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The Vertex PI and Szeged Indices of Chain Graphs

Xianyong Li [a*], **Xiaofan Yang** [a], **Guoping Wang** [b] and **Rongwei Hu** [c]

[a] *College of Computor Science, Chongqing University, Chongqing 400044, P.R.China*

[b] *College of Mathematics Science, Xinjiang Normal University, Urumqi 830054, Xinjiang, P.R.China*

[c] *College of Mathematics and Systems Science, Xinjiang University, Urumqi 830046, Xinjiang, P.R.China*

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Abstract: The vertex Padmakar-Ivan (PI_v) index of a graph G was introduced as the sum over all edges $e = uv$ of G of the number of vertices which are not equidistant to the vertices u and v. In this paper we provide an analogue to the results of T. Mansour and M. Schork [The PI index of bridge and chain graphs, MATCH Commun. Math. Comput. Chem. 61 (2009) 723-734]. Two efficient formulas for calculating the vertex PI index and Szeged index of chain graphs are determined. Using these formulas, the vertex PI index and Szeged index of a spiro chain of hexagons are computed.

1 Introduction

A single number, representing a chemical structure in graph-theoretical terms via the molecular graph, is called a *topological descriptor* and if it in addition correlates with a molecular property it is called *topological index*, which is used to understand physico-chemical properties of chemical compounds. The Wiener index, introduced by H. Wiener [1] in 1947, is one of the oldest and most thoroughly examined molecular graph-based structural descriptor of organic molecule [2]. It is only applicable to acyclic (tree) graphs. For cyclic compounds (graphs), I. Gutman [3] introduced another generalization that

*Corresponding author. E-mail: xian-yong@163.com

is known under the name of Szeged index. Many methods for the calculation of Szeged indices of some systems are considered in [4–9]. Szeged and Wiener indices are the same for acyclic graphs. Consequently, P. V. Khadikar et al. [10, 11] proposed another Szeged-like index called Padmakar-Ivan (PI) index. In recent times, the PI index has been considered for many special graphs, such as product graphs [12, 13], bridge and chain graphs [14], polyomino chains [15] and so on. Since the PI index is viewed as the edge-version, it is natural to introduce another index called vertex PI index which is viewed as vertex-version, see [4, 12, 13]. Very recently, T. Mansour and M. Schork [5] have considered the vertex PI index and Szeged index for bridge graphs. For chain graphs (to be defined more precisely later) the PI index and the Wiener, hyper-Wiener, detour and hyper-detour indices were determined in [14] and [16], respectively.

Suppose that $e = uv$ is an edge of a connected graph $G = (V(G), E(G))$. Then we denote the number of vertices lying closer to the vertex u than to the vertex v by $n_u(e|G)$ and the number of vertices lying closer to v than to u by $n_v(e|G)$. The *vertex Padmakar-Ivan (PI_v)* and *Szeged (Sz) indices* of G are defined as $PI_v(G) := \sum_{e\in E(G)}(n_u(e|G)+n_v(e|G))$ and $Sz(G) := \sum_{e\in E(G)} n_u(e|G)n_v(e|G)$, respectively. Note that in these definitions the vertices equidistant from the two ends of the edge e are not counted. Hence if we let $n_e(G)$ denote the number of vertices of G that are not equidistant from the two end vertices of e, then $n_e(G) = n_u(e|G) + n_v(e|G)$ and $PI_v(G) = \sum_{e\in E(G)} n_e(G)$.

Let us recall the definition of chain graphs; see [14, 16]. If $\{G_i\}_{i=1}^d$ is a set of pairwise disjoint graphs with $v_i, w_i \in V(G_i)$, then the *chain graph* $G = C(G_1, \cdots, G_d; v_1, w_1, \cdots, v_d, w_d)$ of $\{G_i\}_{i=1}^d$ with respect to $\{v_i, w_i\}_{i=1}^d$ is the graph obtained from the graphs $G_1, G_2, \cdots, G_d$ by identifying the vertex w_i and v_{i+1} for $i = 1, 2, \cdots, d-1$, as shown in Fig. 1.

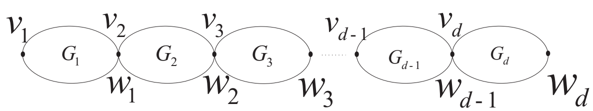

Fig.1

In this paper we will compute exact formulas for the vertex PI index and the Szeged index of the chain graph from the respective indices of the individual graphs. Using these formulas, we also obtain the vertex PI index and Szeged index of a spiro chain of hexagons.

2 Main results

For convenience we introduce the following notation. Let v be a vertex of a graph G. We denote by $M_v(G)$ the set of all edges $xy \in E(G)$ such that $d(x,v) = d(y,v)$. We denote by $|S|$ the cardinality of a set S.

Theorem 1. *Let $G = C(G_1, G_2, \cdots, G_d; v_1, w_1, v_2, w_2, \cdots, v_d, w_d)$ be a chain graph shown in Fig. 1. Then we have*

$$PI_v(G) = \sum_{i=1}^{d} PI_v(G_i) + \sum_{i=2}^{d}(|E(G_i)| - |M_{v_i}(G_i)|)\alpha_i + \sum_{i=1}^{d-1}(|E(G_i)| - |M_{w_i}(G_i)|)\beta_i,$$

where $\alpha_i = \sum_{j=1}^{i-1}|V(G_j)|$, $\beta_i = \sum_{j=i+1}^{d}|V(G_j)|$.

Proof. From the definition we have

$$PI_v(G) = \sum_{i=1}^{d}\sum_{e\in E(G_i)} n_e(G) = \sum_{e\in E(G_1)} n_e(G) + \sum_{i=2}^{d-1}\sum_{e\in E(G_i)} n_e(G) + \sum_{e\in E(G_d)} n_e(G).$$

If $e \in E(G_1) \setminus M_{w_1}(G_1)$, then each vertex in $\cup_{j=2}^{d} V(G_j)$ is not equidistant from the ends of the edge e, and so $n_e(G) = n_e(G_1) + \beta_1$; if $e \in M_{w_1}(G_1)$, then all vertices in $\cup_{j=2}^{d} V(G_j)$ are equidistant from the ends of the edge e, and so $n_e(G) = n_e(G_1)$. Thus we have

$$\sum_{e\in E(G_1)} n_e(G) = PI_v(G_1) + (|E(G_1)| - |M_{w_1}(G_1)|)\beta_1.$$

Similarly, we can obtain

$$\sum_{e\in E(G_d)} n_e(G) = PI_v(G_d) + (|E(G_d)| - |M_{v_d}(G_d)|)\alpha_d.$$

For $e \in E(G_i)$ $(2 \leqslant i \leqslant d-1)$, we distinguish the following four cases.

Case 1. If $e \in M_{v_i}(G_i) \cap M_{w_i}(G_i)$, then all vertices in $V(G)\backslash V(G_i)$ are equidistant from the ends of the edge e, and so $n_e(G) = n_e(G_i)$.

Case 2. If $e \in M_{v_i}(G_i) \setminus M_{w_i}(G_i)$, then all vertices in $\cup_{j=1}^{i-1} V(G_j)$ are equidistant from the ends of the edge e, but all vertices in $\cup_{j=i+1}^{d} V(G_j)$ are not equidistant from the ends of the edge e, and so $n_e(G) = n_e(G_i) + \beta_i$.

Case 3. If $e \in M_{w_i}(G_i) \setminus M_{v_i}(G_i)$, then, as above, we can obtain $n_e(G) = n_e(G_i) + \alpha_i$.

Case 4. If $e \in E(G_i) \setminus (M_{v_i}(G_i) \cup M_{w_i}(G_i))$, then all vertices in $V(G)\backslash V(G_i)$ are not equidistant from the ends of the edge e, and so $n_e(G) = n_e(G_i) + \alpha_i + \beta_i$.

Combining the above arguments we have

$$\sum_{e\in E(G_i)} n_e(G) = \sum_{e\in M_{v_i}(G_i)\cap M_{w_i}(G_i)} n_e(G_i) + \sum_{e\in M_{v_i}(G_i)\setminus M_{w_i}(G_i)} (n_e(G_i)+\beta_i)$$
$$+ \sum_{e\in M_{w_i}(G_i)\setminus M_{v_i}(G_i)} (n_e(G_i)+\alpha_i) + \sum_{e\in E(G_i)\setminus(M_{v_i}(G_i)\cup M_{w_i}(G_i))} (n_e(G_i)+\alpha_i+\beta_i)$$
$$= PI_v(G_i) + (|E(G_i)| - |M_{v_i}(G_i)|)\alpha_i + (|E(G_i)| - |M_{w_i}(G_i)|)\beta_i.$$

Eventually, we obtain the assertion. □

Suppose that v and w are two vertices of a graph H, and let $G_i = H$ and $v_i = v, w_i = w$ for all $i = 1, 2, \cdots, d$. Then, by simple calculations, we can easily obtain the following result.

Corollary 2. *The vertex PI index of the chain graph $G = C(H, H, \cdots, H; v, w, v, w, \cdots, v, w)$ (d times) is given by*

$$PI_v(G) = dPI_v(H) + \binom{d}{2}(2|E(H)| - |M_v(H)| - |M_w(H)|)\ .$$

Suppose that G is a chain graph shown in Fig. 1. Then we further define the four subsets L_{v_i}, R_{v_i}, L_{w_i} and R_{w_i} of $E(G_i)\setminus M_{v_i}(G_i)$ as follows. For $e = uv \in E(G_i)\setminus M_{v_i}(G_i)$, we let $e \in L_{v_i}$ if $d(u, v_i) < d(v, v_i)$ and $e \in R_{v_i}$ otherwise; and $e \in L_{w_i}$ if $d(u, w_i) < d(v, w_i)$ and $e \in R_{w_i}$ otherwise.

Theorem 3. *Let $G = C(G_1, G_2, \cdots, G_d; v_1, w_1, v_2, w_2, \cdots, v_d, w_d)$ be a chain graph shown in Fig. 1. Then we have*

$$Sz(G) = \sum_{i=1}^{d} Sz(G_i) + \sum_{i=1}^{d-1}\beta_i\Big(\sum_{e\in L_{w_i}} n_v(e|G_i) + \sum_{e\in R_{w_i}} n_u(e|G_i)\Big)$$
$$+ \sum_{i=2}^{d}\alpha_i\Big(\sum_{e\in L_{v_i}} n_v(e|G_i) + \sum_{e\in R_{v_i}} n_u(e|G_i)\Big) + \sum_{i=2}^{d-1}(|L_{v_i}\cap R_{w_i}| + |R_{v_i}\cap L_{w_i}|)\alpha_i\beta_i,$$

where $\alpha_i = \sum_{j=1}^{i-1}|V(G_j)|$, $\beta_i = \sum_{j=i+1}^{d}|V(G_j)|$.

Proof. From the definition we have

$$Sz(G) = \sum_{e\in E(G_1)} n_u(e|G)n_v(e|G) + \sum_{i=2}^{d-1}\sum_{e\in E(G_i)} n_u(e|G)n_v(e|G) + \sum_{e\in E(G_d)} n_u(e|G)n_v(e|G).$$

If $e \in M_{w_1}(G_1)$, then each vertex in $\cup_{j=2}^{d}V(G_j)$ is equidistant from the ends of the edge e, and so $n_u(e|G)n_v(e|G) = n_u(e|G_1)n_v(e|G_1)$. Suppose that $e \in E(G_1) \setminus M_{w_1}(G_1)$.

Then each vertex in $\cup_{j=2}^{d} V(G_j)$ is not equidistant from the ends of the edge e. In this case, we further obtain that if $e \in L_{w_1}$ then $n_u(e|G)n_v(e|G) = (n_u(e|G_1) + \beta_1)n_v(e|G_1)$, and if $e \in R_{w_1}$ then $n_u(e|G)n_v(e|G) = n_u(e|G_1)(n_v(e|G_1) + \beta_1)$. Thus we have

$$\begin{aligned}\sum_{e\in E(G_1)} n_u(e|G)n_v(e|G) = &\sum_{e\in M_{w_1}(G_1)} n_u(e|G_1)n_v(e|G_1) + \sum_{e\in L_{w_1}} (n_u(e|G_1)+\beta_1)n_v(e|G_1)\\ &+ \sum_{e\in R_{w_1}} n_u(e|G_1)(n_v(e|G_1)+\beta_1)\\ &= Sz(G_1) + \beta_1(\sum_{e\in L_{w_1}} n_v(e|G_1) + \sum_{e\in R_{w_1}} n_u(e|G_1)).\end{aligned}$$

Similarly, we also have

$$\sum_{e\in E(G_d)} n_u(e|G)n_v(e|G) = Sz(G_d) + \alpha_d(\sum_{e\in L_{v_d}} n_v(e|G_d) + \sum_{e\in R_{v_d}} n_u(e|G_d)).$$

For $e \in E(G_i)$ $(2 \leqslant i \leqslant d-1)$, we distinguish the following four cases:

Case 1. If $e \in M_{v_i}(G_i) \cap M_{w_i}(G_i)$, then all vertices in $V(G) \setminus V(G_i)$ are equidistant from the ends of the edge e, and so $n_u(e|G)n_v(e|G) = n_u(e|G_i)n_v(e|G_i)$.

Case 2. If $e \in M_{v_i}(G_i) \setminus M_{w_i}(G_i)$, then all vertices in $\cup_{j=1}^{i-1} V(G_j)$ are equidistant from the ends of the edge e, but all vertices in $\cup_{j=i+1}^{d} V(G_j)$ are not equidistant from the ends of the edge e. Thus we further know that if $e \in L_{w_i}$ then $n_u(e|G)n_v(e|G) = (n_u(e|G_i) + \beta_i)n_v(e|G_i)$, and if $e \in R_{w_i}$ then $n_u(e|G)n_v(e|G) = n_u(e|G_i)(n_v(e|G_i) + \beta_i)$. Hence we have

$$\begin{aligned}&\sum_{e\in M_{v_i}(G_i)\setminus M_{w_i}(G_i)} n_u(e|G)n_v(e|G)\\ &= \sum_{e\in M_{v_i}(G_i)\setminus M_{w_i}(G_i)} n_u(e|G_i)n_v(e|G_i) + \sum_{e\in M_{v_i}(G_i)\cap L_{w_i}} \beta_i n_v(e|G_i) + \sum_{e\in M_{v_i}(G_i)\cap R_{w_i}} \beta_i n_u(e|G_i).\end{aligned}$$

Case 3. If $e \in M_{w_i}(G_i) \setminus M_{v_i}(G_i)$, then, as above, we can obtain

$$\begin{aligned}&\sum_{e\in M_{v_i}(G_i)\setminus M_{w_i}(G_i)} n_u(e|G)n_v(e|G)\\ &= \sum_{e\in M_{w_i}(G_i)\setminus M_{v_i}(G_i)} n_u(e|G_i)n_v(e|G_i) + \sum_{e\in M_{w_i}(G_i)\cap L_{v_i}} \alpha_i n_v(e|G_i) + \sum_{e\in M_{w_i}(G_i)\cap R_{v_i}} \alpha_i n_u(e|G_i).\end{aligned}$$

Case 4. If $e \in E(G_i) \setminus (M_{v_i}(G_i) \cup M_{w_i}(G_i))$, then all vertices in $V(G) \setminus V(G_i)$ are not equidistant from the ends of the edge e. We can further observe that if $e \in L_{v_i} \cap L_{w_i}$ then $n_u(e|G)n_v(e|G) = (n_u(e|G_i)+\alpha_i+\beta_i)n_v(e|G_i)$, and if $e \in L_{v_i} \cap R_{w_i}$ then $n_u(e|G)n_v(e|G) = (n_u(e|G_i)+\alpha_i)(n_v(e|G_i)+\beta_i)$, and if $e \in R_{v_i} \cap R_{w_i}$ then $n_u(e|G)n_v(e|G) = n_u(e|G_i)(n_v(e|G_i)$

$+\alpha_i+\beta_i)$, and if $e\in R_{v_i}\cap L_{w_i}$ then $n_u(e|G)n_v(e|G)=(n_u(e|G_i)+\alpha_i)(n_v(e|G_i)+\beta_i)$. Thus we have

$$\begin{aligned}
&\sum_{e\in E(G_i)\setminus(M_{v_i}(G_i)\cup M_{w_i}(G_i))} n_u(e|G)n_v(e|G)\\
&=\sum_{e\in E(G_i)\setminus(M_{v_i}(G_i)\cup M_{w_i}(G_i))} n_u(e|G_i)n_v(e|G_i)+\beta_i\sum_{e\in R_{w_i}\cap(E(G_i)\setminus M_{v_i}(G_i))} n_u(e|G_i)\\
&+\beta_i\sum_{e\in L_{w_i}\cap(E(G_i)\setminus M_{v_i}(G_i))} n_v(e|G_i)+\alpha_i\sum_{e\in L_{v_i}\cap(E(G_i)\setminus M_{w_i}(G_i))} n_v(e|G_i)\\
&+\alpha_i\sum_{e\in R_{v_i}\cap(E(G_i)\setminus M_{w_i}(G_i))} n_u(e|G_i)+(|L_{v_i}\cap R_{w_i}|+|R_{v_i}\cap L_{w_i}|)\alpha_i\beta_i.
\end{aligned}$$

Combining the above arguments we obtain

$$\begin{aligned}
\sum_{e\in E(G_i)} n_u(e|G)n_v(e|G)&=Sz(G_i)+\beta_i(\sum_{e\in L_{w_i}} n_v(e|G_i)+\sum_{e\in R_{w_i}} n_u(e|G_i))+\alpha_i(\sum_{e\in L_{v_i}} n_v(e|G_i)\\
&+\sum_{e\in R_{v_i}} n_u(e|G_i))+(|L_{v_i}\cap R_{w_i}|+|R_{v_i}\cap L_{w_i}|)\alpha_i\beta_i.
\end{aligned}$$

Eventually, we obtain the assertion. $\square$

Suppose that v and w are two vertices of a graph H, and let $G_i=H$ and $v_i=v, w_i=w$ for all $i=1,2,\cdots,d$. Then, by a simple calculation, we can easily obtain the following result.

Corollary 4. *The Szeged index of the chain graph $G=C(H,H,\cdots,H;v,w,v,w,\cdots,v,w)$ (d times) is given by*

$$Sz(G)=dSz(H)+\binom{d}{2}(\sum_{e\in R_v\cup R_w} n_u(e|H)+\sum_{e\in L_v\cup L_w} n_v(e|H))+\binom{d}{3}(|L_v\cap R_w|+|R_v\cap L_w|).$$

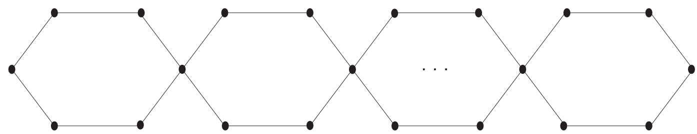

Fig.2

Example 1. The spiro chain of hexagons $G=C(C_6,C_6,\cdots,C_6;v,w,v,w,\cdots,v,w)$ containing the cycle C_6 d times is given in Fig. 2. Since $PI_v(C_6)=36, |M_v(C_6)|=|M_w(C_6)|=0$, by Corollary 2 the vertex PI index of the chain is $PI_v(G)=36d+12\binom{d}{2}=6d^2+30d$. Similarly, using $Sz(C_6)=54, R_v\cup R_w=L_v\cup L_w=E(C_6), |L_v\cap R_w|=|R_v\cap$

$L_w| = 3$, by Corollary 4 the Szeged index of the chain is $Sz(G) = 54d + \binom{d}{2} PI_v(C_6) + 6\binom{d}{3} = d^3 + 15d^2 + 38d$.

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