

ON THE TOPOLOGICAL INDICES OF THORNY-STAR GRAPHS

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ABSTRACT

Let G be the connected graph. The Wiener index $W(G)$ is the sum of all distances between vertices of G , whereas the hyper-Wiener index $WW(G)$ is defined as $WW(G) = W(G) + \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d(u,v)^2$. In this paper we prove some general results on the topological indices of thorny-star graphs and some bounds on it.

Keywords: Molecular graphs, Wiener index and hyper-Wiener index.

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1. INTRODUCTION

In mathematical terms a graph is represented as $G = (V, E)$ where V is the set of vertices and E is the set of edges. Let G be an undirected connected graph without loops or multiple edges with n vertices, denoted by $1, 2, \dots, n$. The topological distance between the vertices u and v of $V(G)$ is denoted by $d(u, v)$ or d_{uv} and it is defined as the number of edges in a minimal path connecting the vertices u and v .

The Wiener index $W(G)$ of a connected graph G is defined as the sum the distances between all unordered pairs of vertices of G . It was put forward by Harold Wiener. The Wiener index is a graph invariant intensively studied both in mathematics and chemical literature, see for details [1, 6, 7, 8, 10 and 12 – 14].

The hyper-Wiener index was proposed by Randić [11] for a tree and extended by Klein *et al.* [2] to a connected graph. It is used to predict physicochemical properties of organic compounds. The hyper-Wiener index defined as,

$$WW(G) = \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv} + 1}{2} = W(G) + \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} d(u,v)^2$$

The hyper-Wiener index is studied both from a theoretical point of view and applications. We encourage the reader to consult [4, 5, 10 and 12 – 15] for further readings. The hyper-Wiener index of complete graph- K_p , path graph- P_n , star graph- $K_{1,(n-1)}$ and cycle graph C_n is given by the expressions

$$WW(K_n) = \frac{n(n-1)}{2}, WW(P_n) = \frac{n^4 + 2n^3 - n^2 - 2n}{24}, WW(K_{1,(n-1)}) = \frac{1}{2}(n-1)(3n-4)$$

And

$$WW(C_n) = \begin{cases} \frac{n^2(n+1)(n+2)}{48}, & \text{if } n \text{ is even} \\ \frac{n(n^2-1)(n+3)}{48}, & \text{if } n \text{ is odd} \end{cases}$$

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2. MAIN RESULTS

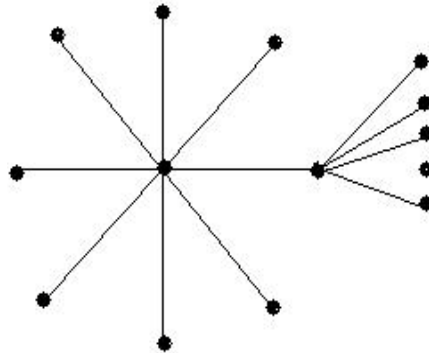
2.1 Wiener and hyper-Wiener indices of Thorny-star graphs in terms of number of vertices in a graph:

Theorem 1: Let H be the star graph on t vertices. The graph G obtained by attaching s-number of pendent vertices to any one pendent vertices of graph H with common vertex then its Wiener and hyper-Wiener indices given by

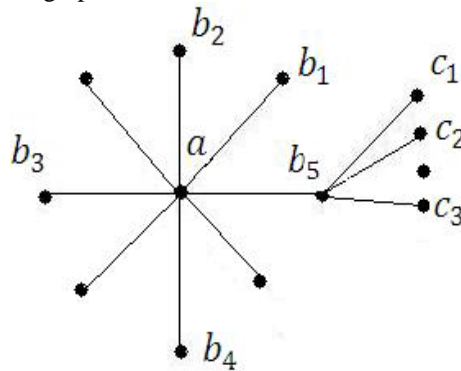
$$W(G) = \frac{1}{2} \{t(2t + 3s - 3) + S(3t + 2s - 5) + 2 - 3s - t\}$$

$$WW(G) = \frac{1}{2} \{t(3t + 6s - 5) + s(6t + 3s - 11) + 4 - 8s - 2t\}$$

where ‘n’ be the number of vertices in G and ‘s’ be the number of pendent vertices. The Schematic representation of G is shown as in below,



Proof: Let us consider the vertex labeled graph,



To find Wiener index of the graph,

$$W(G) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n d(u_i, u_j)$$

$$W(G) = \frac{1}{2} \{d(a | G) + \sum_{i=1}^{t-1} d(b_i | G) + \sum_{j=1}^s d(c_j | G)\}$$

$$W(G) = \frac{1}{2} \left[\left\{ \sum_{i=1}^{t-1} d(a | b_i) + \sum_{j=1}^s d(a | c_j) \right\} + (t-2) \left\{ 1 + \sum_{i=2}^{t-2} d(b_1 | b_i) + \sum_{j=1; b_5 \notin G}^s d(b_1 | c_j) \right\} \right. \\ \left. + \left\{ \sum_{i=1}^s d(b_5 | c_i) + 1 + \sum_{j=1}^{t-2} d(b_5 | b_j) \right\} + s \left\{ 1 + \sum_{i=1}^s d(c_i | c_1) + \sum_{j=1; b_5 \notin G}^{t-2} d(c_1 | b_j) \right\} \right]$$

$$W(G) = \frac{1}{2} \left[\{(t-1) \times 1 + s \times 2\} + (t-2) \{1 + (t-2) \times 2 + s \times 3\} + \{s \times 1 + 1 + (t-2) \times 2\} \right. \\ \left. + s \{1 + s \times 2 + (t-2) \times 3\} \right]$$

Where $d(a | b_1) = 1$; $d(a | c_1) = 2$; $d(b_1 | b_2) = 2$; $d(b_1 | c_1) = 3$;
 $d(b_5 | c_1) = 1$; $d(b_5 | b_1) = 2$; $d(c_1 | c_2) = 2$; $d(c_1 | b_1) = 3$.

$$W(G) = \frac{1}{2} [t - 1 + 2s + (t - 2)(2t + 3s - 3) + (2t + s - 3) + s(3t + 2s - 5)]$$

$$W(G) = \frac{1}{2} [t - 1 + 2s + t(2t + 3s - 3) - 4t - 6s + 6 + 2t + s - 3 + s(3t + 2s - 5)]$$

$$W(G) = \frac{1}{2} \{t(2t + 3s - 3) + S(3t + 2s - 5) + 2 - 3s - t\}$$

To find hyper-Wiener index of the graph,

$$WW(G) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n d(u_i, u_j)^2$$

$$WW(G) = \frac{1}{2} \{d(a | G) + \sum_{i=1}^{t-1} d(b_i | G)^2 + \sum_{j=1}^s d(c_j | G)^2\}$$

$$WW(G) = \frac{1}{2} \left[\left\{ \sum_{i=1}^{t-1} d(a | b_i)^2 + \sum_{j=1}^s d(a | c_j)^2 \right\} + (t-2) \left\{ 1 + \sum_{i=2}^{t-2} d(b_1 | b_i)^2 + \sum_{j=1; b_5 \notin G}^s d(b_1 | c_j)^2 \right\} \right. \\ \left. + \left\{ \sum_{i=1}^s d(b_5 | c_i)^2 + 1 + \sum_{j=1}^{t-2} d(b_5 | b_j)^2 \right\} + s \left\{ 1 + \sum_{i=1}^s d(c_i | c_1)^2 + \sum_{j=1; b_5 \notin G}^{t-2} d(c_1 | b_j)^2 \right\} \right]$$

$$WW(G) = \frac{1}{2} \left[\{(t-1) \times 1 + s \times 3\} + (t-2) \{1 + (t-2) \times 3 + s \times 6\} + \{s \times 1 + 1 + (t-2) \times 3\} \right. \\ \left. + s \{1 + s \times 3 + (t-2) \times 6\} \right]$$

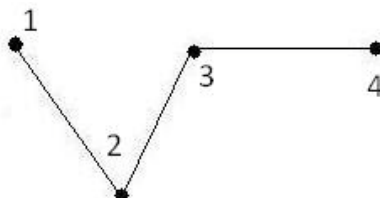
where $d(a | b_1)^2 = 1$; $d(a | c_1)^2 = 3$; $d(b_1 | b_2)^2 = 3$; $d(b_1 | c_1)^2 = 6$;
 $d(b_5 | c_1)^2 = 1$; $d(b_5 | b_1)^2 = 3$; $d(c_1 | c_2)^2 = 3$; $d(c_1 | b_1)^2 = 6$.

$$WW(G) = \frac{1}{2} \{(t-1 + 3s) + (t-2)(1 + 3t - 6 + 6s) + (s + 1 + 3t - 6) + s(1 + 3s + 6t - 12)\}$$

$$WW(G) = \frac{1}{2} \{t + 3s - 1 + (t-2)(3t + 6s - 5) + s(6t + 3s - 11) + 3t + s - 5\}$$

$$WW(G) = \frac{1}{2} \{t(3t + 6s - 5) + s(6t + 3s - 11) + 4 - 8s - 2t\}$$

Example: The molecular graph representing the chemical compound in figure below is 1, 2-Butadiene isomorphic to $S_{3,1}$. Where $S_{3,1}$ is the carbon skeleton of 1, 2-Butadiene.



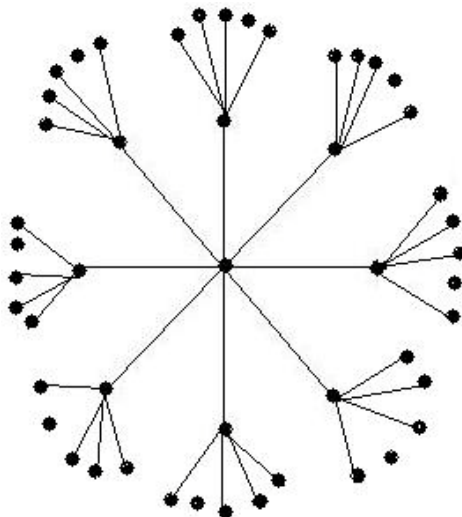
$t = 3, s = 1, W(G) = 10$, and $WW(G) = 15$.

Theorem 2: (Dendrimers) Let H be the star graph on t vertices. The graph G obtained by attaching s-number of pendent vertices to each pendent vertex of H with common vertex then its Wiener and hyper-Wiener index given by

$$W(G) = \frac{1}{2} \{t - 1 + 2p + (t-1)(2t + 3p - 7s - 3 + 3st + 4sp - 2s^2)\}$$

$$WW(G) = \frac{1}{2} \{3p + t - 1 + (t-1)(3t + 6p - 16s - 5 + 6st + 10sp - 7s^2)\}$$

Proof: The Schematic representation of G is shown as in below,



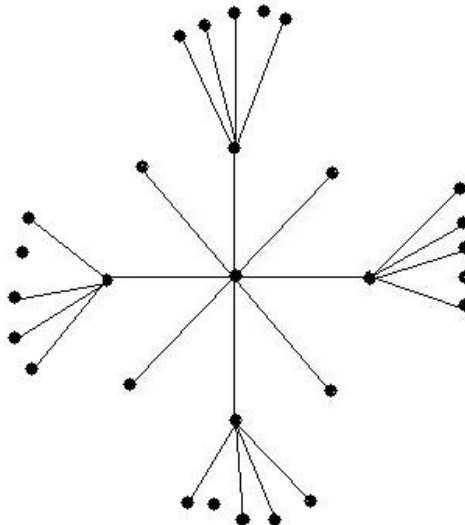
The Proof is similar to above theorem.

Theorem 3: (Dendrimers) Let H be the star graph on t vertices (t – 1 is even). The graph G obtained by attaching s-number of pendent vertices to alternative pendent vertex of graph H with common vertex then its Wiener and hyper-Wiener index given by

$$W(G) = \frac{1}{2} \left\{ \frac{t-1}{2} (4t + 6p - 3s - 5) + 4p^2 + 3pt - 2ps - 3p + t - 1 \right\}$$

$$WW(G) = \frac{1}{2} \left\{ \frac{t-1}{2} (6t + 12p - 6s - 9) + 10p^2 + 6pt - 7ps - 8p + t - 1 \right\}$$

Proof: The Schematic representation of G is shown as in below,



The Proof is similar to above theorem 1.

2.2 Bounds for Wiener and hyper-Wiener indices of acyclic molecular graphs:

Lemma 4: For acyclic molecular graphs following inequalities holds good,

$$1. (a). W(T) \geq \frac{1}{2} \{ t(2t + 3s - 3) + S(3t + 2s - 5) + 2 - 3s - t \}$$

$$(b). WW(T) \geq \frac{1}{2} \{ t(3t + 6s - 5) + s(6t + 3s - 11) + 4 - 8s - 2t \}$$

$$2. (a). W(G) \geq \frac{1}{2} \{ t - 1 + 2p + (t - 1)(2t + 3p - 7s - 3 + 3st + 4sp - 2s^2) \}$$

$$(b). WW(G) \geq \frac{1}{2} \{ 3p + t - 1 + (t - 1)(3t + 6p - 16s - 5 + 6st + 10sp - 7s^2) \}$$

$$3. (a). W(G) \geq \frac{1}{2} \left\{ \frac{t-1}{2} (4t + 6p - 3s - 5) + 4p^2 + 3pt - 2ps - 3p + t - 1 \right\}$$

$$(b). WW(G) \geq \frac{1}{2} \left\{ \frac{t-1}{2} (6t + 12p - 6s - 9) + 10p^2 + 6pt - 7ps - 8p + t - 1 \right\}$$

Proof: To prove, assertion 1. a. We know that among all acyclic graphs, the star $K_{1,(t-1)}$ has a minimum Wiener index and path graph P_n has a maximum Wiener index. So, we can get extreme class of graphs in acyclic molecular trees. Therefore symbolically represented as follows,

$$W(K_{1,(t-1)}) \leq W(G) \leq W(P_n)$$

In the assertion a. Graph under consideration is a star, so above inequality holds good.

$$W(T) \geq \frac{1}{2} \{ t(2t + 3s - 3) + S(3t + 2s - 5) + 2 - 3s - t \}$$

To prove, assertion 1. b. We know that among all acyclic graphs, the star $K_{1,(t-1)}$ has a minimum hyper-Wiener index and path graph P_n has a maximum hyper-Wiener index. So, we can get extreme class of graphs in acyclic molecular trees. Therefore symbolically represented as follows,

$$WW(K_{1,(t-1)}) \leq WW(G) \leq WW(P_n)$$

In the assertion b. Graph under consideration is a star, so above inequality holds good.

$$WW(T) \geq \frac{1}{2} \{ t(3t + 6s - 5) + s(6t + 3s - 11) + 4 - 8s - 2t \}$$

Proofs for results 2 and 3 are similar to 1. a. and 1. b.

We end the paper with the following simple but elegant lemma.

Lemma 5: Let T_1 , T_2 and T_3 are the thorny-star graphs then following inequalities holds good.

- $W(T_1) \leq W(T_3) \leq W(T_2)$
- $WW(T_1) \leq WW(T_3) \leq WW(T_2)$
- $W(T_i) < WW(T_i)$, Where $i = 1,2,3$.

Where

$$W(T_1) = \frac{1}{2}\{t(2t + 3s - 3) + S(3t + 2s - 5) + 2 - 3s - t\}$$

$$WW(T_1) = \frac{1}{2}\{t(3t + 6s - 5) + s(6t + 3s - 11) + 4 - 8s - 2t\}$$

$$W(T_2) = \frac{1}{2}\{t - 1 + 2p + (t - 1)(2t + 3p - 7s - 3 + 3st + 4sp - 2s^2)\}$$

$$WW(T_2) = \frac{1}{2}\{3p + t - 1 + (t - 1)(3t + 6p - 16s - 5 + 6st + 10sp - 7s^2)\}$$

$$W(T_3) = \frac{1}{2}\left\{\frac{t-1}{2}(4t + 6p - 3s - 5) + 4p^2 + 3pt - 2ps - 3p + t - 1\right\}$$

$$WW(T_3) = \frac{1}{2}\left\{\frac{t-1}{2}(6t + 12p - 6s - 9) + 10p^2 + 6pt - 7ps - 8p + t - 1\right\}$$

The proof is straightforward and omitted.

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