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AN ALGEBRAIC METHOD FOR COMPUTING SZEGED INDEX OF TC_4C_8(R/S) NANOTORI

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Let G be a molecular graph and e be an edge of g. Define $N_1(e)$ to be the number of vertices of G lying closer to one end of e and $N_2(e)$ be the number of vertices of G lying closer to the other end of e. Then the Szeged index of G, Sz(G), is defined as the sum of $N_1(e)N_2(e)$ over all edges of G. In this paper, an algebraic method for computing Szeged index of a molecular graph is presented. We apply this method to compute the Szeged index of TUC_4C_8(R/S) nanotori.

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1. Introduction

Graph representation of molecular structures is widely used in computational chemistry [1-3] Trinajstic [1] noted that the roots of chemical graph theory may be found in the works by chemists of 18–19th centuries such as Higgins, Kopp, Crum Brown. First chemical graphs for representing molecules were used by them.

A graph G consists of a set of vertices V(G) and a set of edges E(G). The vertices in G are connected by an edge if there exists an edge $uv \in E(G)$ connecting the vertices u and v in G such that $u, v \in V(G)$. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. The number of vertices and edges in a graph will be denoted by |V(G)| and |E(G)|, respectively.

To identify molecular structures of chemical compound, the molecular graph invariants, called topological indices could be used too. Topological indices are designed basically by transforming a molecular graph into a number. The first use of a topological index was made in 1947 by the chemist Harold Wiener [1]. Wiener introduced the notion of path number of a graph as the sum of distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. Wiener originally defined his index (W) on trees and studied its use for correlations of physico-chemical properties of alkanes, alcohols, amines and their analogous compounds.

Hosoya[5] reformulated the Wiener index in terms of distances between vertices in an arbitrary graph. He defined W as the sum of distances between all pairs of vertices of the graph under consideration, $W(G) = \sum_{u,v} d(u,v)$, where d(u,v) is the number of edges in a minimum path connecting the vertices u and v.

In the 1990s, a large number of other topological indices have been put forward, all being based on the distances between vertices of molecular graphs and all being closely related to W. The Szeged index is one of these topological indices, which is introduced by Ivan Gutma [6].

2. Theoretical

Let G be a simple molecular graph without directed and multiple edges and without loops. If e is an edge of G, connecting the vertices u and v then we write e = uv. Let $N_1(e)$ be the number of vertices of G lying closer to one end of e and $N_2(e)$ be the number of vertices of G lying closer to the other end of e. Edges equidistance from both the ends of an edge are not taken into account. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e \in E(G)} N_1(e)N_2(e)$.

The present authors[7-12] computed the Wiener index of a polyhex, $TUC_4C_8(R)$ and $TUC_4C_8(S)$ nanotori. In the mentioned papers, our method for computing Wiener index of nanotori was geometric. The geometric method is based on distance between vertices of the graph under consideration. In what follows, we show that there is also an algebraic method which is useful for distance based topological indices of trivalent molecular graphs. In algebraic method, some information on the structure of orbits of the automorphism group under its natural action is needed.

We now recall some algebraic definitions that will be used in the paper. Groups are often used to describe symmetries of objects. This is formalized by the notion of a group action: every element of the group acts like a bijective map on some set. To clarify this notion, we assume that G is a group and X is a set. G is said to act on X when there is a map $\varphi : G \times X \rightarrow X$ such that all elements $x \in X$ (i) $\varphi(e,x) = x$, where e is the identity element of G, and,(ii) $\varphi(g,\varphi(h,x)) = \varphi(gh,x)$ for all $g, h \in G$. In this case, G is called a transformation group, X is called a G-set, and φ is called the group action. For simplicity we define $gx = \varphi(g,x)$. In a group action, a group permutes the elements of X .The identity does nothing, while a composition of actions corresponds to the action of the composition. For a given X ,the set $\{gx \mid g \in G\}$, where the group action moves x, is called the group orbit of x. If G has exactly one orbit, then G is said to be vertex transitive.

The goal of this paper is to continue this program to compute the Szeged index of $TC_4C_8(R/S)$. Throughout this paper our notation is standard and taken from the standard book of graph theory. We encourage the readers to consult papers by Diudea and his co-authors[13-17] for background materials as well as basic computational techniques.

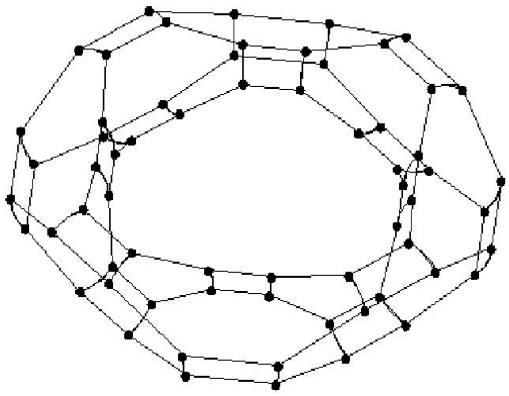

Figure 1. An $TUC_4C_8(S)$ Nanotorus.

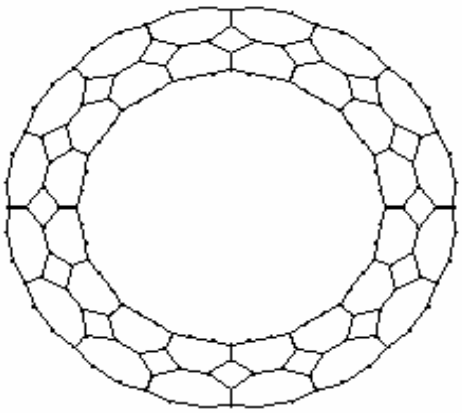

Figure 2. An $TUC_4C_8(R)$ Nanotorus.

3. Results and discussion

In this section, the Szeged index of $TC_4C_8(R)$ and $TC_4C_8(S)$ nanotori are computed. Let us recall some definitions and notations. An automorphism of a graph G is a permutation g of the vertex set V(G) of G with the property that, for any vertices u and v, g(u) and g(v) are adjacent if and only if u is adjacent to v. The set of all automorphisms of a graph G, with the operation of

the composition of permutations, is a permutation group on V(G), denoted Aut(G). We start by stating a result on Szeged index of a polyhex nanotorus.

Theorem 1 ([12]). The molecular graph of a polyhex nanotorus is vertex transitive.

Corollary. If e is an arbitrary edge of T = T[p,q] then $N_1(e) = N_2(e) = pq/2$. In particular, $Sz(T) = 3/8p^3q^3$.

Lemma 1. Suppose G is a graph and $E_1, E_2, ..., E_r$ are orbits of the natural action of Aut(G) on G. If e_i is a representative for the orbit E_i, $1 \leq i \leq r$, then $Sz(G) = |E_1|N_1(e_1)N_2(e_1) + ... + |E_r|N_1(e_r)N_2(e_r)$.

Proof. By definition of Szeged index and main properties of orbits of an action, one can see that:

$$Sz(G) = \sum_e N_1(e)N_2(e) = \sum_{i=1}^{r} \sum_{e \in E_i} N_1(e_i)N_2(e_i) = \sum_{i=1}^{r} |E_i|N_1(e_i)N_2(e_i).$$

We are ready to compute the Szeged index of $TC_4C_8(R/S)$ nanotori, Figures 1 and 2. We first assume that $T_1 = TC_4C_8(S)[m,n]$ is the molecular graph of a $TC_4C_8(S)$ nanotorus with m and n oblique edges in each row and column, Figure 1.

Theorem 2. $Sz(T_1) = 3m^3n^3$.

Proof. From the molecular of T_1, one can see that this graph has exactly 2mn vertices and 3mn edges. The natural action of $Aut(T_1)$ on $V(T_1)$ induces an action of $Aut(T_1)$ on $E(T_1)$. We claim that this action has exactly three orbits determined by a vertical edge, a horizontal edge and an oblique edge of T_1, say e_1, e_2 and e_3, respectively. To do this, we define four permutations π_1, π_2, π_3 and π_4 as follows:

π_1 is a $2\pi/n$ rotation on squares of the first row, through the main axis of T_1, Figure 3.

π_2 is a $2\pi/m$ rotation on squares of the nanotube with 2mn vertices constructed from T_1,

π_3 is the main plane symmetry of the torus,

π_4 is a symmetry obtained from a vertical plane decomposed the torus into two equal nanotube.

It is clear that π_1, π_2, π_3 and π_4 are automorphisms of T_1. Suppose e_1 and e_2 are two horizontal edges of T_1. Then a combination of a power of π_1 and a power of π_2 maps e_1 into e_2. Therefore, horizontal edges of T_1 constitute an orbit of the action. The same argument shows that the vertical edges of T_1 constitute another orbit of the action. Finally, for every edge e_1 and e_2 there is a combination of some powers of π_1, π_2, π_3 and π_4 maps e_1 into e_2 and so oblique edges of T_1 constitute a third orbit for the action. If A, B and C denote these orbits with representatives E_1, E_2, E_3, respectively, then $|A| = |B| = |C| = mn$ and since $|E(T_1)| = 3mn$, these are all the orbits of the

action of $Aut(T_1)$ on $E(T_1)$, see Figure 3. By Lemma 1, $Sz(T_1) = mn[N_1(e_1)N_2(e_1) + N_1(e_1)N_2(e_1) + N_1(e_1)N_2(e_1)] = 3m^3n^3$. ■

In the end of this paper, the molecular graph of $T_2 = TUC_4C_8(R)[m,n]$ nanotorus with exactly n rhombi on the first row and m rhombi on the first column is considered. This graph is bipartite if and only if m and n are even. On the other hand, T_2 has exactly 4mn vertices and 6mn edges. A similar argument as Theorem 2 proves the following theorem:

Theorem 3. $Sz(T_2) = 24m^3n^3$.

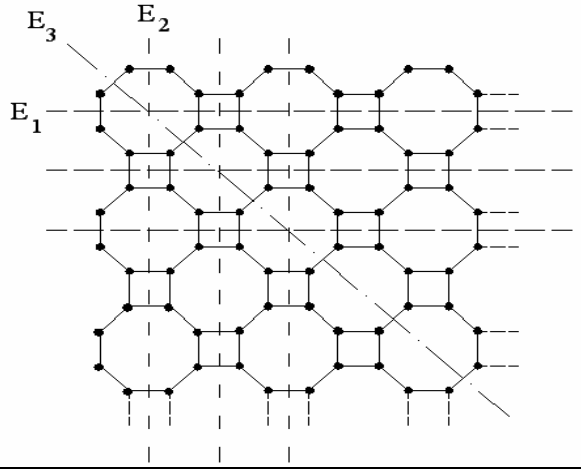

Fig. 3. The 2-Dimensional Lattice of $TUC_4C8(R)[3,3]$ Nanotorus.

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