MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **96** (2026) 625–646
ISSN: 0340–6253
doi: 10.46793/match.96-2.10825

Extremal Hexagonal Chains with Respect to the Kemeny's Constant

Yujun Yang*, **Wei Li**

School of Mathematics and Information Sciences, Yantai University, Yantai 264005, P. R. China

yangyj@ytu.edu.cn, lw0210math@163.com

(Received May 7, 2025)

Abstract

The Kemeny's constant of a graph G, denoted by $\kappa(G)$, is defined as the expected time to travel from a fixed starting vertex to a random destination vertex (according to the stationary distribution). This constant is shown to be a novel resistance distance-based graph invariant, which indicates its crucial application in chemistry. In this paper, comparison result on Kemeny's constant of S,T-isomers is established. Then according to this comparison result, extremal hexagonal chains with maximum and minimum Kemeny's constant are characterized. It turns out that among all hexagonal chains with n hexagons, the linear chain L_n is the unique graph with the maximum Kemeny's constant, whereas the helicene chain H_n is the unique graph with the minimum Kemeny's constant.

1 Introduction

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. The *Kemeny's constant* of G, denoted by $\kappa(G)$, is defined as the expected time

*Corresponding author.

to travel from a fixed starting vertex to a random destination vertex (according to the stationary distribution), averaged over all starting vertices. More precisely, the Kemeny's constant of G is defined as

$$\kappa(G) = \sum_j \frac{d_j^G}{2m} E_i T_j, \tag{1}$$

where d_j^G is degree of vertex j in G and $E_i T_j$ is the expected time for a random walker to arrive at j for the first time when it begins at i. Amazingly, Kemeny and Snell [12] proved that this value is independent of the choice of starting vertex, establishing $\kappa(G)$ as a genuine graph invariant.

In fact, the Kemeny's constant can also be interpreted in terms of resistance distances of graphs. It is well known that the traditional distance function defined on a graph G is the (shortest-path) distance, where the *distance* $d_G(u,v)$ between any two vertices $u, v \in V(G)$ is defined as the length of a shortest path connecting them. Then another novel distance function named resistance distance is defined by Klein and Randić [17]. For $u, v \in V(G)$, the *resistance distance* $\Omega_G(u,v)$ between vertices u and v is defined as the net effective resistance between these two nodes in the corresponding electrical network constructed from G by replacing each edge of G with a 1-ohm resistor. It is proved that $\Omega_G(u,v) < d_G(u,v)$ with equality if and only if u and v are connected by unique path in G. Palacios and Renom [15] established the following nice relation between $\kappa(G)$ and resistance distances of G.

$$\kappa(G) = \frac{1}{4m} \sum_{p \in V(G)} \sum_{q \in V(G)} d_p^G d_q^G \Omega_G(p,q). \tag{2}$$

Note that in [6], Chen and Zhang also defined a resistance distance-based graph invariant called the *multiplicative degree-Kirchhoff index* of G as

$$Kf^*(G) = \frac{1}{2} \sum_{p \in V(G)} \sum_{q \in V(G)} d_p^G d_q^G \Omega_G(p,q). \tag{3}$$

It is interesting to note that $\kappa(G)$ and $Kf^*(G)$ are equal up to a scale factor.

As an intrinsic graph invariant, Kemeny's constant turns out to be a well-established metric for measuring connectivity [2, 20] and criticality [8, 19] of graphs. In addition, Kemeny's constant has been widely used in network analysis [13, 20, 23, 28]. What's more important, as an important resistance distance-based molecular structure descriptor, Kemeny's constant has crucial applications in chemistry. Thus Kemeny's constant has been widely studied in mathematics, chemistry and network science.

Recently, the calculation of the Kemeny's constant of graphs has become a research hotspot. For one thing, Kemeny's constant for graphs adding or reducing one edge, has attracted special attention. Li et al. [14] calculated the maximum possible increase and decrease of Kemeny's constant when adding an edge to a tree with n vertices. Altafini et al. [1] explored the computation of Kemeny's constant for graphs resulting from edge removal. For another, the establishment of the expressions for the Kemeny's constant of certain graphs has drawn attention. For instance, Kooij and Dubbeldam [18] derived formulas for Kemeny's constant of complete bipartite graphs, diameter-constrained trees, and generalized windmill graphs. Zaman et al. [26] established closed-form expressions for Kemeny's constant in hexagonal ring networks. For more information, the readers can refer to the literature [4, 5, 9, 16, 21].

As a fundamental graph invariant, Kemeny's constant has been extensively studied in relation to structural graph properties, with particular interest in its extremal behavior under topological constraints. Recent investigations have focused on characterizing graphs that achieve minimal or maximal Kemeny's constant within given families, revealing profound connections between random walk efficiency and graph structure. For instance, Faught, Kempton and Knudson [10] proved that the path graph attained maximum Kemeny's constant among all connected trees with n vertices. Breen et al. [3] conjectured that the barbell graph attained the maximal Kemeny's constant among all connected graphs with n vertices. Ciardo, Dahl and Kirkland [7] characterized extremal graphs with minimal Kemeny's constant among all trees with fixed order and diameter, and they also gave upper bound for Kemeny's constant among all trees with fixed order and diameter. Jang, Kim and Song [11] gave a necessary condition for a tree to attain maximum Kemeny's constant for trees with fixed diameter. Zeng [27] provided a characterization of weighted tree with maximum and minimum Kemeny's constant. Inspired by these studies on the extremal properties of Kemeny's constant, in this paper, we will characterize the maximum and minimum values of the Kemeny's constant of hexagonal chains.

Hexagonal chains are the graph representations of unbranched cat-acondensed benzenoid hydrocarbons. In graph theoretical language, a hexagonal chain is a connected graph consisting of n regular hexagons $C_1, C_2, \ldots, C_n$ such that (a) for any k, j with $1 \leq k < j \leq n-1$, C_k and C_j have a common edge if and only if $j = k+1$, and (b) each vertex belong to at most two hexagons. Actually, a hexagonal chain with n hexagons could also be obtained from a straight quadrilateral chain with n squares by adding 2 vertices to each square in one of the following three ways: (i) add two vertices to the top edge of the square. (ii) add two vertices to the bottom edge of the square. (iii) add one vertex to the top edge and one vertex to the bottom edge of the square. For convenience, we always assume that C_1 and C_n are formed by the third way. For the remaining hexagons $C_2, C_3, \ldots, C_{n-1}$, we assign a sign of $-$, or 0, or $+$ to each hexagon according to the hexagon is obtained from the square by adding 0, or 1, or 2 vertices to the top edge. In this way, a hexagonal chain with n-hexagons can be uniquely represented by an $(n-2)$-tuple $S = (s_1, s_2, \ldots, s_{n-2})$, where $s_1, s_2, \ldots, s_{n-2}$ are the signs of $C_2, C_3, \ldots, C_{n-1}$. Hence, hereinafter, we will always denote a hexagonal chain with n hexagons as $H(S)$ such that S is a $(n-2)$-tuple taking values from $\{-, 0, +\}$. For a non-terminal hexagon in a hexagonal chain $H(S)$, if the sign of the hexagon is not 0, then we say that there is a *kink* at this hexagon. If $H(S)$ has no kink, i.e. $S = (\underbrace{0, 0, \ldots, 0}_{n-2})$, then we call $H(S)$ a *straight chain* or *linear chain*, and denoted by L_n. For $H(S)$, if S does not contain 0, then $H(S)$ is called a *"all-kink" chain*. In particular, the "all-kink" chain $H(\underbrace{-, -, \ldots, -}_{n-2})$ (isomorphic to $H(\underbrace{+, +, \ldots, +}_{n-2})$) is called a *helicene chain*, which is denoted by H_n. The "all-kink" chain $H(S)$ is called a *zigzag chain* if the signs in S alternate, i.e., $H(\underbrace{+,-,\ldots}_{n-2})$ (isomorphic to $H(\underbrace{-,+,\ldots}_{n-2})$), which is denoted as Z_n. For instance, the hexagonal chains L_5, $H(+,0,-)$, Z_5, and H_5 are illustrated in Fig. 1.

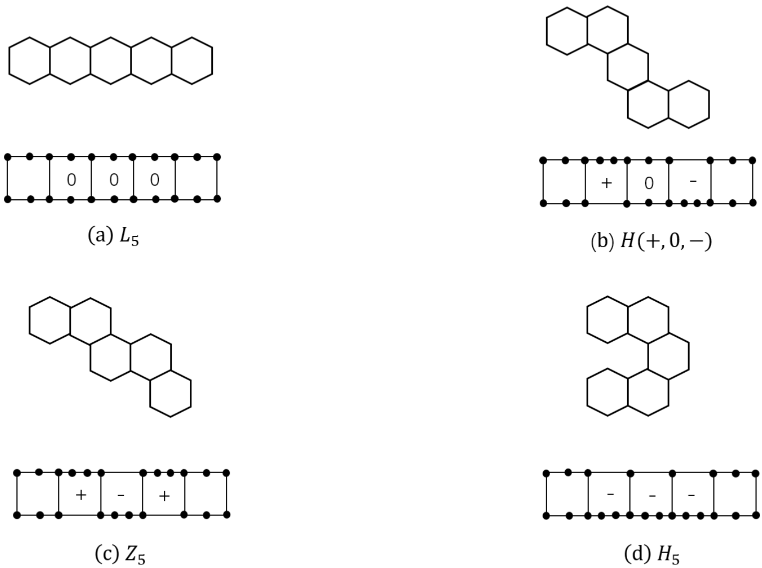

Figure 1. The hexagonal chains L_5, $H(+,0,-)$, Z_5 and H_5.

2 Preliminaries

In this section, we will introduce a few notions,definitions and results that we will use in this paper.

First, we introduce series and parallel connection rules (see Fig. 2) and cut-vertex property on resistance distances.

Definition 1. (Series connection rule) If n resistors with resistances $r_1, r_2, \cdots, r_n$ are connected in series between two vertices u and v, they can be replaced by a single equivalent resistor between u and v. The resistance r_{uv} of this equivalent resistor is calculated as $r_{uv} = r_1 + r_2 + \cdots + r_n$.

Definition 2. (Parallel connection rule) If n resistors with resistances $r_1, r_2, \cdots, r_n$ are connected in parallel between two vertices u and v, they can be substituted with a single equivalent resistor between u and v. The resistance r_{uv} of this equivalent resistor is calculated as $r_{uv} = (\frac{1}{r_1} + \frac{1}{r_2} + \cdots + \frac{1}{r_n})^{-1}$.

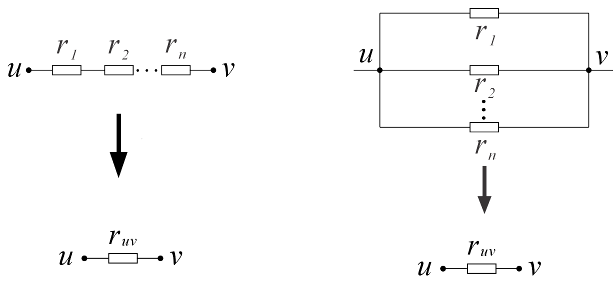

Figure 2. Illustration of series and parallel connection rules.

A cut vertex of G is a vertex whose deletion disconnects G.

Proposition 1. *(Cut-vertex Property [17]) Let G be a connected graph and x a cut vertex of graph G. Suppose u and v are vertices such that they are in different components of $G - x$. Then we have*

$$\Omega_G(u, v) = \Omega_G(u, x) + \Omega_G(x, v). \tag{4}$$

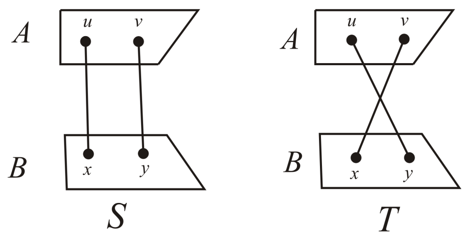

Figure 3. Illustration of S, T-isomers.

Finally, we introduce the concept of S, T-isomers in chemistry. The concept of S, T-isomers was proposed by Polansky and Zander [22] in 1982, which entails a pair of graphical moieties doubly interconnected in two different ways as in Fig. 3. A pair of vertices u and v in moiety A are connected to vertices x and y in moiety B, in one way in the S-isomer, and in the other way in the T-isomer.

3 Extremal hexagonal chains with respect to the Kemeny's constant

Let $H(S)$ be a hexagonal chain consisting of $n+2$ hexagons with $S = (s_1, s_2, \dots, s_n)$. As illustrated in Fig. 4, the hexagons in $H(S)$ are labeled sequentially as $C_1, C_2, \dots, C_{n+2}$, and the common edges of adjacent hexagons are labelled by $h_1 l_1, h_2 l_2, \dots, h_{n+1} l_{n+1}$. For simplicity, we use $\Omega_H(u,v)$ instead of $\Omega_{H(S)}(u,v)$ to denote the resistance distance between vertices u and v in $H(S)$, and use d_v^H instead of $d_v^{H(S)}$ to denote the degree of vertex v in $H(S)$.

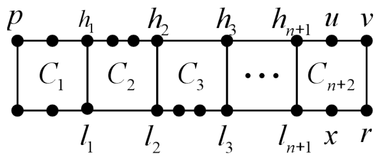

Figure 4. Hexagonal chain $H(S)$ with $n+2$ hexagons.

Lemma 1. *[24] Let $H(S)$ be a hexagonal chain determined by the sequence $S = (s_1, s_2, \dots, s_n)$ as shown in Fig. 4. Denote by u the unique neighbor of h_{n+1} in C_{n+2} and by v the adjacent vertex to u satisfying $v \neq h_{n+1}$. Then for any degree-2 vertex $p \in C_1$, we have*

$$\Omega_H(p,u) < \Omega_H(p,v).$$

In fact, even for the more general case that $H(S)$ is a weighted hexagonal chain, as long as the weight on edge $h_{n+1}l_{n+1}$ is 1, the result in Lemma 1 still holds, as given in the following lemma.

Lemma 2. *[24] Let $H(S)$ be a weighted hexagonal chain such that the weight on edge $h_{n+1}l_{n+1}$ is 1. Denote by u the unique neighbor of h_{n+1} in C_{n+2} and by v the adjacent vertex to u satisfying $v \neq h_{n+1}$. Then for any* *degree-2 vertex* $p \in C_1$*, we have*

$$\Omega_H(p,u) < \Omega_H(p,v).$$

Now we use Lemmas 1 and 2 to prove the following result, which plays an essential rule in proving our main result.

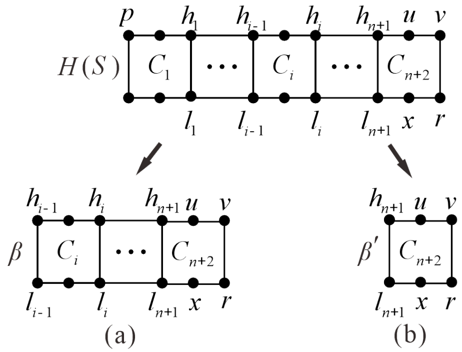

Figure 5. Illustration of network simplifications in the proof of Lemma 3.

Lemma 3. *Let* $H(S)$ *and vertices* u *and* v *be shown in Fig. 4. Then we have*

$$\sum_{p\in V(H(S))} d_p^H[\Omega_H(p,u) - \Omega_H(p,v)] < 0.$$

Proof. Let $V' = V(H(S)) \setminus V(C_{n+2})$, which represents the set of vertices in $H(S)$ that do not belong to C_{n+2}. First, we show that for any $p \in V'$, $\Omega_H(p,u) < \Omega_H(p,v)$. If p is a degree-2 vertex of C_1, then Lemma 1 directly implies that $d_p(\Omega_H(p,u) - \Omega_H(p,v)) < 0$. Now suppose that $p \in V(C_i)$ and $p \notin V(C_{i+1})$ $(2 \le i \le n+1)$, and we compare $\Omega_H(p,u)$ and $\Omega_H(p,u)$. To this end, we make network simplification to $H(S)$. By series and parallel connection rules, it is easily seen that $H(S)$ could be simplified to a weighted hexagonal chain consisting of hexagons $C_i, C_{i+1}, \ldots, C_{n+2}$ such that the weight on the edge $h_{i-1}l_{i-1}$ is $\beta < 1$ and all the other edges still have unit weights, as shown in Fig. 5 (a). Thus by Lemma 2, we have

$\Omega_H(p,u) < \Omega_H(p,v)$. It thus follows that

$$\sum_{p\in V'} d_p^H[\Omega_H(p,u) - \Omega_H(p,v)] < 0. \tag{5}$$

Now we consider $\Omega_H(p,u) - \Omega_H(p,v)$ for $p \in V(C_{n+2})$. As before, we simplify $H(S)$ to a single weighted hexagonal chain which only consists of hexagon C_{n+2} such that the weight on $h_{n+1}l_{n+1}$ is $\beta' < 1$ and all the other edges have unit weights, as illustrated in Fig. 5 (b). Thus by series and parallel connection rules, it is easily get that

$$\Omega_H(h_{n+1},u) = \frac{4+\beta'}{5+\beta'},\ \Omega_H(l_{n+1},u) = \frac{4(1+\beta')}{5+\beta'}, \Omega_H(x,u) = \frac{3(2+\beta')}{5+\beta'},$$
$$\Omega_H(r,u) = \frac{2(3+\beta')}{5+\beta'},\ \Omega_H(v,u) = \frac{4+\beta'}{5+\beta'},$$

and

$$\Omega_H(h_{n+1},v) = \frac{2(3+\beta')}{5+\beta'},\ \Omega_H(l_{n+1},v) = \frac{3(2+\beta')}{5+\beta'}, \Omega_H(x,v) = \frac{2(3+\beta')}{5+\beta'},$$
$$\Omega_H(r,v) = \frac{4+\beta'}{5+\beta'},\ \Omega_H(u,v) = \frac{4+\beta'}{5+\beta'}.$$

Thus it follows that

$$\begin{aligned}
&\sum_{p\in V(C_{n+2})} d_p^H[\Omega_H(p,u) - \Omega_H(p,v)] \\
&= 3[\Omega_H(h_{n+1},u) - \Omega_H(h_{n+1},v)] + 3[\Omega_H(l_{n+1},u) - \Omega_H(l_{n+1},v)] \\
&+ 2[\Omega_H(x,u) - \Omega_H(x,v)] + 2[\Omega_H(r,u) - \Omega_H(r,v)] \\
&+ 2[\Omega_H(v,u) - \Omega_H(v,v)] + 2[\Omega_H(u,u) - \Omega_H(u,v)] \\
&= \frac{4(\beta'-2)}{5+\beta'} < 0.
\end{aligned} \tag{6}$$

According to Eqs. (5) and (6), we get

$$\sum_{p\in V(H(S))} d_p^H[\Omega_H(p,u)-\Omega_H(p,v)] = \sum_{p\in V'} d_p^H[\Omega_H(p,u)-\Omega_H(p,v)]$$
$$+\sum_{p\in V(C_{n+2})} d_p^H[\Omega_H(p,u)-\Omega_H(p,v)] < 0.$$

This completes the proof of Lemma 3. ■

We now consider comparison of Kemeny's constants of S,T-isomers. Comparison result on resistance distances of S,T-isomers is given in the following result.

Lemma 4. *[25] For any two vertices $p,q \in V(S)=V(T)$, if $p,q\in V(A)$ or $p,q\in V(B)$, then*

$$\Omega_S(p,q)=\Omega_T(p,q),$$

whereas if $p\in V(A)$ and $q\in V(B)$, then

$$\Omega_S(p,q)-\Omega_T(p,q)=\frac{[\Omega_A(p,u)-\Omega_A(p,v)][\Omega_B(q,y)-\Omega_B(q,x)]}{2+\Omega_A(u,v)+\Omega_B(x,y)}.$$

By Lemma 4, we could obtain the comparison result on Kemeny's constants of S,T-isomers, as given in the following result.

Lemma 5. *Let S, T , A, B ,u, v, x, y be defined as illustrated in Fig.3. Then*

$$\kappa(S)-\kappa(T)$$
$$=\frac{\left[\sum\limits_{p\in V(A)} d_p^S[\Omega_A(p,u)-\Omega_A(p,v)]\right]\left[\sum\limits_{q\in V(B)} d_q^S[\Omega_B(q,y)-\Omega_B(q,x)]\right]}{2m[2+\Omega_A(u,v)+\Omega_B(x,y)]}.$$

Proof. By Eq. (2) and Lemma 4, we have

$$
\begin{aligned}
&\kappa(S)-\kappa(T)\\
=&\frac{1}{4m}\sum_{p\in V(S)}\sum_{q\in V(S)} d_p^S d_q^S \Omega_S(p,q)-\frac{1}{4m}\sum_{p\in V(T)}\sum_{q\in V(T)} d_p^T d_q^T \Omega_T(p,q)\\
=&\frac{1}{4m}\sum_{p\in V(S)}\sum_{q\in V(S)} d_p^S d_q^S \Omega_S(p,q)-\frac{1}{4m}\sum_{p\in V(S)}\sum_{q\in V(S)} d_p^S d_q^S \Omega_T(p,q)\\
=&\frac{1}{4m}\sum_{p\in V(S)}\sum_{q\in V(S)} d_p^S d_q^S [\Omega_S(p,q)-\Omega_T(p,q)]\\
=&\frac{1}{4m}\left[\sum_{p\in V(A)}\sum_{q\in V(A)}+2\sum_{p\in V(A)}\sum_{q\in V(B)}+\sum_{p\in V(B)}\sum_{q\in V(B)}\right]\\
&\times d_p^S d_q^S [\Omega_S(p,q)-\Omega_T(p,q)]\\
=&\frac{1}{2m}\sum_{p\in V(A)}\sum_{q\in V(B)} d_p^S d_q^S [\Omega_S(p,q)-\Omega_T(p,q)]
\end{aligned}
$$

$$
\begin{aligned}
=&\frac{1}{2m}\sum_{p\in V(A)}\sum_{q\in V(B)}\frac{d_p^S d_q^S[\Omega_A(p,u)-\Omega_A(p,v)][\Omega_B(q,y)-\Omega_B(q,x)]}{2+\Omega_A(u,v)+\Omega_B(x,y)}\\
=&\frac{\left[\sum\limits_{p\in V(A)} d_p^S[\Omega_A(p,u)-\Omega_A(p,v)]\right]\left[\sum\limits_{q\in V(B)} d_q^S[\Omega_B(q,y)-\Omega_B(q,x)]\right]}{2m[2+\Omega_A(u,v)+\Omega_B(x,y)]},
\end{aligned}
$$

which completes the proof. ∎

In the following, we use comparison result on Kemeny's constants of S,T-isomers to characterize hexagonal chains with extremal Kemeny's constant. We first show that if there exist "kinks" in a hexagonal chain $H(S)$, then we could find a hexagonal chain $H(S')$ such that $\kappa(H(S)) < \kappa(H(S'))$. For convenience, we define: $-(-)=+$ and $-(+)=-$.

Lemma 6. *Let $H(S)$ be a hexagonal chain with $S=(s_1,s_2,\dots,s_n)$. If there exists some integer $i\in\{1,2,\dots,n\}$ such that $s_i\neq 0$, then let $S'=$*

$(s_1, \ldots, s_{i-1}, 0, -s_{i+1}, \ldots, -s_n)$ *and we have*

$$\kappa(H(S)) < \kappa(H(S')).$$

Proof. Since $s_i \neq 0$, then either $s_i = -$ or $s_i = +$. We prove that the assertion holds for $s_i = -$, and the case that $s_i = +$ could be proved in the same way.

Now assume that $s_i = -$. Select vertices u, v, x and y in the $(i+1)$-th hexagon of $H(S)$ as shown in Fig. 6. As illustrated in the same

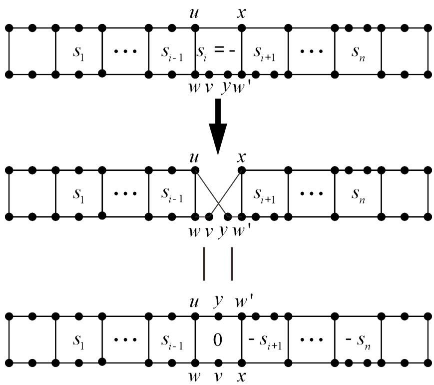

Figure 6. Illustration of hexagonal chains $H(S)$ and $H(S')$ in the proof of Lemma 6.

figure, if we first delete edges $\{ux, vy\}$ from $H(S)$ and then add new edges $\{uy, vx\}$, then we could obtain a new hexagonal chain $H(S')$ with $S' = (s_1, \ldots, s_{i-1}, 0, -s_{i+1}, \ldots, -s_n)$. The only thing left is to prove that $\kappa(H(S')) < \kappa(H(S))$. Clearly $\{ux, vy\}$ and $\{uy, vx\}$ are minimal 2-edge cuts of $H(S)$ and $H(S')$, respectively. Let the two components of $H(S) - \{ux, vy\}$ (also $H(S') - \{uy, vx\}$) are A and B such that the component contains vertices u and v is A. From the construction of $H(S')$, it is obvious that $H(S)$ and $H(S')$ are S, T-isomers. Thus by Lemma 5, we have

$$\kappa(H(S)) - \kappa(H(S'))$$
$$= \frac{\left[\sum\limits_{p\in V(A)} d_p^H[\Omega_A(p,u) - \Omega_A(p,v)]\right]\left[\sum\limits_{q\in V(B)} d_q^H[\Omega_B(q,y) - \Omega_B(q,x)]\right]}{2m[2+\Omega_A(u,v)+\Omega_B(x,y)]}. \tag{7}$$

First, we consider $\sum\limits_{p\in V(A)} d_p^H(\Omega_A(p,u) - \Omega_A(p,v))$. For convenience, we distinguish the following two cases.

Case 1. $p \in V(A)\backslash\{u,v\}$. Suppose that w is the unique neighbor of v in A. Then by the cut-vertex property of resistance distances, we have

$$\Omega_A(p,v) = \Omega_A(p,w) + \Omega_A(w,v) = \Omega_A(p,w) + 1. \tag{8}$$

On the other hand, it is clear that $\Omega_A(u,w) < d_A(u,w) = 1$ since u and w are connected by more than one path in A. Thus by the triangular inequality of resistance distances, we have

$$\Omega_A(p,u) \leq \Omega_A(p,w) + \Omega_A(w,u) < \Omega_A(p,w) + 1. \tag{9}$$

Thus, for any $p \in V(A) \setminus \{u,v\}$, we have

$$\sum_{p\in V(A)\backslash\{u,v\}} d_p^H[\Omega_A(p,u) - \Omega_A(p,v)] < 0. \tag{10}$$

Case 2. $p \in \{u,v\}$. In this case,

$$\begin{aligned}
&\sum_{p\in\{u,v\}} d_p^H[\Omega_A(p,u) - \Omega_A(p,v)] \\
=&d_u^H[\Omega_A(u,u) - \Omega_A(u,v)] + d_v^H[\Omega_A(v,u) - \Omega_A(v,v)] \\
=&2[0 - \Omega_A(u,v)] + 1 \times [\Omega_A(v,u) - 0] \\
=&-\Omega_A(u,v) < 0.
\end{aligned} \tag{11}$$

From Cases 1 and 2, we have

$$\sum_{p\in V(A)} d_p^H[\Omega_A(p,u)-\Omega_A(p,v)] = \sum_{p\in V(A)\setminus\{u,v\}} d_p^H[\Omega_A(p,u)-\Omega_A(p,v)]$$
$$+\sum_{p\in\{u,v\}} d_p^H[\Omega_A(p,u)-\Omega_A(p,v)] < 0. \tag{12}$$

Next, we consider $\sum\limits_{q\in V(B)} d_q^H(\Omega_B(q,y)-\Omega_B(q,x))$. We also distinguish the following two cases.

Case 1. $q\in V(B)\backslash\{x,y\}$. Let w' denote the unique adjacent vertex of y in B. Then by the cut-vertex property, we have

$$\Omega_B(q,y)=\Omega_B(q,w')+\Omega_B(w',y)=\Omega_B(q,w')+1. \tag{13}$$

Since $\Omega_B(x,w')<d_B(x,w')=1$, by the triangular inequality, we have

$$\Omega_B(q,x)\le\Omega_B(q,w')+\Omega_B(w',x)<\Omega_B(q,w')+1=\Omega_B(q,y). \tag{14}$$

Thus, for any $q\in V(B)\setminus\{x,y\}$, $(\Omega_B(q,y)-\Omega_B(q,x)>0$ and it gives that

$$\sum_{q\in V(B)\backslash\{x,y\}} d_q^H[\Omega_B(q,y)-\Omega_B(q,x)]>0. \tag{15}$$

Case 2. $q\in\{x,y\}$. In this case,

$$\begin{aligned}&\sum_{q\in\{x,y\}} d_q^H[\Omega_B(q,y)-\Omega_B(q,x)]\\ =&d_x^H[\Omega_B(x,y)-\Omega_B(x,x)]+d_y^H[\Omega_B(y,y)-\Omega_B(y,x)]\\ =&2[\Omega_B(x,y)-0]+1\times[0-\Omega_B(y,x)]\\ =&\Omega_B(x,y)>0.\end{aligned} \tag{16}$$

From Cases 1 and 2, we get

$$\sum_{q\in V(B)} d_q^H[\Omega_B(q,y)-\Omega_B(q,x)] = \sum_{q\in V(B)\setminus\{x,y\}} d_q^H[\Omega_B(q,y)-\Omega_B(q,x)] + \sum_{q\in\{u,v\}} d_q^H[\Omega_B(q,y)-\Omega_B(q,x)] > 0. \tag{17}$$

Substituting Eqs. (12) and (17) into Eq. (7), we conclude that $\kappa(H(S)) - \kappa(H(S')) < 0$. ■

By Lemma 6, we know that if $H(S)$ has "kinks", then we could find a hexagonal chain $H(S')$ which has one less kink than $H(S)$ but larger Kemeny's constant than $H(S)$. Thus for any non-straight hexagonal chain $H(S)$, the process of removing "kinks" may be iterated. Each such operation strictly increases the Kemeny's constant. This monotonic growth process continues until the hexagonal chain converges to the linear chain. Consequently, we have the following result.

Theorem 2. *Among all hexagonal chains with n hexagons, the linear chain L_n has the maximum Kemeny's constant.*

According to the proof of Lemma 6, we also know that for hexagonal chain $H(S)$ with $S = (s_1, s_2, \ldots, s_n)$, if there exists some integer $i \in \{1, 2, \ldots, n\}$ with $s_i = 0$, then the hexagonal chain $H(S')$ with either $S' = (s_1, \ldots, s_{i-1}, -, -s_{i+1}, \ldots, -s_n)$ or $S' = (s_1, \ldots, s_{i-1}, +, -s_{i+1}, \ldots, -s_n)$ has larger Kemeny's constant than $H(S)$. Hence if a hexagonal chain is not a "all-kink" chain, then the process of adding "kinks" in the hexagonal chain may be iterated, each time reducing the Kemeny's constant, till finally arriving at an "all-kink" chain. Hence we have

Theorem 3. *Among all hexagonal chains, the minimum Kemeny's constant is attained only when the hexagonal chain is an "all-kink" chain.*

In the next section, we will determine which "all-kink" chains have extremal Kemeny's constant among all "all-kink" chains.

4 Extremal "all-kink" chains with respect to the Kemeny's constant

Recall that a hexagonal chain $H(S)$ is defined as an"all-kink" chain if S does not contain element 0. In this section, we aim to characterize the "all-kink" chains that attain maximum and minimum Kemeny's constant among all "all-kink" chains with $(n+2)$ hexagons.

Lemma 7. *Let H be an "all-kink" chain with $S = (s_1, s_2, \ldots, s_n)$. If there exists some integer $i \in \{1, 2, \ldots, n-1\}$ such that $s_i \neq s_{i+1}$, then let $S' = (s_1, \ldots, s_i, -s_{i+1}, \ldots, -s_n)$ and we have*

$$\kappa(H(S')) < \kappa(H(S)).$$

Proof. Since $s_i \neq 0$, either $s_i = -$ or $s_i = +$. We will only prove that the assertion holds for the $s_i = -$, as case for $s_i = +$ can be proved analogously.

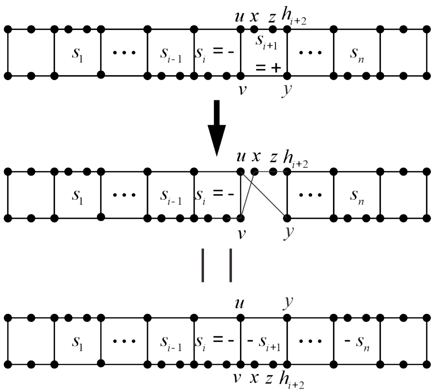

Figure 7. Illustration of "all-kink" chains $H(S)$ and $H(S')$ in the proof of Lemma 7.

Now we suppose $s_i = -$ and $s_{i+1} = +$. Choose vertices u, v, x and y in the $(i+2)$-th hexagon of $H(S)$ as shown in Fig. 7. Deleting edges $\{ux, vy\}$ from $H(S)$ and then adding two new edges $\{uy, vx\}$, we could obtain a new hexagonal chain $H(S')$ with $S' = (s_1, \ldots, s_i, -s_{i+1}, \ldots, -s_n)$ (see Fig. 7). In the following, we show that $\kappa(H(S')) < \kappa(H(S))$. Clearly,

$H(S)$ and $H(S')$ are S,T-isomers. Suppose that the two components of $H(S)-\{ux,vy\}$ are A and B such that A is the component containing u and v. Then by Lemma 5, we have

$$\begin{aligned}&\kappa(H(S))-\kappa(H(S'))\\&=\frac{\left[\sum\limits_{p\in V(A)} d_p^H[\Omega_A(p,u)-\Omega_A(p,v)]\right]\left[\sum\limits_{q\in V(B)} d_q^H[\Omega_B(q,y)-\Omega_B(q,x)]\right]}{2m[(2+\Omega_A(u,v)+\Omega_B(x,y)]}.\end{aligned} \tag{18}$$

We first consider $\sum\limits_{p\in V(A)} d_p^H[\Omega_A(p,u)-\Omega_A(p,v)]$. Observing that A is a hexgonal chain, thus by Lemma 3, we have

$$\sum_{p\in V(A)} d_p^A[\Omega_A(p,u)-\Omega_A(p,v)]<0.$$

Noticing that except for u and v, all the other vertices of A have the same degree in A as in H. Thus

$$\begin{aligned}&\sum_{p\in V(A)} d_p^H[\Omega_A(p,u)-\Omega_A(p,v)]=\sum_{p\in V(A)} d_p^A[\Omega_A(p,u)-\Omega_A(p,v)]\\&+(d_u^H-d_u^A)[\Omega_A(u,u)-\Omega_A(u,v)]+(d_v^H-d_v^A)[\Omega_A(v,u)-\Omega_A(v,v)]\\&=\sum_{p\in V(A)} d_p^A[\Omega_A(p,u)-\Omega_A(p,v)]<0.\end{aligned} \tag{19}$$

Next, we consider $\sum\limits_{q\in V(B)} d_q^H[\Omega_B(q,y)-\Omega_B(q,x)]$. For convenience, we distinguish the following two cases.

Case 1. $q\in V(B)\backslash\{x,y,z\}$. Let z be the unique neighbor of x in B. Then for any $q\in V(B)\setminus\{x,y,z\}$, by cut-vertex property and triangular inequality of resistance distances, we have

$$\Omega_B(q,x)=\Omega_B(q,h_{i+2})+\Omega_B(h_{i+2},x)=\Omega_B(q,h_{i+2})+2, \tag{20}$$

and

$$\Omega_B(q,y) \le \Omega_B(q,h_{i+2}) + \Omega_B(h_{i+2},y) < \Omega_B(q,h_{i+2}) + 1. \qquad (21)$$

It follows from (20) and (21) that

$$\Omega_B(q,y) - \Omega_B(q,x) < -1.$$

Thus we have

$$\sum_{q\in V(B)\setminus\{x,y,z\}} d_q^H[\Omega_B(q,y) - \Omega_B(q,x)] < 0. \qquad (22)$$

Case 2. $q \in \{x,y,z\}$. In this case,

$$\begin{aligned}
&\sum_{q\in\{x,y,z\}} d_p^H[\Omega_B(q,y) - \Omega_B(q,x)] \\
=& d_x^H[\Omega_B(x,y) - \Omega_B(x,x)] + d_y^H[\Omega_B(y,y) - \Omega_B(y,x)] \\
&+ d_z^H[\Omega_B(z,y) - \Omega_B(z,x)] \\
=& 2[\Omega_B(x,y) - 0] + 3[0 - \Omega_B(y,x)] + 2[\Omega_B(z,y) - \Omega_B(z,x)] \\
=& -\Omega_B(x,y) + 2[\Omega_B(z,y) - \Omega_B(z,x)] \\
=& -[2 + \Omega_B(h_{i+2},y)] + 2[1 + \Omega_B(h_{i+2},y) - 1] = -2 + \Omega_B(h_{i+2},y) < 0.
\end{aligned} \qquad (23)$$

From Cases 1 and 2, we obtain:

$$\begin{aligned}
\sum_{q\in V(B)} d_q^H[\Omega_B(q,y) - \Omega_B(q,x)] =& \sum_{q\in V(B)\setminus\{x,y,z\}} d_q^H[\Omega_B(q,y) - \Omega_B(q,x)] \\
+ \sum_{q\in\{x,y,z\}} d_q^H[\Omega_B(q,y) - \Omega_B(q,x)] < 0.&
\end{aligned} \qquad (24)$$

According to Eqs. (19) and (24), we get that $\kappa(H(S)) - \kappa(H(S')) > 0$ as desired. ■

Based on the proof of Lemma 7, we know that for a non-helicene "all-kink" chain, the operation of eliminating "reverse kinks" can be iteratively carried out. With each iteration, the Kemeny's constant decreases, until the helicene chain is ultimately reached. As a direct consequence of Lemma 7, we have the following result.

Theorem 4. *Among all "all-kink" chains with n hexagons, the helicene chain H_n has the minimum Kemeny's constant.*

Since we have proved that among all hexagonal chains, the minimum Kemeny's constant is attained only when the hexagonal chain is an "all-kink" chain. Thus Theorem 4 directly leads to the following result.

Theorem 5. *Among all hexagonal chains with n hexagons, the helicene chain H_n has the minimum Kemeny's constant.*

It is natural to inquire which "all-kink" chain attains the maximum Kemeny's constant. Analogously to the proof of Lemma 7, we can demonstrate that for an "all-kink" chain $H(S)$ with $S = (s_1, s_2, \dots, s_n)$, if there exists some integer $i \in \{1, 2, \dots, n-1\}$ such that $s_i = s_{i+1}$, then the "all-kink" chain $H(S')$ with $S' = (s_1, \dots, s_i, -s_{i+1}, \dots, -s_n)$ has larger Kemeny's constant than $H(S)$. Consequently, if an "all-kink" hexagonal chain is non-zigzag, one can iteratively add "reverse kinks" to the hexagonal chain. Each step strictly increases the Kemeny's constant until the it becomes a zigzag chain. Thus, we have the following result.

Theorem 6. *Among all "all-kink" chains with n hexagons, the zigzag chain Z_n has the maximum Kemeny's constant.*

As an example illustrating the validity of results obtained in this paper, numerical results for Kemeny's constants of all hexagons chains with 5 hexagons are given in the following table. Note that there are 10 different hexagonal chains with 5 hexagons in the sense of isomorphism. It could be seen that hexagonal chains with extremal Kemeny's constants given in the following table coincide with the results given in Theorems 3, 5 and 6.

Since all hexagonal chains with n hexagons have the same number of $m = 4n+2$ edges, the multiplicative degree-Kirchhoff index of a hexagonal chain $H(S)$ with n-hexagon is $2m$ times of its Kemeny's constant. Thus

Table 1. Kemeny's constants of all hexagons chains with 5 hexagons.

G	$\kappa(G)$	G	$\kappa(G)$
$L_5 = H(0,0,0)$	58.4520	$H(0,+,-)$	56.2252
$H(0,0,+)$	57.3870	$H(+,+,0)$	55.7352
$H(0,+,0)$	57.0452	$Z_5 = H(+,-,+)$	55.3839
$H(+,0,-)$	56.3434	$H(+,+,-)$	54.9366
$H(+,0,+)$	56.3007	$H_5 = H(+,+,+)$	54.4039

the extremality results for Kemeny's constant of hexagonal chains also hold for multiplicative degree-Kirchhoff index, which are summerized in the following result.

Theorem 7. *Among all hexagonal chains with n hexagons, the linear chain L_n has the maximum multiplicative degree-Kirchhoff index, whereas the helicene chain H_n has the minimum multiplicative degree-Kirchhoff index. In addition, among all "all-kink" hexagonal chains with n hexagons, the zigzag chain Z_n has the maximum multiplicative degree-Kirchhoff index, whereas the helicene chain H_n has the minimum multiplicative degree-Kirchhoff index.*

***Acknowledgment*:** The authors would like to thank the anonymous referee for carefully reading and valuable comments which improved the final version of the paper. The support of the National Natural Science Foundation of China (through grant no. 12171414) and Taishan Scholars Special Project of Shandong Province is greatly acknowledged.

References

[1] D. Altafini, D. A. Bini, V. Cutini, B. Meini, F. Poloni, An edge centrality measure based on the Kemeny constant, *SIAM J. Matrix Anal. Appl.* **44** (2023) 648–669.

[2] J. Berkhout, B. F. Heidergott, Analysis of Markov influence graphs, *Oper. Res.* **67** (2019) 892–904.

[3] J. Breen, S. Butler, N. Day, C. DeArmond, K. Lorenzen, H. Qian, J. Riesen, Computing Kemeny's constant for barbell-type graphs, *El. J. Lin. Algebra* **35** (2019) 583–598.

[4] J. Breen, E. Crisostomi, S. Kim, Kemeny's constant for a graph with bridges, *Discr. Appl. Math.* **322** (2022) 20–35.

[5] J. Breen, S. Kim, A. L. Fung, A. Mann, A. A. Parfeni, G. Tedesco, Threshold graphs, Kemeny's constant, and related random walk parameters, *Lin. Algebra Appl.* **709** (2025) 284–313.

[6] H. Chen, F. Zhang, Resistance distance and the normalized Laplacian spectrum, *Discr. Appl. Math.* **155** (2007) 654–661.

[7] L. Ciardo, G. Dahl, S. Kirkland, On Kemeny's constant for trees with fixed order and diameter, *Lin. Multilin. Algebra* **70** (2022) 2331–2353.

[8] P. De Meo, F. Messina, D. Rosaci, G. M. Sarné, A. V. Vasilakos, Estimating graph robustness through the Randić index, *IEEE Trans. Cybern.* **48** (2017) 3232–3242.

[9] N. Faught, M. Kempton, A. Knudson, Resistance distance, Kirchhoff index, and Kemeny's constant in flower graphs, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 405–427.

[10] N. Faught, M. Kempton, A. Knudson, A 1-separation formula for the graph Kemeny constant and Braess edges, *J. Math. Chem.* **60** (2022) 49–69.

[11] J. Jang, S. Kim, M. Song, Kemeny's constant and Wiener index on trees, *Lin. Algebra Appl.* **674** (2023) 230–243.

[12] J. G. Kemeny, J. L. Snell, *Finite Markov Chains*, Princeton, Van Nostrand, 1960.

[13] V. Koskin, A. Kells, J. Clayton, A. K. Hartmann, A. Annibale, E. Rosta, Variational kinetic clustering of complex networks, *J. Chem. Phys.* **158** (2023) #104112.

[14] S. Kirkland, Y. Li, J. S. McAlister, X. Zhang, Edge addition and the change in Kemeny's constant, *Discr. Appl. Math.* **373** (2025) 77–90.

[15] J. L. Palacios, J. M. Renom, Broder and Karlin's formula for hitting times and the Kirchhoff index, *Int. J. Quantum Chem.* **111** (2011) 35–39.

[16] S. Kirkl, Z. Zeng, Kemeny's constant and an analogue of Braess' paradox for trees, *El. J. Lin. Algebra* **31** (2016) 444–464.

[17] D. J. Klein, M. Randić, Resistance distance, *J. Math. Chem.* **12** (1993) 81–95.

[18] R. E. Kooji, J. L. A. Dubbeldam, Kemeny's constant for several families of graphs and real-world networks, *Discr. Appl. Math.* **285** (2020) 96–107.

[19] B. Lebichot, S. Marco, A bag-of-paths node criticality measure, *Neurocomputing* **275** (2018) 224–236.

[20] H. Li, L. Wang, Z. Bu, J. Cao, Y. Shi, Measuring the network vulnerability based on Markov criticality, *ACM Trans. Knowl. Discovery Data* **16** (2021) 1–24.

[21] J. L. Palacios, G. Markowsky, Kemeny's constant and the Kirchhoff index for the cluster of highly symmetric graphs, *Appl. Math. Comput.* **406** (2021) #126283.

[22] O. E. Polansky, M. Zander, Topological effects on MO energies, *J. Mol. Struct.* **84** (1982) 361–385.

[23] K. Sricharan, K. Das, Localizing anomalous changes in time-evolving graphs, in: *Proceedings of the 2014 ACM SIGMOD International Conference on Management of Data*, 2014, pp. 1347–1358.

[24] W. Sun, Y. Yang, Minimal hexagonal chains with respect to the Kirchhoff index, *Discr. Appl. Math.* **345** (2022) #113099.

[25] Y. Yang, D. J. Klein, Comparison theorems on resistance distances and Kirchhoff indices of S, T-isomers, *Discr. Appl. Math.* **175** (2014) 87–93.

[26] S. Zaman, A. A. Koam, A. A. Khabyah, A. Ahmad, The Kemeny's constant and spanning trees of hexagonal ring network, *Comput. Mater. Contin.* **73** (2022) 6347–6365.

[27] J. Zeng, On average hitting time and Kemeny's constant for weighted trees, arxiv priprint 2109.09249 (2021).

[28] Y. Zhang, K. W. Ross, On-policy deep reinforcement learning for the average reward criterion, in: M. Meila, T. Zhang (Eds.), *The 38th International Conference on Machine Learning*, 2021, pp. 12535–12545.