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Bounds of Geodetic-Wiener Index on Spirocyclic Graphs

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Abstract. Wiener index has been extensively studied for several decades because of its applications in chemistry. Many variants of Wiener index were defined and their corresponding bounds were explored. In this work, we introduced the concept of geodetic-Wiener index by considering the number of geodesics between any pair of vertices. We used the concept of projection of a vertex to a subgraph to decompose the structure into subtrees. Simple spirocyclic graphs are bicyclic graphs whose cycles share a common vertex. Using the idea of partial Wiener index, we determined the bounds of geodetic-Wiener index with respect to other distance-based topological indices for simple spirocyclic graphs.

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Key Words and Phrases: Topological index, geodetic-Wiener index, spirocyclic graphs

1. Introduction

Topological indices (TIs) are 2D descriptors that consider the internal atomic structure of compounds [1]. They incorporate data on molecular size, shape, branching, occurrence of heteroatoms, and multiple bonds into numeric values [1]. In 1947, Wiener [2] calculated boiling point of paraffin by using a distance-based TI called the Wiener index, which is the sum of distances between all vertex pairs in a graph. Since benzenoid hydrocarbons are fascinating the huge significance of theoretical chemists, the theory of

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the Wiener index of the respective molecular graphs have been extensively developed in the last three decades [2].

Although the Wiener index is the oldest topological index, later on some distance-based topological indices have been defined such as hyper-Wiener index [3], Gutman index [4], Schultz index [5–9], Harary index [10, 11], additively weighted Harary index [12] and multiplicatively weighted Harary index [13].

The idea of Wiener index was introduced by Harold Wiener in 1947 [2]. The Wiener index of a connected graph G as defined in [2] is given by

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

Recently, Lin [14] made a survey of all the extremal results on the Wiener index of trees from 2014 and presented some open problems.

The *generalized Wiener index* of a a connected graph G was introduced by Martinez-Perez and Rodriguez [15] and is given by

$$W_\lambda(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v)^\lambda,$$

where λ is a real number.

The study of *hyper-Wiener index* of a connected graph G was pioneered by Alhevaz et al. [16] and is given by

$$WW(G) = \sum_{\{u,v\}\subseteq V(G)} \binom{d(u,v)+1}{2} = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} [d(u,v)^2 + d(u,v)].$$

The *Gutman index* of G, denoted by $\mathrm{Gut}(G)$, which was introduced by Ivan Gutman in 1994 [17], is given by

$$\mathrm{Gut}(G) = \sum_{\{u,v\}\subseteq V(G)} [d_u d_v] d(u,v).$$

In 2014, Mazorodze et al. [18] established asymptotically sharp bound of the Gutman index for graphs without pendant vertices.

The *Schultz index* of G [19] and is given by

$$S(G) = \sum_{\{u,v\}\subseteq V(G)} [d_u + d_v] d(u,v).$$

The *Harary index* of G [11] is given by

$$H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)}.$$

The *additively weighted Harary index* of G [12] is given by

$$H_A(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{d_u + d_v}{d(u,v)}.$$

The *multiplicatively weighted Harary index* of G was also proposed by Alizadeh et al. [12] as a modification of the Harary index and is given by

$$H_M(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{d_u d_v}{d(u,v)}.$$

Let U and $U^\star$ be nonempty subsets of $V(G)$. The *partial Wiener Index* of G [20] is given by

$$W(U,U^\star;G) = \sum_{(u,v)\in U\times U^\star} d(u,v).$$

In 2017, Jamil [21] first derive closed-form formulas for some distance based topological indices for double graphs in terms of the original graph. Moreover, these formulas are applied for several special kinds of graphs, such as, the complete graph, the path and the cycle.

In 2019, Dobrynin [22] esablished the Wiener index of uniform hypergraphs induced by trees. In the following year, Dobrynin and Estaji [23] investigated the Wiener index of hexagonal chains under some operations on the corresponding binary vectors. The obtained results may be useful in studying of topological indices for sets of hexagonal chains induced by algebraic constructions.

2. Spirocyclic Compounds and Applications

Spiro compounds are organic compounds that have two or more rings with one common atom, the spiro atom. The spiro atom gives a rigid geometry to the rings, which can impose shape and properties on the molecule. Spirocyclic compunds are an interesting group of organic compounds with distinct structural properties, making them suitable for application in many fields, especially medicinal chemistry.

Spirocylic graphs represent a specific class of graphs characterized by unique structural features. These graphs, particularly in the theory of spiro compounds in organic chemistry, are characterized by two or more cycles connected in one common vertex. This particular connectivity pattern imbues the molecules that correspond to it with distinctive properties, thus making them applicable to various chemical and potentially other scientific purposes. If a graph contains exactly two cycles, then we call it *simple spirocyclic* graph [24].

In drug discovery, an essential property of spirocycles is their natural capacity to project functionality to the third dimension [25]. This three-dimensional nature is essential for drug-target interactions since drugs need to fit physically into biological targets, e.g., proteins, which occur in a much more specific and efficient manner than planar sys-

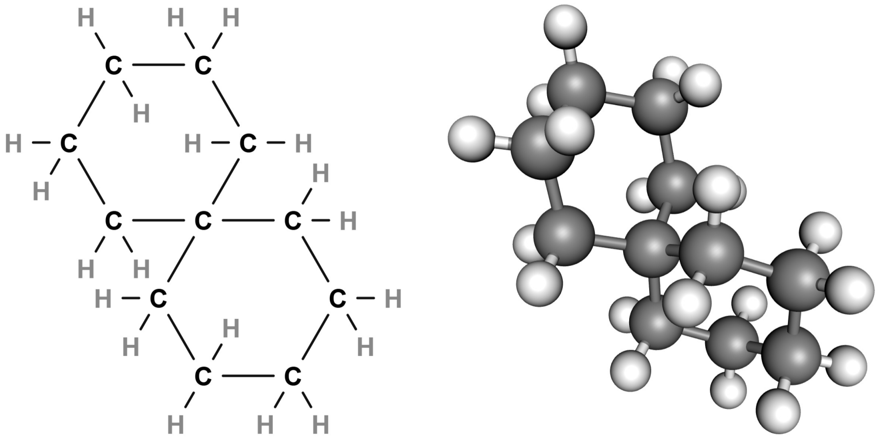

Figure 1: Skeletal formula and molecular structure of spirobicyclohexane

tems [25]. An example of a spiro compound with a simple spirocyclic structure is the spirobicyclohexane ($C_{11}H_{20}$), with skeletal formula and molecular structure [26] shown in Figure 1.

Spirobicyclohexane is a new organic compound whose structure is described by a bicyclic arrangement of two six-membered carbon rings in a spiro orientation. The implication is that the two rings share a common axis, each with three carbon atoms that are not directly bonded. Spirobicyclohexane has a symmetrical and rigid structure, which can be one factor that influences its physical and chemical properties. It is often used as a building block to construct more complex organic molecules. It is used in numerous applications, including pharmaceuticals and materials science because it can impart specific stereochemistry and stability to the molecules it is incorporated into [27].

Bicyclic graphs are graphs that contain exactly two cycles. Simple spirocyclic graphs are bicyclic graphs whose cycles share a common vertex called the *spiro vertex.*

3. Geodetic-Wiener Index Formulation

The study of geodesics is a graph is an important graph-theoretic property to be considered in topological properties of a graph [28]. For example, in a real-world scenario, the idea of considering different shortest routes from station A to station B can be modeled by the number of geodesics between these two stations. In this particular scenario, transporting goods from A to B could take less time by utilizing different transportation services on different shortest routes. The volume of goods that can be transported at the same time is determined by the number of shortest routes from the initial station to the terminal station. In general, the transport of energy from one point to another can be represented by geodesics in a network. These scenarios give us some motivations to study the number of geodesics in a graph and integrate the concept with the Wiener index.

The *distance* $d(u, v)$ between two vertices u and v in a connected graph G is the length of a u-v geodesic in G. A *u-v geodesic* in G is a shortest path joining u and v in G [29].

The *degree of a vertex* u in G is denoted by $d_u = d_G(u)$ [30]. The *minimum degree* δ and the *maximum degree* Δ are, respectively, defined as follows [31]:

$$\delta = \min_{v \in V(G)} \{ d_G(v)\}, \qquad \Delta = \max_{v \in V(G)} \{ d_G(v)\}.$$

The following formulation can be found in [32]. We now introduce a Wiener-type topological index. Consider the function

$$\alpha : V(G) \times V(G) \longrightarrow \mathbb{N},$$

where $\alpha(u, v)$ is counts the number of geodesics between vertices u and v in a graph G as defined in [29]. The *geodetic-Wiener index (g-Wiener index)* of G, as defined in [32], is given by

$$W_g(G) = \sum_{\{u,v\} \subseteq V(G)} \alpha(u, v)d(u, v).$$

In [32], we establish several bounds for geodetic-Wiener index for unicyclic graphs in terms of other distance-based topological indices.

4. The Partitioning

Definition 1. Let G be a connected graph. The *projection* of $u \in V(G)$ onto a subgraph H of G as the set

$$\begin{aligned} P_H(u) &= \{w \in V(H) : d(u, w) = d(u, V(H))\} \\ &= \{w \in V(H) : d(u, w) \leq d(u, z) \text{ for any } z \in V(H)\} \end{aligned}$$

If $P_H(u) = \{w\}$, we simply write $P_H(u) = w$.

Consider a simple spirocyclic graph G with even cycles $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$ and $C_{2t_2} = [u_1 = v_1, v_2, \ldots, v_{2t_2}]$, for some natural numbers $t_1, t_2 \geq 2$. For each $i \in \{1, 2, \ldots, 2t_1\}$, let $U_i = \{u \in V(G) : P_{C_{2t_1} \cup C_{2t_2}}(u) = u_i\}$. Similarly, for each $j \in \{1, 2, \ldots, 2t_2\}$, let $V_j = \{v \in V(G) : P_{C_{2t_1} \cup C_{2t_2}}(v) = v_j\}$. Then the projection operator onto the union of C_{2t_1} and C_{2t_2} generates the tree-partition $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, V_3, \ldots, V_{2t_2}\}$ of $V(G)$. This means that $\langle U_i \rangle$ and $\langle V_j \rangle$ are trees in G for each $i \in \{1, 2, \ldots, 2t_1\}$ and $j \in \{1, 2, \ldots, 2t_2\}$. We call the set $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, V_3, \ldots, V_{2t_2}\}$ the tree-partition of $V(G)$ with respect to its projection onto the union of cycles C_{2t_1} and C_{2t_2}.

In the above illustration, $P_{C_6 \cup C_4}(a) = P_{C_6 \cup C_4}(b) = P_{C_6 \cup C_4}(c) = P_{C_6 \cup C_4}(d) = P_{C_6 \cup C_4}(u_4) = u_4$. This gives $U_4 = \{a, b, c, d, u_4\}$. Also, $U_1 = \{u_1\}$ and $U_3 = \{e, u_3\}$. Moveover, the projection of f onto $C_6 \cup C_4$ is v_2. Note also that $\alpha(u_4, v_3) = 4$.

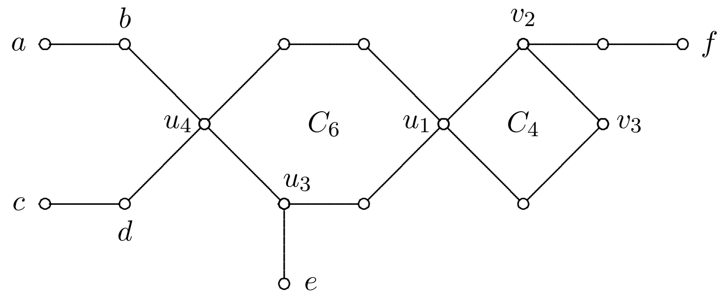

Figure 2: Spirocyclic graph with C_6 and C_4

The geodetic-Wiener index and Wiener index differ only on the number of geodesics between pairs of vertices. Hence, we will consider those pairs where the number of geodesics is at least two. For $u, v \in V(G)$, the value of $\alpha(u, v)$ is determined by the following classes of subsets of $V(G)$.

Lemma 1. *Let G be a simple spirocyclic graph with even cycles $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$ and $C_{2t_2} = [u_1 = v_1, v_2, \ldots, v_{2t_2}]$, for some natural numbers $t_1, t_2 \geq 2$, and $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, V_3, \ldots, V_{2t_2}\}$ is the tree-partition of $V(G)$ with respect to the projection of $V(G)$ onto the union of cycles C_{2t_1} and C_{2t_2}. Then*

(i) $\alpha(u, v) = 2$ *if* $u \in U_i$ *and* $v \in U_{i+t_1}$, *for* $i \in \{1, 2, \ldots, t_1\}$.

(ii) $\alpha(u, v) = 2$ *if* $u \in V_j$ *and* $v \in V_{j+t_2}$, *for* $j \in \{1, 2, \ldots, t_2\}$.

(iii) $\alpha(u, v) = 2$ *if* $u \in V_{t_2+1}$ *and* $v \in U_i$, *for* $i \in \{2, \ldots, t_1\}$.

(iv) $\alpha(u, v) = 2$ *if* $u \in U_{t_1+1}$ *and* $v \in V_j$, *for* $j \in \{2, \ldots, t_2\}$.

(v) $\alpha(u, v) = 4$ *if* $u \in U_{t_1+1}$ *and* $v \in V_{t_2+1}$.

Moreover, if (u, v) is not in the above categories, then $\alpha(u, v) = 1$.

Proof. Let $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$ and $C_{2t_2} = [u_1 = v_1, v_2, \ldots, v_{2t_2}]$ be the cycles in G, for some natural numbers $t_1, t_2 \geq 2$, and $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, V_3, \ldots, V_{2t_2}\}$ is the tree-partition of $V(G)$ with respect to the projection of $V(G)$ onto the union of cycles C_{2t_1} and C_{2t_2}.

(i) Fix $i \in \{1, 2, \ldots, t_1\}$. Let $u \in U_i$ and $v \in U_{i+t_1}$. $\alpha(u, v) = 2$ if $u \in U_i$ and $v \in U_{i+t_1}$. Then there exist u_i, u_{i+t_1} in C_{2t_1} such that $P_{C_{2t_1} \cup C_{2t_2}}(u) = u_i$ and $P_{C_{2t_1} \cup C_{2t_2}}(v) = u_{i+t_1}$. Note that there are exactly 2 geodesics from u_i to u_{i+t_1}. Consequently, there are exactly 2 geodesics from u to v. Accordingly, $\alpha(u, v) = 2$.

(ii) The proof is similar to *(i)*.

(iii) Note that any geodesic from C_{2t_2} to C_{2t_1} passes through $V_1 = U_1$. Here, there are exactly 2 geodesics from a vertex in V_{t_2+1} to any vertex in $V_1 = U_1$. Moreover, for each $i \in \{2, \ldots, t_1\}$, there is only one shortest path from a vertex in U_1 to a vertex in U_i. Consequently, if $u \in V_{t_2+1}$ and $v \in U_i$, for $i \in \{2, \ldots, t_1\}$, then $\alpha(u, v) = 2$.

(*iv*) Similar arguments with (*iii*) gives the desired result.

(*v*) Let $u \in U_{t_1+1}$ and $v \in V_{t_2+1}$. Then any geodesic from u to v passes through $u_1 = v_1$. From (*i*), there are exactly 2 geodesics from u to u_1. Similarly, from (*ii*), there are exactly 2 geodesics from v to v_1. Accordingly, $\alpha(u,v) = 4$.

The following gives the exact relation between g-Wiener and Wiener indices.

Lemma 2. *Let G be a simple spirocyclic graph with even cycles $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$ and $C_{2t_2} = [u_1 = v_1, v_2, \ldots, v_{2t_2}]$, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$\begin{aligned} W_g(G) &= W(G) + \sum_{i=1}^{t_1} W(U_i, U_{i+t_1}; G) + \sum_{j=1}^{t_2} W(V_j, V_{j+t_2}; G) + \sum_{i=2}^{2t_1} W(V_{t_2+1}, U_i; G) \\ &\quad + \sum_{j=2}^{2t_2} W(U_{t_1+1}, V_j; G) + W(U_{t_1+1}, V_{t_2+1}; G). \end{aligned}$$

where $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, \ldots, V_{2t_2}\}$ is the tree-partition of $V(G)$ with respect to the projection of $V(G)$ onto the union of the cycles C_{2t_1} and C_{2t_2}.

Proof. The geodesics in Lemma 1(*i*) are covered in the first and the second quantities. Similarly, the geodesics in Lemma 1(*ii*) are covered in the first and the third quantities. Lemma 1(*iii*) gives the fourth and first quantities. Similarly, Lemma 1(*iv*) are covered in the fifth and the first quantities. The 4 geodesics in Lemma 1(*v*) are covered in the sixth, first, fourth, and fifth quantities.

The result follows.

5. Bounds of g-Wiener Index with Wiener Index

The following result establishes relation between g-Wiener index and Wiener index as defined in [2] for simple spirocyclic graphs.

Theorem 1. *Let G be a simple spirocyclic graph with even cycles $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$ and $C_{2t_2} = [u_1 = v_1, v_2, \ldots, v_{2t_2}]$, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$W(G) + At_1 + Bt_2 \leq W_g(G) \leq W(G) + C diam(G),$$

where $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, \ldots, V_{2t_2}\}$ is the tree-partition of $V(G)$ with respect to the projection of $V(G)$ onto the union of the cycles C_{2t_1} and C_{2t_2}, and

$$A = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + |U_{t_1+1}||V_{t_2+1}|,$$

$$B = \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|,$$

and

$$C = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|.$$

Proof. Let $t_1, t_2 \geq 2$ be a natural numbers. Consider the even cycles $C_{2t_1} = [u_1, u_2, \dots, u_{2t_1}]$ and $C_{2t_2} = [v_1, v_2, \dots, v_{2t_2}]$ in G. Note that $\{u, v\} \subseteq V(G)$, $d(u, v) \leq diam(G)$. Using Lemma 2,

$$\begin{aligned}
W_g(G) &= \sum_{\{u,v\}\subseteq V(G)} \alpha(u, v)d(u, v) \\
&= W(G) + \sum_{i=1}^{t_1} W(U_i, U_{i+t_1}; G) + \sum_{j=1}^{t_2} W(V_j, V_{j+t_2}; G) + \sum_{i=2}^{2t_1} W(V_{t_2+1}, U_i; G) \\
&\quad + \sum_{j=2}^{2t_2} W(U_{t_1+1}, V_j; G) + W(U_{t_1+1}, V_{t_2+1}; G) \\
&= W(G) + \sum_{i=1}^{t_1} \sum_{(u,v)\in U_i\times U_{i+t_1}} d(u, v) + \sum_{j=1}^{t_2} \sum_{(u,v)\in V_j\times V_{j+t_2}} d(u, v) \\
&\quad + \sum_{i=2}^{2t_1} \sum_{(u,v)\in V_{t_2+1}\times U_i} d(u, v) + \sum_{j=2}^{2t_2} \sum_{(u,v)\in U_{t_1+1}\times V_j} d(u, v) + \sum_{(u,v)\in U_{t_1+1}\times V_{t_2+1}} d(u, v) \\
&\leq W(G) + diam(G) \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + diam(G) \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| \\
&\quad + diam(G) \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + diam(G) \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + diam(G)|U_{t_1+1}||V_{t_2+1}| \\
&= W(G) + C diam(G)
\end{aligned}$$

where

$$C = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|.$$

Now, for $(u, v) \in U_i \times U_{i+t_1}$, $d(u, v) \geq t_1$. Also, for $(u, v) \in V_j \times V_{j+t_2}$, $d(u, v) \geq t_2$. Moreover, if $(u, v) \in V_{t_2+1} \times U_i$ for $i \in \{2, 3, \dots, 2t_1\}$, $d(u, v) \geq t_2$ since a $u - v$ geodesic passes through V_1 and the distance between V_1 and V_{t_2+1} is t_2. Similarly, if

$(u,v) \in U_{t_1+1} \times V_j$ for $j \in \{2,3,\ldots,2t_2\}$, $d(u,v) \geq t_1$ since a $u-v$ geodesic passes through U_1 and the distance between U_1 and U_{t_1+1} is t_1. Moreover, for $(u,v) \in U_{t_1+1} \times V_{t_2+1}$, $d(u,v) \geq t_1 + t_2$. Applying Lemma 2 gives

$$\begin{aligned}
W_g(G) &= \sum_{\{u,v\}\subseteq V(G)} \alpha(u,v)d(u,v) \\
&= W(G) + \sum_{i=1}^{t_1} W(U_i, U_{i+t_1}; G) + \sum_{j=1}^{t_2} W(V_j, V_{j+t_2}; G) + \sum_{i=2}^{2t_1} W(V_{t_2+1}, U_i; G) \\
&\quad + \sum_{j=2}^{2t_2} W(U_{t_1+1}, V_j; G) + W(U_{t_1+1}, V_{t_2+1}; G) \\
&= W(G) + \sum_{i=1}^{t_1} \sum_{(u,v)\in U_i \times U_{i+t_1}} d(u,v) + \sum_{j=1}^{t_2} \sum_{(u,v)\in V_j \times V_{j+t_2}} d(u,v) \\
&\quad + \sum_{i=2}^{2t_1} \sum_{(u,v)\in V_{t_2+1} \times U_i} d(u,v) + \sum_{j=2}^{2t_2} \sum_{(u,v)\in U_{t_1+1} \times V_j} d(u,v) + \sum_{(u,v)\in U_{t_1+1} \times V_{t_2+1}} d(u,v) \\
&\geq W(G) + t_1 \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + t_2 \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| \\
&\quad + t_2 \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + t_1 \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + (t_1+t_2)|U_{t_1+1}||V_{t_2+1}| \\
&= W(G) + At_1 + Bt_2,
\end{aligned}$$

where

$$A = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + |U_{t_1+1}||V_{t_2+1}|$$

and

$$B = \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|.$$

The proof is complete.

Theorem 2. *Let G be a simple spirocyclic graph with minimum degree $\delta = 2$ and with even cycles C_{2t_1} and C_{2t_2}, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$W_g(G) = W(G) + 2(t_1 + t_2)^2.$$

Proof. Let $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$ and $C_{2t_2} = [v_1, v_2, \ldots, v_{2t_2}]$ be the cycles in G. Since $\delta = 2$, G has no pendant vertices. Consequently, G is a vertex-gluing of C_{2t_1}

and C_{2t_2}. Assume that $u_1 = v_1$, the spiro vertex. Consider the tree-partition $\{V_1 = U_1, U_2, \ldots, U_{2t_1}, V_2, V_3, \ldots, V_{2t_2}\}$ of $V(G)$ using its projection onto $C_{2t_1} \cup C_{2t_2}$. That is,

$$U_i = \{u \in V(G) : P_{C_{2t_1} \cup C_{2t_2}}(u) = u_i\} \text{ for } i \in \{1, 2, \ldots, 2t_1\}$$

and

$$V_j = \{v \in V(G) : P_{C_{2t_1} \cup C_{2t_2}}(v) = v_j\} \text{ for } j \in \{1, 2, \ldots, 2t_2\}.$$

Then $U_1 = V_1 = \{u_1 = v_1\}, U_2 = \{u_2\}, U_3 = \{u_3\}, \ldots, U_{2t_1} = \{u_{2t_1}\}, V_2 = \{v_2\}, V_3 = \{v_3\}, \ldots, V_{2t_2} = \{v_{2t_2}\}$. Hence, for each $i \in \{1, 2, \ldots, 2t_1\}$, $|U_i| = 1$. Similarly, for each $j \in \{1, 2, \ldots, 2t_2\}$, $|V_j| = 1$.

For each $i \in \{2, 3, \ldots, t_1\}$, $d(U_1, U_i) = d(U_1, U_{2t_1 - i + 2}) = i - 1$. Hence,

$$\sum_{i=2}^{2t_1} \sum_{(u,v) \in V_{t_2+1} \times U_i} d(u,v) = (t_2 + t_1) + 2\sum_{i=2}^{t_1}(t_2 + i - 1) = 2t_1t_2 + t_1^2 - t_2.$$

Similarly, for each $j \in \{2, 3, \ldots, t_2\}$, $d(V_1, V_j) = d(V_1, V_{2t_2 - j + 2}) = j - 1$. Thus,

$$\sum_{j=2}^{2t_2} \sum_{(u,v) \in U_{t_1+1} \times V_j} d(u,v) = (t_1 + t_2) + 2\sum_{j=2}^{t_2}(t_1 + j - 1) = 2t_2t_1 + t_2^2 - t_1.$$

By Lemma 2, we have

$$\begin{aligned}
W_g(G) &= \sum_{\{u,v\} \subseteq V(G)} \alpha(u,v) d(u,v) \\
&= W(G) + \sum_{i=1}^{t_1} W(U_i, U_{i+t_1}; G) + \sum_{j=1}^{t_2} W(V_j, V_{j+t_2}; G) + \sum_{i=2}^{2t_1} W(V_{t_2+1}, U_i; G) \\
&\quad + \sum_{j=2}^{2t_2} W(U_{t_1+1}, V_j; G) + W(U_{t_1+1}, V_{t_2+1}; G) \\
&= W(G) + \sum_{i=1}^{t_1} \sum_{(u,v) \in U_i \times U_{i+t_1}} d(u,v) + \sum_{j=1}^{t_2} \sum_{(u,v) \in V_j \times V_{j+t_2}} d(u,v) \\
&\quad + \sum_{i=2}^{2t_1} \sum_{(u,v) \in V_{t_2+1} \times U_i} d(u,v) + \sum_{j=2}^{2t_2} \sum_{(u,v) \in U_{t_1+1} \times V_j} d(u,v) + \sum_{(u,v) \in U_{t_1+1} \times V_{t_2+1}} d(u,v) \\
&= W(G) + t_1^2 + t_2^2 + [2t_1t_2 + t_1^2 - t_2] + [2t_2t_1 + t_2^2 - t_1] + (t_1 + t_2) \\
&= W(G) + 2(t_1 + t_2)^2.
\end{aligned}$$

6. Bounds of g-Wiener Index with Gutman Index

The following result establishes the extremal bounds for the geodetic-Wiener index of a simple spirocyclic graph G containing even cycles in terms of the Gutman index of G as defined in [17].

Theorem 3. *Let G be a simple spirocyclic graph with even cycles $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$ and $C_{2t_2} = [u_1 = v_1, v_2, \ldots, v_{2t_2}]$, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$\frac{1}{\Delta^2}\mathrm{Gut}(G) + At_1 + Bt_2 < W_g(G) < \frac{1}{\delta^2}\mathrm{Gut}(G) + Cdiam(G),$$

where $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, \ldots, V_{2t_2}\}$ is the tree-partition of $V(G)$ with respect to the projection of $V(G)$ onto the union of the cycles C_{2t_1} and C_{2t_2}, and

$$A = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + |U_{t_1+1}||V_{t_2+1}|,$$

$$B = \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|,$$

and

$$C = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|.$$

Proof. It's enough to show the bounds of Wiener index in terms of the Gutman index and use Lemma 2 and the proof of Theorem 1. Now,

$$\begin{aligned} W(G) &= \sum_{\{u,v\}\subseteq V(G)} d(u,v) \\ &= \sum_{\{u,v\}\subseteq V(G)} d(u,v) \cdot \frac{d_u d_v}{d_u d_v} \\ &< \frac{1}{\delta^2}\mathrm{Gut}(G). \end{aligned}$$

Moreover,

$$\begin{aligned} W(G) &= \sum_{\{u,v\}\subseteq V(G)} d(u,v) \\ &= \sum_{\{u,v\}\subseteq V(G)} d(u,v) \cdot \frac{d_u d_v}{d_u d_v} \\ &> \frac{1}{\Delta^2}\mathrm{Gut}(G). \end{aligned}$$

The strict inequalities in the above result are due to the fact that there exist $u, v \in V(G)$ such that $d_u d_v > \delta^2$.

The following results uses Theorem 2 and the proof of Theorem 3.

Corollary 1. *Let G be a simple spirocyclic graph with minimum degree $\delta = 2$ and with even cycles C_{2t_1} and C_{2t_2}, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$\frac{1}{16}Gut(G) + 2(t_1 + t_2)^2 < W_g(G) < \frac{1}{4}Gut(G) + 2(t_1 + t_2)^2.$$

7. Bounds of g-Wiener Index with Schultz Index

The following result establishes the relation between geodetic-Wiener and Schultz [19] indices for simple spirocyclic graphs containing even cycles.

Theorem 4. *Let G be a simple spirocyclic graph with even cycles $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$ and $C_{2t_2} = [u_1 = v_1, v_2, \ldots, v_{2t_2}]$, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$\frac{1}{2\Delta}S(G) + At_1 + Bt_2 < W_g(G) < \frac{1}{2\delta}S(G) + Cdiam(G),$$

where $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, \ldots, V_{2t_2}\}$ is the tree-partition of $V(G)$ with respect to the projection of $V(G)$ onto the union of the cycles C_{2t_1} and C_{2t_2}, and

$$A = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + |U_{t_1+1}||V_{t_2+1}|,$$

$$B = \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|,$$

and

$$C = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|.$$

Proof. We will establish the bounds of Wiener index in terms of Schultz index and use Lemma 2 together with the proof of Theorem 1.

$$\begin{aligned} W(G) &= \sum_{\{u,v\} \subseteq V(G)} d(u, v) \\ &= \sum_{u,v \in V(G)} d(u, v) \cdot \frac{d_u + d_v}{d_u + d_v} \\ &< \frac{1}{2\delta}S(G). \end{aligned}$$

Moreover,

$$\begin{aligned} W(G) &= \sum_{\{u,v\}\subseteq V(G)} d(u,v) \\ &= \sum_{\{u,v\}\subseteq V(G)} d(u,v)\cdot\frac{d_u+d_v}{d_u+d_v} \\ &> \frac{1}{2\Delta}S(G). \end{aligned}$$

Using Theorem 2 and the proof of Theorem 4, the following is immediate.

The strict inequalities in the above result are due to the fact that there exist $u, v \in V(G)$ such that $d_u + d_v > 2\delta$.

Corollary 2. *Let G be a simple spirocyclic graph with minimum degree $\delta = 2$ and with even cycles C_{2t_1} and C_{2t_2}, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$\frac{1}{8}S(G) + 2(t_1+t_2)^2 < W_g(G) < \frac{1}{4}S(G) + 2(t_1+t_2)^2.$$

8. Bounds of g-Wiener Index with Hyper-Wiener Index

The following result establishes the bounds of geodetic-Wiener index in terms of hyper-Wiener index as defined in [16] for simple spirocyclic graphs with even cycles.

Theorem 5. *Let G be a simple spirocyclic graph with even cycles $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$ and $C_{2t_2} = [u_1 = v_1, v_2, \ldots, v_{2t_2}]$, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$WW(G) + At_1 + Bt_2 < W_g(G) < \frac{2}{diam(G)+1}WW(G) + Cdiam(G)$$

where $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, \ldots, V_{2t_2}\}$ is the tree-partition of $V(G)$ with respect to the projection of $V(G)$ onto the union of the cycles C_{2t_1} and C_{2t_2}, and

$$A = \sum_{i=1}^{t_1}|U_i||U_{i+t_1}| + \sum_{j=2}^{2t_2}|U_{t_1+1}||V_j| + |U_{t_1+1}||V_{t_2+1}|,$$

$$B = \sum_{j=1}^{t_2}|V_j||V_{j+t_2}| + \sum_{i=2}^{2t_1}|V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|,$$

and

$$C = \sum_{i=1}^{t_1}|U_i||U_{i+t_1}| + \sum_{j=1}^{t_2}|V_j||V_{j+t_2}| + \sum_{j=2}^{2t_2}|U_{t_1+1}||V_j| + \sum_{i=2}^{2t_1}|V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|.$$

Proof. The proof is established by taking the bounds of Wiener index in terms of Hyper-Wiener index and using Lemma 2 together with the proof of Theorem 1.

$$\begin{aligned} W(G) &= \sum_{\{u,v\}\subseteq V(G)} d(u,v) \\ &= \sum_{\{u,v\}\subseteq V(G)} d(u,v)\cdot\frac{d(u,v)+1}{d(u,v)+1} \\ &< \frac{2}{diam(G)+1}WW(G). \end{aligned}$$

Moreover,

$$\begin{aligned} W(G) &= \sum_{\{u,v\}\subseteq V(G)} d(u,v) \\ &= \sum_{\{u,v\}\subseteq V(G)} d(u,v)\cdot\frac{d(u,v)+1}{d(u,v)+1} \\ &> WW(G) \end{aligned}$$

The proof is complete.

An immediate result for simple spirocyclic graph with minimum degree $\delta = 2$, which uses Theorem 2 and the proof of Theorem 5, is shown below.

Corollary 3. *Let G be a simple spirocyclic graph with minimum degree $\delta = 2$ and with even cycles C_{2t_1} and C_{2t_2}, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$\frac{2}{t_1+t_2+1}WW(G) + 2(t_1+t_2)^2 < W_g(G) < WW(G) + 2(t_1+t_2)^2.$$

9. Bounds of g-Wiener Index with Harary Index

The following result establishes the relation between g-Wiener index and Harary index for simple spirocyclic graphs.

Theorem 6. *Let G be a simple spirocyclic graph with even cycles $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$ and $C_{2t_2} = [u_1 = v_1, v_2, \ldots, v_{2t_2}]$, for some natural numbers $t_1, t_2 \geq 2$, without a common edge. Then*

$$H(G) + At_1 + Bt_2 < W_g(G) < (diam(G))^2 H(G) + Cdiam(G)$$

where $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, \ldots, V_{2t_2}\}$ is the tree-partition of $V(G)$ with respect to the projection of $V(G)$ onto the union of the cycles C_{2t_1} and C_{2t_2}, and

$$A = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + |U_{t_1+1}||V_{t_2+1}|,$$

$$B = \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|,$$

and

$$C = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|.$$

Proof. It suffices to show the bounds of Wiener index in terms Harary index and use Lemma 2 together with Theorem 1.

$$\begin{aligned} W(G) &= \sum_{\{u,v\}\in V(G)} d(u,v) \\ &= diam(G) \sum_{u,v\subseteq V(G)} \frac{d(u,v)}{d(u,v)} \\ &< diam(G)^2 H(G). \end{aligned}$$

Moreover,

$$\begin{aligned} W(G) &= \sum_{\{u,v\}\subseteq V(G)} d(u,v) \\ &= \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)} \\ &> H(G). \end{aligned}$$

The proof is complete.

For simple spirocyclic graphs with minimum degree $\delta = 2$, the following bounds of Harary index follows by using Theorem 2 and the proof of Theorem 6.

Corollary 4. *Let G be a simple spirocyclic graph with minimum degree $\delta = 2$ and with even cycles C_{2t_1} and C_{2t_2}, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$(t_1+t_2)^2 H(G) + 2(t_1+t_2)^2 < W_g(G) < H(G) + 2(t_1+t_2)^2.$$

10. Bounds of g-Wiener Index with Additively Weighted Harary Index

The following result establishes bounds of g-Wiener index in terms of additively weighted Harary index as defined in [12] for simple spirocyclic graph G containing even cycles.

Theorem 7. *Let G be a simple spirocyclic graph with even cycles $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$*

and $C_{2t_2} = [u_1 = v_1, v_2, \ldots, v_{2t_2}]$*, for some natural numbers* $t_1, t_2 \geq 2$*. Then*

$$\frac{1}{2\Delta} H_A(G) + At_1 + Bt_2 < W_g(G) < \frac{(diam(G))^2}{2\delta} H_A(G) + Cdiam(G)$$

where $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, \ldots, V_{2t_2}\}$ *is the tree-partition of* $V(G)$ *with respect to the projection of* $V(G)$ *onto the union of the cycles* C_{2t_1} *and* C_{2t_2}*, and*

$$A = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + |U_{t_1+1}||V_{t_2+1}|,$$

$$B = \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|,$$

and

$$C = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|.$$

Proof. We use Lemma 2 and the proof of Theorem 1 to simplify the proof. In this case, it is enough to show the bounds of Wiener index in terms of Additively Weighted Harary index.

$$\begin{aligned} W(G) &= \sum_{\{u,v\} \subseteq V(G)} d(u,v) \\ &= diam(G) \sum_{\{u,v\} \subseteq V(G)} \frac{d_u + d_v}{d(u,v)} \cdot \frac{d(u,v)}{d_u + d_v} \\ &< \frac{(diam(G))^2}{2\delta} H_A(G). \end{aligned}$$

Moreover,

$$\begin{aligned} W(G) &= \sum_{\{u,v\} \subseteq V(G)} d(u,v) \\ &= \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)} \cdot \frac{d_u + d_v}{d_u + d_v} \\ &> \frac{1}{2\Delta} H_A(G). \end{aligned}$$

This completes the proof.

The next corollary establishes the bounds of geodetic-Wiener index with additively Weighted Harary index for simple spirocyclic graphs with minimum degree $\delta = 2$ by applying Theorem 2 and the proof of Theorem 7.

Corollary 5. *Let G be a simple spirocyclic graph with minimum degree $\delta = 2$ and with even cycles C_{2t_1} and C_{2t_2}, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$\frac{(t_1+t_2)^2}{4}H_A(G) + 2(t_1+t_2)^2 < W_g(G) < \frac{1}{8}H_A(G) + 2(t_1+t_2)^2.$$

11. Bounds of g-Wiener Index with Multiplicatively Weighted Harary Index

The following result establishes bounds of g-Wiener index in terms of the multiplicatively weighted Harary index as defined in [12] for classes of simple spirocyclic graphs containing even cycles.

Theorem 8. *Let G be a simple spirocyclic graph with even cycles $C_{2t_1} = [u_1, u_2, \ldots, u_{2t_1}]$ and $C_{2t_2} = [v_1, v_2, \ldots, v_{2t_2}]$, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$\frac{1}{\Delta^2}H_M(G) + At_1 + Bt_2 < W_g(G) < \frac{(diam(G))^2}{\delta^2}H_M(G) + Cdiam(G)$$

where $\{U_1 = V_1, U_2, \ldots, U_{2t_1}, V_2, \ldots, V_{2t_2}\}$ is the tree-partition of $V(G)$ with respect to the projection of $V(G)$ onto the union of the cycles C_{2t_1} and C_{2t_2}, and

$$A = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + |U_{t_1+1}||V_{t_2+1}|,$$

$$B = \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|,$$

and

$$C = \sum_{i=1}^{t_1} |U_i||U_{i+t_1}| + \sum_{j=1}^{t_2} |V_j||V_{j+t_2}| + \sum_{j=2}^{2t_2} |U_{t_1+1}||V_j| + \sum_{i=2}^{2t_1} |V_{t_2+1}||U_i| + |U_{t_1+1}||V_{t_2+1}|.$$

Proof. It suffices to establish the bounds of Wiener index in terms of Multiplicatively Weighted Harary and use Lemma 2 together with Theorem 1. Note that in simple spirocyclic graphs, $\delta < \Delta$. Hence,

$$\begin{aligned} W(G) &= \sum_{\{u,v\}\subseteq V(G)} d(u,v) \\ &\leq diam(G) \sum_{\{u,v\}\subseteq V(G)} \frac{d_u d_v}{d(u,v)} \cdot \frac{d(u,v)}{d_u d_v} \\ &< \frac{[diam(G)]^2}{\delta^2} H_M(G). \end{aligned}$$

Moreover,

$$\begin{aligned} W(G) &= \sum_{\{u,v\}\subseteq V(G)} d(u,v) \\ &= \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)} \cdot \frac{d_u d_v}{d_u d_v} \\ &> \frac{1}{\Delta^2} H_M(G). \end{aligned}$$

The proof is complete.

Applying Theorem 2 and the proof of Theorem 8 on the bounds of Wiener index with multiplicatively weighted Harary index yields the following corollary.

Corollary 6. *Let G be a simple spirocyclic graph with minimum degree $\delta = 2$ and with even cycles C_{2t_1} and C_{2t_2}, for some natural numbers $t_1, t_2 \geq 2$. Then*

$$\frac{1}{16} H_M(G) + 2(t_1 + t_2)^2 < W_g(G) < \frac{(t_1 + t_2)^2}{4} H_M(G) + 2(t_1 + t_2)^2.$$

In Theorems 5-8, the strict inequalities are due to the fact that there exist $u, v \in V(G)$ such that $d(u,v) < diam(G)$. In particular, if $uv \in V(G)$, then $d(u,v) = 1 < diam(G)$.

12. Conclusion

In this work, we found some bounds for geodetic-Wiener index in terms of other distance-based topological indices for simple spirocyclic graphs with even cycles by decomposing the structure into subtrees using the concept of projection of $V(G)$ onto the even cycles. Moreover, we have shown that the geodetic-Wiener index of spirocyclic graphs without pendant vertices is equal to the Wiener index plus twice the square of the sum of the diameters of the cycles.

The g-Wiener index captures more structural information compared to standard Wiener index. A concrete example is a spirocyclic compound with even connecting cycles, such as the spirobicyclohexane.

Consider graphs with k even cycles where $k \geq 3$. This will increase the number of geodesics between some vertex pairs in the graph. Also, when an odd cycle is attached to the even cycle, the projection of some vertices to the even cycle may not be unique. This will be another interesting and challenging problem that could be considered. Furthermore, evaluation of g-Wiener index of graphs resulting from some unary and binary graph operations are potential problems that could be considered for further investigations by expressing the g-Wiener index of the graph resulting from the graph operations in terms of the g-Wiener index of the original graph being considered.

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