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A New Method for Computing Wiener Index of Dendrimer Nanostars

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Abstract. Let G be the molecular graph a dendrimer nanostar and $\eta(G) = Sz(G) - W(G)$, where $W(G)$ denotes the Wiener index and $Sz(G)$ denotes the Szeged index of G. In this paper an edge-path matrix for G is presented by which it is possible to compute $\eta(G)$. We apply this number to compute the Wiener index of G.

1 Introduction and Preliminaries

Throughout this article G is a simple connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, the distance between the vertices u and v of G is denoted by $d(u, v)$ and it is defined as the number of edges in a minimal path connecting them. The Wiener index $W(G)$ is defined as the sum of all distances between vertices of G [16]. The Wiener index has noteworthy applications in chemistry and interested readers can be referred to papers [5, 6] and references therein for details.

We now describe some notations which will be kept throughout. Suppose $e = uv$. Define $n_u(e)$ to be the number of vertices of G lying closer to u than v and $n_v(e)$ is defined analogously. The Szeged index of G is defined as $Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e)$. Notice that vertices equidistant from both ends of the edge $e = uv$ are not counted. The Szeged index is a mathematically elegant index defined by Ivan Gutman [7]. Also, the reader can find more information about Szeged index in [8, 9].

Lukovits [13] introduced an all-path version of the Wiener index. To explain, we assume that G is a connected graph with $V(G) = \{1, 2, ..., n\}$. Then $P(G) = \sum\limits_{i<j} \sum\limits_{P\in\pi_{i,j}} |P|$

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is called the "all–path" version of the Wiener index. Here, $\pi_{i,j}$ denotes the set of all path connecting vertices i, j and the summations have to be performed between all pairs of vertices i and j and for all paths between i and j. In the mentioned paper some mathematical properties of $P(G)$ together with its extremal values are investigated. Notice that this matrix is defined in a similar way as "all–path" index of Lukovits.

Suppose G is a connected graph and $e = uv \in E(G)$. Define:

$$\begin{aligned} N_u(e) &= \{x \in V(G) \mid d(x,u) < d(x,v)\}, \\ N_v(e) &= \{x \in V(G) \mid d(x,u) > d(x,v)\}, \\ N_0(e) &= \{x \in V(G) \mid d(x,u) = d(x,v)\}. \end{aligned}$$

Thus $n_u(e) = |N_u(e)|$ and $n_v(e) = |N_v(e)|$. A set $Y = \{P_1, P_2, \cdots, P_{\binom{n}{2}}\}$ of shortest paths in G such that for every vertex $a, b \in V(G)$ and $a \neq b$, there exists a unique path $P \in Y$ connecting vertices a and b is called a complete set of shortest paths of G (CSSP for short). Define the matrix $A_Y = [a_{ij}]$, as follows:

$$a_{ij} = \begin{cases} 1 & e_j \in E(P_i) \\ 0 & e_j \notin E(P_i) \end{cases}.$$

Clearly, if P_i is a path connecting vertices x and y then $d(x,y)$ is the number of non-zero entries in the i^{th} row of A_Y. Thus the summation of entries of the matrix A_Y is equal to the Wiener index of G. In what follows, $P_G(u,v)$ denotes the set of all shortest paths connecting vertices u and v of G and CSSP(G) denotes the set of all CSSP of G.

Suppose G is an $n-$vertex graph with the path-edge matrix A_Y, where Y is a $CSSP$ of G. It is clear that $|Y| = \binom{n}{2}$. If $e = uv$ is an edge of G then we define $\eta_Y(e) = n_u(e)n_v(e) - \sum_i a_{ij}$ and $\eta_Y(G) = \sum_{e \in G} \eta_Y(e)$. It is easy to see that $\eta_Y(G) = Sz(G) - W(G)$ and so the value of $\eta_Y(G)$ is independent from Y. If H is a subgraph of G then we define $\eta_Y(H) = \sum_{e \in E(H)} \eta_Y(e)$. In [12], the presented authors proved the following two theorems which are crucial throughout the paper.

Theorem 1. Suppose G is a graph, $Y, Z \in CSSP(G)$ and B is a block of G. Then $\eta_Y(B) = \eta_Z(B)$.

Theorem 2. Suppose e is an edge of a connected graph G. If $\eta(e) > 0$ then e is belonging to a cycle C_n, $n \geq 4$, or a subgraph isomorphic to $K_4 - e$. If e is an edge of a complete block B of G then $\eta(e) = 0$.

By Theorem 1 and for simplicity, from now on we fix a set Y and write $\eta(e)$ and $\eta(G)$ as $\eta_Y(e)$ and $\eta_Y(G)$, respectively. Throughout this paper our notation is standard and taken mainly from [14, 15]. We let K_n, P_n and C_n denote the complete graph, path and cycle on n vertices, respectively.

2 Main Result

Dendrimers are highly ordered branched macromolecules which have attracted much theoretical and experimental attention [4]. The nanostar dendrimer is part of a new group of macromolecules that seem photon funnels just like artificial antennas and also, it is a great resistant of photo bleaching.

In [1, 2, 10, 11], one of us (ARA) presented a technique for computing Wiener index of dendrimer nanostars by considering some isometric subgraphs $A_1, A_2, \cdots, A_r$ such that we can partition the edge set of the graph into subgraphs isomorphic to one of $A_i, 1 \leq i \leq r$. If $r \leq 4$ then it is possible to calculate the distance matrix of these subgraphs and find a more and less good algorithm for computing Wiener index.

In this paper an efficient method is presented by which it is possible to compute the Wiener index of dendrimer nanostars provided that its Szeged index is known. To do this, we will compute $\eta(G) = Sz(G) - W(G)$ for a given dendrimer nanostar G and since $Sz(G)$ is known the Wiener index of G will be computed immediately. We describe our method by considering a dendrimer nanostar $G[n]$ depicted in Figure 1, where n denotes the number of growth in $G[n]$. Obviously, $N = |V(G[n])| = 18 \times 2^{n-1} - 12$. In Figure 1, the molecular graph of $G[3]$ is depicted.

From Figure 1, one can see that $G[n]$ is constructed from blocks isomorphic to a hexagon or K_2. By Theorem 2, if e is an edge of $G[n]$ outside hexagons then $\eta(e) = 0$. Thus we must compute the values of $\eta(e)$ for edges e, such that there exists a hexagon through e.

It is obvious that every vertex v of H_i of degree 3 is adjacent to a unique cut edge e of $G[n]$. Consider an arbitrary hexagon H_i in the i^{th} step of $G[n]$ with vertex set $V(H_i) = \{v_1, v_2, v_3, v_4, v_5, v_6\}$. Then without loss of generality, we can assume that vertices v_1, v_3 and v_5 have degree 3, and vertices v_2, v_4 and v_6 have degree 2. Define $n_j = m_j + 1$, where m_j is the minimum number of vertices in the components yield by deleting e from $G[n]$, $j = 1, 3, 5$.

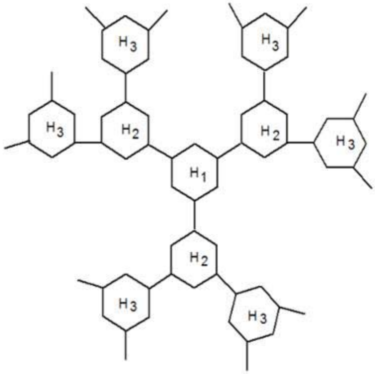

Figure 1: The dendrimer nanostar $G[n]$.

If $deg(v) = 2$ then we define $n_j(v) = 1$. Since H_i is a block, the Theorem 2 implies that η is independent from choosing the shortest path. If $i = n = 1$ then for all j, $1 \le j \le 6$, we define $n_j = 1$. Suppose that $n > 1$. If $i = 1$ then $n_1 = n_3 = n_5 = \frac{N-6}{3} + 1$ $= \frac{N}{3} - 1$ and so $\eta(H_1) = 5(N-3) + 2 \times 3 \times (\frac{N}{3} - 1)^2 + 6 = \frac{2N^2}{3} + 9N$ - 3. If $i = n$ then $n_1 = n_5 = 1$ and $n_3 = N - 5$. Hence $\eta(H_n) = 5(2 + N - 5) + 2(1 + 2(N-5) + 6) = 9(N-3)$. We now assume that $1 < i < n$. Therefore,

$$\begin{aligned} \eta(H_i) &= n_1n_2 + 2n_1n_3 + 3n_1n_4 + 2n_1n_5 + n_1n_6 \\ &+ n_2n_3 + 2n_2n_4 + 3n_2n_5 + 2n_2n_6 \\ &+ n_3n_4 + 2n_3n_5 + 3n_3n_6 \\ &+ n_4n_5 + 2n_4n_6 \\ &+ n_5n_6 \end{aligned}$$

Simplify last equation by the condition $n_2 = n_4 = n_6 = 1$ to prove:

$$\eta(H_i) = 5(n_1 + n_3 + n_5) + 2(n_1n_3 + n_1n_5 + n_3n_5) + 6.$$

On the other hand, $n_1 = n_5 = 6 \times (2^{n-i} - 1) + 1 = 3 \times 2^{n-i+1} - 5$ and so $n_3 = N - 2(3 \times 2^{n-i+1} - 5)$ - 3 $= N - 3 \times 2^{n-i+2} + 7$. Therefore,

$$\begin{aligned} \eta(H_i) &= 5(N-3) + 2[(3 \times 2^{n-i+1} - 5)^2 + 2(3 \times 2^{n-i+1} - 5)(N - 3 \times 2^{n-i+3} + 7)] + 6 \\ &= 3N(2^{n-i+3} - 5) + 9(2^{n-i+5} - 3 \times 2^{2n-2i+3} - 11) \end{aligned}$$

Finally, $\eta(G) = \sum_{e\in E(G)} \eta(e)$ and since for each complete block B and $b \in B$, $\eta(b) = 0$, we have $\eta(G) = \sum_i r_i\eta(H_i)$, where $r_1 = 1$ and for $i > 1$, $r_i = 3 \times 2^{i-2}$ is the number of hexagons in the i^{th} step of $G[n]$. Therefore, $\eta(G[n]) = 162.n.4^n - \frac{783}{2}4^n + 1107.2^{n-1} - 162$. On the other hand, by [3, Theorem 1], $Sz(G[n]) = -30244^n + 5724.2^n + 6480.n.4^n$ - 432. Therefore, we prove our main result as follows:

Theorem. $W(G[n]) = \frac{-1215}{2}.4^n + 1755.2^n - 1 + 243.n.4^n - 270$.

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