $T \in \mathfrak{T}_{n,\beta}(n > 2\beta)$*, then*

$$ESO(T) \leq (n-2\beta+1)(n-\beta+1)\sqrt{1+(n-\beta)^2} + (\beta-1)\Big((n-\beta+2)\sqrt{4+(n-\beta)^2} + 3\sqrt{5}\Big)$$

with equality if and only if $T \cong T_n^{\beta}$ *(see Figure 3.10).*

4. Elliptic Sombor index of unicyclic graphs

In this section, we determine the extremal values of the elliptic Sombor index of unicyclic graphs with order n. Let U_n be the set of unicyclic graphs with n vertices. Let $U_n(t_1, t_2, \ldots, t_k) \in U_n$ be a unicyclic graph with circuit $C_k = v_1v_2\cdots v_kv_1$ such that every component of $G - E(C_k)$ is a star and the component containing v_i has $t_i + 1$ vertices, where $i = 1, 2, \cdots, k$ and $t_1 + t_2 + \cdots + t_k = n - k$.

Lemma 4.1. *Let* $G = U_n(p, q, r)$ *with* $p \geqslant q \geqslant r \geqslant 1$ *and* $p + q + r = n - 3$*. Let* $u, v, w \in V(G)$ *with* $N(u) = \{v, w, u_1, \ldots, u_p\}$, $N(v) = \{u, w, v_1, \ldots, v_q\}$*, and* $N(w) = \{v, u, w_1, \ldots, w_r\}$*. If* $G' = G - \{ww_i : w_i \in N(w)\backslash\{u, v\}\} + \{uw_i : w_i \in N(w)\backslash\{u, v\}\}$*, see Figure 4.1, then* $ESO(G') > ESO(G)$*.*

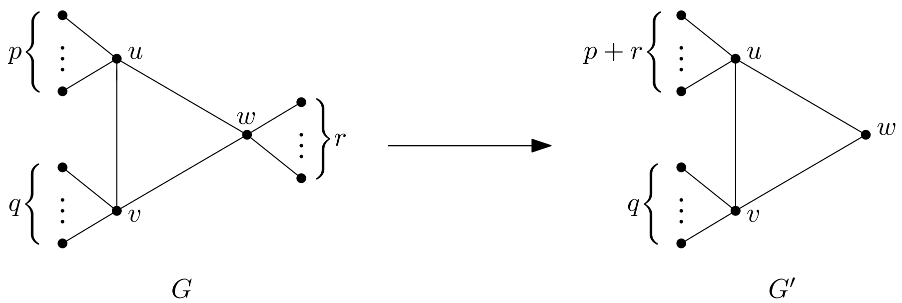

Figure 4.1: The transformation used in Lemma 4.1.

Proof. Note that $d_{G'}(u) = p + r + 2$, $d_{G'}(w) = 2$, and degrees of other vertices remain the same. Hence, we have

$$\begin{aligned}
ESO(G') - ESO(G) = &\Big((d_{G'}(u) + d_{G'}(w))\sqrt{d^2_{G'}(u) + d^2_{G'}(w)} + (d_{G'}(w) + d_{G'}(v))\sqrt{d^2_{G'}(w) + d^2_{G'}(v)} \\
&+ (d_{G'}(u) + d_{G'}(v))\sqrt{d^2_{G'}(u) + d^2_{G'}(v)} + (p+r)(d_{G'}(u) + 1)\sqrt{d^2_{G'}(u) + 1^2} \\
&+ q(d_{G'}(v) + 1)\sqrt{d^2_{G'}(v) + 1^2}\Big) - \Big((d(u) + d(w))\sqrt{d^2(u) + d^2(w)} \\
&+ (d(w) + d(v))\sqrt{d^2(w) + d^2(v)} + (d(u) + d(v))\sqrt{d^2(u) + d^2(v)} \\
&+ p(d(u) + 1)\sqrt{d^2(u) + 1^2} + r(d(w) + 1)\sqrt{d^2(w) + 1^2} + q(d(v) + 1)\sqrt{d^2(v) + 1^2}\Big) \\
= &\Big((p+r+4)\sqrt{(p+r+2)^2 + 4} + (q+4)\sqrt{(q+2)^2 + 4} \\
&+ (p+q+r+4)\sqrt{(p+r+2)^2 + (q+2)^2} + (p+r)(p+r+3)\sqrt{(p+r+2)^2 + 1} \\
&+ q(q+3)\sqrt{(q+2)^2 + 1}\Big) - \Big((p+r+4)\sqrt{(p+2)^2 + (r+2)^2} \\
&+ (q+r+4)\sqrt{(q+2)^2 + (r+2)^2} + (p+q+4)\sqrt{(p+2)^2 + (q+2)^2} \\
&+ p(p+3)\sqrt{(p+2)^2 + 1} + r(r+3)\sqrt{(r+2)^2 + 1} + q(q+3)\sqrt{(q+2)^2 + 1}\Big) \\
> &\, r\sqrt{(p+r+2)^2 + (q+2)^2} + 2pr\sqrt{(p+r+2)^2 + 1} \\
&+ (q+4)\sqrt{(q+2)^2 + 4} - (q+r+4)\sqrt{(q+2)^2 + (r+2)^2} \\
\geqslant &\, 2pr\sqrt{(p+r+2)^2 + 1} + (q+4)\sqrt{(q+2)^2 + 4} - (q+4)\sqrt{(q+2)^2 + (r+2)^2}.
\end{aligned}$$

Note that the function $2pr\sqrt{(p+r+2)^2+1}+(q+4)\sqrt{(q+2)^2+4}-(q+4)\sqrt{(q+2)^2+(r+2)^2}$ is strictly increasing in $r \geqslant 0$ and hence it attains the minimum at $r=0$. Therefore,

$$ESO(G')-ESO(G)>(q+4)\sqrt{(q+2)^2+4}-(q+4)\sqrt{(q+2)^2+4}=0,$$

as desired. □

Lemma 4.2. *Let $G=U_n(p,q,0)$ with $p \geqslant q \geqslant 1$ and $p+q=n-3$. Let $u,v,w \in V(G)$ with $N(u)=\{v,w,u_1,\ldots,u_p\}$, $N(v)=\{u,w,v_1,\ldots,v_q\}$, and $N(w)=\{v,u\}$. If $G'=G-\{vv_i : v_i \in N(v)\backslash\{u,w\}\}+\{uv_i : v_i \in N(v)\backslash\{u,w\}\}$, see Figure 4.2, then $ESO(G')>ESO(G)$.*

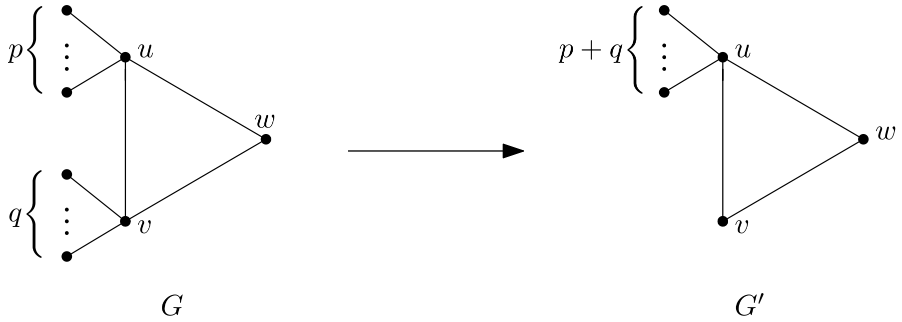

Figure 4.2: The transformation used in Lemma 4.2.

Proof. We note that $d_{G'}(u)=p+q+2$, $d_{G'}(v)=2$, and degrees of other vertices remain the same. Hence, we have

$$\begin{aligned}
ESO(G')-ESO(G)=&\Big((d_{G'}(u)+d_{G'}(v))\sqrt{d^2_{G'}(u)+d^2_{G'}(v)}+(d_{G'}(u)+d_{G'}(w))\sqrt{d^2_{G'}(u)+d^2_{G'}(w)}\\
&+(d_{G'}(v)+d_{G'}(w))\sqrt{d^2_{G'}(v)+d^2_{G'}(w)}+(p+q)(d_{G'}(u)+1)\sqrt{d^2_{G'}(u)+1^2}\Big)\\
&-\Big((d(u)+d(v))\sqrt{d^2(u)+d^2(v)}+(d(u)+d(w))\sqrt{d^2(u)+d^2(w)}\\
&+(d(v)+d(w))\sqrt{d^2(v)+d^2(w)}+p(d(u)+1)\sqrt{d^2(u)+1^2}+q(d(v)+1)\sqrt{d^2(v)+1^2}\Big)\\
=&\Big(2(p+q+4)\sqrt{(p+q+2)^2+4}+8\sqrt{2}+(p+q)(p+q+3)\sqrt{(p+q+2)^2+1}\Big)\\
&-\Big((p+q+4)\sqrt{(p+2)^2+(q+2)^2}+(p+4)\sqrt{(p+2)^2+4}+(q+4)\sqrt{(q+2)^2+4}\\
&+p(p+3)\sqrt{(p+2)^2+1}+q(q+3)\sqrt{(q+2)^2+1}\Big)\\
\geqslant&\,2pq\sqrt{(p+q+2)^2+1}+8\sqrt{2}-2\sqrt{(p+2)^2+4}-2\sqrt{(q+2)^2+4}.
\end{aligned}$$

Note that the function $2pq\sqrt{(p+q+2)^2+1}-2\sqrt{(p+2)^2+4}-2\sqrt{(q+2)^2+4}$ is strictly increasing for $q \geqslant 1$ and attains its minimum at $q=1$. Hence,

$$ESO(G')-ESO(G)\geqslant 2p\sqrt{(p+3)^2+1}+8\sqrt{2}-2\sqrt{(p+2)^2+4}-2\sqrt{13}.$$

The function $2p\sqrt{(p+3)^2+1}-2\sqrt{(p+2)^2+4}$ is strictly increasing for $p \geqslant 1$ and attains its minimum at $p=1$. Therefore,

$$ESO(G')-ESO(G)\geqslant 2\sqrt{17}+8\sqrt{2}-2\sqrt{13}-2\sqrt{13}>0,$$

as desired. □

Theorem 4.1. *If $G \in U_n$ is a unicyclic graph with the maximum elliptic Sombor index, then $G \cong U_n(n-3,0,0)$ and*

$$ESO(G)=2(n-1)\sqrt{(n-1)^2+4}+n(n-3)\sqrt{(n-1)^2+1}+8\sqrt{2}.$$

Proof. By Lemma 2.3 (edge-lifting transformation), G is of the form $U_n(p,q,r)$, with $p \geqslant q \geqslant r \geqslant 0$ and $p+q+r=n-3$. By Lemma 4.1 and Lemma 4.2, $ESO(U_n(p,q,r))<ESO(U_n(p+r,q,0))$ and $ESO(U_n(p,q,0))<ESO(U_n(p+q,0,0))$, respectively. Therefore, $G \cong U_n(n-3,0,0)$. □

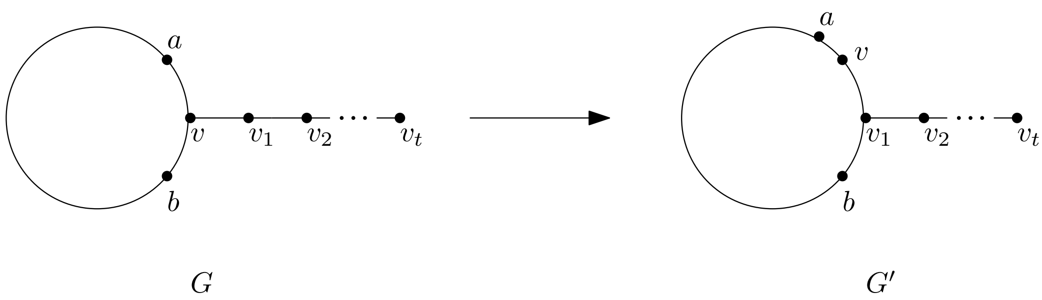

Figure 4.3: The cycle-expanding transformation used in Lemma 4.3.

Lemma 4.3. *Let $G \in U_n$ be a graph and C_k be its unique cycle. Let $v \in V(C_k)$ be a vertex of degree 3 in G such that $N(v) = \{a, b, v_1\}$, where $a, b \in V(C_k)$. If $P_t = vv_1v_2 \dots v_t$, $t \geqslant 1$, is an induced sub-path in G and if $G' = G - vb + v_1b$ (see Figure 4.3), then $ESO(G') \leqslant ESO(G)$.*

Proof. For convenience, let $d(a) = a$ and $d(b) = b$. Certainly, $a, b \geqslant 2$.

Case 1. $t = 1$.
Note that $d(v_1) = 1$, $d_{G'}(v) = 2$, and $d_{G'}(v_1) = 2$. Hence, we have

$$\begin{aligned} ESO(G) - ESO(G') &= \Big((d(v) + d(a))\sqrt{d^2(v) + d^2(a)} + (d(v) + d(v_1))\sqrt{d^2(v) + d^2(v_1)} + (d(v) + d(b))\sqrt{d^2(v) + d^2(b)} \Big) \\ &\quad - \Big((d_{G'}(v) + d_{G'}(a))\sqrt{d^2_{G'}(v) + d^2_{G'}(a)} + (d_{G'}(v) + d_{G'}(v_1))\sqrt{d^2_{G'}(v) + d^2_{G'}(v_1)} \\ &\quad + (d_{G'}(v_1) + d_{G'}(b))\sqrt{d^2_{G'}(v_1) + d^2_{G'}(b)} \Big) \\ &= \Big((a+3)\sqrt{a^2+9} + 4\sqrt{10} + (b+3)\sqrt{b^2+9} \Big) - \Big((a+2)\sqrt{a^2+4} + 8\sqrt{2} + (b+2)\sqrt{b^2+4} \Big) \\ &\geqslant (a+3)\sqrt{a^2+9} - (a+2)\sqrt{a^2+4} + 4\sqrt{10} - 8\sqrt{2} > 0. \end{aligned}$$

Case 2. $t \geqslant 3$.
In this case, we have $d(v_1) = d(v_2) = 2$, $d_{G'}(v) = 2$, and $d_{G'}(v_1) = 3$. Hence,

$$\begin{aligned} ESO(G) - ESO(G') = &\Big((d(v) + d(a))\sqrt{d^2(v) + d^2(a)} + (d(v) + d(v_1))\sqrt{d^2(v) + d^2(v_1)} \\ &+ (d(v_1) + d(v_2))\sqrt{d^2(v_1) + d^2(v_2)} \Big) \\ &- \Big((d_{G'}(v) + d_{G'}(a))\sqrt{d^2_{G'}(v) + d^2_{G'}(a)} + (d_{G'}(v) + d_{G'}(v_1))\sqrt{d^2_{G'}(v) + d^2_{G'}(v_1)} \\ &+ (d_{G'}(v_1) + d_{G'}(v_2))\sqrt{d^2_{G'}(v_1) + d^2_{G'}(v_2)} \Big) \\ = &(a+3)\sqrt{a^2+9} - (a+2)\sqrt{a^2+4} + 8\sqrt{2} - 5\sqrt{13} \\ \geqslant &5\sqrt{13} - 8\sqrt{2} + 8\sqrt{2} - 5\sqrt{13} = 0. \end{aligned}$$

Case 3. $t = 2$.
Note that $d(v_1) = 2$, $d(v_2) = 1$, $d_{G'}(v) = 2$, and $d_{G'}(v_1) = 3$. Hence, we have

$$\begin{aligned} ESO(G) - ESO(G') = &\Big((d(v) + d(a))\sqrt{d^2(v) + d^2(a)} + (d(v) + d(v_1))\sqrt{d^2(v) + d^2(v_1)} \\ &+ (d(v_1) + d(v_2))\sqrt{d^2(v_1) + d^2(v_2)} \Big) \\ &- \Big((d_{G'}(v) + d_{G'}(a))\sqrt{d^2_{G'}(v) + d^2_{G'}(a)} + (d_{G'}(v) + d_{G'}(v_1))\sqrt{d^2_{G'}(v) + d^2_{G'}(v_1)} \\ &+ (d_{G'}(v_1) + d_{G'}(v_2))\sqrt{d^2_{G'}(v_1) + d^2_{G'}(v_2)} \Big). \end{aligned}$$

Consequently, we have

$$ESO(G) - ESO(G') = \left((a+3)\sqrt{a^2+9} + 5\sqrt{13} + 3\sqrt{5}\right) - \left((a+2)\sqrt{a^2+4} + 5\sqrt{13} + 4\sqrt{10}\right)$$
$$\geqslant (a+3)\sqrt{a^2+9} - (a+2)\sqrt{a^2+4} + 3\sqrt{5} - 4\sqrt{10} > 0.$$

In all three cases, we obtained the desired inequality. □

Theorem 4.2. *If $G \in U_n$ is a unicyclic graph with the minimum elliptic Sombor index, then $G \cong C_n$ and $ESO(G) = 8n\sqrt{2}$.*

Proof. By Lemma 2.3 (path-lifting inverse transformation) and Lemma 4.3 (cycle-expanding transformation), C_n is the graph with the minimum elliptic Sombor index in U_n. □

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