

ON THE HYPER-WIENER INDEX OF TREES

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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 hyper-Wiener index of trees and some bounds on it.

Keywords: acyclic graphs, molecular graphs 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 Randic [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_n , path graph- P_n , star graph- $K_{1,(n-1)}$ and cycle graph C_n is given by the expressions

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

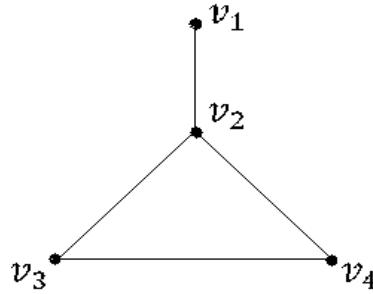
And

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

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For example: Consider a graph G with vertices v_1, v_2, v_3 and v_4 as labeled in the figure below.



Here $d(v_1, v_2) = 1, d(v_1, v_3) = 2, d(v_1, v_4) = 2, d(v_2, v_3) = 1, d(v_2, v_4) = 1, d(v_3, v_4) = 1$.

$$\begin{aligned} \text{Therefore } WW(G) &= \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv} + 1}{2} \\ &= \frac{2 \times 1}{2} + \frac{3 \times 2}{2} + \frac{3 \times 2}{2} + \frac{2 \times 1}{2} + \frac{2 \times 1}{2} + \frac{2 \times 1}{2} \\ &= 1 + 3 + 3 + 1 + 1 + 1 \\ &= 10 \end{aligned}$$

2. MAIN RESULTS

Claim 1: If $\beta_1(T) = 2$, then $3 \leq \text{diam}(T) \leq 4$.

If $\beta_1(T) = 2$ then we have following two trees of diameter 3 and 4 and which we denote them by $A_n(k)$ and $B_n(k)$ respectively.

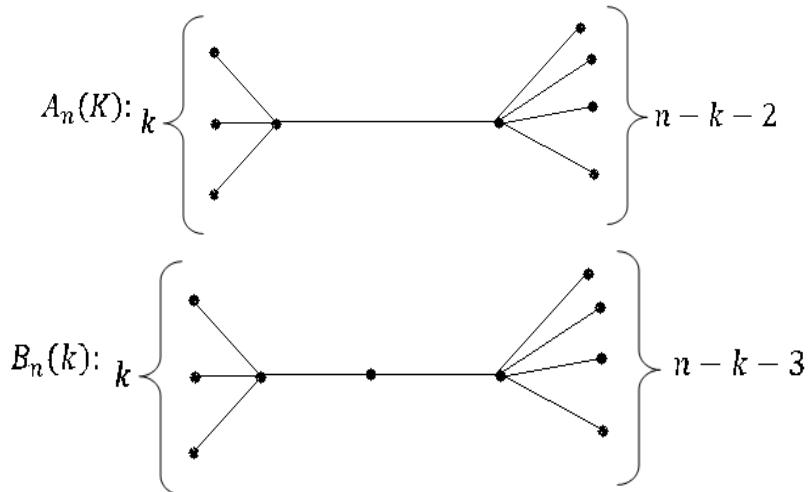


Figure-1

Lemma 2.1: Let $A_n(k)$ and $B_n(k)$ are the trees of order n , then its hyper wiener index given by

- (i) $WW(A_n(k)) = \frac{1}{2}[k(6n - 3k - 11) + (n - k - 2)(3n + 3k - 5) + 4n - 6]$
- (ii) $WW(B_n(k)) = \frac{1}{2}[k(10n - 7k - 23) + (n - k - 3)(3n + 7k - 2) + 10n - 20]$

Proof: To find hyper wiener index of: $A_n(k)$

$$\begin{aligned} WW(A_n(k)) &= \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv} + 1}{2} \\ &= \frac{1}{2} \left\{ \underbrace{(6n - 3k - 11) + \dots + (6n - 3k - 11)}_{k \text{ times}} + (3n - 2k - 5) + (n + 2k - 1) \right. \\ &\quad \left. + \underbrace{(3n + 3k - 5) + \dots + (3n + 3k - 5)}_{(n - k - 2) \text{ times}} \right\} \end{aligned}$$

$$WW(A_n(k)) = \frac{1}{2}[k(6n - 3k - 11) + (3n - 2k - 5) + (n + 2k - 1) + (n - k - 2)(3n + 3k - 5)]$$

$$WW(A_n(k)) = \frac{1}{2}[k(6n - 3k - 11) + (n - k - 2)(3n + 3k - 5) + 4n - 6]$$

To find hyper wiener index of: $B_n(k)$

$$\begin{aligned} WW(B_n(k)) &= \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv} + 1}{2} \\ &= \frac{1}{2} [(\underbrace{(10n - 7k - 23) + \dots + (10n - 7k - 23)}_{k \text{ times}}) \\ &\quad + (6n - 5k - 14) + (3n - 7) + (n + 5k + 1) \\ &\quad + (\underbrace{(3n + 7k - 2) + \dots + (3n + 7k - 2)}_{(n - k - 3) \text{ times}})] \end{aligned}$$

$$\begin{aligned} WW(B_n(k)) &= \frac{1}{2} [k(10n - 7k - 23) + (6n - 5k - 14) + (3n - 7) + (n + 5k + 1) + (n - k - 3)(3n + 7k - 2)] \\ WW(B_n(k)) &= \frac{1}{2} [k(10n - 7k - 23) + (n - k - 3)(3n + 7k - 2) + 10n - 20] \end{aligned}$$

Remark 1: Above result of the graph $A_n(k)$ used to find hyper-Wiener index of following chemical trees, Butane, 2-Methylbutane, 2, 2-Dimethylbutane, 2, 2, 3-Trimethylbutane, etc.

Theorem 2.2: Let $A_n(k)$ and $B_n(k)$ are the trees of orders n, as in figure 1. Then

- (i) $WW(A_n(1)) < WW(A_n(2)) < WW(A_n(3)) \dots < WW\left[A_n\left(\left\lfloor \frac{n-2}{2} \right\rfloor\right)\right]$
- (ii) $WW(B_n(1)) < WW(B_n(2)) < WW(B_n(3)) \dots < WW\left[B_n\left(\left\lfloor \frac{n-3}{2} \right\rfloor\right)\right]$

Proof: The integer valued function $f(n, k) = \frac{1}{2}[k(6n - 3k - 11) + (n - k - 2)(3n + 3k - 5) + 4n - 6]$ has the maximum value if $k = \left\lfloor \frac{n-2}{2} \right\rfloor$ and also it is strictly increasing one and thus we have

$$WW(A_n(1)) < WW(A_n(2)) < WW(A_n(3)) \dots < WW\left[A_n\left(\left\lfloor \frac{n-2}{2} \right\rfloor\right)\right]$$

Similarly, $\Phi(n, k) = \frac{1}{2}[k(10n - 7k - 23) + (n - k - 3)(3n + 7k - 2) + 10n - 20]$ achieves maximum value, if $k = \left\lfloor \frac{n-3}{2} \right\rfloor$ and it is also increasing one. Hence we have,

$$WW(B_n(1)) < WW(B_n(2)) < WW(B_n(3)) \dots < WW\left[B_n\left(\left\lfloor \frac{n-3}{2} \right\rfloor\right)\right]$$

Theorem 2.3: If $n > k + 3$, then $WW(A_n(k)) < WW(B_n(k))$

Proof: Let $n > k + 3$ and assume, to the contrary, that $WW(A_n(k)) \not< WW(B_n(k))$.

Thus $WW(A_n(k)) \geq WW(B_n(k))$. Since

$$WW(A_n(k)) = \frac{1}{2}[k(6n - 3k - 11) + (n - k - 2)(3n + 3k - 5) + 4n - 6] \text{ and}$$

$$WW(B_n(k)) = \frac{1}{2}[k(10n - 7k - 23) + (n - k - 3)(3n + 7k - 2) + 10n - 20]$$

Now consider $n=5$ and $k=1$, since $n > k + 3$. We obtain $WW(A_n(k)) = 28$ and $WW(B_n(k)) = 35$, it contradicts the fact that $WW(A_n(k)) \geq WW(B_n(k))$. Therefore If $n > k + 3$, then $WW(A_n(k)) < WW(B_n(k))$

Theorem 2.4: If $n > k + 2$, then $WW(A_n(k + 1)) < WW(B_n(k))$

Proof: Let $n > k + 2$ and assume, to the contrary, that $WW(A_n(k + 1)) \not< WW(B_n(k))$.

Thus $WW(A_n(k + 1)) \geq WW(B_n(k))$. Since

$$WW(A_n(k + 1)) = \frac{1}{2}[(k + 1)(6n - 3k - 11) + (n - k - 2)(3n + 3k - 5) + 4n - 6] \text{ and}$$

$$WW(B_n(k)) = \frac{1}{2}[k(10n - 7k - 23) + (n - k - 3)(3n + 7k - 2) + 10n - 20]$$

Now consider $n=5$ and $k=1$, since $n > k + 2$. We obtain $WW(A_n(k + 1)) = 28$ and $WW(B_n(k)) = 35$, it contradicts the fact that $WW(A_n(k + 1)) \geq WW(B_n(k))$. Therefore If $n > k + 2$, then $WW(A_n(k + 1)) < WW(B_n(k))$

Claim 2: If $\beta_1(T) = 3$, then $4 \leq \text{diam}(T) \leq 6$.

If $\beta_1(T) = 3$ then we have following six trees of diameter 4, 5 and 6 and which we denote them by $C_n(l, m, k)$, $D_n(l, m, k)$, $E_n(k)$, $F_n(l, m, k)$, $G_n(k)$ and $H_n(l, m, k)$ respectively.

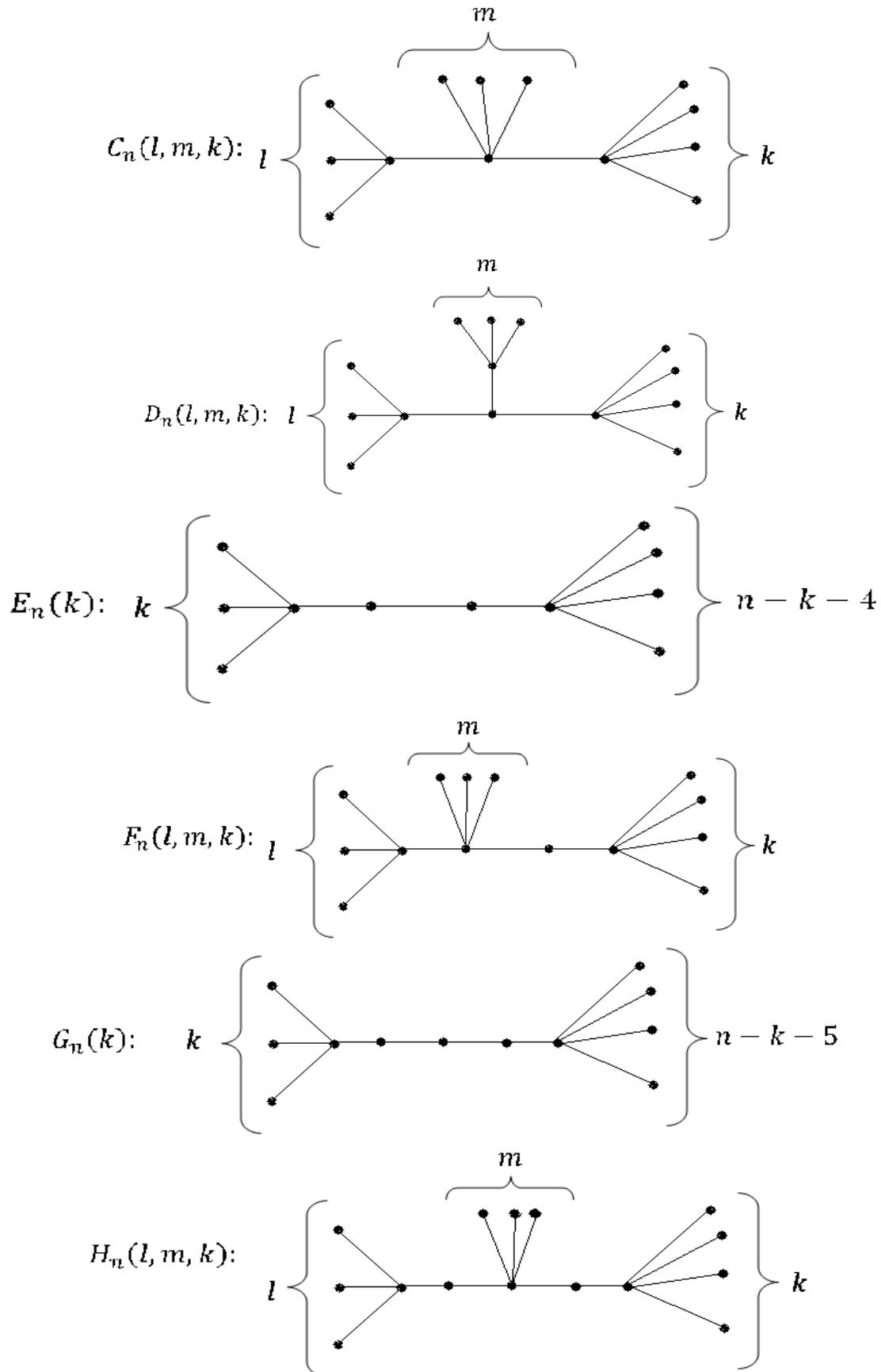


Figure-2

Lemma 2.5: Let $C_n(l, m, k)$, $D_n(l, m, k)$, $E_n(k)$, $F_n(l, m, k)$, $G_n(k)$ and $H_n(l, m, k)$ are the trees of orders n, then its hyper wiener index given by

- (i) $WW(C_n(l, m, k)) = \frac{1}{2} [l(3l + 6m + 10k + 7) + m(6l + 3m + 6k + 4) + k(10l + 6m + 3k + 7) + 10l + 7m + 10k + 10]$, Where $l + m + k + 3 = n$
- (ii) $WW(D_n(l, m, k)) = \frac{1}{2} [l(3l + 10m + 10k + 13) + m(10l + 3m + 10k + 13) + k(10l + 10m + 3k + 13) + 16l + 16m + 16k + 24]$, Where $l + m + k + 4 = n$
- (iii) $WW(E_n(k)) = \frac{1}{2} [k(15n - 12k - 43) + (n - k - 4)(3n + 12k + 5) + 20n - 50]$
- (iv) $WW(F_n(l, m, k)) = \frac{1}{2} [l(3l + 6m + 15k + 17) + m(6l + 3m + 10k + 10) + k(15l + 10m + 3k + 17) + 20l + 13m + 20k + 30]$, Where $l + m + k + 4 = n$
- (v) $WW(G_n(k)) = \frac{1}{2} [k(21n - 18k - 73) + (n - k - 5)(3n + 18k + 17) + 35n - 105]$
- (vi) $WW(H_n(l, m, k)) = \frac{1}{2} [l(3l + 10m + 21k + 32) + m(10l + 3m + 10k + 16) + k(21l + 10m + 3k + 32) + 35l + 19m + 35k + 70]$, Where $l + m + k + 5 = n$

Proof: To find hyper wiener index of: $C_n(l, m, k)$

$$\begin{aligned} WW(C_n(l, m, k)) &= \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv} + 1}{2} \\ &= \frac{1}{2} [\underbrace{(3l + 6m + 10k + 7) + \dots + (3l + 6m + 10k + 7)}_{l \text{ times}} + (l + 3m + 6k + 4) \\ &\quad + \underbrace{(3l + m + 3k + 2) + (6l + 3m + 6k + 4) + \dots + (6l + 3m + 6k + 4)}_{m \text{ times}} \\ &\quad + \underbrace{(6l + 3m + k + 4) + (10l + 6m + 3k + 7) + \dots + (10l + 6m + 3k + 7)}_{k \text{ times}}] \\ WW(C_n(l, m, k)) &= \frac{1}{2} [l(3l + 6m + 10k + 7) + (l + 3m + 6k + 4) + (3l + m + 3k + 2) \\ &\quad + m(6l + 3m + 6k + 4) + (6l + 3m + k + 4) + k(10l + 6m + 3k + 7)] \\ WW(C_n(l, m, k)) &= \frac{1}{2} [l(3l + 6m + 10k + 7) + m(6l + 3m + 6k + 4) + \\ &\quad k(10l + 6m + 3k + 7) + 10l + 7m + 10k + 10] \end{aligned}$$

To find hyper wiener index of: $D_n(l, m, k)$

$$\begin{aligned} WW(D_n(l, m, k)) &= \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv} + 1}{2} \\ &= \frac{1}{2} [\underbrace{(3l + 10m + 10k + 13) + \dots + (3l + 10m + 10k + 13)}_{l \text{ times}} \\ &\quad + \underbrace{(l + 6m + 6k + 7) + (3l + 3m + 3k + 3) + (6l + m + 6k + 7)}_{m \text{ times}} \\ &\quad + \underbrace{(10l + 3m + 10k + 13) + \dots + (10l + 3m + 10k + 13)}_{k \text{ times}}] \\ &+ (6l + 6m + k + 7) \\ &+ \underbrace{(10l + 10m + 3k + 13) + \dots + (10l + 10m + 3k + 13)}_{k \text{ times}} \\ WW(D_n(l, m, k)) &= \frac{1}{2} [l(3l + 10m + 10k + 13) + (l + 6m + 6k + 7) + (3l + 3m + 3k + 3) \\ &\quad + (6l + m + 6k + 7) + m(10l + 3m + 10k + 13) + (6l + 6m + k + 7) \\ &\quad + k(10l + 10m + 3k + 13)] \end{aligned}$$

$$\begin{aligned} WW(D_n(l, m, k)) &= \frac{1}{2} [l(3l + 10m + 10k + 13) + m(10l + 3m + 10k + 13) \\ &\quad + k(10l + 10m + 3k + 13) + 16l + 16m + 16k + 24] \end{aligned}$$

To find hyper wiener index of: $E_n(k)$

$$\begin{aligned} WW(E_n(k)) &= \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv} + 1}{2} \\ &= \frac{1}{2} \left[\underbrace{(15n - 12k - 43) + \dots + (15n - 12k - 43)}_{k \text{ times}} + (k + 10n - 10k - 30) \right. \\ &\quad +(3k + 6n - 6k - 19) + (6k + 3n - 3k - 7) + (n + 9k + 6) \\ &\quad \left. + \underbrace{(3n + 12k + 5) + \dots + (3n + 12k + 5)}_{(n - k - 4) \text{ times}} \right] \end{aligned}$$

$$WW(E_n(k)) = \frac{1}{2} [k(15n - 12k - 43) + (n - k - 4)(3n + 12k + 5) + (10n - 9k - 30) \\ + (6n - 3k - 19) + (3n + 3k - 7) + (n + 9k + 6)]$$

$$WW(E_n(k)) = \frac{1}{2} [k(15n - 12k - 43) + (n - k - 4)(3n + 12k + 5) + 20n - 50]$$

To find hyper wiener index of: $F_n(l, m, k)$

$$\begin{aligned} WW(F_n(l, m, k)) &= \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv} + 1}{2} \\ WW(F_n(l, m, k)) &= \frac{1}{2} \left[\underbrace{(3l + 6m + 15k + 17) + \dots + (3l + 6m + 15k + 17)}_{l \text{ times}} \right. \\ &\quad +(l + 3m + 10k + 10) + (3l + m + 6k + 5) \\ &\quad + \underbrace{(6l + 3m + 10k + 10) + \dots + (6l + 3m + 10k + 10)}_{m \text{ times}} \\ &\quad +(6l + 3m + 3k + 5) + (10l + 6m + k + 10) \\ &\quad \left. + \underbrace{(15l + 10m + 3k + 17) + \dots + (15l + 10m + 3k + 17)}_{k \text{ times}} \right] \end{aligned}$$

$$WW(F_n(l, m, k)) = \frac{1}{2} [l(3l + 6m + 15k + 17) + (l + 3m + 10k + 10) + (3l + m + 6k + 5) \\ + m(6l + 3m + 10k + 10) + (6l + 3m + 3k + 5) + (10l + 6m + k + 10) \\ + k(15l + 10m + 3k + 17)]$$

$$WW(F_n(l, m, k)) = \frac{1}{2} [l(3l + 6m + 15k + 17) + m(6l + 3m + 10k + 10) \\ + k(15l + 10m + 3k + 17) + 20l + 13m + 20k + 30]$$

To find hyper wiener index of: $G_n(k)$

$$\begin{aligned} WW(G_n(k)) &= \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv} + 1}{2} \\ WW(G_n(k)) &= \frac{1}{2} \left[\underbrace{(21n - 18k - 73) + \dots + (21n - 18k - 73)}_{k \text{ times}} + (15n - 14k - 55) \right. \\ &\quad +(10n - 7k - 39) + (6n - 22) + (3n + 7k - 4) + (n + 14k + 15) \\ &\quad + \underbrace{(3n + 18k + 17) + \dots + (3n + 18k + 17)}_{(n - k - 5) \text{ times}} \left. \right] \end{aligned}$$

$$WW(G_n(k)) = \frac{1}{2} [k(21n - 18k - 73) + (15n - 14k - 55) + (10n - 7k - 39) + (6n - 22) \\ + (3n + 7k - 4) + (n + 14k + 15) + (n - k - 5)(3n + 18k + 17)]$$

$$WW(G_n(k)) = \frac{1}{2} [k(21n - 18k - 73) + (n - k - 5)(3n + 18k + 17) + 35n - 105]$$

To find hyper wiener index of: $H_n(l, m, k)$

$$WW(H_n(l, m, k)) = \sum_{\{u,v\} \subseteq V(G)} \binom{d_{uv} + 1}{2}$$

$$WW(H_n(l, m, k)) = \frac{1}{2} [\underbrace{(3l + 10m + 21k + 32) + \dots + (3l + 10m + 21k + 32)}_{l \text{ times}}]$$

$$\begin{aligned} &+ (l + 6m + 15k + 20) + (3l + 3m + 10k + 11) + (6l + m + 6k + 8) \\ &+ \underbrace{(10l + 3m + 10k + 16) + \dots + (10l + 3m + 10k + 16)}_{m \text{ times}} \\ &+ (10l + 3m + 3k + 11) + (15l + 6m + k + 20) \\ &+ (21l + 10m + 3k + 32) + \dots + (21l + 10m + 3k + 32)] \end{aligned}$$

$$\begin{aligned} WW(H_n(l, m, k)) = \frac{1}{2} [&l(3l + 10m + 21k + 32) + (l + 6m + 15k + 20) \\ &+ (3l + 3m + 10k + 11) + (6l + m + 6k + 8) \\ &+ m(10l + 3m + 10k + 16) + (10l + 3m + 3k + 11) \\ &+ (15l + 6m + k + 20) + k(21l + 10m + 3k + 32)] \end{aligned}$$

$$\begin{aligned} WW(H_n(l, m, k)) = \frac{1}{2} [&l(3l + 10m + 21k + 32) + m(10l + 3m + 10k + 16) \\ &+ k(21l + 10m + 3k + 32) + 35l + 19m + 35k + 70] \end{aligned}$$

Remark 2: Above results of the graphs $B_n(k)$ and $C_n(l, m, k)$ used to find hyper-Wiener index of Pentane, 2, 4-Dimethylpentane, 2,2-Dimethylpentane, etc.

Remark 3: Similar way the results of the graphs $D_n(l, m, k)$, $E_n(k)$, $F_n(l, m, k)$, $G_n(k)$ and $H_n(l, m, k)$ used to find hyper-Wiener index of 3,3-Dimethylpentane, 2,3-Dimethylpentane, etc.

Theorem 2.6: For trees of the classes $C_n(l, m, k)$, $D_n(l, m, k)$, $E_n(k)$, $F_n(l, m, k)$, $G_n(k)$ and $H_n(l, m, k)$ following relations holds good

- (i) $WW(C_n(1, n - 5, 1)) \leq WW(C_n(l, m, k))$ for all $l, m, k \geq 1$ where $l + m + k + 3 = n$.
- (ii) $WW(D_n(1, n - 6, 1)) \leq WW(D_n(l, m, k))$ for all $l, m, k \geq 1$ where $l + m + k + 4 = n$.
- (iii) $WW(F_n(1, n - 6, 1)) \leq WW(F_n(l, m, k))$ for all $l, m, k \geq 1$ where $l + m + k + 4 = n$.
- (iv) $WW(H_n(1, n - 7, 1)) \leq WW(H_n(l, m, k))$ for all $l, m, k \geq 1$ where $l + m + k + 5 = n$.

Proof is similar to that of **theorem 2.4**

Theorem 2.7: Let $WW(E_n(k))$ and $WW(G_n(k))$ are trees as in the figure 2, then,

- (iii) $WW(E_n(1)) < WW(E_n(2)) < WW(E_n(3)) \dots < WW\left[E_n\left(\left\lfloor \frac{n-4}{2} \right\rfloor\right)\right]$
- (iv) $WW(G_n(1)) < WW(G_n(2)) < WW(G_n(3)) \dots < WW\left[G_n\left(\left\lfloor \frac{n-5}{2} \right\rfloor\right)\right]$

Proof is similar to that of **theorem 2.2**

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