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On topological properties of the line graphs of subdivision graphs of certain nanostructures

Muhammad Faisal Nadeem [a], Sohail Zafar [b,*], Zohaib Zahid [b]

[a] Department of Mathematics, Comsat Institute of Information Technology, Lahore, Pakistan
[b] University of Management and Technology, Lahore, Pakistan

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ABSTRACT

In the study of QSAR/QSPR, topological indices such as Shultz index, generalized Randic index, Zagreb index, general sum-connectivity index, atom-bond connectivity (ABC) index and geometric–arithmetic (GA) index are exploited to estimate the bioactivity of chemical compounds. A topological index attaches a chemical structure with a numeric number. There are numerous applications of graph theory in this field of research. In this paper we computed generalized Randic, general Zagreb, general sum-connectivity, ABC, GA, ABC_4 and GA_5 indices of the line graphs of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p, q]$ by using the concept of subdivision.

1. Introduction and preliminaries

In this article we will consider only simple graphs without loop and multiple edges. Let G be a simple graph, with vertex set $V(G)$ and edge set $E(G)$. The degree d_u of a vertex u is the number of edges that are incident to it and $S_u = \sum_{v\in N_u} d_v$ where $N_u = \{v \in V(G)|uv \in E(G)\}$. N_u is also known as the set of neighbor vertices of u. 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 graph G is the graph whose vertices are the edges of G, two vertices e and f are incident if and only if they have a common end vertex in G. For any natural number l, we define $V_l = \{u \in V(G) \mid S_u = l\}$.

Topological indices are the mathematical measures which correspond to the structures of any simple finite graph. They are invariant under the graph isomorphisms. The significance of topological indices is usually associated with quantitative structures property relationship (QSPR) and quantitative structure activity relationship (QSAR) (see [28]).

The idea of topological index appears from work done by Wiener (see [37]) in 1947 although he was working on boiling point of paraffin. He called this index as Wiener index and then theory of topological index started.

The Wiener index of graph G is defined as

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

where (u, v) is any ordered pair of vertices in G and $d(u, v)$ is $u - v$ geodesic. The reader can find more information about the Wiener index in [4,15,18,19].

* Corresponding author. Tel.: +92 3214242349.
E-mail addresses: mfaisalnadeem@ymail.com (M.F. Nadeem), sohailahmad04@gmail.com (S. Zafar), zohaib_zahid@hotmail.com (Z. Zahid).

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Table 1
Numbers of vertices and edges.

Graph	Number of vertices	Number of edges
$2D$-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 first degree-based connectivity index for graphs developed by using vertex degrees is Randić index [23]. The Randić index of graph G is defined as

$$R(G)=\sum_{uv\in E(G)}(d_u d_v)^{-1/2}.$$

Later, this index was generalized for any real number α, and known as the generalized Randić index $R_\alpha(G)$:

$$R_\alpha(G)=\sum_{uv\in E(G)}(d_u d_v)^{\alpha}. \tag{1}$$

For further study of Randić index of various graph families, see [10,16,25,29].

Li and Zhao introduced the first general Zagreb index in [17]:

$$M_\alpha(G)=\sum_{u\in V(G)}(d_u)^{\alpha}. \tag{2}$$

For more results on Zagreb index, see [1,8,11,13,20,34,36].

In 2010, the general sum-connectivity index $\chi_\alpha(G)$ has been introduced in [39]:

$$\chi_\alpha(G)=\sum_{uv\in E(G)}(d_u+d_v)^{\alpha}. \tag{3}$$

The atom-bond connectivity (ABC) index was introduced by Estrada et al. in [3]. The ABC index of graph G is defined as

$$ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_u d_v}}. \tag{4}$$

D. Vukicevic and B. Furtula introduced the geometric arithmetic (GA) index in [35]. The GA index for graph G is defined as

$$GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_u d_v}}{d_u+d_v}. \tag{5}$$

The fourth member of the class of ABC index was introduced by Ghorbani and Hosseinzadeh in [6]:

$$ABC_4(G)=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_u S_v}}. \tag{6}$$

The 5th GA index was introduced by Graovac et al. in [7]:

$$GA_5(G)=\sum_{uv\in E(G)}\frac{2\sqrt{S_u S_v}}{S_u+S_v}. \tag{7}$$

For more details on the topological indices we refer to the articles [2,5,9,12,14,21,24,30,32,33,38].

2. Topological indices of $L(S(G))$

In 2011, Ranjini et al. calculated the explicit expressions for the Shultz indices of the subdivision graphs of the tadpole, wheel, helm and ladder graphs [27]. They also studied the Zagreb indices of the line graphs of the tadpole, wheel and ladder graphs with subdivision in [26]. In 2015, Su and Xu calculated the general sum-connectivity indices and co-indices of the line graphs of the tadpole, wheel and ladder graphs with subdivision in [31]. In [22], Nadeem et al. computed ABC_4 and GA_5 indices of the line graphs of the tadpole, wheel and ladder graphs by using the notion of subdivision.

In this paper, we computed generalized Randic, general Zagreb, general sum-connectivity, ABC, GA, ABC_4 and GA_5 indices of the line graphs of subdivision graphs of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$. Let 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 of $TUC_4C_8[p,q]$ as shown in Fig. 1(a), (b), and (c) respectively.

The numbers of vertices and edges of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ are given in Table 1.

In order to find the number of edges of the arbitrary graph the following lemma is important for us.

Lemma 2.1. *Let G be a graph. Then* $\sum_{u\in V(G)} d_u = 2|E(G)|$.

This is also known as handshaking lemma.