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On edge detour index polynomials

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Abstract. The edge detour index polynomials were recently introduced for computing the edge detour indices. In this paper we find relations among edge detour polynomials for the 2-dimensional graph of $TUC_4C_8(S)$ in a Euclidean plane and $TUC_4C_8(S)$ nanotorus.

Keywords: Detour index, Edge detour indices, Edge detour index polynomials, Line graph, Nanotube.

1. Introduction

A graph $G = (V, E)$ is a combinatorial object consisting of an arbitrary set $V = V(G)$ of vertices and a set $E = E(G)$ of unordered pairs $x, y = xy$ of distinct vertices of G called edges. In a molecular graph, vertices are atoms while the edges represent covalent bonds.

Among the topological indices, the Wiener number is the oldest and probably the most important one [1]. The Wiener index, a distance-based invariant, was introduced by H. Wiener. Topological indices have found applications in communication, facility location, cryptology, etc. [2].

The detour index was introduced in graph theory some time ago by F. Harary in describing the connectivity in directed graphs [3]. The detour index, in contrast to the Wiener index (that counts the length of the shortest path between pair vertices), considers

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the length of the longest path between each pair of vertices. This index has recently received some attention in the chemical literature [4, 5]. The detour index certainly carries some interesting structural information for cyclic compounds. For acyclic structures the Wiener index and the detour index are the same, since there is only a single possible path connecting any pair of vertices [1]. The detour index is defined as follows:

$$D(G) = \sum_{\{u,v\} \subseteq V(G)} \Delta(u, v) \tag{1}$$

where $\Delta(u, v)$ denotes the detour between the vertices u and v (i.e. the number of edges on the longest path joining them).

The detour index polynomial of a graph G was introduced recently [6]. The detour index polynomial of G is

$$D(G; x) = \sum_{\{x,y\} \subseteq V(G)} x^{\Delta(x,y)} \tag{2}$$

Also, the edge versions of detour index are the sum of distances between edges of a connected graph G on the longest path as follow [7]:

The first edge-detour index is:

$$D_{e0}(G) = \sum_{\{e,f\} \in E(G)} \Delta_0(e, f) = \sum_{\{e,f\} \in V(L(G))} \Delta_0(e, f) \tag{3}$$

where $\Delta_0(u, v)$ is the detour index in the Line graph (also called the edge intersection graph) $L(G)$, where vertices correspond to edges of G and vertices in $L(G)$ are adjacent if the corresponding edges share an angle.

The second edge-detour index is:

$$D_{e3}(G) = \sum_{\{e,f\} \in E(G)} \Delta_3(e, f) \tag{4}$$

Where

$$\Delta_3(e, f) = \begin{cases} \Delta_1(e, f) + 1 & , e \neq f \\ 0 & , e = f \end{cases}$$

and

$$\Delta_1(e, f) = \min\{\Delta(u, x), \Delta(u, y), \Delta(v, x), \Delta(v, y)\}$$

where $e = uv$ and $f = xy$.

The third edge-detour index is:

$$D_{e4}(G) = \sum_{\{e,f\} \subseteq E(G)} \Delta_4(e, f) \tag{5}$$

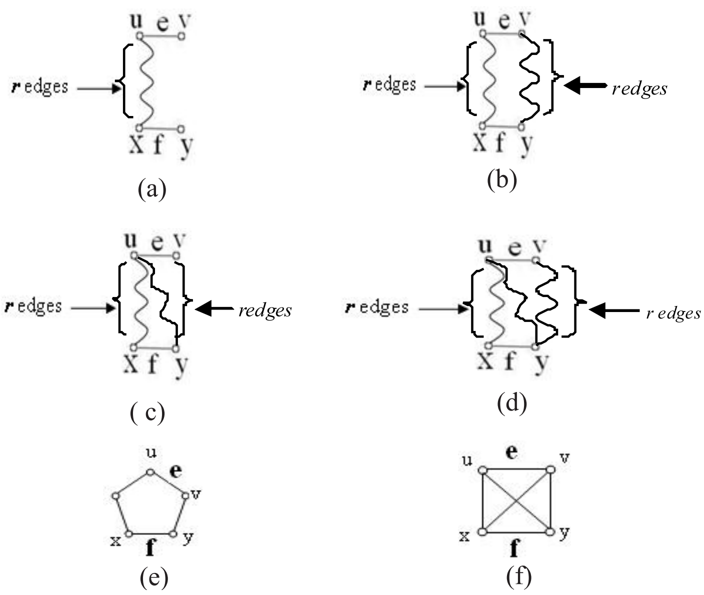

Figure 1. The quantity $\Delta'_P(e,f)$ is r for shapes (a,b,c and d) and is 1 for shapes (e and f).

Where

$$\Delta_4(e,f) = \begin{cases} \Delta_2(e,f)+1 & , e \neq f \\ 0 & , e = f \end{cases}$$

and

$$\Delta_2(e,f) = \max\{\Delta(u,x), \Delta(u,y), \Delta(v,x), \Delta(v,y)\}$$

where $e = uv$ and $f = xy$.

In addition, the edge detour index polynomials are introduced recently as follows [8]:

$$D_{ei}(G;x) = \sum_{\{e,f\} \in E(G)} x^{\Delta_i(e,f)} \quad \text{where } i = 0,3,4. \tag{6}$$

Due to the applications of nanostructures in particular nanotorus and edge detour index polynomials, we present here the relations among edge detour index polynomials for the 2-dimensional graph of $TUC_4C_8(S)$ in a Euclidean planeand $TUC_4C_8(S)$ nanotorus.

2. Result and discussion

Definition 2.1 Let $e, f \in E(G)$, $e = uv$ and $f = xy$. Fix a longest path between edges e and f and name it P. We define the quantity $\Delta'_P(e,f)$ as follows [8]:

$$\Delta'_P(e,f) = \min\{\Delta_P(u,x), \Delta_P(u,y), \Delta_P(v,x), \Delta_P(v,y)\}$$

where Δ_P is length of the path P. If the edge detour is defined as the longest path between edges, we can imagine six cases (Figure 1). Therefore, we partition the set of pair edges into the following subsets.

$$A_1 = \{\{e, f\} \subseteq E(G) | e, f, \text{Figure 1(a)}\};\ A_2 = \{\{e, f\} \subseteq E(G) | e, f, \text{Figure 1(b)}\}$$
$$A_3 = \{\{e, f\} \subseteq E(G) | e, f, \text{Figure 1(c)}\};\ A_4 = \{\{e, f\} \subseteq E(G) | e, f, \text{Figure 1(d)}\}$$
$$A_5 = \{\{e, f\} \subseteq E(G) | e, f, \text{Figure 1(e)}\};\ A_6 = \{\{e, f\} \subseteq E(G) | e, f, \text{Figure 1(f)}\}$$

Then, we find the edge detours as follows:

Lemma 2.2 [8] Let $e, f \in E(G)$, $e = uv$ and $f = xy$. Then,

$$\Delta_0(e, f) = \begin{cases} \Delta'(e, f) + 1 & \{e, f\} \in A_1 \\ \Delta'(e, f) + 1 & \{e, f\} \in A_2 \\ \Delta'(e, f) + 2 & \{e, f\} \in A_3 \\ 3\Delta'(e, f) + 1 & \{e, f\} \in A_4 \\ \Delta'(e, f) + 2 & \{e, f\} \in A_5 \\ 4\Delta'(e, f) + 1 & \{e, f\} \in A_6 \end{cases}$$

and

$$\Delta_3(e, f) = \begin{cases} \Delta'(e, f) + 1 & \{e, f\} \in A_1 \\ \Delta'(e, f) + 2 & \{e, f\} \in A_2 \\ \Delta'(e, f) + 2 & \{e, f\} \in A_3 \\ \Delta'(e, f) + 2 & \{e, f\} \in A_4 \\ \Delta'(e, f) + 3 & \{e, f\} \in A_5 \\ 3\Delta'(e, f) + 1 & \{e, f\} \in A_6 \end{cases}$$

and

$$\Delta_4(e, f) = \begin{cases} \Delta'(e, f) + 2 & \{e, f\} \in A_1 \\ \Delta'(e, f) + 2 & \{e, f\} \in A_2 \\ \Delta'(e, f) + 2 & \{e, f\} \in A_3 \\ 3\Delta'(e, f) & \{e, f\} \in A_4 \\ \Delta'(e, f) + 3 & \{e, f\} \in A_5 \\ 3\Delta'(e, f) & \{e, f\} \in A_6 \end{cases}$$

Theorem 2.3 [8] The relations between edge-detour index polynomials are:

$$\begin{aligned} D_{e0}(G;x) - D_{e3}(G;x) = (1-x) &\sum_{\{e,f\}\in A_2} x^{(\Delta'(e,f)+1)} \\ &+ \sum_{\{e,f\}\in A_4} x^{(\Delta'(e,f)+2)} \left(x^{(2\Delta'(e,f)-1)} - 1\right) \\ &+ (1-x) \sum_{\{e,f\}\in A_5} x^{(\Delta'(e,f)+2)} \\ &+ \sum_{\{e,f\}\in A_6} x^{(\Delta'(e,f)+1)} \left(x^{\Delta'(e,f)} - 1\right). \end{aligned} \tag{7}$$

and

$$\begin{aligned} D_{e0}(G;x) - D_{e4}(G;x) = (1-x) &\sum_{\{e,f\}\in A_1} x^{(\Delta'(e,f)+1)} + (1-x) \sum_{\{e,f\}\in A_2} x^{(\Delta'(e,f)+1)} \\ &+ (x-1) \sum_{\{e,f\}\in A_4} x^{(3\Delta'(e,f))} + (1-x) \sum_{\{e,f\}\in A_5} x^{(\Delta'(e,f)+2)} \\ &+ \sum_{\{e,f\}\in A_6} x^{(3\Delta'(e,f))} \left(x^{(\Delta'(e,f)+1)} - 1\right). \end{aligned} \tag{8}$$

■

In the following, we mention the relation between edge detour index polynomials $D_{e3}(G;x)$ and $D_{e4}(G;x)$ as a result of Theorem 2.3.

Corollary 2.4 [9] The relations between edge detour index polynomials $D_{e3}(G;x)$ and $D_{e4}(G;x)$ are:

$$\begin{aligned} D_{e4}(G;x) - D_{e3}(G;x) = -(1-x) &\sum_{\{e,f\}\in A_1} x^{(\Delta'(e,f)+1)} \\ &+ \sum_{\{e,f\}\in A_4} x^{\Delta'(e,f)} \left(x^{2\Delta'(e,f)} - x^2\right) \\ &+ \sum_{\{e,f\}\in A_6} x^{(3\Delta'(e,f))}(1-x). \end{aligned} \tag{9}$$

■

Now, the relations among edge detour indices and their polynomials are computed for the 2-dimensional graph of $TUC_4C_8(S)$ in a Euclidean planeand $TUC_4C_8(S)$ nanotorus. In the following figures, we mention to some examples of the 2-dimentional graph of $TUC_4C_8(S)$ in a Euclidean planeand $TUC_4C_8(S)$ nanotorus, also we denote the number of rows of squares by q and number of squaresin one row by p. For convenience, we denote the two-dimensional graph of $TUC_4C_8(S)$ in a Euclidean plane by K as shown in Figure 2. Accordingly $|E(K)| = 12pq-2p-2q$. We denote $TUC_4C_8(S)$ nanotube by Gas shown in Figure 3. Accordingly, $|E(G)| = 12pq$.

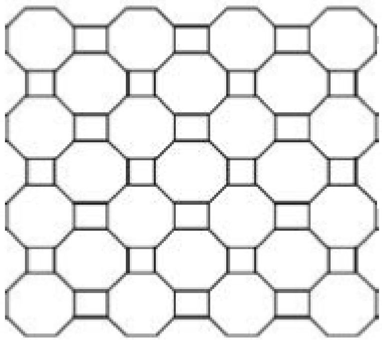

Figure 2. two-dimensional graph of $TUC_4C_8(S)$ in a Euclidean plane, $p = 4$, $q = 4$.

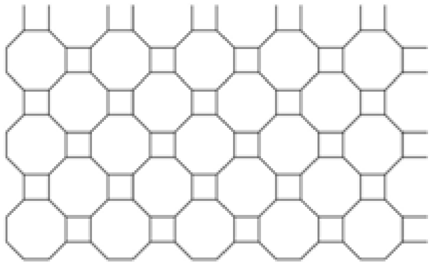

Figure 3. The $TUC_4C_8(S)$ nanotorus, $p = 5$, $q = 3$.

Theorem 2.5 The relations among edge detour index polynomials for graph K are:

$$D_{e0}(K;x) - D_{e3}(K;x) = (1-x) \sum_{\{e,f\} \in A_2} x^{(\Delta'(e,f)+1)} \tag{10}$$

$$D_{e0}(K;x) - D_{e4}(K;x) = (1-x) \sum_{\{e,f\} \subseteq E(G)} x^{(\Delta'(e,f)+1)} \tag{11}$$

$$D_{e4}(K;x) - D_{e3}(K;x) = -(1-x) \sum_{\{e,f\} \in A_1} x^{(\Delta'(e,f)+1)} \tag{12}$$

Proof. Due to the Figure 2, the subsets A_3, A_4, A_5 and A_6 are empty and then, we can get results by using the equations 7, 8 and 9. Then, we can conclude the desire results.

Theorem 2.6 The relations among edge detour index polynomials for graph G are:

$$D_{e0}(G;x) - D_{e3}(G;x) = (1-x) \sum_{\{e,f\} \in A_2} x^{(\Delta'(e,f)+1)} \tag{13}$$

$$D_{e0}(G;x) - D_{e4}(G;x) = (1-x) \sum_{\{e,f\} \subseteq E(G)} x^{(\Delta'(e,f)+1)} \tag{14}$$

$$D_{e4}(G;x) - D_{e3}(G;x) = -(1-x) \sum_{\{e,f\} \in A_1} x^{(\Delta'(e,f)+1)} \tag{15}$$

Proof. Due to the Figure 3, the subsets A_3, A_4, A_5 and A_6 are empty and then, we can get results by using the equations 7, 8 and 9. Then, we can conclude the desire results.

3. Conclusions

The relations among edge detour index polynomials of the 2-dimensional graph of $TUC_4C_8(S)$ in a Euclidean planeand $TUC_4C_8(S)$ nanotorushave been computed, mainly by using the relations between the detour distances of edges in the molecular graph. Also, we concluded that their relations only depended to two sets of 2-subsets ofedges, A_1 and A_2.

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