The PI Index of polyomino chains

Lixing Xu\textsuperscript{a,},* Shubo Chen\textsuperscript{b}

\textsuperscript{a} Department of Science and Information Science, Shaoyang University, Shaoyang, Hunan 422000, PR China
\textsuperscript{b} Department of Mathematics and Computer Science, Hunan City University, Yiyang, Hunan 413000, PR China

Received 5 October 2006; received in revised form 11 November 2007; accepted 11 December 2007

Abstract

The PI index is a graph invariant defined as the summation of the sums of $n_{eu}(e|G)$ and $n_{ev}(e|G)$ over all the edges $e = uv$ of a connected graph $G$, i.e., $\text{Pl}(G) = \sum_{e \in E(G)}[n_{eu}(e|G) + n_{ev}(e|G)]$, where $n_{eu}(e|G)$ is the number of edges of $G$ lying closer to $u$ than to $v$ and $n_{ev}(e|G)$ is the number of edges of $G$ lying closer to $v$ than to $u$. An efficient formula for calculating the PI index of polyomino chains is given, and the bounds for the PI index of polyomino chains are established.

\textcopyright{} 2008 Elsevier Ltd. All rights reserved.

Keywords: Graph invariant; PI index; Polyomino chain; Square lattice; Segment

1. Introduction

The structure of a molecule could be represented in a variety of ways. The information on the chemical constitution of molecule is conventionally represented by a molecular graph. And graph theory was successfully provided the chemist with a variety of very useful tools, namely, topological indices. One of the oldest and most thoroughly examined molecular graph-based structural descriptor of organic molecule is the Wiener index or Wiener number [1,2]. The Wiener index (W) is applicable to acyclic (tree) graphs only. For cyclic compounds a novel molecular-graph-based descriptor, referred to as the Szeged index (Sz) is put forward by Gutman [3] and coworkers [4]. This is considered as the modification of W to cyclic graph. It is based on distance in the molecular graph but is not of the same type as W. For acyclic systems (trees) Sz and W coincide. Consequently, one of the authors (PVK) introduced yet another index called Padmakar-Ivan (PI) index [5,6]. The PI index of a graph $G$ is defined as

$$\text{Pl}(G) = \sum_{e \in E(G)}[n_{1}(e) + n_{2}(e)]$$

where for edge $e = xy$, $n_{1}(e)$ is the number of edges of $G$ lying closer to $x$ than $y$, $n_{2}(e)$ is the number of edges of $G$ lying closer to $x$ than $y$ and summation goes over all edges of $G$. The edges equidistant from $x$ and $y$ are not consider for the calculation of PI index. Since the PI index is different for acyclic graphs, several applications of the PI
index are reported in the literature [6–8]. Many methods for the calculation of PI indices of some systems are reported in [9–13]. In this paper, we calculate the PI index of polyomino chains.

2. Calculation of the PI index of polyomino chains

A polyomino system is a finite 2-connected plane graph such that each interior face (or say a cell) is surrounded by a regular square of length one. In other words, it is an edge-connected union of cells in the planar square lattice. For the origin of polyominoes we quote Klarner [14]: “Polyominoes have a long history, going back to the start of the 20th century, but they were popularized in the present era initially by Golomb, i.e. [15,16], then by Gardner in his Scientific American columns.” At the present time they are widely known by mathematicians, physicists, chemists and have been considered in many different applications [17]. A polyomino chain is a polyomino system, in which the joining of the centres of its adjacent regular forms a path \( c_1 c_2 \cdots c_n \), where \( c_i \) is the centre of the \( i \)-th square.

Let \( B_n \) be the set of polyomino chains with \( n \) squares. \( B_n \in B_n \). If the subgraph of \( B_n \) induced by the vertices with degree 3 is a graph with exactly \( n - 2 \) squares, then \( B_n \) is called a linear chain and denoted by \( L_n \). If the subgraph of \( B_n \) induced by the vertices with a degree bigger than two is a path with \( n - 1 \) edges, then \( B_n \) is called a zig-zag chain and denoted by \( Z_n \). Fig. 1(a) and (b) illustrate \( L_n \) and \( Z_n \), respectively.

For calculating the PI index of polyomino chains, we introduce some conceptions in a polyomino chain. A kink of a polyomino chain is the branched or angularly connected squares. A segment of a polyomino chain is a maximal linear chain in the polyomino chains, including the kinks and/or terminal squares at its end. The number of squares in a segment \( S \) is called its length and is denoted by \( l(S) \). For any segment \( S \) of a polyomino chain with \( n \geq 2 \) squares, \( 2 \leq l(S) \leq n \). Particularly, a polyomino chain is a linear chain one if and only if it contains only one segment; a polyomino chain is a zig-zag chain one if and only if the length of each segment is 2.

A polyomino chain consists of a sequence of segments \( S_1, S_2, \ldots, S_s \), \( s \geq 1 \), with lengths \( l(S_i) = l_i, i = 1, 2, \ldots, s \), where \( l_1 + l_2 + \cdots + l_{s} = n + s - 1 \)(where \( n \) denote the number of squares of a polyomino chain) since two neighbouring segments have always one square in common. Then the PI index of polyomino chain may be calculated from these structural parameters.

**Theorem 1.** Let \( B_n \) be a polyomino chain with \( n \) squares and consisting of \( s \) segments \( S_1, S_2, \ldots, S_s \) \((s \geq 1)\) with lengths \( l_1, l_2, \ldots, l_s \). Then

\[
\text{PI}(B_n) = 9n^2 + s - 1 - \sum_{i=1}^{s} l_i^2.
\]

**Proof.** For any edge \( e \) which is cut across by the straight line passed through the centres of the squares of \( S_i \), we have

\[
n_1(e) + n_2(e) = (3n + 1) - (l_i + 1)
\]

where \( 3n + 1 \) is the number of edges in \( B_n \). And for the other edges of \( S_i \), we have

\[
n_1(e) + n_2(e) = (3n + 1) - 2 = 3n - 1,
\]

\( i = 1, 2, \ldots, s \). Therefore, the sum of the contributions of all the edges will give the PI index for \( B_n \)

\[
\text{PI}(B_n) = \sum_{i=1}^{s} (l_i + 1)(3n + 1) - (l_i + 1)] + 2(n - s + 1)(3n - 1)
\]

Fig. 1. A linear chain and a zig-zag chain.
Proof.  Theorem 3.

Corollary 2. (i) $\text{PI}(L_n) = 8n^2$; (ii) $\text{PI}(Z_n) = 9n^2 - 3n + 2$.

3. Bounds for the PI indices of polyomino chains

In this section, we give the bounds of the PI indices of polyomino chains.

Theorem 3. For any polyomino chain $B_n$ with $n$ squares,

$$8n^2 \leq \text{PI}(B_n) \leq 9n^2 - 3n + 2$$

with the left (right) equality if and only if $B_n$ is a linear (zig-zag) polyomino chain.

Proof. Let $B_n$ be a polyomino chain consisting of $s$ segments of lengths $l_1, l_2, \ldots, l_s$, where $l_1 + l_2 + \cdots + l_s = n + s - 1$ and $l_i \geq 2$, $i = 1, 2, \ldots, s$. From Theorem 1,

$$\text{PI}(B_n) = 9n^2 + s - 1 - \sum_{i=1}^{s} l_i^2.$$  

(i) By the Root Mean Square-Arithmetic Mean Inequality, $\sum_{i=1}^{s} l_i^2 \geq \frac{1}{s} (n + s - 1)^2 = s + (n - 1)^2 \frac{1}{s} + 2(n - 1) \geq 4(n - 1)$ with the equality if and only if $s = n - 1$ and $l_1 = l_2 = \cdots = l_s = 2$, we have

$$\text{PI}(B_n) = 9n^2 + s - 1 - \sum_{i=1}^{s} l_i^2$$

$$\leq 9n^2 + s - 1 - 4(n - 1)$$

$$\leq 9n^2 - 3n + 2 \quad \text{(since } s \leq n - 1\text{)}$$

with the equality if and only if $s = n - 1$ and $l_1 = l_2 = \cdots = l_s = 2$, i.e. $B_n$ is a zig-zag polyomino chain.

(ii) If $s > 1$, then

$$[l_1^2 + l_2^2 + \cdots + l_s^2] - [l_1^2 + \cdots + l_{s-2}^2 + (l_{s-1} + l_s - 1)^2] = 2(l_{s-1} + l_s) - 2l_{s-1}l_s - 1 < 0$$

and

$$l_1^2 + l_2^2 + \cdots + l_s^2 < l_1^2 + \cdots + l_{s-2}^2 + (l_{s-1} + l_s - 1)^2$$

$$< l_1^2 + \cdots + l_{s-3}^2 + (l_{s-2} + l_{s-1} + l_s - 2)^2$$

$$< \cdots$$

$$< (l_1 + l_2 + \cdots + l_s - s + 1)^2 = n^2.$$  

$$\text{PI}(B_n) = 9n^2 + s - 1 - \sum_{i=1}^{s} l_i^2$$

$$\geq 9n^2 + s - 1 - n^2 \quad \text{(since } s \geq 1\text{)}$$

$$\geq 8n^2$$

with the equality if and only if $s = 1$, i.e. $B_n$ is a linear polyomino chain.  \(\square\)

References


