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HARARY INDEX OF AN INFINITE FAMILY OF DENDRIMER NANOSTARS

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ABSTRACT. Let G be a simple graph. The Harary index of G is defined as the sum of reciprocal distances.Dendrimer nanostars form a new group of macromolecules that show photon funnels just like artificial antennas and also are resistant to photo-bleaching. In this paper we compute the Harary index for an infinite family of dendrimer nanostars.

Keywords: *Harary index; Wiener index; Dendrimer nanostar.*

INTRODUCTION

A simple graph $G=(V,E)$ is a finite nonempty set $V(G)$ of objects called vertices, together with a (possibly empty) set $E(G)$ of unordered pairs of distinct vertices of G called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds.

In theoretical chemistry, molecular structure descriptors (also called topological indices) are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds [1,2]. There exist several types of such indices, especially those based on graph theoretical distances. In 1993 Plavsic et al. [3] and Ivanciuc et al. [4] independently introduced a new topological index, named Harary index, in honor of Frank Harary on the occasion of his 70th birthday. This topological index is derived from the reciprocal distance matrix and is related to a number of interesting physico-chemical properties [5-9].

The Harary index is defined as the half-sum of the elements in the reciprocal distance matrix (also called the Harary matrix [10]):

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

where $d(u,v)$ denotes the distance between vertices u and v and the sum goes over all the pairs of vertices.

The Wiener index of a connected graph G is denoted by $W(G)$ and is defined as the sum of distances between all pairs of vertices in G [11]:

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

Dendrimers are a new class of polymeric materials. They are highly branched, mono-disperse macromolecules. The structure of these materials has a great impact on their physical and chemical properties. As a result of their unique behavior, dendrimers are suitable for a wide range of biomedical and industrial applications. Recently some people investigated the mathematical properties of these nanostructures [12-22].

In the next section, we present a method to compute the Harary index for an infinite family of dendrimer nanostars.

MAIN RESULTS

In this section we shall compute the Harary index for a family of dendrimer nanostars. We consider the dendrimer grown n steps denoted $D_1[n]$. Figure 1 shows $D_1[4]$. Note that there are three edges between each two hexagons in this dendrimer.

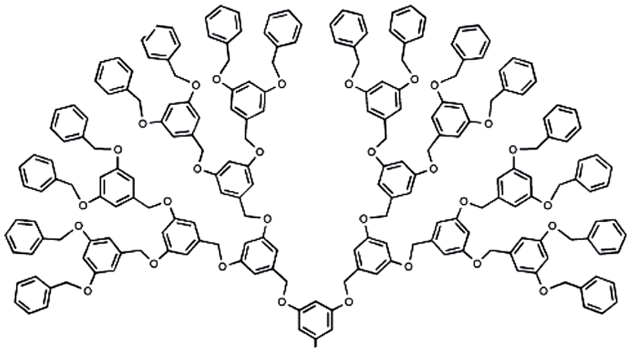

Figure 1. Dendrimer $D_1[4]$ of generation 1-4.

Recall that in computer science, a binary tree is a tree data structure in which each node has at most two child nodes, usually distinguished as “left” and “right”. Nodes with children are parent nodes, and child nodes may contain references to their parents. Outside the tree, there is often a reference to the “root” node (the ancestor of all nodes), if it exists. Any node in the data structure can be reached by starting at root node and repeatedly following references to either the left or right child.

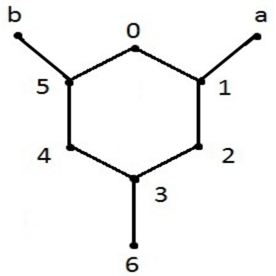

Figure 2. Labeled hexagon.

We label each vertices of hexagon with three pendant edges as shown in Figure 2. Let us denote the first hexagon (root) of $D_1[n]$ by symbol O We also denote the right child and the left child of O by $O(1)$ and $O(2)$, respectively. Let $O(x_1 \ldots x_{k-1})$ be a dendrimer which has grown until $(k-1)$-th stage. As was shown above, we shall denote its left and right child by $O(x_1 \ldots x_{k-1}1)$ and $O(x_1 \ldots x_{k-1}2)$, respectively. Now suppose that $x, y \in \{0,1,\ldots,6,a,b\}$. By $x(O(x_1 \ldots x_i))$, we mean the vertex x in hexagon $O(x_1 \ldots x_i)$. We shall compute the distance of two arbitrary vertices $x(O(x_1 \ldots x_i))$ and $y(O(y_1 \ldots y_j))$.

Theorem 1. *The distance of two arbitrary vertices* $x(O(x_1 \ldots x_i))$ *and* $y(O(y_1 \ldots y_j))$ *is obtained as follows:*

1. $d(x(O), y(O(y_1 \ldots y_j)) = \begin{cases} d(x,a) + d(y,6) + 5j - 4; & y_1 = 1, \\ d(x,b) + d(y,6) + 5j - 4; & y_1 = 2; \end{cases}$
2. $d(x(O(x_1 \ldots x_k)), y(O(x_1 \ldots x_k x_{k+1} \ldots x_j)) = d(x(O), y(O(x_{k+1} \ldots x_j)))$.
3. $d(x(O(x_1 \ldots x_k)), y(O(y_1 \ldots y_j)) = d(x,6) + d(y,6) + 5(j + i - 2r) + 6$,

where r is defined as $r = min\{i : x_i \neq y_i\}$.

Proof. It is straightforward and follows from the construction of $D_1[n]$.

Now we try to compute the Harary index of $D_1[n]$. Consider the following polynomial as Harary polynomial of which value at $x=1$ gives the Harary index of a graph.

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

The following theorem gives the coefficient of x^i of $H(D_1[n],x)$ for $1 \le i \le 5$. Our method led us to develop an approach for computing the coefficient x^i in $H(D_1[n],x)$ for $i \ge 6$ (see Theorem 4).

Theorem 2.

1. The coefficient of x in $H(D_1[n],x)$ is $2^{n+4}-9$.
2. The coefficient of x^2 in $H(D_1[n],x)$ is $12\times 2^n - 8$.
3. The coefficient of x^3 in $H(D_1[n],x)$ is $\frac{27\times 2^n - 22}{3}$.
4. The coefficient of x^4 in $H(D_1[n],x)$ is $\frac{23\times 2^n - 22}{4}$.
5. The coefficient of x^5 in $H(D_1[n],x)$ is $\frac{28(2^n - 1)}{5}$.

Proof.

1. The coefficient of x in $H(D_1[n],x)$ is the number of edges of $D_1[n]$. It is easy to see that the number of its edges is $2^{n+4}-9$.

2. To evaluate the coefficient of x^2, we compute the number of pair vertices which have distance 2 and are in different hexagons. So we have to consider two cases of Part (i) of Theorem 1, that is $d(x,a)+d(y,6)+5j-4=2$ or $d(x,b)+d(y,6)+5j-4=2$. In the both cases $j=1$. In the first case $\{d(x,a),d(y,6)\}=\{0,1\}$ or for the second case $\{d(x,b),d(y,6)\}=\{0,1\}$. Obviously $y=6$ is one of the answers. For this case there are two cases $(1,6)$ and $(5,6)$. Also if $d(y,6)=1$, then $y=3$ and $x=a$ or $x=b$. Therefore we have four solutions: $(a(O),3(O(1)),(b(O),3(O(2))),(1(O),6(O(1)))$ and $(5(O),6(O(2)))$. Now by considering the Part (ii) of the Theorem 1 all of the pair vertices of distance 2 are:

$$\begin{matrix}(a(O(x_1...x_k)),3(O(x_1...x_k1))),(1(O(x_1...x_k)),6(O(x_1...x_k1))),\\(b(O(x_1...x_k)),3(O(x_1...x_k2))),(5(O(x_1...x_k)),6(O(x_1...x_k2)))\end{matrix}\quad(1\le k\le n-1).$$

Therefore the number of solutions are $4(2^n-1)$. By the other hand, there are 12 pair vertices of distance 2 in any hexagon, and so the coefficient of x^2 is

$$\frac{1}{2}(4(2^n-1)+12(1+2+...+2^{n-1})+8(2^n))=\frac{4(2^n-1)+12(2^n-1)+8(2^n)}{2}=12\times 2^n-8$$

3. The proof of part (iii), (iv), and (v) are similar to proof of part(ii).

Theorem 3.

1. The diameter of $D_1[n]$ is $10n+4$. 2. The radius of $D_1[n]$ is $5n+4$.

Proof.

1. It is obvious that the most distances between two vertices of this graph are between $x\in O(x_1...x_n)$ and $y\in O(y_1...y_n)$, where $x_1\neq y_1$ and $x=y=0$. By Theorem 1(iii) we have

$$d(0O(x_1,...x_n),0O(y_1,...y_n))=2d(0,6)+5((2n-2)+6)=10n+4.$$

2. Note that the radius of a graph G is $r(G)=min_x max_y\{d(x,y)\mid y\in V(G)\}$. This minimum occurs when $x=6\in O$ and the maximum of $\{d(6,y)\mid y\in V(D_1[n])\}=5n+4$ and this occurs when $y=0O(x_1...x_n))$ by Theorem 1(i).

Now we shall compute the coefficient of x^l in $H(D_1[n],x))=\frac{1}{l}\sum x^l$, where $l\geq 6$.We need the following lemma, of which proof can be obtained directly by considering all the possibilities.

Lemma 1. *Let x,y,a and 6 be vertices of hexagons of $D_1[n]$ with the positions shown in Figure 2. Then we have the following table:*

Case	Equation	No. of solutions
1	$d(x,a)+d(y,6)=4$	13
2	$d(x,6)+d(y,6)=4$	14
3	$d(x,a)+d(y,6)=0$	1
4	$d(x,a)+d(y,6)=5$	13
5	$d(x,6)+d(y,6)=5$	14
6	$d(x,a)+d(y,6)=6$	18
7	$d(x,6)+d(y,6)=1$	2
8	$d(x,6)+d(y,6)=6$	16

Case	Equation	No. of solutions
9	$d(x,a)+d(y,6)=2$	5
10	$d(x,6)+d(y,6)=7$	12
11	$d(x,6)+d(y,6)=2$	5
12	$d(x,6)+d(y,6)=7$	12
13	$d(x,a)+d(y,6)=3$	8
14	$d(x,a)+d(y,6)=8$	9
15	$d(x,6)+d(y,6)=3$	8
16	$d(x,6)+d(y,6)=8$	9

Proof. It is straightforward and is obtained directly by considering all the possibilities.

Here we state the main theorem of this paper which gives the coefficients of x^l in $H(D_1[n],x)$ for $l \geq 6$. First we use the following notations:

$$A = 2^{n+1} - 2^q,\ B = 2^{n+1} - 2^{q+1},\ C = 2^{n+1} - 2^{q+2},$$
$$D = \sum_{r=0}^{\lfloor \frac{2n-q+3}{2} \rfloor}(2n-q-2r+1),\ E = \sum_{r=0}^{\lfloor \frac{2n-q+2}{2} \rfloor}(2n-q-2r-2).$$

Theorem 4. *Suppose that the Harary polynomial of* $D_1[n]$ *is*

$$H(D_1[n],x) = \sum_{u,v\in V} \frac{1}{d(u,v)} x^{d(u,v)} = \frac{1}{d(u,v)} \sum_{l=1}^{10n+4} a_l x^l.$$

Then for every $l \geq 6$*, we have*

$$a_l = \begin{cases} 13A+14D; & if\ l \equiv 0\ (\ mod\ 5), \\ B+13C+14D; & if\ l \equiv 1\ (\ mod\ 5) \\ 18A+16D+2E; & if\ l \equiv 2\ (\ mod\ 5) \\ 12A+5B+12D+5E; & if\ l \equiv 3\ (\ mod\ 5) \\ 8B+9D+8E; & if\ l \equiv 4\ (\ mod\ 5)\ . \end{cases}$$

Proof. We prove the theorem for case $l \equiv 0(\ mod\, 5)$. Let $l = 5q$, for some $q \in$ N Therefore we have $d(x,a)+d(y,6)+5j-4=5q$ and so $d(x,a)+d(y,6)=4$. By Lemma 1 there are 13 cases. By solving the equation of Theorem 1 (i) we will have $q = j$, and by Part (ii) of this theorem the number of all possibilities are

$$13\times 2^q(1+2+\ldots+2^{n-q}) = 13(2^{n+1}-2^q) = 13A.$$

Now by considering the part (iii) of Theorem 1, we have to find the number of solutions of $d(x,6)+d(y,6)+5(i+j-2r)+6=5q$. When $d(x,6)+d(y,6)=4$ this equation has solution, and this occurs for 14 different cases by Lemma 1. With substituting in this equation we have $i+j=q+2r-2$, where $r \le i, j \le n$. This equation is equivalent to $i'+j'=q-2$, $(0 \le i', j' \le n-r)$ or equivalent to $i''+j''=2n-2r-q+2$, where i'' and j'' are non-negative. By inclusion-exclusion principle the number of solutions of this equation is

$$D=\sum_{r=0}^{\lfloor \frac{2n-q+3}{2} \rfloor}(2n-q-2r+1).$$

Since there are 14 cases for this part, we have $a_l = 13A+14D$ and the proof is complete.

We have the following result:

Corollary 1. *The Harary index of* $D_1[n]$ *is*

$$H(D_1[n])=(2^{n+4}-9)+\frac{1}{2}(24\times 2^n-16)+\frac{1}{3}(27\times 2^n-22)+\frac{1}{4}(23\times 2^n-22)+\frac{1}{5}(28(2^n-1))+\frac{1}{l}\sum_{l=6}^{10n+4}a_l x^l,$$

where a_l is obtained in Theorem 4.

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