Computing a new edge-Wiener index of $TUC_4C_8(S)$ nanotubes and $TUC_4C_8(R)$ nanotorus

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Let G be a connected graph. Distance between two edges of G is the distance between the corresponding vertices in the line graph of G. The edge-Wiener index of a graph G is defined the sum of distances between all pairs of edges of the graph G. In this paper at first we defined a new distance between two edges of the graph G, and then in according to this definition, we define the edge-Wiener index of a graph G. Then we obtain the edge Wiener index of some well-known graphs and the nanotubs $TUC_4C_8(R)$ and $TUC_4C_8(S)$ nanotorus.

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1. Introduction

Throughout this paper $G=(V,E)$ will denote a simple connected graph with n vertices and m edges. The Wiener index equal to the sum of distances between all pairs of vertices of G, that is,

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

where $d(u,v)$ denotes the distance between of vertices u and v.

This index was introduced by the chemist Harold Wiener [1] within the study of relation between the structure of organic compounds and their properties. The first mathematical paper on W was published somewhat later [2]. Many papers published in related of computation of some topological indices of nanotubes. For example see [3-18].

Definition 1. Let S be any set. The distance is a mapping $\delta : S\times S \to R$ such that for any $a,b,c\in S$,

1°. $\delta(a,b)\ge 0$

2°. $\delta(a,b)=0 \Leftrightarrow a=b$

3°. $\delta(a,b)=\delta(b,a)$

4°. $\delta(a,b)+\delta(b,c)\ge \delta(a,c)$

Definition 2. The edge-Wiener index of the graph G is denoted by $W_e(G)$ and defined as follows:

$$W_e=W_e(G)=\sum_{\{e,f\}\subseteq E(G)} d(e,f)$$

where $d(e,f)$ is a distance between edges e and f of the graph G.

Since the edge-Wiener index of the graph G deal with distance between of two edges in different ways. For example in [], they defined two edge-Wiener index with the symbol $W_{e0}(G)$ and $W_{e4}(G)$ index. Also, in [8], they defined the edge-Wiener index of graph G according the line graph G.

2. Results and discussions

Now, we define a new distance between two edges of the graph G as follows:

Definition 3. Let G be a connected graph and $e,f\in E(G)$ such that $e=(u,v)$, $f=(x,y)$, we define $d(e,f)=\max\{\deg u,\deg v,\deg x,\deg y\}$, where $\deg i$ is the vertex degree of i.

d is not distance because, if e=f, then $d(e,f)\neq 0$, condition 2° of definition 1 is violated.

We now proceed to amend the above definition.

Definition 4.

$$d_A(e,f)=\begin{cases} d(e,f) & e\neq f \\ 0 & e=f \end{cases}$$

Lemma 5. Let G be a connected graph and $e, f, g \in E(G)$ such that $e=(u,v)$, $f=(x,y)$, $g=(h,t)$, the quantity d_A, defined by the above definition is a true distance.

Proof. Clearly d_A satisfies condition 1°, 2°, 3° of definition 1. We now consider the condition 4°, We must to show that: $d_A(e,f)+d_A(f,g)\geq d_A(e,g)$, so we show that the below correlation is true:

$$\begin{aligned}&\max\{\deg u,\deg v,\deg x,\deg y\}\\&+\max\{\deg x,\deg y,\deg h,\deg t\}\geq\\&\max\{\deg u,\deg v,\deg h,\deg t\}\end{aligned} \quad (1)$$

On the right-hand side of (1) compute the maximum quantities appearance at two sets and the compute their maximum. So is true relation (1).

Definition 6.

$$W_{eA}=W_{eA}(G)=\sum_{\{e,f\}\subseteq E(G)} d_A(e,f)$$

We called this index degree-edge index.

Let, as usual, P_n, C_n, K_n and S_n be the n-vertex path, cycle, complete graph and star, respectively. Let $K_{a,b}$ be the complete bipartite graph on at $a+b$ vertices.

Theorem 7.

(a). $W_{eA}(C_n)=n(n-1)\, for n\geq 3$

(b). $W_{eA}(P_n)=(n-1)(n-2)$

(c). $W_{eA}(S_n)=\frac{1}{2}(n-1)^2(n-2)$

(d). $W_{eA}(K_n)=\frac{1}{8}n(n+1)(n-1)^2(n-2)$

(e). $W_{eA}(K_{a,b})=\frac{1}{2}ab^2(ab-1)$

$for b\geq a$

Proof.

(a). $$\begin{aligned}W_{eA}(C_n)&=[(n-1)+(n-2)+.....+2+1]\\&=\frac{1}{2}n(n-1)\times 2=n(n-1)\qquad for\quad n\geq 3\end{aligned}$$

(b). $$\begin{aligned}W_{eA}(P_n)&=2[(n-2)+(n-3)+.....+2+1]\\&=(n-2)(n-1)\end{aligned}$$

(c). $$\begin{aligned}&W_{eA}(S_n)=[(n-2)+(n-3)+....\\&.+2+1](n-1)=\frac{1}{2}(n-2)(n-1)^2\end{aligned}$$

(d). $$\begin{aligned}&W_{eA}(K_n)=[(\binom{n}{2}-1)+(\binom{n}{2}-2)+...\\&..+2+1](n-1)=\frac{1}{2}[\binom{n}{2}-1]\binom{n}{2}(n-1)\\&=\frac{1}{8}n(n+1)(n-1)^2(n-2)\end{aligned}$$

(e). $$\begin{aligned}W_{eA}(K_{a,b})&=\left((ab-1)+.....+2+1\right)b\\&=\frac{1}{2}ab^2(ab-1)\end{aligned}$$ for $b>a$

Theorem 8. Let G be a tree of order n. then

$$W_{eA}(G)\leq\frac{1}{2}(n-1)^2(n-2) \quad (1),$$

with equality if and only if G is star of order n-1.

Proof. Let Δ be a maximum degree of the graph G. Clearly;

$$W_{eA}(G)\leq\Delta\binom{n-1}{2} \qquad becaus \quad .$$

$$|E(G)|=n-1$$

If $\Delta=n-1$, then n-1 is the maximum quantity of the set degree vertices of all tree G. so

$$W_{eA}(G)\leq(n-1)\binom{n-1}{2}=,$$

$$\frac{1}{2}(n-1)^2(n-2)$$

If G is star, then by theorem 7, the equality is obtained.

Converse, if G is a tree, so there is $\binom{n-1}{2}$ comparison between edges of the graph G and relation (1) shown that $d_A(e,f)=n-1$ for each $\{e,f\}\subseteq E(G)$, so there is a vertex of the graph G (for example $v\in V(G)$) that $\deg v=n-1$ and hence G is a star.

3. Conclusions

In this section, we obtain the edge-degree index of $TUC_4C_8(R)$ nanotorus and $TUC_4C_8(S)$ nanotubes.

(ι). Computing the edge-degree index of $TUC_4C_8(R)$ nanotorus. $C_4C_8(R)$ net is a trivalent decoration made by alternating squares C_4 and octagons C_8. It can cover either by a cylinder or a torus. $T = T(m,n)$ denotes an arbitrary $C_4C_8(R)$ nanotorus in which n is the number of rhombs on the level 1 and the length of torus is m. To compute the edge-degree index of this graph, we consider the 2-dimensional lattice of T (Fig. 1). By this figure, it is obvious that T has exactly 4 mn vertices, 6 mn edges. Thus

$$W_{eA}(T[m,n]) = 3\binom{6mn}{2}$$

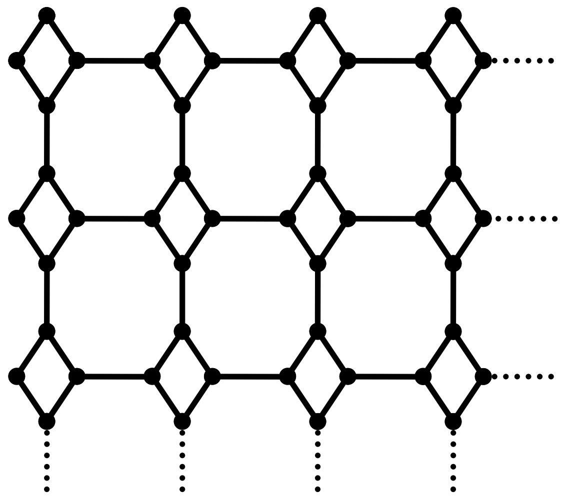

Fig. 1. The 2-Dimensional lattice of $TUC_4C_8(R)$ nanotorus with m=3 and n=4.

(u). Computing the edge-degree index of $TUC_4C_8(S)$ nanotubes

Carbon nanotubes, one-dimensional carbon allotropes, were first discovered in 1991, by Iijima [19] and next in 1993 by the Iijima's group [4] and the Bethune's group [20]. Diudea et al. [21] constructed TUC_4C_8 nanotubes, tubules tessellated by square C_4 and octagon C_8 in different ways. Among them, there is one highly symmetric special case of interest: $TUC_4C_8(S)$ nanotube. About mathematical aspects related to the counting of distance sums of the special case we can refer to [9]. The 2-dimensional lattice of $TUC_4C_8(S)$ nanotubes graph is denoted by $G = GTUC[p,q]$ (Fig. 2). It is easy to see that $|V(G)| = 8pq$, $|E(G)| = 12pq - 2p$, so

$$W_{eA}(GTUC(p,q)) = 3\binom{12pq-2p}{2} - \binom{2p}{2}$$

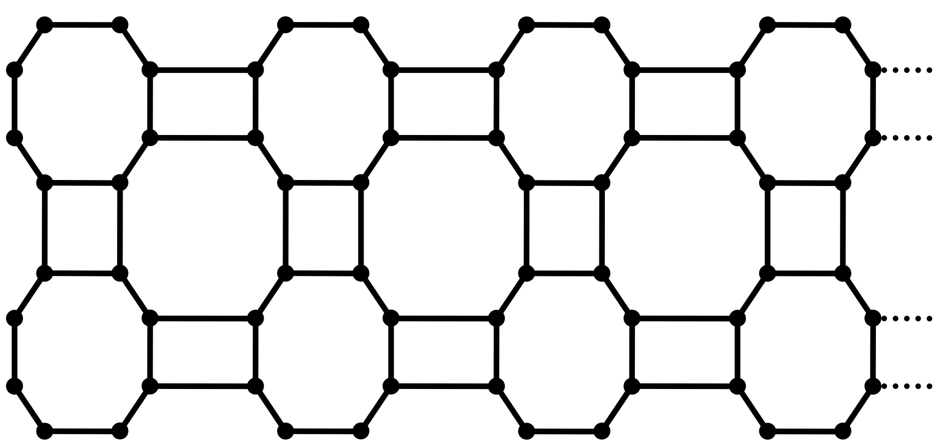

Fig. 2. The graph of $TUC_4C_8(S)$ nanotube $G = GTUC[p,q]$ with p=4 and q=2.

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