Two Types of Geometric-Arithmetic Indices of Nanotubes and Nanotori

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Abstract

The concept of geometric-arithmetic indices was introduced in the chemical graph theory. These indices are defined as

\[ GA(G) = \sum_{uv \in E(G)} 2 \sqrt{Q_u Q_v} / (Q_u + Q_v), \]

where \( Q_u \) is some quantity that in a unique manner can be associated with the vertex \( u \) of graph \( G \). In this paper, exact formulas for two types of geometric-arithmetic index of \( TUC_4C_8(S) \) nanotube and \( TC_4C_8(S) \) nanotorus are given.

1. Introduction

Throughout this section \( G \) is a simple connected graph with vertex and edge sets \( V(G) \) and \( E(G) \), respectively. A topological index is a numeric quantity from the structure of a graph which is invariant under automorphisms of the graph under consideration.

A topological index is a numeric quantity from the structural graph of a molecule. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffin. The Wiener index of \( G \) is the sum of distance between all unordered pair of vertices of \( G \),

\[ W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v), \]

where \( d_G(u,v) \) and is defined as the number of edges in a minimal path connecting the vertices \( u \) and \( v \), see [1]. The concept of geometric-arithmetic indices was introduced in the chemical graph theory. These indices generally are defined as

\[ GA_{general} = GA_{general}(G) = \sum_{uv \in E(G)} 2 \sqrt{Q_u Q_v} / (Q_u + Q_v), \]

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where $Q_u$ is some quantity that in a unique manner can be associated with the vertex $u$ of graph $G$.

The first type of geometric-arithmetic index is denoted by $GA_1$ and defined as

$$GA_1 = GA_1(G) = \frac{2d_u d_v}{d_u + d_v},$$

where $uv$ is an edge of the molecular graph $G$ and $d_u$ stand for the degree of the vertex $u$, see [2]. The $GA_1$ index has been introduced less than a year ago [2]. However, a few papers are appeared dealing with this quantity, see [3-5].

The second type of geometric-arithmetic index is denoted by $GA_2$ and defined as

$$GA_2 = GA_2(G) = \frac{2n_u n_v}{n_u + n_v},$$

where $n_u$ is the number of vertices of $G$ lying closer to $u$ than to $v$ and $n_v$ is the number of vertices of $G$ lying closer to $v$ than to $u$, see [6]. For $uv \in E(G)$, let $m_u$ is the number of edges of $G$ lying closer to $u$ than to $v$ and $m_v$ is the number of edges of $G$ lying closer to $v$ than to $u$.

The third member of the class of $GA_{general}$ by setting $Q_u (Q_v)$ to be the number $m_u (m_v)$ for the edge $uv$ of the graph $G$ is defined as

$$GA_3 = GA_3(G) = \frac{2\sqrt{m_u m_v}}{m_u + m_v},$$

it has been introduced in the paper [7]. A $C_4C_8$ net is a trivalent decoration made by alternating squares $C_4$ and octagons $C_8$. In recent years, some researchers are interested to topological indices of $C_4C_8$ nanotubes and nanotori, see [8-21] for details. They computed some distance based topological indices of these nanotubes and nanotori.

The $TUC_4C_8(S)$ nanotube is a mathematically beautiful object constructed from squares and octagons, Figure 1 (a). The aim of this article is to compute $GA_2$ and $GA_3$ indices of $TUC_4C_8(S)$ nanotube and $TC_4C_8(S)$ nanotorus that obtained from $TUC_4C_8(S)$ nanotube by gluing its ends, Figure 1 (b).

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure1.png}
\caption{(a) $TUC_4C_8(S)$ nanotube, (b) $TC_4C_8(S)$ nanotorus.}
\end{figure}
Throughout this paper $T = T[p, q]$ denotes an arbitrary $TUC_4C_8(S)$ nanotube in terms of the number of octagons in a fixed row ($p$) and the number of octagons in a fixed column ($q$), in the two-dimensional lattice of $T$, Figure 2. We also denote a $TC_4C_8(S)$ nanotorus, Figure 3, by $S = S[p, q]$.

![Figure 2. Two Dimensional Lattice $TUC_4C_8(S)$ nanotube, with $p=5$ and $q=3$.](image1)

![Figure 3. Two Dimensional Lattice $TC_4C_8(S)$ nanotorus, with $p=5$ and $q=3$.](image2)

### 2. Main Results

In this section, $GA_2$ and $GA_3$ indices of the molecular graph of $TUC_4C_8(S)$ nanotube and $TC_4C_8(S)$ nanotorus are computed. It is easy to see that

$$|V(T)| = |V(T[p, q])| = 8pq \quad \text{and} \quad |E(T)| = |E(T[p, q])| = 12pq - 2p,$$

$$|V(S)| = |V(S[p, q])| = 8pq \quad \text{and} \quad |E(S)| = |E(S[p, q])| = 12pq.$$

In the following theorem the $GA_2$ index of $TUC_4C_8(S)$ nanotube is obtained.
Theorem 1. The $GA_k$ index of $T=T[p,q]$ is computed as follows:

$$GA_k(T) = \begin{cases} 
4pq + \frac{1}{4pq} \sum_{i=1}^{p} \sqrt{(p+k-l)(p+k)|V(T)| - (p+k-l)(p+k)} & p \leq \frac{q}{2} \\
+ \frac{1}{2q} \sum_{i=1}^{2p+1} \sqrt{4pk(|V(T)| - 4pk)} & p > \frac{q}{2} \\
+ \frac{1}{2q} \sum_{i=1}^{2p+1} \sqrt{4pk(|V(T)| - 4pk)} & p > \frac{q}{2} 
\end{cases} $$

Proof. One can see that there are three separate types of edges of $TUC_4C_8(S)$ nanotube and the number of edges is different. Suppose $e_1$, $e_2$ and $e_3$ are representative edges for these types.

![Figure 4](image.png)

**Figure 4.** The set $E_1(T)$ (The edges of type $e_1$).

We partition the edges of $TUC_4C_8(S)$ nanotube into three subsets $E_1(T)$, $E_2(T)$ and $E_3(T)$, as follows:

- $E_1(T) = \{ e \mid e$ is the type of $e_1 \}$,
- $E_2(T) = \{ e \mid e$ is the type of $e_{2,k}$ for $1 \leq k \leq 2q \}$,
- $E_3(T) = \{ e \mid e$ is the type of $e_3 \}$. 
The sets $E_1(T)$, $E_2(T)$ and $E_3(T)$ are shown by dashed lines in Figures 4, 5 and 6, respectively.

Figure 5. The set $E_2(T)$ (The edges of type $e_2$).

Figure 6. The set $E_3(T)$ (The edges of type $e_3$).

Therefore, by definition of $GA_2$ index,

$$GA_2(T) = \sum_{e \in E_1(T)} \frac{2\sqrt{n_u n_v}}{n_u + n_v} + \sum_{e \in E_2(T)} \frac{2\sqrt{n_u n_v}}{n_u + n_v} + \sum_{e \in E_3(T)} \frac{2\sqrt{n_u n_v}}{n_u + n_v}.$$ 

We evaluate each sums separately. For evaluating the first sum, we know that for $e = uv \in E_1(T)$, we have $n_u = n_v = \frac{|V(T)|}{2}$. Also $|E_1(T)| = 4pq$, then $\sum_{e \in E_1(T)} 2\sqrt{n_u n_v} = 4pq$.

For each $e = uv \in E_2(T)$, we have $n_u + n_v = 8pq$. Obviously, for every $e_{2,1} = uv$, we have $n_u = p(p+1), n_v = 8pq - p(p+1)$, for every $e_{2,2} = uv$, we have $n_u = (p+1)(p+2), n_v = 8pq - (p+1)(p+2)$, ..., for every $e_{2,j} = uv$, we have
By the same method when $p > \frac{q}{2}$, we can compute $\sum_{uv \in E_1(T)} \frac{2\sqrt{n_u n_v}}{n_u + n_v}$.

Finally for computing the third sum, we attend, for each $e = uv \in E_3(T)$ in $k$-th row, $n_u = 4pk$ and $n_v = 8pq - 4pk$ and the number of edges of third type in each row is $2p$. Since $TUC_4C_8(S)$ nanotube is bipartite then for each $e = uv \in E_3(T)$, we have $n_u + n_v = |V(T)|$. Then

$$\sum_{uv \in E_3(T)} \frac{2\sqrt{n_u n_v}}{n_u + n_v} = \frac{1}{4pq} \sum_{uv \in E_3(T)} \sqrt{n_u n_v} = \frac{2p}{4pq} \sum_{i=1}^{2q-1} \sqrt{(4pk)(|V(T)| - 4pk)}$$

$$= \frac{1}{2q} \sum_{i=1}^{2q-1} \sqrt{(4pk)(|V(T)| - 4pk)}.$$

This completes the proof. □

**Theorem 2.** The $GA_4$ index of $T = T[p, q]$ is given by:

$$GA_4(T) = 4pq + \sum_{uv \in E_2(T)} \frac{2\sqrt{m_u m_v}}{m_u + m_v} + \frac{2p}{12pq - 4p} \sum_{i=0}^{2q-2} (4p + 6kp)(12pq - 8p - 6kp),$$

where the elements of $E_4(T)$ are shown in Figure 4.

**Proof.** We can now state the analogue of Theorem 1. Then

$$GA_4(T[p, q]) = \sum_{uv \in E_1(T)} \frac{2\sqrt{m_u m_v}}{m_u + m_v} + \sum_{uv \in E_2(T)} \frac{2\sqrt{m_u m_v}}{m_u + m_v} + \sum_{uv \in E_3(T)} \frac{2\sqrt{m_u m_v}}{m_u + m_v}.$$

For each $e = uv \in E_1(T)$, $m_u = m_v = \frac{m - 2q}{2}$, then $\sum_{uv \in E_1(T)} \frac{2\sqrt{m_u m_v}}{m_u + m_v} = 4pq$. We can partition $E_2(T)$ into $2q$ subsets such as $E_{2,1}$, $E_{2,2}$, ..., $E_{2,2q}$ such that $E_{2,k} = \{ e | e \text{ is the type of } e_{2,k} \}$, for $1 \leq k \leq 2q$. Therefore

$$\sum_{uv \in E_2(T)} \frac{2\sqrt{m_u m_v}}{m_u + m_v} = 2 \sum_{k=1}^{q} \sum_{uv \in E_{2,k}} \frac{2\sqrt{m_u m_v}}{m_u + m_v}.$$

By calculation we have the following results. Suppose $i$ is an odd positive integer, such that $1 \leq i \leq q$, for each $e = uv \in E_{2,i}$,
Suppose $i$ is an even positive integer, such that $1 \leq i \leq q$, for each $e = uv \in E_{3i}$,

$$m_i(e) = \begin{cases} (p + i - 1)^2 + \left\lfloor \frac{p^2}{2} \right\rfloor + (i - 1)p + \frac{i - 1}{2} & p < 2q - 2\left\lfloor \frac{i - 1}{2} \right\rfloor \\ 6p - 6q^2 + (6i - 4)q - 2p + 2\left\lfloor \frac{p}{2} \right\rfloor - i & p \geq 2q - 2\left\lfloor \frac{i - 1}{2} \right\rfloor \end{cases}$$

and

$$m_s(e) = \begin{cases} |E(T)| - m_s(e) - (2p + 2i - 2) & p < 2q - 2\left\lfloor \frac{i - 1}{2} \right\rfloor \\ |E(T)| - m_s(e) - 4pq & p \geq 2q - 2\left\lfloor \frac{i - 1}{2} \right\rfloor \end{cases}.$$

For $e = uv \in E_{3}(T)$, in $k$-th row, $m_u + m_v = 12pq - 4p$ and then, $m_u = 4p + 6pk, m_v = 12pq - 8p - 6pk$. Hence $\sum_{e \in E(T)} \frac{2\sqrt{m_u m_v}}{m_u + m_v} = \frac{2p}{12pq - 4p} \sum_{i=0}^{2q-2} \sqrt{(4p + 6pk)(12pq - 8p - 6pk)}$. This completes the proof.

**Theorem 3.** The $GA_2$ and $GA_4$ indices of $S = S[p, q]$ are equal and computed as follows:

$$GA_2(S) = GA_4(S) = |E(S)|.$$

**Proof.** Since $TC_4C_8(S)$ nanotri is bipartite then for each $e = uv \in E(S)$, we have $n_u + n_v = |V(S)|$. Moreover for each $e = uv \in E(S)$, $n_u = n_v = \frac{|V(S)|}{2}$, therefore by definition of
GA\(_2\) index we conclude that, \(GA_2(S) = \sum_{uv \in E(S)} \frac{2\sqrt{m_u m_v}}{n_u + n_v} = |E(S)|\). Now for obtaining the \(GA_3\) index, it is sufficient to show that for each \(e = uv \in E(S)\), \(m_u = m_v\). Such as Theorem 1, we partition the edge set of \(S = \{p, q\}\) into three subsets \(E_1(S)\), \(E_2(S)\) and \(E_3(S)\), these subsets are shown in Figure 7 by dashed lines.

For each \(e = uv \in E_1(S)\), \(m_u = m_v = \frac{|E(S)| - 2q}{2}\). For second type of edges for each \(e = uv \in E_2(S)\), \(m_u = m_v = \frac{|E(S)| - (10 + 6(r - 2))}{2} = \frac{|E(S)| + 2 - 6r}{2}\), where \(r = \min\{p, q\}\). Finally for each \(e = uv \in E_3(S)\), \(m_u = m_v = \frac{|E(S)| - 2p}{2}\). By above argument, we conclude that

\[
GA_3(S) = \sum_{uv \in E_1(S)} \frac{2\sqrt{m_u m_v}}{m_u + m_v} + \sum_{uv \in E_2(S)} \frac{2\sqrt{m_u m_v}}{m_u + m_v} + \sum_{uv \in E_3(S)} \frac{2\sqrt{m_u m_v}}{m_u + m_v} = |E_1(S)| + |E_2(S)| + |E_3(S)| = |E(S)|,
\]

and this complete the proof.

\[\square\]

**Figure 7.** The partition of \(E(S)\) into \(E_1(S)\), \(E_2(S)\) and \(E_3(S)\).

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