Wiener Index of a Cycle in the Context of Some Graph Operations

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Abstract. The Wiener index is one of the oldest molecular-graph-based structure-descriptors. It was first proposed by American Chemist Harold Wiener in 1947 as an aid to determining the boiling point of paraffin. The study of Wiener index is one of the current areas of research in mathematical chemistry. It also gives good correlations between Wiener index (of molecular graphs) and the physico-chemical properties of the underlying organic compounds. That is, the Wiener index of a molecular graph provides a rough measure of the compactness of the underlying molecule. The Wiener index \( W(G) \) of a connected graph \( G \) is the sum of the distances between all pairs (ordered) of vertices of \( G \).

\[ W(G) = \frac{1}{2} \sum_{u \neq v} d(u, v) \]

In this paper, we give theoretical results for calculating the Wiener index of a cycle in the context of some graph operations. These formulas will pave the way to demonstrate the Wiener index of molecular structures.

Keywords: Cycle, Distance, Wiener index

AMS Mathematics Subject Classification (2010): 05C12, 05C85

1. Introduction

Molecular descriptor is a final result of a logic and mathematical procedure which transforms chemical information encoded in a symbolic representation of a molecule into a useful number or the result of some standardized experiment. The Wiener index \( W(G) \) is a distance-based topological invariant is also a molecular descriptor, it much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds introduced by Harold Wiener in 1947 for predicting boiling points \((b, p)\) of alkanes based on the formula \( b, p = aW + \beta w(3) + \gamma \), where \( a, \beta, \gamma \) are empirical constants, and \( w(3) \) is called path number. It is defined as the half sum of the distances between all pairs of vertices of \( G \).

\[ W(G) = \frac{1}{2} \sum_{u \neq v} d(u, v) \]
Notation:

\[ W(G) = \frac{1}{2} \sum_{u,v} d(u,v) = \sum_{u<v} d(u,v) = \sum_{i<j} d(u_i, u_j) \]

Our notation is standard and mainly taken from standard books of graph theory \[2, 6\]. All graphs considered in this paper are simple and connected. The vertex and edge sets of a graph \( G \) are denoted by \( V(G) \) and \( E(G) \) respectively. The distance\( d(u,v) \) between the vertices \( u \) and \( v \) of the graph \( G \) is equal to length of the shortest path that connects \( u \) and \( v \). The Wiener index of the cycle is defined by

\[ W(C_n) = \begin{cases} \frac{1}{8} n^3 & \text{when } n \text{ is even} \\ \frac{1}{8} (n-1)n(n+1) & \text{when } n \text{ is odd} \end{cases} \]

In this paper we have investigated some new results on cycle in the context of some graph operations.

2. Cycle with one diameter and twin diameter\[4\]

Definition 2.1. A chord of cycle \( C_n \) is an edge joining two non-adjacent vertices.

Let \( V(C_n) = \{v_1, v_2, \ldots, v_n\} \) and \( n \) be even then the chord \( (v_i, v_{i+n/2}) \), where \( 1 \leq i \leq 2n \) of a cycle \( C_n \) is called one diameter. It is denoted by \( C_{1d}(n) \)

Definition 2.2. Two chords of a cycle \( C_n \) with \( n \) odd vertices are said to be twin diameter if the chord between the vertices \( (v_{i}, v_{i+(n-1)/2}) \) and \( (v_{i}, v_{i+(n+1)/2}) \) of cycle \( C_n \) (i.e.) the chords are joining the vertices at diameter distance and they form a triangle with an edge of cycle \( C_n \). It is denoted by \( C_{2d}(n) \).

\[ \text{Figure 1: } C_6 \text{ with one diameter } C_7 \text{ with twin diameter} \]

Theorem 1. Consider the cycle with \( n \geq 4 \) vertices

\[ W(C_{2d}(n)) = \frac{1}{32} \left[ 3n^3 + 18n^2 + 143n - 1124 \right] n \equiv 1 \text{ mod}(4) \text{ when } n \text{ be odd} \]

\[ = \frac{1}{32} \left[ n^3 + n^2 - n - 1 \right] n \equiv 3 \text{ mod}(4) \]
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\[ W(C_{id}(n)) = \frac{1}{32} \left(3n(n^2 + 2n - 8) + 32\right), \text{ when } n \text{ be even} \]

\[ = \frac{1}{32} \left(3n(n^2 + 2n - 4) + 8\right), \text{ when } n \equiv 2 \text{ mod}(4) \]

**Proof:** It follows immediately from the basic definition of \( W(G) \).

3. **Vertex duplication** [10]

**Definition 3.1.** Duplication of a vertex \( v \) by a new edge = \( v'v'' \) in a graph \( G \) produces a new graph \( G' \) such that \( N(v') = \{v_k; v''\} \) and \( N(v'') = \{v_k; v'\} \).

![Figure 2: The graph obtained by duplicating all the vertices by edges in cycle \( C_7 \)](image)

**Theorem 2.** Wiener index of the graph obtained by duplication of all the vertices by new edges in cycle \( C_n \) is

\[ W(VD(C_n)) = W(C_n) + n{n^2 + 6n - 4}, \text{ when } n \text{ be odd} \]

\[ W(VD(C_n)) = W(C_n) + n{n^2 + 6n - 3}, \text{ when } n \text{ be even} \]

**Proof:** Let \( u_1, u_2, \ldots, u_n \) be vertices and \( e_1, e_2, \ldots, e_n \) be edges of cycle \( C_n \). Let the graph obtained by duplicating all the vertices by edges in cycle \( C_n \) is \( G \). Then \( |V(G)| = 3n \), \( |E(G)| = 4n \).

We can consider the following two cases

**Case 1:** When \( n \) is odd

\[ W(VD(C_n)) = \sum_{u_i \in C, e \in \emptyset G} d(u_i, v_j) = \sum_{u_i, u_j \in G} d(u_i, u_j) + \sum_{u_i, v_j \in G} d(u_i, v_j) + \sum_{v_i, v_j \in G} d(v_i, v_j) \]

\[ = W(C_n) + \left[4n \left[3 + 4 + \ldots + \left(\frac{n+3}{2}\right)\right] + n\right] + \left[4n \left[2 + 3 + \ldots + \left(\frac{n+1}{2}\right)\right] + 2n\right] \]
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\[ W(C_n) + n[n^2 + 6n - 4] = \]

**Case 2:** When \( n \) is even

\[
W(\text{VD}(C_n)) = \sum_{u,v \in E} d(u,v) = \sum_{u \in V(C)} \sum_{v \in V(C)} d(u,v) + \sum_{v \in V(C)} d(v,v)
\]

\[
= W(C_n) + 4n \left[ 3 + 4 + \ldots + \left( \frac{n + 2}{2} \right) \right] + n[n + 4] + n
\]

\[
+ 4n \left[ 2 + 3 + \ldots + \left( \frac{n}{2} \right) \right] + n(n + 2) + 2n
\]

\[ = W(C_n) + n[n^2 + 6n - 3] \]

**Note:** In particular, the duplication of all the vertices by new edges in cycle \( C_n \) is also called as corona product \( C_n \circ K_2 \), where the corona product \( G \circ H \) is obtained by taking one copy of \( G \) and \( |V(G)| \) copies of \( H \); and by joining each vertex of the \( i \)-th copy of \( H \) to the \( i \)-th vertex of \( G \), \( i = 1, 2, \ldots, |V(G)| \).

**4. Edge duplication** [10]

**Definition 4.1.** Duplication of an edge \( e = v_i v_{i+1} \) by a vertex \( v' \) in a graph \( G \) produces a new graph \( G' \) such that \( N(v') = \{ v_i, v_{i+1} \} \).

**Figure 3:** The graph obtained by duplicating all the edges by vertices in cycle \( C_5 \)

**Theorem 3.** Wiener index of the graph obtained by duplication of all the edges by new vertices in cycle \( C_n \) is

\[
W(\text{ED}(C_n)) = 4W(C_n) + n^2, \text{ when } n \text{ be odd}
\]

\[
= 4W(C_n) + n^2 - \frac{1}{2}n, \text{ when } n \text{ be even}
\]
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**Proof:** Let \( u_1, u_2, \ldots, u_n \) be vertices and \( e_1, e_2, \ldots, e_n \) be edges of cycle \( C_n \). Let the graph obtained by duplicating all the edges by vertices in cycle \( C_n \) be \( G \). Then \(|V(G)| = 2n \) and \(|E(G)| = 3n\).

We can consider the following two cases

**Case 1:** When \( n \) is odd

\[
W(ED(C_n)) = \sum_{u_i, v_j \in G} d(u_i, v_j) = \sum_{u_i, v_j \in G} d(u_i, u_j) + \sum_{u_i, v_j \in G} d(v_i, v_j) + \sum_{u_i, v_j \in G} d(u_i, v_j)
\]

\[
= W(C_n) + W(C_n) + \binom{n}{2} + n \left[ \frac{n+1}{2} \right]^2 = \frac{1}{4} [8W(C_n) + n^3 + 4n^2 - n]
\]

\[
W(ED(C_n)) = 4W(C_n) + n^2
\]

**Case 2:** When \( n \) is even

\[
W(ED(C_n)) = \sum_{u_i, v_j \in G} d(u_i, v_j) = \sum_{u_i, v_j \in G} d(u_i, u_j) + \sum_{u_i, v_j \in G} d(v_i, v_j) + \sum_{u_i, v_j \in G} d(u_i, v_j)
\]

\[
= W(C_n) + W(C_n) + \binom{n}{2} + n^2 \left[ \frac{n+2}{4} \right] = \frac{1}{4} [8W(C_n) + n^3 + 4n^2 - 2n]
\]

\[
W(ED(C_n)) = 4W(C_n) + n^2 - \frac{1}{2} n
\]

5. Alternative method

In this paper, we characterize the cycle graph with respect to the duplication of a molecule, molecular bond, in continuation of the paper [9]. Let \( G \) be a graph with \( n \) vertices. Let \( \lambda_1, \lambda_2, \ldots, \lambda_n \) be its eigen values, then **Energy** of the graph \( G \) is defined by

\[
E = E(G) = \sum_{i=1}^{n} |\lambda_i|.
\]

A graph \( G \) on \( n \) vertices is said to be **hyperenergetic** if \( E > 2n - 2 \). A graph \( G \) on \( n \) vertices is said to be **hypoenergetic** if \( E(G) < n \). Graphs for which \( E(G) \geq n \) are said to be **non-hypoenergetic**. In theoretical chemistry, the \( \pi \)-electron energy of a conjugated carbon molecule, computed using the Hückel theory, coincides with the energy as defined here. Hence results on graph energy assume special significance [3, 7].

If \( G \) is a molecular graph with \( n \) nodes, then its adjacency matrix \( A_{ij} \) is a square matrix of order \( n \) defined as

\[
a_{ij} = \begin{cases} 1, & \text{if there is an link between } i\text{th and } j\text{th nodes} \\ 0, & \text{if there is no link between them} \end{cases}
\]
The eigenvalues of the adjacency matrix of G are usually called to be the eigenvalues of G. The largest eigenvalue of G, referred to as the spectral radius of G, will be labeled by $\lambda_1$. Using $\lambda_1$ as a measure of branching was proposed by one of the present authors as early as in 1977. For decades this branching index has not attracted much attention of theoretical chemists. Recently, studies of the spectral radius as the measure of branching became attractive again. W depends on the size (number of carbon atoms) of the molecules examined, it is purposeful to restrict the consideration to classes of alkane isomers. Our investigation of the relation between W and $\lambda_1$ is being performed on certain class of graphs with respect to the duplication of a molecule, molecular bond of the graph [8].

5.1. Programme
The following MATLAB program illustrates the characterization of Cycle with one, twin chords with Wiener Index, with the extension of the earlier finding [9].

```matlab
clc
clear all
n= input('Cycle with vertices n=');
d1 = zeros(1,n-1);
d2 = ones(1,n-2);
C= diag(d1) + diag(d2,1) + diag(d2,-1);
if rem(n,2)==0
  D=zeros(1,n-1);
  for i=1:n-1
    D(1,1)=1;
    D(1,n-1)=1;
    D(1,n/2)=1;
  end
  D;
  A1=[0 D;D' C]
  disp('Eigen value1')
  EV1=eig(A1)
  SpectralRadiusofG =max(EV1)
  E1 = abs(EV1);
  Energy1=sum(sum(E1))
  G1 = sparse(A1);
  disp('Distance matrix')
  DM1 = graphallshortestpaths(G1,'directed',false)
  M1=sum(sum(DM1));
  fprintf('Wiener index of cycle with one dia: W = %d \n', M1/2);
  UG1 = tril(G1 + G1');
  view(biograph(UG1,[],'ShowArrows','off','ShowWeights','off'))
  if Energy1>(2*n)-2
    disp('G1 is Hyper energetic')
  elseif Energy1<=(2*n)-2
    disp('G1 is NonHyper energetic')
```
6. Discussion

1. $W(C_{id}(n)) < W(C_n) < W(ED(C_n)) < W(VD(C_n))$, where $i = 1, 2$
2. $C_{1d}(n), C_{2d}(n)$ are nonhyper, nonhypo energetic for all $n \geq 4$
3. $VD(C_n)$ is hyperenergetic for all $n \geq 3$
   $VD(C_n)$ is nonhypoenergetic for all $n \geq 3$
   $VD(C_n)$ has constant spectral radius 3 for all $n \geq 3$
4. $\text{ED}(C_n)$ is hyperenergetic for all $n \geq 3$
$\text{ED}(C_n)$ is nonhypoenergetic for all $n \geq 3$
$\text{ED}(C_n)$ has constant spectral radius 3.2361 for all $n \geq 3$

**Structural Relation between $C_n$, $C_{1d}(n)$, $C_{2d}(n)$, $\text{VD}(C_n)$, $\text{ED}(C_n)$ graphs**

<table>
<thead>
<tr>
<th>Graph Class</th>
<th>Notation</th>
<th>Total no. of vertices</th>
<th>Total no. of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cycle graph</td>
<td>$C_n$</td>
<td>$N$</td>
<td>$N$</td>
</tr>
<tr>
<td>Cycle with one diameter</td>
<td>$C_{1d}(n)$</td>
<td>$N$</td>
<td>$n+1$</td>
</tr>
<tr>
<td>Cycle with twin diameter</td>
<td>$C_{2d}(n)$</td>
<td>$N$</td>
<td>$n+2$</td>
</tr>
<tr>
<td>Vertex duplication of a cycle</td>
<td>$\text{VD}(C_n)$</td>
<td>$3n$</td>
<td>$4n$</td>
</tr>
<tr>
<td>Edge duplication of a cycle</td>
<td>$\text{ED}(C_n)$</td>
<td>$2n$</td>
<td>$3n$</td>
</tr>
</tbody>
</table>

**Table 1.** Comparing $W(C_n)$ with the Wiener index of $C_{1d}(n)$, $C_{2d}(n)$, $\text{VD}(C_n)$, $\text{ED}(C_n)$ graphs

<table>
<thead>
<tr>
<th>$G$</th>
<th>$C_n$</th>
<th>$C_{1d}(n)$</th>
<th>$C_{2d}(n)$</th>
<th>$\text{VD}(C_n)$</th>
<th>$\text{ED}(C_n)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n=$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>-</td>
<td>72</td>
<td>21</td>
<td></td>
</tr>
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<td>4</td>
<td>8</td>
<td>7</td>
<td>156</td>
<td>46</td>
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<td>25</td>
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<td>141</td>
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<tr>
<td>9</td>
<td>90</td>
<td>74</td>
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<td>441</td>
<td></td>
</tr>
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<td>10</td>
<td>125</td>
<td>109</td>
<td>1695</td>
<td>595</td>
<td></td>
</tr>
</tbody>
</table>

**Table 2.** Illustrates Wiener indices for $n = 3 \leq 10$

7. **Conclusion**

In this paper, we have determined the Wiener index of a cycle in the context of some graph operations such as Cycle with one diameter and twin diameter, Vertex duplication, Edge duplication and classified its characterization like Energy, Spectral radius using MATLAB.

**REFERENCES**

Wiener Index of a Cycle in the Context of Some Graph Operations


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