Chemical Indices of Generalized Petersen Graph*

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Abstract

The generalized Petersen graph $GP(n, k)$ is a graph whose vertex and edge sets are $\{u_1, u_2, \cdots, u_n, v_1, v_2, \cdots, v_n\}$ and $\{u_i u_{i+1}, u_i v_i, v_i v_{i+k} | i \in [n]\}$, respectively. In this paper, for $k \in [4]$, the Wiener polarity index and the Wiener index of generalized Petersen graph $GP(n, k)$ are obtained; for $k \in [2]$, the Szeged index, the edge-Szeged index, and the PI index are educed; for $k \geq 1$, the exact values about the Randić index, the Gutman index, first and second zagreb index, and Harmonic index are gained.

Keywords: Generalized Petersen graphs; Wiener polarity index; Wiener index; Szeged index; Randić index

1 Introduction

All graphs considered in this paper are finite, undirected, and simple. For integers $a, b$, a positive integer $k$ and a real number $x$, let $[a, b] = \{a, a+1, \cdots, b-1, b\}$, $[k] = \{1, 2, \cdots, k\}$, $[x]$ and $\lfloor x \rfloor$ denote the smallest integer not less than $x$ and the largest integer not greater than $x$, respectively. In recent years, many parameters and classes of graphs are studied. For example, in [2], the restricted connectivity of Cartesian product graphs is obtained, in [7, 11], some results on 3-equitable labeling and the $n$-dimensional cube-connected complete graph are gained, and in [9], graph energy is studied.

The generalized Petersen graph [1, 4, 13, 14, 16, 17] $GP(n,k)$ is a graph whose vertex set and edge set are $\{u_1, u_2, \cdots, u_n, v_1, v_2, \cdots, v_n\}$ and $\{u_i u_{i+1}, u_i v_i, v_i v_{i+k} | i \in [n]\}$, respectively, where the indices are taken modular $n$ and all of them belong to $[n]$. The most famous Petersen graph is $GP(5,2)$. In fact, $GP(n, k) = GP(n, n-k)$. Therefore, Petersen graphs is also $GP(5,3)$, and we just consider $k \leq \frac{n}{2}$ in this paper.

For $k < \frac{n}{2}$, the generalized Petersen graph $GP(n,k)$ is a cubic graph whose outer ring is a regular polygon, which is the cycle $C_n$, inner ring is a $n$-pointed stars, which is the circulant graph $C_n(k)$, respectively, and the corresponding vertices are connected. The generalized Petersen graphs were first found by Coxeter in 1950 and named by Watkins in 1969. Later, many scholars studied generalized Petersen graphs, including their hamiltonian path [14], hamiltonian cycle [1], coloring [4], metric dimension [13] and domination number [16].

The Wiener polarity index [12] and Wiener index [6, 8, 15] are related to the distance of vertices, and the Wiener index can be used to explain the physical and chemical property of molecules, which was first proposed by Harold Wiener in 1947. Later, many mathematicians studied the Wiener index.

In this paper, some chemical indices of generalized Petersen graphs are studied, such as the Wiener polarity index, the Wiener index, generalized Randić index, et cetera.

2 The Wiener (polarity) index of generalized Petersen graphs

In the following, let $n, k, x$ be all nonnegative integers.

Definition 2.1. The Wiener polarity index of $G$ is denoted by $W_p(G)$ and defined as the number of the pairs of vertices whose distances are 3:

$$W_p(G) = \left| \{u, v \in V(G) \mid d(u, v) = 3, u, v \in V(G)\} \right|,$$

where $d(u, v)$ denotes the distance between the vertices $u, v$.

The Wiener index of a graph $G$, is defined as

$$W(G) = \sum_{u, v \in V(G)} d(u, v).$$

The Wiener polarity index of generalized Petersen graph $GP(n, k)$ is denoted by $W_p(n, k)$, and the Wiener index is denoted by $W(n, k)$.

According to the definition, the Wiener polarity index is 0 when the diameter of $G$ is less than 3. Therefore, we just consider $W_p(n, k)$ ($n > 6$).

Theorem 2.2 For $k \geq 1$, we have

$$W_p(n, k) = \begin{cases} 
4n, & \text{for } k = 1 \text{ and } n > 6, \\
7n, & \text{for } k = 2, \text{ and even } n > 12, \\
9n, & \text{for } k = 3, 3|n \text{ and } n > 18, \\
12n, & \text{for } k = 4, 4|n \text{ and } n > 24,
\end{cases}$$

and $W_p(n, k) \leq 12n$ if $n - k$ is large enough.

Proof. (1) For $k = 1$, from the definition of generalized Petersen graphs, when $n > 6$, the vertex on outer...
ring whose distance to \( u_i \) is 3 is \( u_{i+3} \), and the vertices on inner ring are \( v_{i+2} \) and \( v_{i-2} \). The vertex on inner ring whose distance to \( v_i \) is 3 is \( v_{i+3} \). (Although the distance between \( u_i \) and \( u_{i-3} \) is also 3, to avoid repeated calculation, we just consider \( u_{i+3} \), similarly hereafter.) Therefore, \( W_p(n, 1) = n + 2n + n = 4n \).

(2) For \( k = 2 \), if \( n \) is odd and \( n > 7 \), or \( n \) is even and \( n > 12 \), then the vertex on outer ring whose distance to \( u_i \) is 3 is \( u_{i+3} \), the vertices on inner ring are \( v_{i+4}, v_{i-4}, v_{i+3} \) and \( v_{i-3} \). The vertices on inner ring whose distance to \( v_i \) is 3 are \( v_{i+1} \) and \( v_{i+9} \). Therefore,

\[
W_p(n, 2) = n + 4n + 2n = 7n.
\]

(3) For \( k = 3 \), if \( 3|n \) and \( n > 18 \), or \( 3 \mid n, n > 11 \) and \( n \) is odd, then the vertex on outer ring whose distance to \( u_i \) is 3 is \( u_{i+3} \), the vertices on inner ring are \( v_{i+2}, v_{i-2}, v_{i+4}, v_{i-4}, v_{i+3} \) and \( v_{i-3} \). The vertices on inner ring whose distance to \( v_i \) is 3 are \( v_{i+1} \) and \( v_{i+9} \). Therefore,

\[
W_p(n, 3) = n + 6n + 2n = 9n.
\]

(4) For \( k = 4 \), if \( 4|n \) and \( n > 24 \), or \( 4 \mid n, n > 15 \) and \( n \) is odd, then the vertex on outer ring whose distance to \( u_i \) is 3 are \( u_{i+3}, u_{i+4} \), and the vertices on inner ring are \( v_{i+2}, v_{i-2}, v_{i+5}, v_{i-5}, v_{i+8}, v_{i-8}, v_{i+3} \) and \( v_{i-3} \). The vertices on inner ring whose distance to \( v_i \) is 3 are \( v_{i+1} \) and \( v_{i+12} \). Therefore,

\[
W_p(n, 4) = 2n + 8n + 2n = 12n.
\]

(5) Assume that both \( n \) and \( k \) are large enough so that the vertices whose distance to \( u_i \) is 3 are maximum. Since \( GP(n, k) \) is a cubic graph, for \( u_i \), three branches can be found to take count of the vertices whose distance to \( u_i \) is 3. Obviously, the distance between each pair of vertices \( u_{i+1}, v_{i+1}, u_{i-1} \) and \( u_i \) is 1. There are two branches in each of three vertices above and as well as the next vertices. All of the vertices whose distance to \( u_i \) is 3 can be found by doing so.

Table 1 is the total process of the work and there are 12 such vertices. Vertices whose distance to \( v_i \) is 3 can be found like this and there are 12 of those, too. Analyzing every vertex of \( GP(n, k) \), each pair of vertices whose distance is 3 is calculated twice. Therefore, the Wiener polarity index of generalized Petersen graph is at most

\[
W_p(n, k) = (12n + 12n) \times \frac{1}{2} = 12n.
\]

That is to say, \( W_p(n, k) \leq 12n \).

For the Wiener index, we have the following results.

**Theorem 2.3** If \( k = 1 \), then

\[
W(n, 1) = \begin{cases} \frac{n^3}{3} + n^2, & \text{if } n \text{ is even}, \\ \frac{n^3}{3} + n^2 - \frac{n}{2}, & \text{if } n \text{ is odd}. \end{cases}
\]

**Proof.** (1) If \( n \) is even, then the number of pairs whose distance is 1 is \( 3n \). The number of pairs whose distance is 2, 3, \( \cdots \), \( \frac{n}{2} - 2 \) or \( \frac{n}{2} - 1 \) are all \( 4n \). The number of pairs whose distance is \( \frac{n}{2} \) is 3n and the number of pairs whose distance is \( \frac{n}{2} + 1 \) is \( n \). Therefore, we have

\[
W(n, 1) = 3n \times 1 + 4n \times 2 + 4n \times 3 + \cdots + 4n \times \left( \frac{n}{2} - 1 \right) + 3n \times \frac{n}{2} + n \times \left( \frac{n}{2} + 1 \right) = 4n(1 + 2 + 3 + \cdots + \frac{n}{2} - 1 + \frac{n}{2} + n) = 4n \times \frac{(\frac{n}{2} - 1 + \frac{n}{2} + n) \times \frac{n}{2}}{2} + 2n^2 = \frac{n^3}{2} + n^2.
\]

(2) If \( n \) is odd, then the number of pairs whose distance is 1 is \( 3n \). The number of pairs whose distance is 2, 3, \( \cdots \), \( \frac{n+3}{2} \), or \( \frac{n-1}{2} \), are all \( 4n \). The number of pairs whose distance is \( \frac{n+3}{2} \) is 2n. Therefore, we obtain that

\[
W(n, 1) = 3n \times 1 + 4n \times 2 + 4n \times 3 + \cdots + 4n \times \left( \frac{n-1}{2} + \frac{n-1}{2} \right) + 2n \times \frac{n+1}{2} + n^2 = 4n \times \frac{(\frac{n-1}{2} + \frac{n-1}{2}) \times (\frac{n-1}{2} + n) + n^2}{2} = \frac{n^3}{2} + n^2 - \frac{n}{2}.
\]

**Theorem 2.4** Suppose that \( n > 6 \). Then

\[
W(n, 2) = \begin{cases} \frac{1}{3}n^3 + 3n^2 - 5n \text{ for even } n, \\ 16x^3 + 36x^2 - 46x + 9 \text{ for } n = 4x - 1 \\ and \ x \geq 2, \\ 16x^3 + 60x^2 - 2x - 4 \text{ for } n = 4x + 1 \\ and \ x \geq 2. \end{cases}
\]

**Proof.** The Wiener index \( W(n, 2) \) of generalized Petersen graph \( GP(n, 2) \) is related to \( n \). Assume that \( W(n, 2) = a_n \cdot n \), then it is obvious that \( a_n \) is double the average distance of \( GP(n, 2) \). So the main problem is to get \( a_n \).

(1) When \( n \) is even, it is obvious that \( a_n \) meet the condition

\[
(a_{n+2} - a_n) - (a_n - a_{n-2}) = 2.
\]

Assume that \( b_n = a_n - a_{n-2} \) (\( n \geq 10 \) and is even), then \( b_n - b_{n-2} = 2 \). Using accumulation twice, we have
\[
b_n = n+5 \text{ and } a_n = \frac{1}{2}n^2+3n-5, \text{ respectively. Therefore } W(n,2) = a_n \cdot n = \frac{1}{2}n^3+3n^2-5n.
\]

(2) When \( n \) is odd, let \( x \geq 2 \). Then \( n = 4x-1 \) or \( n = 4x+1 \). Assume that \( b_n = a_n - a_{n-2} \), then we can know that
\[
\begin{cases}
  b_{4x+1} - b_{4(x-1)+1} = 4, \\
  b_{4x-1} = b_{4x+1} + 8 - 3.
\end{cases}
\]
Therefore,
\[
\begin{cases}
  b_{4x+1} = 2 \cdot (4x+1) - 5 = 8x - 3, \\
  b_{4x-1} = 8x - 3.
\end{cases}
\]
Thus
\[
\begin{cases}
  a_{4x+1} = 4x^2 + 14x - 4, \\
  a_{4x-1} = 4x^2 + 10x - 9.
\end{cases}
\]
Because \( W(n,2) = a_n \cdot n \), we have
\[
W(4x - 1, 2) = (4x^2 + 10x - 9)(4x - 1) = 16x^3 + 36x^2 - 46x + 9
\]
if \( n = 4x - 1 \), and
\[
W(4x + 1, 2) = (4x^2 + 14x - 4)(4x + 1) = 16x^3 + 60x^2 - 2x - 4
\]
if \( n = 4x + 1 \).

By Theorem 2.4, we can obtain that \( W(n,2) < W(n+1,2) \); we only consider the case of even \( n \) since the other case is similar. If \( n = 4x - 2 \), then
\[
W(4x - 2, 2) = \frac{1}{2}(4x^2 - 2)^2 + 3 \cdot (4x^2 - 2)(4x - 2) - 5 \cdot (4x - 2) = 16x^3 + 24x^2 - 56x + 20,
\]
and
\[
W(4x - 1, 2) = 16x^3 + 36x^2 - 46x + 9
\]
for \( x \geq 2 \). If \( n = 4x \), then
\[
W(4x, 2) = \frac{1}{2}(4x^2 + 3 \cdot (4x)^2 - 5 \cdot 4x^2 - 20x) = 16x^3 + 48x^2 - 20x,
\]
and
\[
W(4x + 1, 2) = 16x^3 + 60x^2 - 2x - 4
\]
for \( x \geq 2 \).

**Theorem 2.5** For \( n > 7, k = 3, x \geq 1 \), we have
\[
W(n,3) = \begin{cases}
  36x^3 + 144x^2 - 30x, & \text{for } n = 6x, \\
  36x^3 + 162x^2 + 2x - 4, & \text{for } n = 6x + 1, \\
  36x^3 + 180x^2 + 56x, & \text{for } n = 6x + 2, \\
  36x^3 + 198x^2 + 132x + 21, & \text{for } n = 6x + 3, \\
  36x^3 + 216x^2 + 200x + 48, & \text{for } n = 6x + 4, \\
  36x^3 + 234x^2 + 254x + 70, & \text{for } n = 6x + 5.
\end{cases}
\]

**Proof.** Assume that \( W(n,3) = a_n \cdot n \). For \( n > 7 \), it is well known that \( n = 6x + i \) for \( i \in [0,5] \). Suppose that \( b_n = a_n - a_{n-2} \), then
\[
\begin{cases}
  b_{6x+6} - b_{6x} = 6, \\
  b_{6x+3} = b_{6x}.
\end{cases}
\]
Using accumulation, we have
\[
\begin{cases}
  b_{6x} = 6x + 12, \\
  b_{6x+3} = 6x + 12.
\end{cases}
\]
Thus,
\[
\begin{cases}
  a_{6x} = 6x^2 + 24x - 5, \\
  a_{6x+3} = 6x^2 + 30x + 7,
\end{cases}
\]
and the Harmonic index of generalized Petersen graphs

**Definition 3.1** The Randić index of \( G \) is defined as
\[
R(G) = \sum_{uv \in E(G)} \frac{1}{\deg(u) \cdot \deg(v)};
\]
the first zagreb index of \( G \) is defined as
\[
M_1(G) = \sum_{u \in V(G)} \deg(u)^2;
\]
the second zagreb index is defined as
\[
M_2(G) = \sum_{u \in E(G)} \deg(u) \cdot \deg(v);
\]
the connectivity index of \( G \) is defined as
\[
\chi(G) = \sum_{uv \in E(G)} [\deg(u) + \deg(v)]^{-\frac{1}{2}},
\]
and the Harmonic index of \( G \) is defined as
\[
H(G) = \sum_{uv \in E(G)} \frac{2}{\deg(u) + \deg(v)}.
\]

We simply use \( H(n,k) \) to denote the Harmonic index of generalized Petersen graph \( GP(n,k) \), similarly for other indices.
Theorem 3.2 (1) If \( n \neq 2k \), then \( R(n, k) = n \), 
\( M_1(n, k) = 18n \), \( M_2(n, k) = 27n \), and \( \chi(n, k) = \frac{\sqrt{6n}}{2} \).

(2) If \( n = 2k \), then \( R(2k, k) = \frac{7+2\sqrt{5}}{6}k \), \( M_1(2k, k) = 26k \), 
\( M_2(2k, k) = 34k \), and 
\[ \chi(2k, k) = \frac{10\sqrt{6} + 12\sqrt{5} + 15}{30} k. \]

(3) \( H(n, k) = n \) if \( n \neq 2k \), and \( H(n, k) = \frac{37}{15} k \) if \( n = 2k \).

Proof. (1) If \( n \neq 2k \), then \( GP(n, k) \) is a cubic graph. Thus we have 
\[ R(n, k) = \sum_{uv \in E(GP)} \frac{1}{\sqrt{\deg(u) \cdot \deg(v)}} = 3n \cdot \frac{1}{3} = n, \]
\[ M_1(n, k) = \sum_{u \in V(GP)} \deg(u)^2 = 2n \cdot 9 = 18n, \]
\[ M_2(n, k) = \sum_{uv \in E(GP)} \deg(u) \cdot \deg(v) = 3n \cdot 9 = 27n, \]
and
\[ \chi(n, k) = \sum_{uv \in E(GP)} [\deg(u) + \deg(v)]^{-\frac{1}{2}} = 3n \cdot \frac{1}{\sqrt{6}} = \frac{\sqrt{6n}}{2}. \]

(2) If \( n = 2k \), then there are \( n \) edges with two ends whose degrees are 3 in \( GP(2k, k) \), \( n \) edges with two ends whose degrees are 2 and 3, respectively, and \( \frac{n}{2} \) edges with two ends whose degrees are 2. Thus, 
\[ R(2k, k) = \sum_{uv \in E(GP)} \frac{1}{\sqrt{\deg(u) \cdot \deg(v)}} = n \cdot \frac{1}{3} + n \cdot \frac{1}{\sqrt{6}} + \frac{n}{2} \cdot \frac{1}{2} = \frac{7 + 2\sqrt{5}}{6} k, \]
\[ M_1(2k, k) = \sum_{u \in V(GP)} \deg(u)^2 = n \cdot 9 + n \cdot 6 + \frac{n}{2} \cdot 4 = 13n = 26k, \]
\[ M_2(2k, k) = \sum_{uv \in E(GP)} \deg(u) \cdot \deg(v) = n \cdot 9 + n \cdot 6 + \frac{n}{2} \cdot 4 = 17n = 34k, \]
and 
\[ \chi(2k, k) = \sum_{uv \in E(GP)} [\deg(u) + \deg(v)]^{-\frac{1}{2}} = n \cdot \frac{1}{\sqrt{6}} + n \cdot \frac{1}{\sqrt{6}} + n \cdot \frac{1}{2} \cdot \frac{1}{2} = \frac{10\sqrt{6} + 12\sqrt{5} + 15}{30} k. \]

(3) If \( n \neq 2k \), then 
\[ H(n, k) = \sum_{uv \in E(GP)} \frac{2}{\deg(u) + \deg(v)} = 3n \cdot \frac{2}{6} = n. \]
If \( n = 2k \), then 
\[ H(n, k) = \sum_{uv \in E(GP)} \frac{2}{\deg(u) + \deg(v)} = n \cdot \frac{2}{6} + n \cdot \frac{1}{3} + n \cdot \frac{2}{4} = \frac{37}{15} k. \]
For \( e = uv \in E(G) \), let \( n_u(e) \) denote the number of vertices of \( G \) whose distance to \( u \) is smaller than the one to \( v \) and \( n_v(e) \) the number of edges whose distance to \( u \) is smaller than the one to \( v \), respectively.

Definition 3.3 [3] The Gutman index and generalized terminal Wiener index are denoted by \( Gut(G) \) and \( TW_r(G) \), respectively, and are defined as follows:
\[ Gut(G) = \sum_{e \in V(G)} \deg(u) \deg(v) d(u, v), \]
\[ TW_r(G) = \sum_{e \in V(G)} d(u, v). \]
The Szeged index \( S_G(G) \), edge-Szeged index \( S_{Z_e}(G) \), and PI index \( PI(G) \) of \( G \) are defined as
\[ S_G(G) = \sum_{e \in V(G)} n_u(e) n_v(e), \]
\[ S_{Z_e}(G) = \sum_{e \in V(G)} m_u(e) m_v(e), \]
and
\[ PI(G) = \sum_{e \in V(G)} [m_u(e) + m_v(e)], \]
respectively.

Let \( S_{G}(n, k) \), \( S_{Z_e}(n, k) \), \( PI(n, k) \), \( Gut(n, k) \) and \( TW_r(n, k) \) denote the Szeged index, edge-Szeged index, PI index, the Gutman index and generalized terminal Wiener index of generalized Petersen graph, respectively.

Theorem 3.4 (1) If \( n \neq 2k \), then \( Gut(n, k) = 9W(n, k) \);
(2) If \( n = 2k \), then 
\[ Gut(2k, k) = \begin{cases} 9k^3 + 5k^2 + 28k - 16 & \text{for even } k, \\ 9k^3 + 5k^2 + 38k - 21 & \text{for odd } k. \end{cases} \]

Proof. (1) If \( n \neq 2k \), then \( \deg(u) = \deg(v) = 3 \). Thus 
\[ Gut(n, k) = \sum_{u, v \in V(GP)} \deg(u) \deg(v) d(u, v) = 9W(n, k). \]
(2) If \( n = 2k \), then for any \( u \in V(GP) \), either \( \deg(u) = 2 \) or \( \deg(u) = 3 \).

1° If \( \deg(u) = \deg(v) = 3 \), then both \( u \) and \( v \) are on the outer ring of \( GP(n, k) \). Thus 
\[ \sum_{\deg(u) = \deg(v) = 3} \deg(u) \deg(v) d(u, v) = 9 \sum d(u, v) \]
\[ = 9 \times \frac{9}{2} \cdot [1 \times 2 + 2 \times 2 + \cdots + (\frac{9}{2} - 1) \times 2 + \frac{9}{2} \times 1] \]
\[ = 9 \times \frac{9}{2} \cdot \frac{(\frac{9}{2} - 1)}{2} \times 2 + \frac{9}{2} \times \frac{9}{2} \times 3 = 9k^3. \]

2° If \( \deg(u) = 3 \) and \( \deg(v) = 2 \), then \( u \) is on the outer ring of \( GP(n, k) \), and \( v \) is on the inner ring of \( GP(n, k) \). Thus 
\[ \sum_{\deg(u) = 3, \deg(v) = 2} \deg(u) \deg(v) d(u, v) = 6 \sum d(u, v). \]
Case 1. If \( \frac{n}{2} = k \) is even, then
\[
\sum d(u, v) = 1 \times 1 + 2 \times 3 + 3 \times 4 + \cdots + (\frac{n}{2} + 1) \times 4 \\
= 7 + 4 \times \left(\frac{n+2}{2}\right) (\frac{n}{2} + 1) \\
= \frac{2n^2}{4} + \frac{n^2}{2} + 1 = \frac{1}{4} k^2 + 3k - 1.
\]

Case 2. If \( \frac{n}{2} = k \) is odd, then
\[
\sum d(u, v) = 1 \times 1 + 2 \times 3 + 3 \times 4 + \cdots + (\frac{n+2}{2}) \times 4 + (\frac{n+2}{2} + 1) \times 2 \\
= 7 + 4 \times \left(\frac{n+2}{2}\right) (\frac{n+2}{2} + 1) + \frac{n^2}{2} + 2 \\
= \frac{2n^2}{4} + \frac{n^2}{2} n - \frac{1}{2} = \frac{1}{2} k^2 + 3k - \frac{1}{2}.
\]

Therefore, we have
\[
\sum_{\deg(u) = \deg(v) = 3} \deg(u) \deg(v) d(u, v) = 6 \sum d(u, v) \\
= \begin{cases} 
3k^2 + 18k - 6, & \text{if } k \text{ is even}, \\
3k^2 + 18k - 3, & \text{if } k \text{ is odd}.
\end{cases}
\]

3. If \( \deg(u) = \deg(v) = 2 \), then both \( u \) and \( v \) are on the inner ring of \( GP(n, k) \). Thus
\[
\sum_{\deg(u) = \deg(v) = 2} \deg(u) \deg(v) d(u, v) = 4 \sum d(u, v).
\]

Case 1. If \( \frac{n}{2} = k \) is even, then
\[
\sum d(u, v) = 1 \times 1 + 3 \times 2 + 4 \times 4 + \cdots + (\frac{n}{2} + 2) \times 4 \\
= 7 + 4 \times \left(\frac{n}{2} + 1\right) (\frac{n}{2} + 2) \\
= \frac{1}{8} n^2 + \frac{3}{2} n - \frac{5}{2} = \frac{1}{8} k^2 + 5k - 5.
\]

Case 2. If \( \frac{n}{2} = k \) is odd, then
\[
\sum d(u, v) = 1 \times 1 + 3 \times 2 + 4 \times 4 + \cdots + (\frac{n+2}{2} + 1) \times 4 + (\frac{n+2}{2} + 2) \times 2 \\
= 7 + 4 \times \left(\frac{n+2}{2}\right) (\frac{n+2}{2} + 2) + \frac{n^2}{2} + 2 \\
= \frac{1}{8} n^2 + \frac{3}{2} n - \frac{5}{2} = \frac{1}{2} k^2 + 5k - \frac{5}{2}.
\]

Therefore, we have
\[
\sum_{\deg(u) = \deg(v) = 2} \deg(u) \deg(v) d(u, v) = 4 \sum d(u, v) \\
= \begin{cases} 
2k^2 + 10k - 10, & \text{if } k \text{ is even}, \\
2k^2 + 20k - 18, & \text{if } k \text{ is odd}.
\end{cases}
\]

In a word, we obtain that
\[
\text{Gut}(2k, k) = \sum_{u, v \in V(GP)} \deg(u) \deg(v) d(u, v) \\
= \begin{cases} 
9k^3 + 5k^2 + 28k - 16, & \text{if } k \text{ is even}, \\
9k^3 + 5k^2 + 38k - 21, & \text{if } k \text{ is odd}
\end{cases}
\]
for \( n = 2k \).

By the proof of Theorem 3.4, we arrive at the following conclusions.

Corollary 3.5 If \( n \neq 2k \), then \( TW_2(n, k) = 0 \) and \( TW_3(n, k) = W(n, k) \). Moreover, we have
\[
TW_2(2k, k) = \begin{cases} 
\frac{1}{2} k^2 + 5k - \frac{5}{2}, & \text{if } k \text{ is even}, \\
\frac{5}{2} k + \frac{1}{2} - 1 = \frac{1}{2} k^2 + 3k - 1,
\end{cases}
\]
and
\[
TW_3(2k, k) = k^3.
\]

The Szeged index \( S_Z(G) \), edge-Szeged index \( S_Z_e(G) \), and PI index \( PI(G) \) of \( G \) are important indexes in computer science.

Theorem 3.6 For the Szeged index, we have
\[
S_Z(n, 1) = \left\{ \begin{array}{ll} 
3n^3 - 4n^2 + 2n, & \text{if } n \text{ is odd}, \\
3n^3, & \text{if } n \text{ is even},
\end{array} \right.
\]
and
\[
S_Z(n, 2) = \left\{ \begin{array}{ll} 
3n^3 - 12n^2 + 12n, & \text{if } n \text{ is even}, \\
3n^3 - 16n^2 + 22n, & \text{if } n \text{ is odd}.
\end{array} \right.
\]

Proof. (1) The edges of \( GP(n, 1) \) can be divided into three types, that is, \( e_1 = u_i u_{i+1}, e_2 = v_i v_{i+1} \) or \( e_3 = u_i v_i \). Then we have
\[
n_{u_i}(e_1) = n_{u_{i+1}}(e_1) = \left\{ \begin{array}{ll} 
n - 1, & \text{if } n \text{ is odd}, \\
n, & \text{if } n \text{ is even}
\end{array} \right.
\]
and
\[
n_{v_i}(e_2) = n_{v_{i+1}}(e_2) = \left\{ \begin{array}{ll} 
n - 1, & \text{if } n \text{ is odd}, \\
n, & \text{if } n \text{ is even}
\end{array} \right.
\]
and \( n_{u_i}(e_3) = n_{v_i}(e_3) = n \).

According to the definition, we have
\[
S_Z(n, 1) = \sum_{e = u_i v_i \in GP} n_e(e) \\
= n \cdot [n_{u_i}(e_1) \cdot n_{u_{i+1}}(e_1)] \\
+ n \cdot [n_{v_i}(e_2) \cdot n_{v_{i+1}}(e_2)] \\
+ n \cdot [n_{u_i}(e_3) \cdot n_{v_i}(e_3)] \\
= \left\{ \begin{array}{ll} 
3n^3 - 4n^2 + 2n, & \text{if } n \text{ is odd}, \\
3n^3, & \text{if } n \text{ is even}.
\end{array} \right.
\]

(2) If \( k = 2 \) and \( n > 9 \), then divide the edges of \( GP(n, 2) \) into three parts as (1) similarly, i.e., \( e_1 = u_i u_{i+1}, e_2 = v_i v_{i+1}, e_3 = u_i v_i \). It can be easily known that apart from the vertices whose distance to \( u \) is equal to the distance to \( v \), the number of \( GP(n, 2) \)’s vertices with a shorter distance to \( u \) than to \( v \) is equal to the number of vertices with a longer distance to \( u \) than to \( v \). Firstly, the vertices whose distance to \( u \) is equal to the distance to \( v \) should be found.

Case 1. Assume that \( n \) is even.

For \( e_1 = u_i u_{i+1} \), the set of vertices whose distance to \( u_i \) is equal to the distance to \( u_{i+1} \) is \( \{v_{i-1}, v_{i-3}, v_{i+2}, v_{i+4}\} \), then \( n_{u_i}(e_1) = n_{u_{i+1}}(e_1) = \frac{2n-4}{2} = n - 2 \).

For \( e_2 = u_i v_i \), the set of vertices whose distance to \( u_i \) is equal to the distance to \( v_i \) is \( \{v_{i+2}, v_{i+3}, u_{i-2}, u_{i-3}\} \), then \( n_{u_i}(e_2) = n_{v_i}(e_2) = \frac{2n-4}{2} = n - 2 \).

If \( e_3 = v_i v_{i+2}, \) the set of vertices whose distance to \( v_i \) is equal to the distance to \( v_{i+2} \) is \( \{u_{i+1}, v_{i+1}, u_{i+1} + \frac{2}{3}, v_{i+1} + \frac{2}{3}\} \), then \( n_{v_i}(e_3) = n_{v_{i+1}}(e_3) = \frac{2n-4}{2} = n - 2 \).

Case 2. Assume that \( n \) is odd.
For $e_1 = u_1u_{i+1}$, the set of vertices whose distance to $u_i$ is equal to the distance to $u_{i+1}$ is $\{v_{i-1}, v_{i-3}, v_{i+1}, v_{i+4}, u_{i+1}+\frac{3}{2}, v_{i+1}+\frac{3}{2}\}$, then $n_{u_i}(e_1) = n_{u_{i+1}}(e_1) = \frac{2n-6}{2} = n - 3$.

For $e_2 = u_i v_i$, the set of vertices whose distance to $u_i$ is equal to the distance to $v_i$ is $\{u_{i+2}, u_{i+3}, u_{i-2}, u_{i-3}\}$, then $n_{u_i}(e_2) = n_{v_i}(e_2) = \frac{2n-4}{2} = n - 2$.

If $e_3 = v_i v_{i+2}$, the set of vertices whose distance to $v_i$ is equal to the distance to $v_{i+2}$ is $\{u_{i+1}, v_{i+1}, u_{i+1}+\frac{3}{2}, v_{i+1}+\frac{3}{2}, u_{i+1}+\frac{3}{2}, v_{i+1}+\frac{3}{2}\}$, then $n_{v_i}(e_3) = n_{v_{i+2}}(e_3) = \frac{2n-4}{2} = n - 3$.

According to the definition, we have

$$S_z(n, 2) = \sum_{e = uv \in E(GF)} n_u(e)n_v(e)$$

$$= n \cdot [n_{u_i}(e_1) \cdot n_{u_{i+1}}(e_1)] + n \cdot [n_{v_i}(e_2) \cdot n_{v_{i+1}}(e_2)] + n \cdot [n_{u_i}(e_3) \cdot n_{v_{i+2}}(e_3)]$$

$$= \begin{cases} 3n^3 - 12n^2 + 12n, & \text{if } n \text{ is even}, \\ 3n^3 - 16n^2 + 22n, & \text{if } n \text{ is odd}. \end{cases}$$

**Theorem 3.7** For edge-Szeged index and PI index, we have

$$S_{ze}(n, 1) = \begin{cases} \frac{11}{2} n^3 - 9n^2 + \frac{9}{2} n, & \text{if } n \text{ is odd}, \\ \frac{11}{2} n^3 - 12n^2 + 8n, & \text{if } n \text{ is even}. \end{cases}$$

$$PI(n, 1) = \begin{cases} 8n^2 - 6n, & \text{if } n \text{ is odd}, \\ 8n^2 - 8n, & \text{if } n \text{ is even}. \end{cases}$$

$$S_{ze}(n, 2) = \begin{cases} \frac{27}{2} n^3 - 36n^2 + 50n, & \text{if } n = 4x, \\ \frac{27}{2} n^3 - 39n^2 + 57n, & \text{if } n = 4x + 2, \\ \frac{27}{2} n^3 - \frac{27}{4} n^2 + \frac{27}{4} n, & \text{if } n \text{ is odd}, \end{cases}$$

and

$$PI(n, 2) = \begin{cases} 9n^2 - 24n, & \text{if } n = 4x, \\ 9n^2 - 26n, & \text{if } n = 4x + 2, \\ 9n^2 - 21n, & \text{if } n \text{ is odd.} \end{cases}$$

**Proof.** (1) The edge set of $GP(n, 1)$ can be divided into three categories as in Theorem 3.6, then we may get the following results.

**Case 1.** If $n$ is odd, then

$$m_{u_i}(e_1) = m_{u_{i+1}}(e_1) = \frac{n - 1}{2} + \frac{n - 1}{2} + \frac{n - 1}{2} = \frac{3n - 3}{2},$$

$$m_{v_i}(e_2) = m_{v_{i+1}}(e_2) = \frac{n - 1}{2} + \frac{n - 1}{2} + \frac{n - 1}{2} = \frac{3n - 3}{2},$$

and

$$m_{u_i}(e_3) = m_{v_i}(e_3) = n.$$

Therefore, we have

$$S_{ze}(n, 1) = \sum_{e = uv \in E(GP)} m_u(e)m_v(e)$$

$$= n \cdot [m_{u_i}(e_1) \cdot m_{u_{i+1}}(e_1)] + n \cdot [m_{v_i}(e_2) \cdot m_{v_{i+1}}(e_2)] + n \cdot [m_{u_i}(e_3) \cdot m_{v_i}(e_3)]$$

$$= \frac{11}{2} n^3 - 9n^2 + \frac{9}{2} n,$$

and

$$PI(n, 1) = \sum_{e = uv \in E(GP)} [m_u(e) + m_v(e)]$$

$$= n \cdot [m_{u_i}(e_1) + m_{u_{i+1}}(e_1)] + n \cdot [m_{v_i}(e_2) + m_{v_{i+1}}(e_2)] + n \cdot [m_{u_i}(e_3) + m_{v_i}(e_3)]$$

$$= 8n^2 - 6n.$$

**Case 2.** If $n$ is even, then

$$m_{u_i}(e_1) = m_{u_{i+1}}(e_1) = \frac{n - 2}{2} + \frac{n - 2}{2} + \frac{n - 2}{2} = \frac{3n - 4}{2},$$

$$m_{v_i}(e_2) = m_{v_{i+1}}(e_2) = \frac{n - 2}{2} + \frac{n - 2}{2} + \frac{n - 2}{2} = \frac{3n - 4}{2},$$

and

$$m_{u_i}(e_3) = m_{v_i}(e_3) = n.$$

Therefore, we have

$$S_{ze}(n, 1) = \sum_{e = uv \in E(GP)} m_u(e)m_v(e)$$

$$= n \cdot [m_{u_i}(e_1) \cdot m_{u_{i+1}}(e_1)] + n \cdot [m_{v_i}(e_2) \cdot m_{v_{i+1}}(e_2)] + n \cdot [m_{u_i}(e_3) \cdot m_{v_i}(e_3)]$$

$$= \frac{11}{2} n^3 - 12n^2 + 8n,$$

and

$$PI(n, 1) = \sum_{e = uv \in E(GP)} [m_u(e) + m_v(e)]$$

$$= n \cdot [m_{u_i}(e_1) + m_{u_{i+1}}(e_1)] + n \cdot [m_{v_i}(e_2) + m_{v_{i+1}}(e_2)] + n \cdot [m_{u_i}(e_3) + m_{v_i}(e_3)]$$

$$= 8n^2 - 8n.$$

(2) It can be easily known that apart from the primitive edge and the edges whose distance to $u$ is equal to the distance to $v$, the number of $GP(n, 2)$’s edges of with a shorter distance to $u$ than to $v$ is equal to the number of edges with a longer distance to $u$ than to $v$. First, the edges whose distance to $u$ is equal to the distance to $v$ should be found and they are related to the vertices whose distance to $u$ is equal to the distance to $v$.

**Case 1.** Assume that $n$ is even.

If $e_1 = u_iu_{i+1}$, then the set of edges whose distance to $u_i$ is equal to the distance to $u_{i+1}$ is $\{v_{i-1}v_{i-3}, v_{i-3}v_{i-5}, v_{i+1}v_{i+2}, v_{i+2}v_{i+4}, v_{i+4}v_{i+6}, v_{i+6}v_{i+8}, v_{i+8}v_{i+10}, v_{i+10}v_{i+12}\}$, so $m_{e_i}(u_i) = m_{e_i}(u_{i+1}) = \frac{3n-8}{2}$.

If $e_2 = u_iv_i$, then the set of edges whose distance to $u_i$ is equal to the distance to $v_i$ is $\{u_{i+2}u_{i+3}, u_{i+3}u_{i+4}, u_{i+4}u_{i+5}, u_{i+5}u_{i+6}, u_{i+6}u_{i+7}, u_{i+7}u_{i+8}, u_{i+8}u_{i+9}, u_{i+9}u_{i+10}, u_{i+10}u_{i+11}, u_{i+11}u_{i+12}\}$, so $m_{e_2}(u_i) = m_{e_2}(v_i) = \frac{3n-10}{2}$.

For $e_3 = v_iv_{i+2}$, if $\frac{n}{2}$ is even, then the set of edges whose distance to $v_i$ is equal to the distance to $v_{i+2}$ is $\{v_{i+1}v_{i+3}, v_{i+3}v_{i+5}, v_{i+5}v_{i+1+}v_{i+7}, v_{i+7}v_{i+9}, v_{i+9}v_{i+1+}, v_{i+11}v_{i+12}\}$.
Thus $m_{e_3}(v_1) = m_{e_3}(v_{i+2}) = \frac{3n-6}{2}$. If $n$ is odd, then the set of edges whose distance to $v_i$ is equal to the distance to $v_{i+2}$ is

$$\left\{ u_{i+1}v_{i+1}, u_{i+1}v_{i+3}, u_{i-1}v_{i+1}, u_{i+1}\frac{3}{2}v_{i+1+\frac{3}{2}}, v_{i+\frac{3}{2}}v_{i+2+\frac{3}{2}}, u_{i+\frac{1}{2}}u_{i+\frac{3}{2}}u_{i+\frac{1}{2}}u_{i+3}, u_{i+3}u_{i+2} \right\}.$$  

Hence $m_{e_3}(v_1) = m_{e_3}(v_{i+2}) = \frac{3n-6}{2}$.  

**Case 2.** Assume that $n$ is odd.  

If $e_1 = u_iu_{i+1}$, then the set of edges whose distance to $u_i$ is equal to the distance to $u_{i+1}$ is

$$\left\{ u_{i-1}v_{i-3}, u_{i-3}v_{i-5}, u_{i+1}v_{i+4}, u_{i+4}v_{i+4}, v_{i+4}v_{i+6}, u_{2i+3}\left( v_{i}^{\frac{3}{2}}v_{i+\frac{3}{2}}v_{i+1}\right) \right\},$$

thus $m_{e_2}(u_i) = m_{e_2}(u_{i+1}) = \frac{3n-6}{2}$.

If $e_2 = u_iv_i$, then the set of edges whose distance to $u_i$ is equal to the distance to $v_i$ is

$$\left\{ u_{i+2}u_{i+3}, u_{i+3}u_{i+1}, u_{i}v_{i+4}, u_{i-2}v_{i-3}, u_{i-3}v_{i-4}, u_{i-3}v_{i-3} \right\},$$

so $m_{e_2}(u_i) = m_{e_2}(v_i) = \frac{3n-7}{2}.$

If $e_3 = v_iv_{i-1}$, the set of edges whose distance to $v_i$ is equal to the distance to $v_{i+2}$ is

$$\left\{ u_{i+1}v_{i+1}, u_{i}v_{i+1}, u_{i+1}v_{i+3}, u_{i+\frac{3}{2}}u_{i+1+\frac{3}{2}} \right\},$$

then $m_{e_3}(v_i) = m_{e_3}(v_{i+2}) = \frac{3n-5}{2}.$

Therefore, we have

$$S_{Ze}(n,2) = \sum_{e=uv \in E(GP)} m_u(e)m_v(e) = n \cdot m_u(e_1) \cdot m_v(e_1) + n \cdot m_u(e_2) \cdot m_v(e_2) + n \cdot m_u(e_3) \cdot m_v(e_3)$$

$$= \begin{cases} \frac{2n^3}{3} - 36n^2 + 50n, & \text{if even } n = 4x, \\ \frac{2n^3}{3} - 39n^2 + 57n, & \text{if } n = 4x + 2, \\ \frac{2n^3}{3} - 63n^2 + 155n, & \text{if } n \text{ is odd.} \end{cases}$$

and

$$P_I(n,2) = \sum_{e=uv \in E(GP)} [m_u(e) + m_v(e)]$$

$$= n \cdot [m_u(e_1) + m_v(e_1)] + n \cdot [m_u(e_2) + m_v(e_2)] + n \cdot [m_u(e_3) + m_v(e_3)]$$

$$= \begin{cases} 9n^2 - 24n, & \text{if even } n = 4x, \\ 9n^2 - 26n, & \text{if even } n = 4x + 2, \\ 9n^2 - 21n, & \text{if } n \text{ is odd.} \end{cases}$$

Hence Theorem 3.7 is proved. 

**References**


