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On Topological Properties of the Line Graphs of Subdivision Graphs of Certain Nanostructures - II

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Strictly as per the compliance and regulations of :

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17. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972), 535–538.

On Topological Properties of the Line Graphs of Subdivision Graphs of Certain Nanostructures - II

Sunilkumar M. Hosamani

Abstract- In this note, we give expressions for the first(second) Zagreb coindex, second Zagreb index(coindex), third Zagreb index and first hyper-Zagreb index of the line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of TUC_4C_8 *[p, q]* and obtain upper bounds for Wiener index and degree-distance index of these graphs. This note continue the program of computing certain topological indices of the line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p, q]$ [25] [M. F. Nadeem, S. Zafar, Z. Zahid, *On topological properties of the line graphs of subdivision graphs of certain nanostructures*, *Appl. Math. Comput.* 273(2016) 125{130].

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I. Introduction

Let G be a simple graph. The order of a graph is $|V(G)|$, its number of vertices denoted by n. The size of a graph is $|E(G)|$, its number of edges denoted by m. The degree of a vertex v, denoted by $d_G(v)$. The complement of a graph G, denoted by $\overline{G}$, is a simple graph on the same set of vertices $V(G)$ in which two vertices u and v are connected by an edge uv, if and only if they are not adjacent in G. Obviously, $E(G) \cup E(\overline{G}) = E(K_n)$ where K_n is complete graph of order n, and $|E(\overline{G})| = \frac{n(n-1)}{2} - m$. The subdivision graph $S(G)$ is the graph attained from G by replacing each of its edges by a path of length 2. The line graph $L(G)$ of a graph is the graph derived from G in such a way that the edges in G are replaced by vertices in $L(G)$ and two vertices in $L(G)$ are connected whenever the corresponding edges in G are adjacent [19].

The Zagreb indices were first introduced by Gutman [17], they are important molecular descriptors and have been closely correlated with many chemical properties [29] and defined as:

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2 \qquad \text{and} \tag{1}$$

$$M_2(G) = \sum_{uv \in E(G)} d_G(u)\, d_G(v), \tag{2}$$

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In fact, one can rewrite the first Zagreb index as

$$M_1(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v)\right].$$

Noticing that contribution of nonadjacent vertex pairs should be taken into account when computing the weighted Wiener polynomials of certain composite graphs (see [6]) defined first Zagreb coindex and second Zagreb coindex as

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} \left[d_G(u) + d_G(v)\right] \quad \text{and}$$

$$\overline{M_2}(G) = \sum_{uv \notin E(G)} d_G(u)\, d_G(v), \tag{4}$$

respectively.

The third Zagreb index was first introduced by Fath-Tabar [13]. This index is defined as follows:

$$M_3(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)| \tag{5}$$

The hyper-Zagreb index was first introduced in [28]. This index is defined as follows:

$$HM(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))^2 \tag{6}$$

In fact the idea of topological index appears from work done by Wiener [31] in 1947 although he was working on boiling point of paraffin. He called this index as Wiener index then theory of topological index started. The Wiener index of graph G is defined as

$$W(G) = \frac{1}{2} \sum_{(u,v)} d(u, v) \tag{7}$$

where (u, v) is any ordered pair of vertices in G and $d(u, v)$ is $u - v$ geodesic.

The degree distance index for graphs developed by Dobrynin and Kochetova [12] and Gutman [14] as a weighted version of the Wiener index. The degree distance of G, denoted by $DD(G)$, is defined as follows

$$DD(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v)[d_G(u) + d_G(v)]. \tag{8}$$

For more details on the topological indices we refer to the articles [2–5,17,20,21,24,30,32].

Ref

6. T. Došlić, Vertex-weighted Wiener polynomials for composite graphs, Ars Mathematica Contemporanea 1 (2008) 66–80.

II. Nanostructures

In a series of papers, Diudea and co-authors studied the structure and topological indices of some chemical graphs related to some nanostructures [1,7–11,23]. Rajani et. al derived the expressions for the Shultz indices of the subdivision graphs of the tadpole graph, wheel, helm and ladder graphs [27]. The expressions for the line graphs of subdivision graphs of the tadpole, wheel and ladder graphs can be seen in [26] and [14]. Recently Nadeem et. al [25] obtained expressions for certain topological indices for the line graph of subdivision graphs 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$, where p and q denote the number of squares in a row and the number of rows of squares, respectively in 2D-lattice, nanotube and nanotorus.

In Fig. 1, 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ are depicted. The order

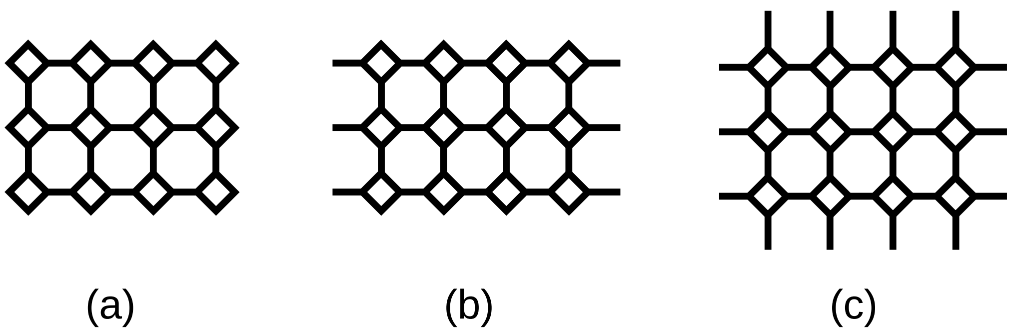


Figure 1: (a) 2D−lattice of $TUC_4C_8[4, 3]$; (b) $TUC_4C_8[4, 3]$ nanotube; (c) $TUC_4C_8[4, 3]$ nanotorus

and size of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ are given in the Table 1.

Table 1: Order and size

Graph	Order	Size
$2D$ − lattice of $TUC_4C_8[p,q]$	$4pq$	$6pq-p-q$
$TUC_4C_8[p,q]$ nanotube	$4pq$	$6pq-p$
$TUC_4C_8[p,q]$ nanotorus	$4pq$	$6pq$

The goal of this paper is to continue this program to compute the first (second) Zagreb coindex, second Zagreb index (coindex), third Zagreb index and first hyper-Zagreb index of the line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ and to obtain upper bounds for Wiener index and degree-distance index of these graphs.

III. Main Results

We begin with the following straightforward, previously known, auxiliary results.

Lemma 1. [18] *For any graph G of order n and size m, the subdivision graph $S(G)$ of G is a graph of order $n+m$ and size $2m$.*

Lemma 2. [18] *Let G be a graph of order n and size m, then the line graph $L(G)$ of G is a graph of order m and size $\frac{1}{2}M_1(G)-m$.*

Ref

27. P.S.Ranjini, V.Lokesha, M.A.Rajan, On the Shultz index of the subdivision graphs, Adv. Stud. Contemp. Math. 21(3)(2011) 279-290.

Theorem 1. [15] *Let G be a graph of order n and size m. Then*

$$\begin{aligned} M_1(\overline{G}) &= M_1(G) + n(n-1)^2 - 4m(n-1) && (9) \\ \overline{M_1}(G) &= 2m(n-1) - M_1(G) && (10) \\ \overline{M_1}(\overline{G}) &= 2m(n-1) - M_1(G) && (11) \end{aligned}$$

Theorem 2. [16] *Let G be a graph of order n and size m. Then*

$$\begin{aligned} M_2(\overline{G}) &= \frac{1}{2}n(n-1)^3 - 3m(n-1)^2 + 2m^2 + \frac{2n-3}{2}M_1(G) - M_2(G) && (12) \\ \overline{M_2}(G) &= 2m^2 - \frac{1}{2}M_1(G) - M_2(G) && (13) \\ \overline{M_2}(\overline{G}) &= m(n-1)^2 - (n-1)M_1(G) + M_2(G) && (14) \end{aligned}$$

Theorem 3. [22] *Let G be a graph of order n and size m. Then*

$$\overline{M_1}(G) \geq 2W(G) - 2M_1(G) + 6m(n-1) - n^3 + n^2 \quad (15)$$

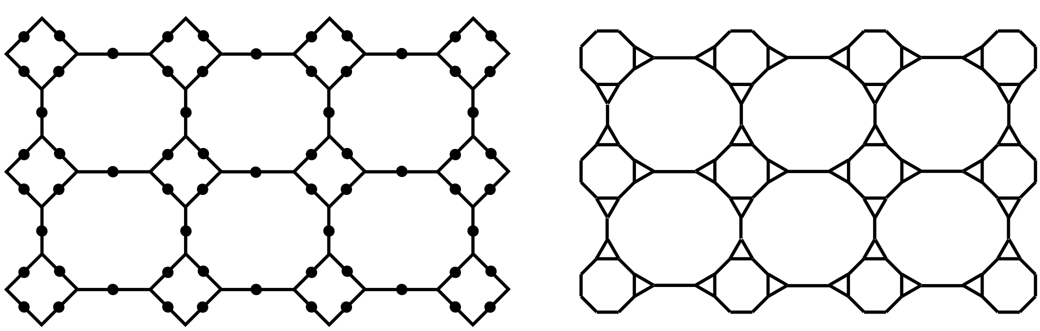
Theorem 4. [22] *Let G be a nontrivial graph of diameter $d \geq 2$. Then*

$$\overline{M_1}(G) \leq \frac{DD(G) - M_1(G)}{2} \quad (16)$$

with equality if and only if $d = 2$.

IV. Topological Indices of Line Graph of the Subdivision Graph of 2D-Lattice of $TUC_4C_8[P, Q]$

In Fig. 2 (b) the line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$ is depicted.



(a) (b)

Figure 2: (a) Subdivision of 2*D*-lattice of $TUC_4C_8[4;3]$; (b) Line graph of the subdivision graph of 2*D*-lattice of $TUC_4C_8[4;3]$.

Theorem 5. Let G be the line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$. Then

Notes

Notes

1. $M_3(G) = 4(p+q-2)$;
2. $HM(G) = 648pq - 264(p+q) + 8$;
3. $\overline{M_1}(G) = \overline{M_1}(\overline{G}) = 2[18pq-5p-5q][12pq-2p-2q-1] + 38(p+q) - 108pq$;
4. $M_1(\overline{G}) = 2[6pq-p-q][4(6pq-p-q)^2 - 4(6pq-p-q)+1] - 2[36pq-10(p+q)][6pq-p-q-1] + 108pq - 38(p+q)$;
5. $M_2(G) = 162pq - 67(p+q) + 4$;
6. $M_2(\overline{G}) = (6pq-p-q)[12pq-2p-2q-1]^3 - 3(18pq-5p-5q)[12pq-2p-2q-1]^2 + (24pq-4p-4q-3)[8(p+q)+27(2pq-p-q)] + 2[18pq-5p-5q]^2 - (162pq-67(p+q)+4)^2$;
7. $\overline{M_2}(G) = 2[18pq-5p-5q]^2 + 86(p+q) - 216pq - 4$;
8. $\overline{M_2}(\overline{G}) = (18pq-5p-5q)[12pq-2p-2q-1]^2 - (12pq-2p-2q-1)[108pq-38(p+q)] + 162pq - 67(p+q) + 4$;
9. $W(G) \leq (18pq-5p-5q)(12pq-2p-2q-1) - 3(18pq-5p-5q)(12pq-2p-2q-1) + 4(12pq-2p-2q-1)[6pq-p-q]^2 + 54pq - 19(p+q)$;
10. $DD(G) \leq 4(18pq-5p-5q)(12pq-2p-2q-1) - 32pq + 114(p+q)$.

Proof. The 2D-lattice of $TUC_4C_8[p,q]$ is a graph of order $4pq$ and size $6pq-p-q$. Then by Lemma 1, the subdivision graph of 2D-lattice of $TUC_4C_8[p,q]$ have order $10pq-p-q$ and size $2[6pq-p-q]$ (see Fig. 2 (a)). Therefore by Lemma 2, G will have order $2[6pq-p-q]$ and size $18pq-5p-5q$. Further notice that in a graph G there are $4(p+q)$ vertices are of degree 2 and remaining all the vertices of degree 3. Hence we can partition the edge set of a graph G as shown in Table 2.

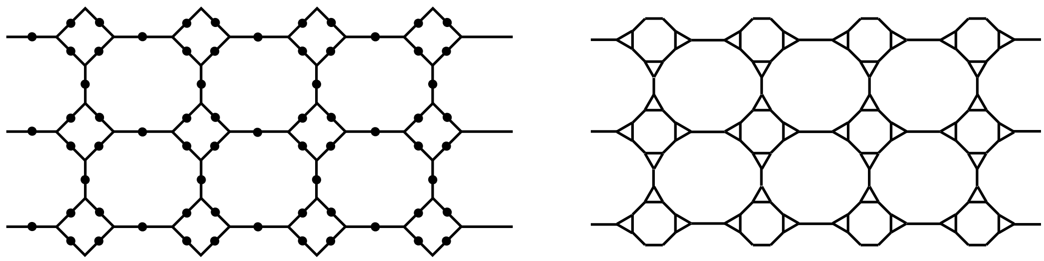
Table 2: The edge partition of the graph G

(d_u, d_v) where $uv \in E(G)$	$(2,2)$	$(2,3)$	$(3,3)$
Number of edges	$2p+2q+4$	$4p+4q-8$	$18pq-11p-11q+4$

We apply Formulas (1)-(8) and by employing the Equations (9)-(16) we can obtain the required results. □

V. Topological Indices of Line Graph of the Subdivision Graph of $TUC_4C_8[P,Q]$ Nanotube

In Fig. 3 (b), the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube is depicted.



(a) (b)

Figure 3: (a) Subdivision of $TUC_4C_8[4,3]$ nanotube; (b) Line graph of subdivision of $TUC_4C_8[4,3]$ nanotube

Theorem 6. Let G be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ of nanotube. Then

1. $M_3(G) = 4p$;
2. $HM(G) = 648pq - 264p$;
3. $\overline{M_1}(G) = \overline{M_1}(\overline{G}) = 2[18pq - 5p][12pq - 2p - 1] + 38p - 108pq$;
4. $M_1(\overline{G}) = 2(6pq - p - q)[12pq - 2p]^2 - 4(18pq - 5p)(12pq - 2p - 1) + 120pq - 38p$;
5. $M_2(G) = 162pq - 67p$;
6. $M_2(\overline{G}) = (6pq - p)[12pq - 2p - 1]^3 - 3(18pq - 5p)[12pq - 2p - 1]^2 + (24pq - 4p - 3)[57pq - 19p] + 2[18pq - 5p]^2 - 162pq + 67p$;
7. $\overline{M_2}(G) = 2[18pq - 5p]^2 + 86p - 216pq$;
8. $\overline{M_2}(\overline{G}) = (18pq - 5p)[12pq - 2p - 1]^2 - (12pq - 2p - 1)[108pq - 38p)] + 162pq - 67p$;
9. $W(G) \leq (18pq - 5p)(12pq - 2p - 1) - 3(18pq - 5p)(12pq - 2p - 1) + (12pq - 2p)^2(12pq - 2p - 1) + 54pq - 19p$;
10. $DD(G) \leq 4(18pq - 5p)(12pq - 2p - 1) - 108pq + 6p$.

Proof. The $TUC_4C_8[p,q]$ of nanotube is a graph of order $4pq$ and size $6pq - p$. Then by Lemma 1, the subdivision graph of $TUC_4C_8[p,q]$ of nanotube of order $10pq - p$ and size $12pq - 2p$ (see Fig. 3 (a)). Therefore by Lemma 2, G will have order $12pq - 2p$ and size $18pq - 5p$. Further notice that in a graph G there are $4p$ vertices are of degree 2 and remaining all the vertices of degree 3. Hence we can partition the edge set of a graph G as shown in Table 3.

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Notes

Table 3: The edge partition of the graph G

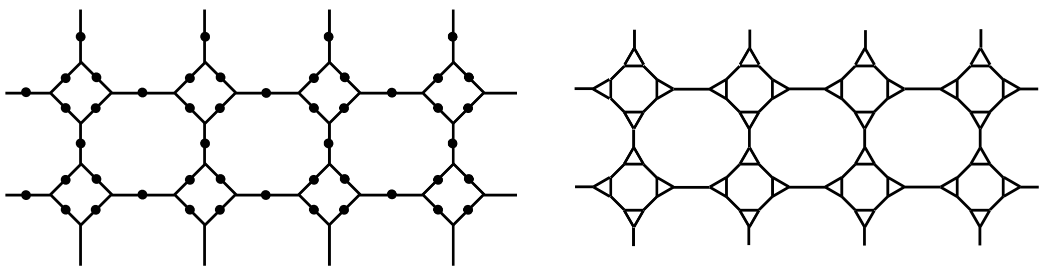
(d_u, d_v) where $uv \in E(G)$	$(2,2)$	$(2,3)$	$(3,3)$
Number of edges	$2p$	$4p$	$18pq - 11p$

We apply Formulas (1)-(8) and by employing the Equations (9)-(16) we can obtain the required results. □

Notes

VI. Topological Indices of Line Graph of the Subdivision Graph of TUC_4C_8 [P, Q] Nanotorus

In Fig. 4 (b) the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotorus is depicted.



(a) (b)

Figure 4: (a) Subdivision of TUC_4C_8[4, 2] nanotorus; (b) Line graph of Subdivision of TUC_4C_8[4, 2] nanotorus

Theorem 7. *Let G be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotorus. Then*

1. $M_3(G) = 0$;
2. $HM(G) = 648pq$;
3. $\overline{M_1}(G) = \overline{M_1}(\overline{G}) = 432p^2q^2 - 144pq$;
4. $M_1(\overline{G}) = 12pq(12pq-1)^2 - 72pq(12pq-1) + 108pq$;
5. $M_2(G) = 162pq$;
6. $M_2(\overline{G}) = 6pq[12pq-1]^3 - 64pq[12pq-1]^2 + 54pq(24pq-3) + 324p^2q^2 - 162pq$;
7. $\overline{M_2}(G) = 648p^2q^2 - 216pq$;
8. $\overline{M_2}(\overline{G}) = (18pq(12pq-1)^2 - (12pq-1)108pq + 162pq$;
9. $W(G) \leq 6p^2q^2[288pq+12] - 54pq(12pq-1) + 36pq$;
10. $DD(G) \leq 864p^2q^2 - 396pq$.

Proof. The $TUC_4C_8[p,q]$ of nanotorus is a graph of order $4pq$ and size $6pq$. Then by Lemma 1, the subdivision graph of $TUC_4C_8[p,q]$ of nanotorus have order $10pq$ and size $12pq$ (see Fig. 4 (a)). Therefore by Lemma 2, G will have $12pq$ vertices and $18pq$ edges. Further note that the degree of each vertex is 3 in G. Hence we can partition the edge set of a graph G as shown in Table 4.

Table 4: The edge partition of the graph G

(d_u, d_v) where $uv \in E(G)$	$(3,3)$
Number of edges	$18pq$

We apply Formulas (1)-(8) and by employing the Equations (9)-(16) we can obtain the required results. □

Notes

Conclusion: In this paper, we continue the study certain degree based topological indices for the line graph of subdivision graph of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ and obtained upper bounds for Wiener index and degree distance index of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ respectively.

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