Some Aspects of the Wiener Index for Sun Graphs

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Abstract

The Wiener index $W(G)$ is the sum of distances of all pairs of vertices of the graph $G$. The Wiener polarity index $W_p(G)$ of a graph $G$ is the number of unordered pairs of vertices $u$ and $v$ of $G$ such that the distance $d_G(u,v)$ between $u$ and $v$ is 3. In this paper the Wiener and the Wiener polarity indices of sun graphs are computed. A relationship between those indices with some other topological indices are presented. Finally, we find the Hosoya (Wiener) polynomial for sun graphs.

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1 Introduction

In theoretical chemistry, distance based molecular structure descriptors are used for modeling physical, pharmacologic, biologic and others properties of chemical compounds [13, 14].

Let $G = (V,E)$ be a finite undirected connected graph. The distance between two vertices $u$ and $v$ in $G$, denoted by $d_G(u,v)$, is the length of a shortest path between $u$ and $v$ in $G$. A tree is a connected acyclic graph. Let $d_G(v)$ of a vertex $v$ be the sum of all distances between $v$ and all other vertices of $G$.

The Wiener index $W(G)$ of $G$ is defined by

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

One can define the Wiener index also in a slightly different way

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} d_G(v).$$
The Wiener polarity index $W_P(G)$ of a graph $G$ of order $n$ is defined as the number of unordered pairs of vertices $u$ and $v$ of $G$ such that the distance $d_G(u, v)$ between $u$ and $v$ is 3. $W_P(G)$ was recently introduced and receive more attention. The authors in [12] demonstrated quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons by using $W_P(G)$. Hosoya [9] found a physical-chemical interpretation of $W_P(G)$. Recently, [5] gives all trees (resp. unicyclic graphs) of order $n$ minimizing and maximizing the Wiener polarity. Some extremal properties on particular trees were given in [4] [2] [3] [11].

A $k$–sun graph ($k \geq 3$), is the graph on $2k$ vertices obtained from a clique $c_1, ..., c_k$ on $k$ vertices and an independent set $s_1, ..., s_k$ on $k$ vertices. The set of edges is defined by couples $s_ic_i, s_ic_{i+1}$, $1 \leq i < k$, and $s_kc_k, s_kc_1$, see figure 1.

![Figure 1: A $k$–Sun graph](image)

The paper is organized as follow, the Wiener and the Wiener polarity indices of sun graphs are computed in section 2. In section 3, a relationship between those indices with some other topological indices are presented. Finally, in section 4 we find the Hosoya (Wiener) polynomial for sun graphs.

## 2 Exact Wiener and Wiener Polarity Index of $k$-sun graphs

Let $G = (V, E)$ be a $k$-sun graph for $k \geq 3$, obtained from a clique $c_1, ..., c_k$ on $k$ vertices and an independent set $s_1, ..., s_k$.

**Theorem 1** Let $G$ be a $k$–sun graph ($k \geq 3$) then, $W(G) = k(4k - 5)$.

**Proof.** We have by definition

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} d_G(v),$$

$$= \frac{1}{2} \sum_{v \in U(G)} d_G(v) + \frac{1}{2} \sum_{v \in C(G)} d_G(v).$$

2
Theorem 2

Let \( C(G) \) a clique \( c_1, ..., c_k \) on \( k \) vertices and \( U(G) \) an independent set \( s_1, ..., s_k \) of \( G \).

Let \( U = \sum_{v \in U(G)} d_G(v) \) and \( C = \sum_{v \in C(G)} d_G(v) \). Then, for a vertex \( u_i \) chosen arbitrarily, then

\[
U = k(d(u_i, c_i) + d(u_i, c_{i+1}) + d(u_i, u_{i+1}) + d(u_i, u_{i-1}) + (k-2)d(u_i, c_j) + (k-3)d(u_i, u_j))
\]

with \( d(u_i, c_i) = 1, d(u_i, c_{i+1}) = 1, d(u_i, u_{i+1}) = 2, d(u_i, u_{i-1}) = 2, d(u_i, c_j) = 2 \)
and \( d(u_i, u_j) = 3 \). Hence, \( U = k(5k - 7) \).

Moreover, for a vertex \( c_i \) chosen arbitrarily, we have
\( C = k((k-1)d(c_i, c_j) + d(c_i, u_i) + d(c_i, u_{i+1}) + (k-2)d(c_i, u_j)) \)
with \( d(c_i, c_j) = 1, d(c_i, u_i) = 1, d(c_i, u_{i+1}) = 1, d(c_i, u_j) = 2 \).

Then, \( C = k(3k - 3) \), proving a result.

**Theorem 2** Let \( G \) be a \( k \)-sun graph then \( W_P(G) = \frac{k(k-3)}{2} \).

**Proof.** If \( k = 3 \), then \( W_P(G) = 0 \) since \( diam(G) = 2 \).

Let \( G = (V, E) \) be a \( k \)-sun graph for \( k \geq 4 \).

Let compute \( W_P(G) = |\{\{u, v\} \mid d_G(u, v) = 3, u, v \in V\}| \).

All distances of all pairs of vertices \( \{u, v\} \) such that \( d_G(u, v) = 3 \) are resumed below

- If \( u = c_i \) and \( v = c_j \) then \( d_G(u, v) \leq 1 \) for \( 1 \leq i \leq k, 1 \leq j \leq k \),
- If \( u = s_i \) and \( v = c_i \) then \( d_G(u, v) = 1 \) for \( 1 \leq i \leq k \),
- If \( u = s_i \) and \( v = c_{i+1} \) then \( d_G(u, v) = 2 \) for all \( u = s_i, v = c_j, j \neq i+1, i \neq k \) and \( j \neq 1 \), with \( 1 \leq i \leq k, 1 \leq j \leq k \),
- \( d_G(u, v) = 2 \), for all \( u = s_i, v = c_j, j \neq i+1, i \neq k \) and \( j \neq 1 \), with \( 1 \leq i \leq k \),
- Finally, \( d_G(u, v) = 3 \) if and only if \( u = s_i, v = s_j \), with \( i \neq j, j \neq i+1, 1 \leq i \leq k, 1 \leq j \leq k \), \(|\{u, v\}/d_G(u, v) = 3\}| = k - 3 \), proving the result.

# 3 Relation between Wiener and Wiener Polarity index

The first Zagreb index \( M_1(G) \), is defined as the summation of squares of the degrees of the vertices, and the second Zagreb index \( M_2(G) \), is the sum of the products of the degrees of pairs of adjacent vertices of the graph \( G \). These topological indices were introduced by Gutman and Trinajstić [4].
In [10] and for $d \geq 1$, authors define a generalization of Wiener polarity index as the number of unordered pairs of vertices $\{u, v\}$ of $G$ such that the shortest distance between $u$ and $v$ is $d$.

$$W_d(G) = |\{u, v\} \mid d_G(u, v) = d, u, v \in V\}.$$ 

So we have

$$W(G) = \sum_{d=1}^{\text{diam}(G)} W_d(G).$$

**Lemma 3** [1] Let $G$ be a graph then

$$W_p(G) \leq \frac{n(n - 1)}{2} - \frac{1}{2} M_1(G),$$

with equality if $\text{diam}(G) = 3$.

**Corollary 4** [1] If $\text{diam}(G) \leq 3$ then $W(G) = \frac{3n(n - 1)}{2} - \frac{1}{2} M_1(G) - m$.

This corollary is valid for sun graphs since their diameter is $\leq 3$ with $n = 2k$.

**Corollary 5** Let $G$ be a sun graph then $W(G) = \frac{3n(n - 1)}{2} - \frac{1}{2} M_1(G) - m$.

**Proposition 6** Let $G$ be a sun graph then $W(G) = n(n - 1) + W_p(G) - m$.

**Proof.** From corollary 1, 2 and lemma 1, we have

$$M_1(G) = n(n - 1) + W_p(G) - m,$$

$$W(G) = \frac{3n(n - 1)}{2} - \frac{1}{2} n(n - 1) + W_p(G) - m - m,$$

hence $W(G) = n(n - 1) + W_p(G) - m$.

### 4 The Hosoya (Wiener) polynomial of sun graphs

The Hosoya (Wiener) polynomial of graphs is defined by:

$$H(G, t) = \sum_{k=1}^{D} d(G, k)t^k.$$ 

The wiener index of a graph $G$ can be determined as the first derivative of the polynomial $H(G, t)$ at $t = 1$, such that $W(G) = \sum_{k=1}^{D} k.t^k$.
Theorem 7 Let $G$ be a sun graph, then we have
\[ H(G, t) = \frac{1}{2} k(k + 3) t + k(k - 1) t^2 + \frac{k(k - 3)}{2} t^3. \]

Proof.
We have $H(G, t) = \sum_{k=1}^{3} d(G, k) t^k$, since $G$ is a sun graph.

We have $d(G, 1) = |\{(u, v) \ d(u, v) = 1\}|$, the pairs are $\{u_i, c_i\}_{i=1}^{k}$; $\{c_i, u_{i+1}\}_{i=1}^{k}$, and
$\{c_i, c_j\}_{i,j=1}^{k}$. Then $d(G, 1) = k + k + \frac{k(k - 1)}{2}$.

$d(G, 2) = |\{(u, v) \ d(u, v) = 2\}|$, the pairs are $\{u_i, u_{i+1}\}_{i=1}^{k}$; $\{u_i, c_j\}_{i=1, j \neq 1, k}^{k}$. Then $d(G, 2) = k + k(k - 2) = k(k - 1)$.

$d(G, 3) = |\{(u, v) \ d(u, v) = 3\}|$, the pairs are $\{u_i, u_j\}_{i=1, j \neq i+1, i, i-1}^{k}$. Then $d(G, 3) = \frac{k(k - 3)}{2}$, proving the result.

Remark 8 The wiener index of a sun graph $G$ can be calculated in another way such as the first derivative of the polynomial $H(G, t)$ at $t = 1$, then
\[ W(G) = \frac{1}{2} k(k + 3) + 2k(k - 1) + 3 \frac{k(k - 3)}{2} = k(4k - 5) \]

Corollary 9 Let $G = S_3$ be the 3-sun graph, then $H(S_3, t) = 9 t + 6 t^2$.

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