Short Communication

The Wiener index of odd graphs

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Abstract

The Wiener index of a graph G is defined to be $\frac{1}{2}\sum_{u,v\in V(G)} d(u,v)$, where $d(u, v)$ is the distance between the vertices u and v in G. In this paper, we obtain an explicit expression for the Wiener index of an odd graph.

Keywords: Wiener index, odd graph.

1. Introduction

Let $G = (V, E)$ be a simple connected undirected graph with $|V(G)| = n$ and $|E(G)| = m$. Given two distinct vertices u, v of G, let $d(u, v)$ denote the distance (= the number of edges on a shortest path between u and v) between u and v. The Wiener index $W(G)$ of the graph G is defined by

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

where the summation extends over all possible pairs of distinct vertices u and v in $V(G)$.

Given the structure of an organic compound, the corresponding (molecular) graph is obtained by replacing the atoms by vertices and covalent bonds by edges (double and triple bonds also correspond to single edges unless specified otherwise). The Wiener index is one of the oldest molecular-graph-based structure-descriptors, first proposed by the chemist Harold Wiener [1] as an aid to determining the boiling point of paraffins. The study of Wiener index is one of the current areas of research in mathematical chemistry (see, for example, [2] and [3]). It is now recognised that there are good correlations between Wiener index (of molecular graphs) and the physico-chemical properties of the underlying organic compounds. For more details on the computation of Wiener index and its application to chemistry, see [4]. Two recent surveys on the topic are [5] and [6]. Our notation and terminology are as in [7].

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In this note, we present a simple proof (based on mathematical induction) for an expression for the Wiener index of odd graphs. It is known that odd graphs have interesting combinatorial properties (see e.g. [8]). First, we recall the definition of an odd graph. For a positive integer $k \geq 2$, let X be any set of cardinality $2k - 1$ and V, the collection of all $(k - 1)$-subsets of X. The odd graph O_k has V as its vertex set, and two vertices of O_k are adjacent if and only if the corresponding $(k - 1)$-subsets are disjoint. It is well known that O_3 is the Petersen graph. Apart from possessing interesting combinatorial properties, odd graphs have found applications in the design of interconnection networks for high-performance parallel computing systems (see [9]).

2. Wiener index of O_k

It is clear that if A and B are distinct vertices of O_k, then $|A \cap B| = i$ for some $i \in \{0, 1, \ldots, k - 2\}$.

Lemma 1:

Let $k \geq 2$. Fix $A_0 \in V(O_k)$. Then for any $A \in V(O_k)$, the distance $d(A_0, A) = i$ in O_k iff

$$|A_0 \cap A| = \begin{cases} \frac{i-1}{2} & \text{if } i \text{ is odd}, \\ k - \left(\frac{i+2}{2}\right) & \text{if } i \text{ is even}. \end{cases}$$

Hence $diam(O_k) = k - 1$.

Proof. If $k = 2$, $O_k = C_3$, and the result is true. So assume that $k \geq 3$. We prove the result by induction on $d(A_0, A)$. Now, $d(A_0, A) = 0$ iff $A = A_0$, and $d(A_0, A) = 1$ iff $A \cap A_0 = \phi$. Hence the result is true for $i = 0$ and $i = 1$.

Now consider the case when $d(A_0, A) = 2$. Then there exists $A_1 \in V(O_k)$ such that A_0A_1A is a path of length 2 in O_k. This means that $A_0 \cap A_1 = \phi = A_1 \cap A$. Hence $A_0 \cup A \subseteq X \backslash A_1$, and so $k - 1 = |A_0| \leq |A_0 \cup A| \leq |X \backslash A_1| = (2k - 1) - (k - 1) = k$. Consequently, $k - 1 \leq |A_0 \cup A| \leq k$. But $A_0 \neq A$ and so $|A_0 \cup A| \neq k - 1$. Thus $|A_0 \cup A| = k$ and $|A_0 \cap A| = |A_0| + |A| - |A_0 \cup A| = (k - 1) + (k - 1) - k = k - 2$. Thus $d(A_0, A) = 2$ implies that

$$|A_0 \cap A| = k - 2. \tag{1}$$

Conversely, assume that $|A_0 \cap A| = k - 2$. Set $Y = A_0 \cap A$. Then $A_0 = Y \cup \{y_0\}$, and $A = Y \cup \{y\}$ for same y_0, y in $X \backslash Y$, $y_0 \neq y$. Let $B = X \backslash (Y \cup \{y_0, y\})$. Then $B \in V(O_k)$ and $A \cap B = \phi = A_0 \cap B$. Hence A_0BA is a path of length 2 in O_k, and $d(A_0, A) \leq 2$. But $A_0 \cap A \neq \phi$ and so A is nonadjacent to A_0 in O_k. Thus $d(A_0, A) = 2$. Therefore

$$d(A_0, A) = 2 \quad \text{iff} \quad |A_0 \cap A| = k - 2. \tag{2}$$

So assume that $d(A_0, A) = i > 2$ and that the result is true if $d(A_0, A) \leq i - 1$.

Case 1: i odd

There exist vertices $A_1, A_2, \ldots, A_{i-1}$ of O_k such that $A_0A_1 \ldots A_{i-1}A$ is a path of length i in O_k. As $d(A_0, A_{i-1}) = d(A_1, A) = i - 1$, by our induction assumption (as $i - 1$ is even)

$$|A_0 \cap A_{i-1}| = |A_1 \cap A| = k - \frac{i+1}{2}. \tag{3}$$

Since $A_1 \cap A_0 = \phi$, we have by (3)

$$|A_0 \cap A| \leq |A| - |A \cap A_1| = (k-1) - \left(k - \frac{i+1}{2}\right) = \frac{i-1}{2}. \tag{4}$$

Moreover, as $d(A_0, A) = i$, we have $d(A_0, A) \notin \{1, 3, \ldots, i-2\}$ (by induction assumption), we get, $|A_0 \cap A| = \frac{i-1}{2}$.

Conversely, assume that $|A_0 \cap A| = \frac{i-1}{2}$. Set $Y = A_0 \cap A$, and $s = k - \frac{i+1}{2}$. Let $A_0 = Y \cup \{a_1, \ldots, a_s\}$, and $A = Y \cup \{b_1, \ldots, b_s\}$, where $\{a_1, \ldots, a_s\} \cap \{b_1, \ldots, b_s\} = \phi$. Further assume that $Z = X \backslash (A_0 \cup A)$. Now choose $\{z_1, z_2\} \in Z$, (since $i > 2$, $|Z| \geq 2$) and $y \in Y$ and set

$$B = Z \backslash \{z_1, z_2\} \cup \{a_1, \ldots, a_s, y\}.$$

Then

$$|B| = |Z| - 1 + s = \frac{i+1}{2} - 1 + \left(k - \frac{i+1}{2}\right) = k - 1.$$

Thus $B \in V(O_k)$, and $|A_0 \cap B| = s + 1 = k - \frac{(i-3)+2}{2}$, and $|A \cap B| = 1$. Now as i is odd, $i - 3$ is even, and by the induction hypothesis, $d(A_0, B) = i - 3$. We can take $A = \{y, x_1, \ldots, x_{k-2}\}$, and $B = \{y, y_1, \ldots, y_{k-2}\}$ (where no x_i is equal to any y_j). Let $X \backslash (A \cup B) = \{v, w\}$. If we take $A_1 = \{v, y_1, \ldots, y_{k-2}\}$, and $A_2 = \{w, x_1, \ldots, x_{k-2}\}$, then AA_1A_2B is a path of length 3 in O_k. Hence $d(A, B) \leq 3$, and therefore, $d(A_0, A) \leq d(A_0, B) + d(A, B) \leq (i-3) + 3 = i$. By induction hypothesis, this implies that $d(A_0, A) = i$.

Case 2: *i* even

Let $d(A_0, A) = i$. Then there exist vertices $A_1, \ldots, A_{i-1}$ of O_k such that $A_0A_1 \ldots A_{i-1}A$ is a path of length i in O_k. As i is even, by induction assumption, $|A_0 \cap A_{i-2}| = k - \frac{i}{2}$, and $|A_0 \cap A_{i-1}| = \frac{i-2}{2}$. Therefore $|A_0 \cap A_{i-2}| + |A_0 \cap A_{i-1}| = (k - \frac{i}{2}) + \frac{i-2}{2} = k - 1 = |A_0|$. This means, since $A_{i-1} \cap A_{i-2} = \phi$, that $A_0 = (A_0 \cap A_{i-1}) \cup (A_0 \cap A_{i-2})$. Again, as $A \cap A_{i-1} = \phi$, we have

$$\begin{aligned} A \cap A_0 &= A \cap [(A_0 \cap A_{i-1}) \cup (A_0 \cap A_{i-2})] \\ &= A \cap A_0 \cap A_{i-2} \subseteq A_0 \cap A_{i-2}. \end{aligned} \tag{5}$$

Now, $A_0 \cap A \neq A_0 \cap A_{i-2}$. Otherwise, by induction hypothesis, (as $d(A_0, A_{i-2}) = i - 2$), $|A_0 \cap A_{i-2}| = k - \frac{i}{2} = |A_0 \cap A|$ and hence $d(A_0, A) = i - 2$, a contradiction. Thus

$$|A_0 \cap A| \leq k - \frac{i+2}{2}. \tag{6}$$

Again since $d(A_{i-2}, A) = 2$, $|A \cap A_{i-2}| = k - 2$.

Table I
Distance $d(A_0, A)$ and corresponding $|A_0 \cap A|$

$d(A_0, A)$	0	1	2	3	4	5	…	$k-1$
$\lvert A_0 \cap A\rvert$	$k-1$	0	$k-2$	1	$k-3$	2	…	$\lfloor \frac{k-2}{2} \rfloor$

Hence there exist $x \in A$ and $y \in A_{i-2}$ such that

$$A \cap A_{i-2} = A \backslash \{x\} = A_{i-2} \backslash \{y\}. \tag{7}$$

Now, from (7), $A_{i-2} \backslash \{y\} \subseteq A$, $(A_0 \cap A_{i-2}) \backslash \{y\} \subseteq A_0 \cap A$, and hence

$$|A_0 \cap A| \geq |A_0 \cap A_{i-2}| - 1 = k - \frac{i}{2} - 1 = k - \left(\frac{i+2}{2}\right). \tag{8}$$

From (6) and (8), it follows that if $d(A_0, A) = i$, (i even), then $|A_0 \cap A| = k - \frac{i+2}{2}$.

Conversely, assume that

$$|A_0 \cap A| = k - \frac{i+2}{2}. \tag{9}$$

Let $Y = A_0 \cap A$, and $A_0 = Y \cup \{\alpha_1, \ldots, \alpha_s\}$, and $A = Y \cup \{\beta_1, \ldots, \beta_s\}$, where $s = i/2$.

Let $Z_0 = Y \cup \{\alpha_1, \beta_2, \ldots \beta_s\}$. Then $Z_0 \in V(O_k)$, $|A_0 \cap Z_0| = k - \frac{i}{2}$, and $|A \cap Z_0| = k - 2$.

By assumption, these imply that

$$d(A_0, Z_0) = i - 2, \quad \text{and} \quad d(Z_0, A) = 2.$$

Hence $d(A_0, A) \leq i$. But by (9) and by induction assumption, we have $d(A_0, A) \geq i$. Thus $d(A_0, A) = i$. ■

Table I which has been constructed using Lemma 1 gives the possible values for $d(A_0, A)$ for a fixed vertex A_0 of O_k and the corresponding numbers $|A_0 \cap A|$.

Remark 1:

Table I shows that the diameter of the odd graph O_k is $k - 1$. Indeed, if $V(O_k) = \{v_0, \ldots, v_{2k-2}\}$, one diametral path is given by $A_0 A_1 \ldots A_{k-1}$, where

$$A_i = \{v_j: \ \tfrac{i}{2} \leq j \leq \tfrac{i}{2} + k - 2 \quad \text{if } i \text{ is even, and}$$

$$k + \tfrac{i-1}{2} \leq j \leq 2k + \tfrac{i-1}{2} - 2 \quad \text{if } i \text{ is odd, } (j \text{ taken modulo } 2k-1)\}.$$

Remark 2:

Fix $A_0 \in V(O_k)$. Let $0 \leq j \leq k - 2$. Then the number of vertices B of O_k such that $|A_0 \cap B| = j$ is equal to

$$\binom{k-1}{j}\binom{k}{k-1-j} = \binom{k-1}{j}\binom{k}{1+j} = \frac{k}{1+j}\binom{k-1}{j}^2.$$

Remark 3:

From Table I, it is clear that if $|A_0 \cap A| = j \le \lfloor \frac{k-2}{2} \rfloor$, then $d(A_0, A) = (2j + 1)$, and if $|A_0 \cap A| = j \ge \lfloor \frac{k-2}{2} \rfloor + 1$, then $d(A_0, A) = 2(k - 1 - j)$.

These remarks enable us to compute the Wiener index $W(O_k)$ of the odd graph O_k.

Theorem 1:

$$W(O_k) = \frac{1}{2}\binom{2k-1}{k-1}\left[\sum_{j=0}^{\lfloor \frac{k-2}{2} \rfloor} \frac{(2j+1)k}{(1+j)}\binom{k-1}{j}^2 + \sum_{j=1+\lfloor \frac{k-2}{2} \rfloor}^{k-2} \frac{2(k-1-j)k}{(1+j)}\binom{k-1}{j}^2\right].$$

Proof. By Remarks (2) and (3), the sum of the distances from a fixed vertex A_0 to all the vertices of O_k is

$$D = \sum_{j=0}^{\lfloor \frac{k-2}{2} \rfloor} \frac{(2j+1)k}{(1+j)}\binom{k-1}{j}^2 + \sum_{j=1+\lfloor \frac{k-2}{2} \rfloor}^{k-2} \frac{2(k-1-j)k}{(1+j)}\binom{k-1}{j}^2. \tag{10}$$

As the expression in (10) is independent of the vertex A_0, we get

$$W(O_k) = \frac{1}{2}\binom{2k-1}{k-1} D. \qquad \blacksquare$$

Remark 4:

Taking $k = 3$ and 4, we get $W(O_3 = \text{Petersen graph}) = 75$, and $W(O_4) = 1435$.

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References

1. H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.*, **69**, 17–20 (1947).
2. S. Bajaj, S. S. Sambi, and A. K. Madan, Models for prediction of anti-neoplastic activity of 1,2-bis(sulfonyl)-1-methylhydrazines: Computational approach using Wiener's indices, *MATCH Commun. Math. Comput. Chem.*, **55**, 193–204 (2006).
3. L. Xu, and X. Guo, Catacondensed hexagonal systems with large Wiener numbers, *MATCH Commun. Math. Comput. Chem.*, **55**, 137–158 (2006).
4. I. Gutman, and O. Polansky, *Mathematical concepts in organic chemistry*, Springer-Verlag (1986).
5. A. A. Dobrynin, R. Entringer, and I. Gutman, Wiener index of trees: Theory and applications, *Acta Appl. Math.*, **66**, 211–249 (2001).
6. A. A. Dobrynin, I. Gutman, S. Klavžar, and P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.*, **72**, 247–294 (2002).
7. R. Balakrishnan, and K. Ranganathan, *A textbook of graph theory*, Springer (2000).
8. N. L. Biggs, *Algebraic graph theory*, Cambridge University Press (1974).
9. A. Ghafoor, and T. R. Bashkow, A study of odd graphs as fault-tolerant interconnection networks, *IEEE Trans. Comput.*, **40**, 225–232 (1991).