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The Topological Indices of some Dendrimer Graphs

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ABSTRACT

In this paper, the Wiener and hyper Wiener indices of two kinds of dendrimer graphs are computed. Using the Wiener index formula, the Szeged, Schultz, PI and Gutman indices of these graphs are also determined.

1. INTRODUCTION

Let $\boldsymbol{G} = (V,E)$ be a simple connected graph with vertex set V and edge set E. A topological index of a simple connected graph G is a graph invariant which is related to the structure of the graph. The Wiener index is one of the best known topological index of a simple connected graph which is studied in both mathematical and chemical literature and it's definition is in terms of distances between arbitrary pairs of vertices, see for example [1, 2, 3, 4]. The Wiener index of G is denoted by $W(G)$ and it is defined by:

$$W(G)=\sum_{\{u,v\}\subseteq V(G)} d(u,v)=\frac{1}{2}\sum_{u\in V} d(u),$$

where $d(u,v)$ is the distance between vertices u and v and $d(u)=\sum_{v\in V} d(u,v)$.

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The Szeged index [5, 6] is another invariant of a graph which is based on the distribution of the vertices and introduced by Ivan Gutman and it is the same with the Wiener index in the case that G is a tree. The set of vertices of graph G which are closer to u (resp. v) than v (resp. u) is denoted by $N_u(e|G)$ (resp. $N_v(e|G)$). This index is defined as the summation of ($n_u(e|G)\ n_v(e|G)$) where $n_u(e|G)$ (resp. $n_v(e|G)$), is the number of vertices of graph G closer to u (resp. v) than v (resp. u), over all edges $e = uv$ of graph. Now, the Szeged index of G which is denoted by $Sz(G)$ is defined as:

$$Sz(G) = \sum_{e=uv\in E} (n_u(e|G).n_v(e|G)).$$

The Padmaker-Ivan (PI) index [7, 8] is another topological index of a simple connected graph that takes into account the distribution of edges so is closely related to Szeged index. The PI index of G is defined by

$$PI(G) = \sum_{e=uv\in E} (n_{eu}(e|G) + n_{ev}(e|G)),$$

where $(n_{eu}(e|G)$ (resp. $(n_{ev}(e|G)$) is the number of edges of the subgraph of G which has the vertex set $N_u(e|G)$ (resp. $N_v(e|G)$).

The molecular topological index (Schultz index) was introduced by Schultz and Schultz [9, 10]. In addition to the chemical applications, the Schultz index attracted some attention that in the case of a tree it is related to the Wiener index [11]. It is denoted by $S(G)$ and defined as follows:

$$S(G) = \sum_{\{u,v\}\subseteq V} (\rho(u) + \rho(v)),$$

where $\rho(u)$ (resp. $\rho(v)$) is the degree of vertex u (resp. v).

The Gutman index which attracts more attention recently is defined by Klavžar and Gutman in [11, 12]. This index is also known as the Schultz index of the second kind but in this paper the first name is used. Gutman [11] has proved that if G is a tree then there is a relation between Wiener and Gutman indices of G that we will mention this in Section 2. The Gutman index of G is denoted by $Gut(G)$ and is defined as follows:

$$Gut(G) = \Sigma_{\{u,v\}\subseteq V} (\rho(u)\rho(v))$$

The hyper–Wiener index is one of the graph invariants, used as a structure descriptor related to physicochemical properties of compounds. This index was introduced by Randić in 1993 as extension of Wiener index [13] and it has come to be known as the hyper–Wiener index by Klein [14]. The hyper–Wiener index of G is denoted by $WW(G)$ and is defined as follows:

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

Here we mainly try to determine the Wiener, hyper Wiener and PI indices of two kinds of dendrimer graphs (explained in Section 2), then the Schultz, Szeged and Gutman indices are obtained as results of the relation between the Wiener index with both the Schultz and Gutman indices.

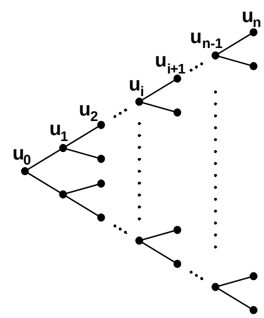

Figure 1. The first dendrimer graph G_n .

2. Calculating the Wiener, Hyper-Wiener and PI Indices of the First Dendrimer Graph G_n

Let G = (V,E) be the graph with vertex set V and edge set E as in Figure 1. This graph begins with one vertex u_0 which connects to two other vertices such that each one of these two vertices connects to two other vertices and so on. The vertices which have the same distance from u_0 are located on a branch. Let G have $(n+1)$ branches so there are 2^i vertices in the i'-th branch ($0 \le i \le n$). We denote this graph by G_n .

Proposition 2.1. Let $G_n = (V, E)$ be the dendrimer graph in Figure 1, then:

$$W(G_n) = 4^{(n+1)} (n - 2) + 2^{(n+1)} (n + 4).$$

Proof. From definitions we have:

$$W(G_n) = \sum_{\{u,v\}\subseteq V(G)} d(u,v) = \frac{1}{2} \sum_{u\in V} d(u).$$

This graph has $n+1$ branches and there are 2^i vertices in the i'–th branch, so we denote the vertex set of this branch by V_i, hence we have: $V = \bigcup_{i=0}^{n} V_i$. Because of the symmetric structure of the graph G_n (Figure l), for every vertex u in the n'th branch, $d(u)$ is constant and doesn't depend on u . So we choose u_i as representative of the i'–th branch ($0 \le i \le n$).

$$d(u_n)=\sum_{v\in V_n} d(u_n,v)+\sum_{v\in V-V_n} d(u_n,v). \tag{1}$$

2^{n-1} vertices which are in lower branch of Figure l, are of the same distance from u_n and this value equals to:

$$2d(u_n, u_0)=2n.$$

Also 2^{n-2} vertices are of the same distance from u_n and this value equals to:

$$2d(u_n,u_1)=2(n-1).$$

Finally continuing in this way the distance between u_n to the last vertex in the n'–th branch is equals to:

$$2d(u_n,u_{n-1})=2\,.$$

So we have:

$$\begin{aligned}\sum_{v\in V_n} d(u_n,v) &= 2^{n-1}\times 2n+2^{n-2}\times 2(n-1)+...+2^{(1-1)}2\\ =\sum_{v\in V_n} d(u_n,v) &= n2^{n}\times(n-1)2^{(n-1)}+...+1.2\\ =\sum_{i=1}^{n} i2^{i} &= 2(1+(n-1)2^{n}).\end{aligned} \tag{2}$$

For computing the second part of the summation in (1), note that because the graph G_n is a tree, for every vertex $v\in\bigcup_{i=0}^{n}V_i$ we have:

$$d(u_n,v)=1+d(u_{n-1},v)$$

$$\sum_{v\in\bigcup_{i=0}^{n-1}V_i} d(u_n,v)-\sum_{v\in\bigcup_{i=0}^{n-1}V_i} d(u_{(n-1)},v)=\sum_{i=0}^{n-1}2^{i}. \tag{3}$$

Considering (2) and (3):

$$d(u_n)-d(u_{n-1})=\sum_{i=0}^{n-1}2^{i}+2(1+(n-1)2^{n})=2n2^{n}-2^{n}+1\,.$$

Because, $d(u_o)=0.$ Hence :

$$d(u_n)=\sum_{i=1}^{n}(d(u_i)-d(u_{i-1}))=\sum_{i=1}^{n}2i2^{i}-2^{i}+1=(2n-3)2^{n+1}+n+6. \tag{4}$$

By multiplying 2^n in $d(u_n)$ the distance between vertices in the n'–th branch is considered twice, so if the Wiener index of G_n with n (resp. $n+1$) branch is denoted by $W(n+1)$ (resp. $W(n)$) we have:

$$\begin{aligned}W(n)-W(n-1) &= 2^{n}((2n-3)2^{n+1}+(n+6))-\sum_{\{u,v\}\subseteq V_n} d\ (u,v)\\ &= 2^{n}(2n-3)2^{(n+1)}+2^{n}(n+6)-2^{n}(1+(n-1)2^{n})\\ &= (3n-5)2^{2n}+(n+5)2^{n}.\end{aligned}$$

So,

$$W(n) = \sum_{i=1}^{n} (3k-5)2^{2k} + (k+5)2^{k} = 4^{(n+1)}\,(n-2) + 2^{(n+1)}\,(n+4). \qquad \blacksquare$$

Corollary 2.2. $Sz(G_n) = 4^{(n+1)}\,(n-2) + 2^{(n+1)}\,(n+4)$.

Proof. The graph G_n is a tree, so by [11] the result is obtained. ■

Corollary 2.3. $S(G_n) = 4^{(n+1)}\,(4n-9) + 2^{(n+1)}\,(4n+19) - 2$.

Proof. Because G_n is a tree by [11] we have: $S(G_n) = 4W(G_n) - n(n-1)$, where n is the number of vertices of G_n. Now by replacing the closed form of $W(G_n)$ which was obtained from proposition 2.1, the proof is completed. ■

Corollary 2.4. $Gut(G_n) = 4^{(n+1)}\,(4n-10) + 2^{(n+1)}\,(4n+19) + 10$.
Proof. Because G_n is a tree, by [11] we have, $Gut(G_n) = 4W(G_n) - (2n-1)(n-1)$ where n is the number of vertices of G_n and by proposition 2.1 it is done. ■

Corollary 2.5. $PI(G_n) = (2^{(n+1)} - 3)(2^{(n+1)} - 2)$.
Proof. Because G_n is a tree so for every edge $e = uv$ of G_n we have:

$$n_u(e \mid G_n) + n_v(e \mid G_n) = |V| = 2^{n+1} - 1.$$

Subgraphs of G_n with vertex sets $N_u(e \mid G_n)$ and $N_v(e \mid G_n)$ both are trees and whose number of edges are $n_u(e \mid G_n) - 1$ and $n_v(e \mid G_n) - 1$ respectively. Then we have:

$$\begin{aligned}
n_{eu}(e \mid G_n) + n_{ev}(e \mid G_n) &= n_u(e \mid G_n) + n_v(e \mid G_n) - 2 = 2^{n+1} - 3 \\
|E|(2^{(n+1)} - 3) &= (2^{(n+1)} - 2)(2^{(n+1)} - 3) \\
PI(G_n) &= |E|(2^{(n+1)} - 3) = (2^{(n+1)} - 2)(2^{(n+1)} - 3)
\end{aligned}$$

Proposition 2.6. The hyper–Wiener index of G_n in Figure 1 is:

$$WW(G_n) = 4^{n}(4n^2 - 14n + 24) + 2^{n}(n^2 - 3n - 31) - 1.$$

Proof. By definition we have:

$$WW(G) = \frac{1}{2}\Big(W(G) + \sum_{\{u,v\} \subseteq V} d^2(u,v)\Big). \qquad (5)$$

Because of the symmetric structure of the graph G_n in Figure l, d(u) for every vertex u in the n'–th branch is constant and doesn't depend on u, so we choose u_i as representative of the i'–th branch ($0 \le i \le 1$).

$$d^2(u_n) = \sum_{v\in V} d^2(u_n, v) = \sum_{v\in\bigcup_{i=0}^{n-1}V_i} d^2(u_n, v) + \sum_{v\in Vn} d^2(u_n, v). \tag{6}$$

The graph G_n is a tree, so, for every vertex, $v \in \bigcup_{i=0}^{n-1} V_i$:

$$d(u_n, v) = 1 + d(u_{n-1}, v) .$$

Now by (6) we have:

$$\begin{aligned} d^2(u_n) &= \sum_{v\in\bigcup_{i=0}^{n-1}V_i} (d\ \ (u_{n-1}, v) + 1)^2 + \sum_{v\in Vn} d^2(u_n, v) \\ &= \sum_{v\in\bigcup_{i=0}^{n-1}V_i} d^2(u_{n-1}, v) + 2\sum_{v\in\bigcup_{i=0}^{n-1}V_i} d\ \ (u_{n-1}, v) + \sum_{v\in V_n} d^2(u_n, v) + 2^n - 1 \\ &= d^2(u_{n-1}) + 2d(u_{n-1}) + \sum_{v\in Vn} d^2(u_n, v) + 2^n - 1. \end{aligned} \tag{7}$$

2^n vertices are in the n'–th branch and by symmetric structure of the graph G_n we have :

$$\begin{aligned} \sum_{v\in V_n} d^2(u_n, v) &= 2^{n-1}(2n)^2 + 2^{n-2}(2n-2)^2 + \ldots + 2^0(2)^2 \\ &= \sum_{i=1}^{n} 2^{i+1} i^2 = 2^{n+2}(n^2 - 2n + 3) - 12. \end{aligned} \tag{8}$$

By (4) in the proof of the proposition 2.1, and considering (7), (8):

$$\begin{aligned} d^2(u_n) &= \sum_{i=1}^{n} d^2(u_i) - d^2(u_{i-1}) \\ &= \sum_{i=1}^{n} (4i^2 - 4i + 3)2^i + 2i - 3 = 2^{n+1}(4n^2 - 12n + 19) + n^2 - 2n - 38 \end{aligned}$$

Therefore:

$$\begin{aligned} \Sigma_{\{u,v\}\subseteq V} d^2(u,v) - \Sigma_{\{u,v\}\subseteq\bigcup_{i=0}^{n-1}V_i} d^2(u,v) &= 2^n\ \ d^2(u_n) - \Sigma_{\{u,v\}\subseteq V_n} d^2(u,v) \\ &= 2^n\ \ d^2(u_n) - 2^{n-1}\Sigma_{v\in V_n} d^2(u_n, v) \\ &= 2^{2n+1}(3n^2 - 10n + 16) + 2n(n^2 - 2n - 32). \end{aligned}$$

Now let,

$$F(i) = \sum_{\{u,v\}\subseteq\bigcup_{i=0}^{i}V_j} d^2(u,v).$$

So,

$$\sum_{\{u,v\}\subseteq V} d^2(u,v) = \sum_{i=1}^{n} (F(i) - F(i-1)) = \sum_{i=1}^{n} 2^{2i+1}(3i^2 - 10i + 16) + 2^i(i^2 - 2i - 32)$$

$$= 4^{n+1}.2(n^2 - 4n + 7) + 2^{n+1}(n^2 - 4n - 27) - 2. \tag{9}$$

Now considering (9) and the formula of $W(G_n)$ which was computed in proposition 2.1, and replacing those in (5), the proof is done. ■

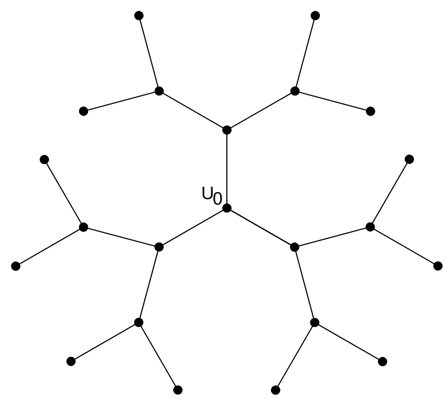

Figure 2. The second dendrimer graph H_n.

3. Calculating the Wiener, Hyper–Wiener and PI Indices of the Second Dendrimer Graph H_n

Let $G = (V,E)$ be the graph with vertex set V and edge set E, that begins with one vertex u_0 in Figure 2 that connects to three vertices which form the first branch and each one of these three vertices connects to two other vertices in second branch and so on. It means that any vertex but u_0 in the i'–th branch joins to the two vertices in the (i+1)'–th branch, so the vertices which have the same distance from u_0 are located on one branch. Let G have $n+1$ branches therefore, there are $3\times 2^{i-1}$vertices in the i'–th branch ($0 < \mathrm{i} \le n$). The graph G is another kind of dendrimer graph which have $n+1$ branches, which is denoted by H_n.

Proposition 3.1. Let $H_n = (V,E)$ be the dendrimer graph in Figure 2, then:

$$W(H_n) = 3(3\mathrm{n}-5)4^{\mathrm{n}} + 18\times 2^{\mathrm{n}} - 3.$$

Proof. The graph H_n consists of a starting vertex u_0 and n+1 branches such that the vertex set of the i'–th branch ($i > 0$), has $3\times 2^{i-1}$ vertices and is denoted by V_i and $|V_0|=1$. So we have:

$$|V| = 1 + |\bigcup_{i=0}^{n} V_i| = 1 + 3\sum_{i=0}^{n-1} 2^i = 3\times 2^n - 2.$$

Because of the symmetric structure of the graph G in Figure 2, $d(u)$ for every vertex u in the n'–th branch is constant and doesn't depend on u, so we choose u_i as representative of the i'–th branch ($0 \le \mathrm{i} \le n$).

$$d(u_n) = \sum_{v\in V_n} d(u_n, v) + \sum_{v\in V-V_n} d(u_n, v). \tag{10}$$

2/3 vertices in n'–th branch have the same distance from u_i which is:

$$2d(u_n, u_0) = 2n .$$

And the distance of 1/2 of the rest vertices in this branch from u_n is:

$$2d(u_n, u_1) = 2(n-1) .$$

By continuing in this way we have:

$$\begin{aligned}\sum_{v\in V_n} d(u_n, v) &= \frac{2}{3}(3\times 2^{n-1})\times 2d(u_n, u_0) + \frac{1}{2}\times\frac{1}{3}(3\times 2^{n-1})\times 2d(u_n, u_1)\\ &+\frac{1}{4}\times\frac{1}{3}(3\times 2^{n-1})\times 2d(u_n, u_2) + \ldots + \frac{1}{2^{n-1}}\times\frac{1}{3}(3\times 2^{n-1})2d(u_n, u_{n-1})\\ &2n\times 2^n + 2(n-1)\times 2^{n-2} + 2(n-2)\times 2^{n-3} + \ldots + 2\times 2^0\\ &n\times 2^n + \sum_{i=1}^{n} i2^i = 2 + (3n-2)\times 2^n.\end{aligned} \tag{11}$$

Now because H_n is a tree, the path between any two vertices is unique and for every vertex $v \in \bigcup_{i=0}^{n} V_i$ we have:

$$d(u_n, v) = 1 + d(u_{n-1}, v) .$$

So:

$$\sum_{v\in\bigcup_{i=0}^{n-1}V_i} d(u_n, v) - \sum_{v\in\bigcup_{i=0}^{n-1}V_i} d(u_{(n-1)}, v) = |\bigcup_{i=0}^{n-1} V_i| = 3\times 2^{n-1} - 2. \tag{12}$$

By (10), (11) and (12) we have:

$$\begin{aligned} d(u_n) - d(u_{n-1}) &= \sum_{v\in V_n} d(u_n, v) - \sum_{v\in V-V_n} d(u_{(n-1)}, v)\\ 2 + (3n-2)2^n + (3\times 2^{(n-1)}) - 2 &= (6n-1)2^{n-1} - 2^n + 1\\ d(u_n) &= \sum_{i=1}^{n} d(u_i) - d(u_{i-1}) = 7 + (6n-7)2^n \end{aligned}$$

If the Wiener index of H_n with $n+1$ branches is denoted by $W(n)$, we have:

$$\begin{aligned} W(n) - W(n-1) &= 3\times 2^{(n-1)}\left(7 + (6n-7)2^n\right) - \frac{1}{2}(3\times 2^{n-1})(2 + (3n-2)2^n)\\ &18\times 2^{n-1}((3n-4).2^{n-2} + 1) \end{aligned}$$

Therefore,

$$W(n) = \sum_{i=0}^{n} 18\times 2^{i-1}((3i-4).2^{i-2} + 1) = 3(3n-5)4^n + 18\times 2^n - 3 .$$

And the proof is completed. ■

Corollary 3.2. $Sz(H_n) = 3(3\mathrm{n} - 5)4^{\mathrm{n}} + 18 \times 2^{\mathrm{n}} - 3$.

Proof. The graph H_n is a tree so, by [11] the result is obtained. ■

Corollary 3.3. $S(H_n) = 4^{\mathrm{n}}(36\mathrm{n} - 69) + 87(2^{\mathrm{n}}) - 18$.

Proof. Because H_n is a tree by [11] we have, $S(G_n) = 4W(G_n) - \mathrm{n}(\mathrm{n}-1)$, where n is the number of vertices of H_n. Now by replacing the closed form of $W(H_n)$ which was obtained from proposition 3.1, the proof is completed. ■

Corollary 3.4. $Gut(G_n) = 4^{\mathrm{n}}(36\mathrm{n} - 78) + 105(2^{\mathrm{n}}) - 97$.

Proof. Because H_n is a tree by [11] we have, $Gut(G_n) = 4W(G_n) - (2\mathrm{n}-1)(\mathrm{n}-1)$ which n is the number of vertices of H_n and by proposition 3.1 it is done. ■

Corollary 3.5. $PI(H_n) = (3 \times 2^{\mathrm{n}} - 3)(3 \times 2^{\mathrm{n}} - 4)$.

Proof. Because H_n is a tree so for every edge $e = uv$ of H_n we have:

$$n_u(e \mid \mathrm{H_n}) + n_v(e \mid \mathrm{H_n}) = |V| = 3 \times 2^{\mathrm{n}} - 2.$$

Subgraphs of H_n with vertex sets $N_u(e \mid \mathrm{H_n})$ and $N_v(e \mid H_n)$ both are trees, so the number of edges of them are $n_u(e \mid \mathrm{H_n}) - 1$ and $n_v(e \mid \mathrm{H_n}) - 1$ respectively. Then we have*:*

$$\begin{aligned} n_{eu}(e \mid \mathrm{H_n}) + n_{ev}(e \mid \mathrm{H_n}) &= n_u(e \mid \mathrm{H_n}) + n_v(e \mid \mathrm{H_n}) - 2 = 3 \times 2^{\mathrm{n}} - 2 \\ PI(H_n) = |E|(3 \times 2^{\mathrm{n}} - 4) &= (3 \times 2^{\mathrm{n}} - 3)(3 \times 2^{\mathrm{n+1}} - 4) \end{aligned}$$

Proposition 3.6. The hyper–Wiener index of H_n is:

$$WW(H_n) = \frac{1}{2}\left((18\mathrm{n}^2 - 51\mathrm{n} + 81)4^{\mathrm{n}} - 87(2^{\mathrm{n}}) + 6\right).$$

Proof. By the definition we have:

$$WW(H_n) = \frac{1}{2}\left(W(H_n) + \sum_{\{u,v\} \subseteq V} d^2(u,v)\right). \tag{14}$$

Because of the symmetric structure of the graph H_n Figure 2, *d(u)* for every vertex *u* in the *n*'–th branch is constant and doesn't depend on *u*, so we choose u_i as representative of the *i*'–th branch ($0 \le \mathrm{i} \le 1$).

$$d^2(u_n) = \sum_{v \in V} d^2(u_n, v) = \sum_{v \in \bigcup_{i=0}^{n-1} V_i} d^2(u_n, v) + \sum_{v \in Vn} d^2(u_n, v). \tag{15}$$

The graph H_n is a tree so, for any vertex $v \in \bigcup_{i=0}^{n-1} V_i$:

$$d(u_n, v) = 1 + d(u_{n-1}, v)$$

Now by (15) we have:

$$\begin{aligned} d^2(u_n) &= \sum_{v \in \bigcup_{i=0}^{n-1} V_i} (d\ (u_{n-1}, v) + 1)^2 + \sum_{v \in Vn} d^2(u_n, v) \\ &= \sum_{v \in \bigcup_{i=0}^{n-1} V_i} d^2(u_{n-1}, v) + 2\sum_{v \in \bigcup_{i=0}^{n-1} V_i} d\ (u_{n-1}, v) + \sum_{v \in V_n} d^2(u_n, v) + 3 \times 2^{n-1} - 2 \\ &= d^2(u_{n-1}) + 2d(u_{n-1}) + \sum_{v \in Vn} d^2(u_n, v) + 3 \times 2^{n-1} - 2. \end{aligned} \tag{16}$$

2/3 vertices of the n'–th branch have the same distance from u_n which is:

$$2d(u_n, u_0) = 2n,$$

and the distance of 1/2 of the rest vertices in this branch from u_n is:

$$\begin{aligned} \sum_{v \in V_n} d^2(u_n, v) &= \frac{2}{3}(3 \times 2^{n-1})(2n)^2 + \frac{1}{2}.\frac{1}{3}(3 \times 2^{n-1})(2n-2)^2 \\ &+ \frac{1}{4}.\frac{1}{3}(3 \times 2^{n-1})(2n-4)^2 + \ldots + 2^0(2)^2 \\ &2^{n+2}n^2 + 2^n(n-1)^2 + 2^{(n-1)}(n-2)^2 + \ldots + 2^0(2)^2 \\ &= 2^{n+1}n^2 + \sum_{i=1}^{n} 2^{i+1} i^2 = 2^{n+1}(3n^2 - 4n + 6) - 12. \end{aligned} \tag{17}$$

By (13) in the proof of the proposition 3.1, and considering (16), (17):

$$\begin{aligned} d^2(u_n) &= \sum_{i=1}^{n} d^2(u_i) - d^2(u_{i-1}) \\ &= \sum_{i=1}^{n} 2^{i-1}(12i^2 - 4i + 1) = (12n^2 - 28n + 41)2^n - 41 \end{aligned}$$

Therefore:

$$\begin{aligned} \sum_{\{u,v\} \subseteq V} d^2(u, v) - \sum_{\{u,v\} \subseteq \bigcup_{i=0}^{n-1} V_i} d^2(u, v) &= (3 \times 2^n \ - 2) d^2(u_n) - \sum_{\{u,v\} \subseteq V_n} d^2(u, v) \\ &= (3 \times 2^n \ - 2) d^2(u_n) - (3 \times 2^{n-2}) \sum_{v \in V_n} d^2(u_n, v). \end{aligned}$$

Now let,

$$F(i) = \sum_{\{u,v\} \subseteq \bigcup_{j=0}^{i} V_j} d^2(u, v).$$

So, we have:

$$\sum_{\{u,v\} \subseteq V} d^2(u, v) = \sum_{i=1}^{n} F(i) - F(i-1) = 6(3n^2 - 10n + 16)4^n - 105(2^n) + 9. \tag{18}$$

Now considering (18) and the formula of $W(H_n)$ which was computed in Proposition 3.1, and replacing those in (14), the proof is done. ■

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