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Harary Index of Dendrimer Nanostar $NS_2[n]$

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Abstract

Let G be a simple graph. The Harary index of G is defined as

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

where $d(u,v)$ denotes the distance between disjoint vertices u and v. The dendrimer nanostar is a part of a new group of macromolecules that seem photon funnels just like artificial antennas and also is a great resistant of photo bleaching. In this paper we compute the Harary index for an infinite family of dendrimer nanostar.

1 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 [16, 17]. There exist several types of such indices, especially those based on graph theoretical distances. In 1993 Plavsic et al. in [15] and Ivanciuc et al. in [11] independently introduced a new topological index, which was 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 has a number of interesting chemicalphysics properties [12]. The Harary index and its related molecular descriptors have shown some success in structure-property correlations [3–5, 8].

The Harary index is defined as the half-sum of the elements in the reciprocal distance matrix (also called the Harary matrix [18]),

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

where $d(u,v)$ denotes the distance between disjoint 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 defined as the sum of distances between all pairs of vertices in G ([9]), i.e.,

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

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 [13]. Recently some people investigated the mathematical properties of this nanostructures in [1, 2, 6, 7, 10, 14, 18].

In this paper, we compute Harary index of an infinite family of nanostar dendrimer. In Section 2 we compute the Harary index of a graph with inductive structure denoted by $NS_1'[n]$ which is a branch of an infinite family of dendrimer $NS_2[n]$. In Section 3 we use results in Section 2 to compute the Harary index of an infinite family of dendrimer nanostar $NS_2[n]$.

As usual we denote diameter and radius of a graph G by $diam(G)$ and $r(G)$, respectively.

2 Harary index of $NS_2'[n]$

In this section we introduce a graph with inductive structure denoted by $NS_2'[n]$ which is useful for the study of an infinite family of dendrimer. We need some definitions. Figure 1 show $NS_2'[3]$.

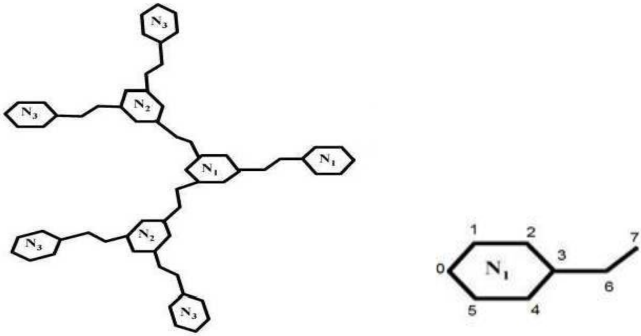

Figure 1. $NS_2'[3]$ and labeled hexagon, respectively.

We 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.

We label every vertices of hexagon with pendant path as shown in Figure 1. Let to denote the first hexagon (root) of $NS_2'[n]$ by symbol O. We also denote the right child and the left child of O by $O(1)$ and $O(2)$, respectively. Let $O(x_1...x_{k-1})$ be dendrimer which has grown until $(k-1)$-th stage. As know we shall denote its left and right child by $O(x_1...x_{k-1}1)$ and $O(x_1...x_{k-1}2)$, respectively. Now suppose that $x, y \in \{0,1,\ldots,7\}$. We mean $x(O(x_1...x_i))$ a vertex x in hexagon $O(x_1...x_i)$. We shall compute the distance of two arbitrary vertices $x(O(x_1...x_i))$ and $y(O(y_1...y_j))$. We obtain the following theorem which its proof follows from the construction of $NS_2[n]$ and left to reader.

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

1. $d(x(O), y(O(y_1...y_j)) = d(x,0) + d(y,7) + 5j - 4$

2. $d(x(O(x_1...x_k)), y(O(x_1...x_k x_{k+1}...x_j)) = d(x,1) + d(y,7) + 5(j-k) - 4$, where $x_{k+1} = 1$

and

$d(x(O(x_1...x_k)), y(O(x_1...x_k x_{k+1}...x_j)) = d(x,5) + d(y,7) + 5(j-k) - 4$, where $x_{k+1} = 2$.

3. $d(x(O(x_1...x_k)), y(O(y_1...y_j)) = d(x,7) + d(y,7) + 5(k + j - 2r) + 4$, where r is defined as $r = min\{i : x_i \neq y_i\}$.

Now we try to compute the Harary index of $NS_2'[n]$. Let to consider the following polynomial as Harary polynomial which its value at $x = 1$ give us 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 $H(NS_2'[n], x)$ for $1 \leq i \leq 4$. Our method in the following theorem lead us to follow an approach for computing of the coefficient x^i of $H(NS_2'[n], x)$ for $i \geq 5$ in Theorem 4.

Theorem 2 .

1. The coefficient of x in $H(NS_2'[n], x)$ is $9 \times 2^n - 3$.
2. The coefficient of x^2 in $H(NS_2'[n], x)$ is $3 \times 2^{n+1} - 3$.
3. The coefficient of x^3 in $H(NS_2'[n], x)$ is $2^{n+2} - 3$.
4. The coefficient of x^4 in $H(NS_2'[n], x)$ is $\frac{23 \times 2^{n-1} - 13}{4}$.

Proof.

1. The coefficient of x in $H(NS_2'[n], x)$ is the number of edges of $NS_2'[n]$. It is easy to see that the number of its edges is $9 \times 2^n - 3$.

2. To compute the coefficient of x^2, we compute the number of pair of 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 $d(x,0) + d(y,7) + 5j - 4 = 2$. In this case $j = 1$. Then

$\{d(x,0),d(y,7)\}=\{0,1\}$. Obviously $y=7$ is one of the answer. For this case there are two cases $(1,7)$ and $(5,7)$. Also if $d(y,7)=1$, then $y=6$ and $x=0$. Therefore we have three solutions $(0(O),6(O(1)),(1(O),7(O(2))$ and $(5(O),7(O(1)))$.

Now by considering the Part (ii) of the Theorem 1 all of the pair of the vertices of distance 2 are in form:

$$\begin{array}{l}(1(O(x_1...x_k)),6(O(x_1...x_k1))),(2(O(x_1...x_k)),7(O(x_1...x_k1))),\\ (0(O(x_1...x_k)),7(O(x_1...x_k1))),(5(O(x_1...x_k)),6(O(x_1...x_k2))),\quad (1\le k\le n-1).\\ (0(O(x_1...x_k)),7(O(x_1...x_k2))),(4(O(x_1...x_k)),5(O(x_1...x_k2)))\end{array}$$

Therefore the number of solutions are $6(2^{n-1}-1)$. In other hand there are 6 pairs of vertices of distance 2 in first hexagon and 9 pairs of vertices of distance 2 in other hexagon, so the coefficient of x^2 is

$$\frac{1}{2}(3+6(2^{n-1}-1)+9(1+2+...+2^{n-1})+6)=\frac{6(2^{n-1}-1)+9(2^n-1)+9}{2}=3\times 2^{n+1}-3.$$

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

Theorem 3 .

1. $diam(NS_2'[1])=9$ and for every $n\ge 2$, $diam(NS_2'[n])=10n-6$.
2. $r(NS_2'[1])=5$, $r(NS_2'[2])=8$ and for every $n\ge 3$, $r(NS_2'[n])=5n-3$.

Proof.

1. When $n=1$, the most distances between two vertices is $d(3(O),0(O(1)))=9$.

When $n\ge 2$,it is obvious that the most distances between two vertices of this graph is between $x\in O(x_1...x_n)$ and $y\in O(y_1...y_n)$, where $x_2\ne y_2$ and $x=y=0$. By Theorem 1(iii) we have $d(0(O(x_1,...x_n)),0(O(y_1,...y_n)))=2d(0,7)+5(2n-4)+4=10n-6$.

2. Note that the radius of a graph G is $r(G)=min_x max_y\{d(x,y)\mid y\in V(G)\}$.

When $n=1$,this minimum occur when $x=7\in O(1)$ and $y=0\in O(1)$ or $x=6\in O(1)$ and $y=3\in O$, therefore in the both cases we have $r(G)=5$.

when $n=2$, this minimum occur when $x=1$ or $5\in O(1)$ and $y=3\in O$, therefore we have $r(G)=8$.

When $n \geq 3$, this minimum occur when $x = 0 \in O(1)$ and the maximum of $\{d(0, y) \mid y \in V(NS_1'[n])\} = 5n-3$ and this occur when $y = 7 \in O(x_1 \cdots x_n)$, by Theorem 1(ii). ■

Now we shall compute the coefficient of x^l in $H(NS_1'[n], x)) = \frac{1}{l}\sum x^l$, where $l \geq 5$.

We need to the following lemma which its proof can be obtain directly by considering all the possibilities.

Lemma 1 . *Let x and y be vertices of hexagons of $NS_2'[n]$ with position shown in Figure 0. Then we have the following table:*

Case	Equation	The number of solutions
1	$d(x,0)+d(y,7)=4$	9
2	$d(x,1)+d(y,7)=4$	11
3	$d(x,5)+d(y,7)=4$	11
4	$d(x,7)+d(y,7)=1$	2
5	$d(x,7)+d(y,7)=6$	7
6	$d(x,0)+d(y,7)=5$	10
7	$d(x,1)+d(y,7)=5$	12
8	$d(x,5)+d(y,7)=5$	12
9	$d(x,7)+d(y,7)=2$	3
10	$d(x,7)+d(y,7)=7$	10
11	$d(x,0)+d(y,7)=6$	8
12	$d(x,1)+d(y,7)=6$	11
13	$d(x,7)+d(y,7)=3$	6
14	$d(x,7)+d(y,7)=8$	8
15	$d(x,0)+d(y,7)=7$	4
16	$d(x,1)+d(y,7)=7$	8
17	$d(x,5)+d(y,7)=7$	8
18	$d(x,7)+d(y,7)=4$	9

19	$d(x,7)+d(y,7)=9$	6
20	$d(x,0)+d(y,7)=8$	1
21	$d(x,1)+d(y,7)=8$	4
22	$d(x,5)+d(y,7)=8$	4
23	$d(x,7)+d(y,7)=5$	10
24	$d(x,7)+d(y,7)=10$	1

Here we state the main theorem of this paper which gives the coefficients of x^l in $H(NS'_2[n],x)$ for $l \geq 5$. First we use the following notations:

$$A = 2^{q-1},\ B = 2^q + 2^{q+1} + \ldots + 2^n,$$

$$C = \sum_{r=2}^{n}(2n-q-2r+2),$$

$$D = \sum_{r=2}^{n}(2n-q-2r+3).$$

Theorem 4 . *Suppose that the Harary polynomial of* $NS'_2[n]$ *is*

$H(NS'_2[n],x) = \sum_{u,v\in V}\frac{1}{d(u,v)}x^{d(u,v)} = \frac{1}{d(u,v)}\sum_{l=1}^{10n-6}a_l x^l$. *Then for every* $l \geq 5$, *we have*

$$a_l = \begin{cases} 9A+11B+2C+7D; & if\ l \equiv 0\ (\ mod\ 5), \\ 10A+12B+3C+10D; & if\ l \equiv 1\ (\ mod\ 5)\ , \\ 8A+11B+6C+8D; & if\ l \equiv 2\ (\ mod\ 5)\ , \\ 4A+8B+9C+4D; & if\ l \equiv 3\ (\ mod\ 5)\ , \\ A+4B+10C+D; & if\ l \equiv 4\ (\ mod\ 5)\ . \end{cases}$$

Proof. We prove the theorem for case $l \equiv 0(\ mod\ 5)$. Another cases prove similarly. Let $l = 5q$, for some $q \in \mathbb{N}$. Therefore we have $d(x,0)+d(y,7)+5j-4=5q$ and so $d(x,0)+d(y,7)=4$. By Lemma 1 , there are 9 cases. By solving of the equation of Theorem 1 (i) we will have $q = j$, and by Part (ii) of this theorem the number of all possibilities cases is

$$9\times 2^{q-1} + 11\times(2^q + \ldots + 2^n) = 9A + 11B.$$

Now by considering the part (iii) of Theorem 1, we have to find the number of solution of

$d(x,7)+d(y,7)+5(i+j-2r)+4=5q$. we have two cases.

Case 1: When $d(x,7)+d(y,7)=1$ this equation has solution, and this occur for 2 different cases by Lemma 1. With substituting in equation we have $i+j=q+2r-1$, where $r\le i,j\le n$. This equation is equivalent to $i'+j'=q-1$, $(0\le i',j'\le n-r)$ .This equation has $q-2(q-n+r-1)=2n-2r-q+2$ solutions by Inclusion-Exclusion principle.since r can choose every element between 2 and n ,the number of possible cases is:

$$C=\sum_{r=2}^{n}(2n-2r-q+2).$$

Since there are 2 pair x,y for this part, we have $2C$ of possible cases.

Case 2: When $d(x,7)+d(y,7)=6$ this equation has solution, and this occur for 7 different cases by Lemma 1. With substituting in equation we have $i+j=q+2r-2$, where $r\le i,j\le n$. This equation is equivalent to $i'+j'=q-2$, $(0\le i',j'\le n-r)$ .This equation has $(q-1)-2(q-n+r-2)=2n-2r-q+3$ solutions by Inclusion-Exclusion principle.since r can choose every element between 2 and n ,the number of possible cases is:

$$D=\sum_{r=2}^{n}(2n-2r-q+3).$$

Since there are 7 pair x,y for this part, we have $7D$ of possible cases, and proof is complete. ■

We obtained the following result:

Corollary 1 . *The Harary index of* $NS_2'[n]$ *is* $H(NS_2'[n])=H(NS_2'[n],x)_{x=1}$ *and*

$$H(NS_2'[n],x)=(9\times 2^{n}-3)x+(3\times 2^{n+1}-3)x^{2}+(2^{n+2}-3)x^{3}+\frac{1}{4}(23\times 2^{n-1}-13)x^{4}+\frac{1}{l}\sum_{l=5}^{10n-6}a_l x^{l}$$

, where a_l *is obtained in Theorem 4.*

3 Harary index of dendrimer $NS_2[n]$

In this section we use our results in Section 2 to compute the Harary polynomial of a dendrimer nanostar. We consider the first kind of dendrimer which has grown n steps denoted $NS_2[n]$. Figure 2 show $NS_2[3]$.

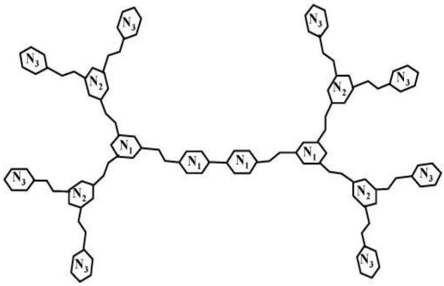

Figure 2. The first kind of dendrimer of generation 1-3 has grown 3 stages

It is easy to see that we are able to construct $NS_2[n]$ from two copies of $NS_2'[n]$.

Theorem 5 .

1. $diam(NS_2[n]) = 10n + 9$.
2. $r(NS_2[n]) = 5(n+1)$.

Proof.

1. The most distances between two vertices of this graph is $0(O(x_1,...,x_{n-1},1))$ and $0(P(x_1,...,x_{n-1},1))$.

By Theorem1(i) we have $d(0(O(x_1,...x_{n-1},1)),0(P(x_1,...x_{n-1},1)))$

$= 2d(3(O),0(O(x_1,...,x_{n-1},1))) + 1 = 2(d(3,0) + d(0,7) + 5n - 4) + 1 = 10n + 9$.

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 occur when $x = 3 \in O$ and $y = 0 \in P(x_1,...,x_n)$, therefore by Theorem 1(i) we have

$$r(NS_2[n]) = d(3(O),0(p(x_1,...,x_n))) = d(3(O) + 0(O(x_1,...,x_n))) + 1 = d(3,0) + d(0,7) + 5n - 4 + 1 = 5(n+1).$$ ■

Here we compute the Harary polynomial of $NS_2[n]$. For this purpose let

$g(x)=\sum_i g_i x^i$, where g_i is the number of vertices which have distance i from $3(O)$ in $NS_1'[n]$.

Remark 1: Obviously the degree of $g(x)$ is finite, but simply we suppose that its degree is infinite and we consider $g(x)$ as a series in the rest of paper.

We state and prove the following lemma which is about $g(x)$:

Lemma 2 . $g(x)=\dfrac{1+2x+2x^2+x^3+x^4-x^5-3x^6-2x^7+x^9}{1-2x^5}$

Proof. Clearly we have $g_0=1$, $g_1=g_2=2$ and $g_3=g_4=1$. By Theorem 1 we have $d(3(O),y(O(x_1,...,x_k)))=d(3,0)+d(y,7)+5k-4=d(y,7)+5k-1$.

Suppose that $i=d(y,7)+5k-1$, $i\geq 5$. We have the following cases:

1. $i=5k$. In this case $k=t$, $y=6$.
2. $i=5k+1$. In this case $k=t$, $y=3$.
3. $i=5k+2$. In this case $k=t$, $y\in\{2,4\}$.
4. $i=5k+3$. In this case $k=t$, $y\in\{1,5\}$.
5. $i=5k+4$. In this case $k=t$, $y\in\{0,7(O(x_1,...,x_t,1)),7(O(x_1,...,x_t,2))\}$.

If $i=5t$ or $i=5t+1$, then the number of possibilities of y is 2^{t-1},

If $i=5t+2$ or $i=5t+3$, then the number of possibilities of y is 2^t and

If $i=5t+4$, then the number of possibilities of y is $3(2^{t-1})$. Therefore

$$g(x)=1+2x+2x^2+x^3+x^4+x^5(1+x+2x^2+2x^3+3x^4)+2x^{10}(1+x+2x^2+2x^3+3x^4)+...$$

We put $l(x)=1+x+2x^2+2x^3+3x^4$. So we have

$$g(x)=(l(x)+x-x^3-2x^4)+x^5(l(x))+2x^{10}(l(x))+2^2x^{15}(l(x))+...$$

$$=l(x)+x-x^3-2x^4+\frac{l(x)}{2}(2x^5+(2x^5)^2+(2x^5)^3+...)$$

$$=l(x)+x-x^3-2x^4+\frac{l(x)}{2}\left(\frac{2x^5}{1-2x^5}\right)$$

$$=\frac{1+2x+2x^2+x^3+x^4-x^5-3x^6-2x^7+x^9}{1-2x^5}\ \blacksquare$$

Now we are ready to state and prove the main theorem of this paper. Observe that the statement in the following theorem is a polynomial, because we need to consider the coefficients x^i of $g(x)$ just for $0 \le i \le 10n-6$.

Theorem 6 . *Let* $H(NS_2[n],x)=\frac{1}{l}\sum_{l=1}^{10n+9} b_l x^l$ *and* $H(NS_1'[n],x)=\frac{1}{l}\sum_{l=1}^{10n-6} a_l x^l$. *Then we have* $H(NS_2[n],x)=\frac{1}{l}(2lH(NS_1'[n],x)+(g(x))^2)$, where

$$g(x)=\frac{1+2x+2x^2+x^3+x^4-x^5-3x^6-2x^7+x^9}{1-2x^5}.$$

Proof. By definition of Harary polynomial b_l is the number of pairs of vertices with distance l in $NS_2[n]$. This pair can be in the one of the $NS_1'[n]$. Since in every $NS_1'[n]$ the number of these kind of pairs is a_l , we have $2a_l$ pairs of vertices with distance l in one of the $NS_1'[n]$. Now we consider two vertices x and y such there are in different $NS_1'[n]$. If $d(x,3(O))=j$ and $d(y,3(O))=i$, then $j+i=l$. The number of these kind of vertices is the coefficient of x^l in $(g(x))^2$. Therefore $H(NS_2[n],x)=\frac{1}{l}(2lH(NS_1'[n],x)+(g(x))^2)$.■

Corollary 2 . *The Harary index of* $NS_2[n]$ *is* $H(NS_2[n])=H(NS_2[n],x)_{x=1}$.

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