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ON ESTRADA INDEX OF TWO CLASSES OF DENDRIMERS

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ABSTRACT. Suppose G = (V, E) is a graph. The sequence $v_1v_2\ldots v_t(v_t = v_1)$ is called a closed walk with length t – 1 in G if v_i's are in V(G) and $v_iv_{i+1} \in$ E(G). In this paper, the number of closed walks with length k, $C_w(G,k)$, for two classes of denderimers are computed.

Keywords: *Dendrimer, closed walk.-graph spectrum, Estrada index.*

INTRODUCTION

Dendrimers are polymeric macromolecules composed of multiple perfectly-branched monomers radially emanating from a central core, Figures 1, 2. The number of branching points increases upon moving from the dendrimer core to its surface and defines dendrimer generations. They are being investigated for possible uses in nanotechnology, gene therapy, and other fields [1-5].

In this paper, the word graph refers to a finite, undirected graph without loops and multiple edges. Suppose G is a graph. The vertices and edges of G are denoted by V(G) and E(G), respectively. A walk in G is an alternating sequence of graph vertices and edges such that any subsequent two edges are adjacent. A closed walk is a walk in which the first and the last vertices are the same. We encourage to the reader to consult papers [6-11] for background material, as well as basic computational techniques. Our notation is standard and mainly taken from the standard book of graph theory [12].

MAIN RESULTS AND DISCUSSION

Let $D_1[n]$ and $D_2[n]$ be the molecular graphs of the dendrimers depicted in Figures 1 and 2, respectively. In this section, some formulas are derived for the number of closed walks of length k, $C_w(G,k)$, where $1 \le k \le 10$ and G is one of the molecular graphs $D_1[n]$ and $D_2[n]$. For the sake of completeness, we mention here a well-known theorem in algebraic graph theory as follows:

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THEOREM 1. $C_w(D_1[n], 2k–1) = 0$ and $C_w(D_2[n], 2k–1) = 0$.

In the following theorems, the number of walks, of even length, are computed.

THEOREM 2. $C_w(D_1[n], 2) = 4 \times 3^{n+1} - 4$ and $C_w(D_2[n], 2) = 2 \times 3^{n+1} - 4$.

PROOF. Since for every graph G, $C_w(G, 2) = 2m$ we have $C_w(D_1[n], 2) = 4 \times 3^{n+1} - 4$ and $C_w(D_2[n], 2) = 2 \times 3^{n+1} - 4$.

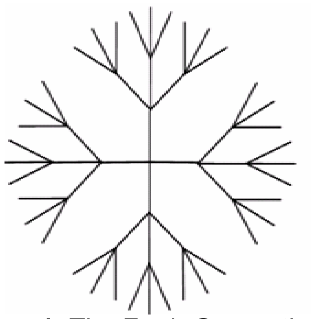

Figure 1. The Forth Generation of Dendrimer Molecule $D_1[4]$

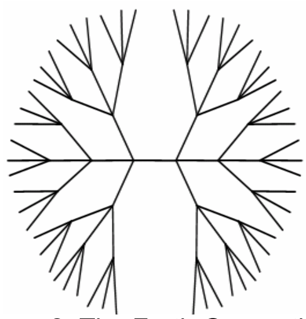

Figure 2. The Forth Generation of Dendrimer Molecule $D_2[4]$

THEOREM 3. $C_w(D_1[n], 4) = 48 \times 3^n + 24$ and $C_w(D_2[n], 4) = 24 \times 3^{n+1} - 66$.

PROOF. Every closed walk of length 4 in the dendrimer molecules $D_1[n]$ and $D_2[n]$ are constructed from one edge or a path of length 2. Therefore, we must count the following type of sequences:

a) $v_1v_2v_1v_2v_1$;
b) $v_1v_2v_3v_2v_1$;
c) $v_2v_1v_2v_3v_2$.

There are $4 \times 3^{n+1} - 4$ sequences of type (a) in $D_1[n]$, $2 \times 3^{n+1} - 4$ sequences of type (a) in $D_2[n]$, $24 \times 3^n + 12$ sequences of type (b) in $D_1[n]$ and $12 \times 3^n - 33$ sequences of type (b) in $D_2[n]$. So, there are $24 \times 3^n + 12$ sequences of type (c) in $D_1[n]$ and $12 \times 3^n - 33$ sequences of type (c) in $D_2[n]$. These facts imply that $C_w(D_1[n],4) = 48 \times 3^{n+1} + 24$ and $C_w(D_2[n], 4) = 24 \times 3^{n+1} - 66$.

THEOREM 4. $C_w(D_1[n], 6) = 534 \times 3^n - 210$ and $C_w(D_2[n], 6) = 144 \times 3^n - 376$.

Proof. We apply a similar argument as in Theorem 1 to count the number of closed walk of length 6 in $D_1[n]$ and $D_2[n]$. Such walks constructed from an edge, a path of length 2, a path of length 3 or a star S_4. The number of closed walks of length 6 in $D_1[n]$ and $D_2[n]$ on an edge is $4 \times 3^{n+1} - 4$ and $2 \times 3^{n+1} - 4$, respectively. The number of closed walks of length 6 in $D_1[n]$ and $D_2[n]$ on a path with length 2 is $144 \times 3^n - 72$ and $72 \times 3^n - 216$, respectively and the number of closed walks of length 6 in $D_1[n]$ and $D_2[n]$ on a path with length 3 is $294 \times 3^n - 36$ and $18 \times 3^n - 108$, respectively. Finally, the number of closed walks of length 6 in $D_1[n]$ and $D_2[n]$ on a star S_4 is $84 \times 3^n - 48$ and $48 \times 3^n - 48$, respectively. Therefore, by a simple calculation, one can see that $C_w(D_1[n], 6) = 534 \times 3^n - 210$ and $C_w(D_2[n], 6) = 144 \times 3^n - 376$.

THEOREM 5. Suppose k, $k \geq 8$, is an even integer. Then

$$534 \times 3^n - 210 < C_w(D_1[n], k) < 2(4^k .3^{n+1} - 4^k), \qquad (1)$$

$$144 \times 3^n - 376 < C_w(D_2[n], k) < (4^k \times 3^{n+1} - 4^k). \qquad (2)$$

PROOF. For proving the left sides of inequalities (1) and (2), we note that $C_w(G, 2k) > C_w(G, 2(k-1))$, $k > 3$. Thus $C_w(G, 2k) > C_w(G, 6)$ and so $C_w(D_1[n], 2k) > C_w(D_1[n], 6) = 534 \times 3^n - 210$ and $C_w(D_1[n], 2k) > C_w(D_1[n], 6) = 144 \times 3^n - 376$. By an elementary fact in algebraic graph theory, the number of closed walks of length k connecting the i-th and j-th vertices of G is equal to the ij-th entry of A^k, where A denotes the adjacency matrix of G. Therefore, for an arbitrary eigenvalue λ, we have $|\lambda| \leq 4$. Thus, $C_w(D_1[n], k) < 2(4^k \times 3^{n+1} - 4^k)$ and $C_w(D_1[n], k) < (4^k \times 3^{n+1} - 4^k)$. A similar argument proves the same for $D_2[n]$. This completes the proof.

Using calculations given above, it is possible to evaluate the Estrada index of this class of dendrimers. To explain this topological index, we assume that G is a simple graph on n vertices. The adjacency matrix of G is the $n \times n$ matrix where the entry a_{ij} is 1 if vertex i is adjacent to vertex j, otherwise a_{ij} is 0. The eigenvalues of the adjacency matrix of G are said to be the eigenvalues of G and to form the spectrum of G [13]. A graph of order n has exactly n eigenvalues not necessarily distinct, but necessarily real-valued. We denote these eigenvalues by $\lambda_1, \lambda_2, \ldots, \lambda_n$. A graph-spectrum-based invariant, recently proposed by Estrada is defined as $EE = EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$ [14-16]. We encourage the interested readers to consult papers [17,18] and references therein for more information on Estrada index and its computational techniques.

THEOREM 6. Consider the molecular graphs of dendrimers $D_1[n]$ and $D_2[n]$. Then there are constants c_i, $1 \leq i \leq 2 \times 3^{n+2} - 1$, and d_j, $1 \leq j \leq 3^{n+1} - 1$, such that $-4 \leq c_i, d_j \leq 4$ and the Estrada index of these graphs are computed as follows:

1) $EE(D_1[n]) = \frac{1769}{120} 3^n - \frac{55}{24} + \sum_{i=1}^{2\times 3^{n+1}-1} \frac{\lambda_i^8 e^{c_i}}{8!}$,
2) $EE(D_2[n]) = \frac{31}{5} 3^n - \frac{1129}{180} + \sum_{i=1}^{3^{n+1}-1} \frac{\lambda_i^8 e^{d_i}}{8!}$.

CORROLAY 7. The Estrada index of dendrimers $D_1[n]$ and $D_2[n]$ are bounded above as follows:

1) $EE(D_1[n]) \leq \frac{1769}{120} 3^n - \frac{55}{24} + \frac{32e^4}{7!}(2 \times 3^{n+1} - 1)$,
2) $EE(D_2[n]) \leq \frac{31}{5} 3^n - \frac{1129}{180} + \frac{32e^4}{7!}(3^{n+1} - 1)$.

CONCLUSIONS

In this paper, a simple method enabling to compute the closed walks of dendrimers was presented. By our calculation it is possible to evaluate the Estrada index of these dendrimers. It is possible to extend our method in other classes of dendrimers.

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