Wiener index of a type of composite graph *

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Abstract

Wiener index, one of the oldest molecular topological descriptors used in mathematical chemistry, was well-studied during the past decades. For a graph G, its *Wiener index* is defined as $W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u, v)$, where $d_G(u, v)$ is the distance between two vertices u and v in G. In this paper, we study Wiener index of a class of composite graph, namely, double graph. We reveal the relation between the Wiener index of a given graph and the one of its double graph as well as the relation between Wiener index of a given graph and the one of its k-iterated double graph. As a consequence, we determine the graphs with the maximum and minimum Wiener index among all double graphs and k-iterated double graphs of connected graphs of same order, respectively.

Keywords: Distance in graphs; Wiener index; double graph; extremal graphs.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For a graph G, we let $d_G(v)$ be the degree of a vertex v in G and $d_G(u, v)$ be the distance between two vertices u and v in G.

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One of the oldest and well-studied distance-based graph invariants associated with a connected graph G is the Wiener number $W(G)$, also termed as *Wiener index* in chemical or mathematical chemistry literature, which is defined [11] as the sum of distances over all unordered vertex pairs in G, namely,

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

Up to now, there are a lot of mathematical and chemical literatures dealing with Wiener index; many results were achieved (see the recent papers [2, 3, 4, 5, 6, 9, 10, 12] and the references quoted therein). Despite of the results obtained above, there are few results dealing with Wiener index of composite graphs (see [7, 8, 13]).

In this paper, we study Wiener index of a class of composite graph, namely, double graph. We reveal the relation between the Wiener index of a given graph and the one of its double graph as well as the relation between Wiener index of a given graph and the one of its k-iterated double graph. As a consequence, we determine the graphs with the maximum and minimum Wiener index among all double graphs and k-iterated double graphs of connected graphs of same order, respectively.

Before proceeding, we introduce some further notation and terminology.

The *diameter* of a connected graph is the greatest distance between any pair of vertices in this graph. The *eccentricity* of a vertex v in a graph G is defined to be $ec_G(v) = \max\{d_G(u, v) | u \in V(G)\}$. Denoted by P_n and K_n the path and complete graph on n vertices, respectively. Other notation and terminology not defined here will conform to those in [1].

For a fixed vertex v, let $n_v(k)$ denote the number of vertices in G at distance k from v. Then we can rewrite the Wiener index as

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{k=1}^{ec_G(v)} k n_v(k), \tag{1}$$

where $ec_G(v)$ is the eccentricity of vertex v and $\sum_{k=1}^{ec_G(v)} n_v(k) = n - 1$.

2 Wiener index of double graph and k-th iterated double graph

The *double graph* G^* of a given graph G is constructed by making two copies of (including the initial edge set of each) and adding edges u_1v_2 and u_2v_1 for every edge uv of G.

For each vertex u in G, we call the corresponding vertices u_1 and u_2, in G^*, the *clone vertices* of u.

Theorem 1. *Let G be a nontrivial connected graph of order n and G^* its double graph. Then*

$$W(G^*) = 4W(G) + 2n.$$

Proof. For the sake of convenience, we label vertices of G as $\{v_1, \ldots, v_n\}$. Suppose that x_i and y_i are the corresponding clone vertices, in G^*, of v_i for each $i = 1, \ldots, n$. Given a vertex v_i in G. According to the definition of double graph, for any vertex v_j, different from v_i, in G, we have $d_{G^*}(x_i, x_j) = d_{G^*}(x_i, y_j) = d_{G^*}(y_i, x_j) = d_{G^*}(y_i, y_j) = d_G(v_i, v_j)$. So $ec_{G^*}(x_i) = ec_{G^*}(y_i) = ec_G(v_i)$.

For a given vertex v_i in G, let $n_{v_i}(k)$ denote the number of k-paths starting from v_i ($k = 1, \ldots, ec_G(v_i)$). Then the number of k-paths starting from x_i (or y_i) in G^* is just $2n_{v_i}(k)$ for $k \neq 2$ and the number of 2-paths starting from x_i (or y_i) in G^* is just $2n_{v_i}(2) + 1$. By symmetry and the equation (1), we have

$$
\begin{aligned}
W(G^*) &= \sum_{\{u,v\}\subseteq V(G^*)} d_{G^*}(u,v) \\
&= \frac{1}{2}\left(2\sum_{i=1}^{n}\sum_{v\in V(G^*)} d_{G^*}(x_i,v)\right) \\
&= \sum_{i=1}^{n}\sum_{v\in V(G^*)} d_{G^*}(x_i,v) \\
&= \sum_{i=1}^{n}\left[\sum_{k=1,\,k\neq 2}^{ec_{G^*}(x_i)} k\cdot 2n_{v_i}(k) + 2\cdot(2n_{v_i}(2)+1)\right] \\
&= 2\sum_{i=1}^{n}\sum_{k=1}^{ec_G(v_i)} kn_{v_i}(k) + 2n \\
&= 4W(G) + 2n,
\end{aligned}
$$

as expected. □

Example 1. *Consider Wiener index of H_{2n}, obtained from the complete graph K_{2n} by removing an n-matching. It is obvious that H_{2n} can be viewed as the double graph of K_n. Then by Theorem 1, we have*

$$W(H_{2n}) = 4W(K_n) + 2n = 4\cdot\frac{n(n-1)}{2} + 2n = 2n^2.$$

For a graph G, its *k-th iterated double graph* G^{k*}, is defined as

$$G^{1*} = G^* \text{ and } G^{k*} = (G^{(k-1)*})^* \text{ for } k \geq 2.$$

For consistence, we let $G^{0*} = G$.

Theorem 2. *Let G be a nontrivial connected graph of order n and G^{k*} its k-th iterated double graph. Then*

$$W(G^{k*}) = 4^k W(G) + 2^k(2^k - 1)n.$$

Proof. Note that G^{k*} has $2^k n$ vertices. By Theorem 1 and the definition of k-th iterated double graph, for $k \geq 1$, we have the following recursive relation:

$$W(G^{k*}) = 4W(G^{(k-1)*}) + 2\cdot 2^{k-1}n = 4W(G^{(k-1)*}) + 2^k n.$$

By the recursive relations above, we thus have

$$\begin{aligned}
W(G^{k*}) &= 4W(G^{(k-1)*}) + 2^k n \\
&= 4(4W(G^{(k-2)*}) + 2^{k-1}n) + 2^k n \\
&= 4^2 W(G^{(k-2)*}) + 2^{k+1}n + 2^k n \\
&= 4^3 W(G^{(k-3)*}) + 2^{k+2}n + 2^{k+1}n + 2^k n \\
&= \ldots \\
&= 4^k W(G^{0*}) + 2^{2k-1}n + \ldots + 2^{k+2}n + 2^{k+1}n + 2^k n \\
&= 4^k W(G) + 2^{2k-1}n + \ldots + 2^{k+2}n + 2^{k+1}n + 2^k n \\
&= 4^k W(G) + 2^k(2^k - 1)n.
\end{aligned}$$

□

Recall that among all connected graphs of order n, K_n has the minimum Wiener index, while P_n has the maximum Wiener index. By means of Theorems 1 and 2, we thus have

Corollary 1. *Among all double graphs of connected graphs of order n, the double graph of K_n has the minimum Wiener index, while the double graph of P_n has the maximum Wiener index.*

Corollary 2. *Among all k-th iterated double graphs of connected graphs of order n, the k-th iterated double graph of K_n has the minimum Wiener index, while the k-th iterated double graph of P_n has the maximum Wiener index.*

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