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On the Wiener Index of Quasi-Total Graph and Its Complement

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Abstract: The *Wiener index* of a graph G denoted by $W(G)$ is the sum of distances between all (unordered) pairs of vertices of G. In practice G corresponds to what is known as the *molecular graph* of an organic compound. In this paper, we obtain the Wiener index of quasi-total graph and its complement for some standard class of graphs, we give bounds for Wiener index of quasi-total graph and its complement also establish Nordhaus-Gaddum type of inequality for it.

Key Words: Wiener index, quasi-total graph, complement of quasi-total graph.

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§1. Introduction

Let G be a simple, connected, undirected graph with vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \cdots, e_m\}$. The distance between two vertices v_i and v_j, denoted by $d(v_i, v_j)$ is the length of the shortest path between the vertices v_i and v_j in G. The shortest $v_i - v_j$ path is often called *geodesic*. The *diameter* $diam(G)$ of a connected graph G is the length of any longest geodesic. The *degree* of a vertex v_i in G is the number of edges incident to v_i and is denoted by $d_i = deg(v_i)$ [2].

The *Wiener index* (or *Wiener number*) [8] of a graph G denoted by $W(G)$ is the sum of distances between all (unordered) pairs of vertices of G.

$$W(G) = \sum_{i<j} d(v_i, v_j).$$

The *Wiener index* $W(G)$ of the graph G is also defined by

$$W(G) = \frac{1}{2} \sum_{v_i, v_j \epsilon V(G)} d(v_i, v_j),$$

where the summation is over all possible pairs $v_i, v_j \in V(G)$.

The *Wiener polarity index* [8] of a graph G denoted by $W_P(G)$ is equal to the number of

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unordered vertex pairs of distance 3 of G. In [8], Wiener used a linear formula of $W(G)$ and $W_P(G)$ to calculate the boiling points t_B of the paraffins, i.e.,

$$t_B = aW(G) + bW_P(G) + c,$$

where a, b and c are constants for a given isomeric group.

Line graphs, total graphs and middle graphs are widely studied transformation graphs. Let $G = (V(G), E(G))$ be a graph. The *line graph* $L(G)$ [11] of G is the graph whose vertex set is $E(G)$ in which two vertices are adjacent if and only if they are adjacent in G.

The *middle graph* $M(G)$ [11] of G is the graph whose vertex set is $V(G) \cup E(G)$ in which two vertices x and y are adjacent if and only if at least one of x and y is an edge of G, and they are adjacent or incident in G. The *quasi-total graph* $P(G)$ of a graph G is the graph whose vertex set is $V(G) \cup E(G)$ and two vertices are adjacent if and only if they correspond to two nonadjacent vertices of G or to two adjacent edges of G or one is a vertex and other is an edge incident with it in G. This concept was introduced in [6]. The *complement* of G, denoted by $\overline{G}$, is the graph with the same vertex set as G, but where two vertices are adjacent if and only if they are nonadjacent in G. We denote the *complement of quasi-total graph* $P(G)$ of G by $\overline{P(G)}$. Its vertex set is $V(G) \cup E(G)$ and two vertices are adjacent if and only if they correspond to two adjacent vertices of G or to two nonadjacent edges of G or one is a vertex and other is an edge nonincident with it in G. In [9], it is interesting to see that the transformation graph G^{-++} is exactly the quasi-total graph $P(G)$ of G, and G^{+--} is the complement of $P(G)$. Many papers are devoted to quasi-total graphs [1, 3, 6, 9, 10].

In the following we denote by C_n, P_n, S_n, W_n and K_n the cycle , the path, the star, the wheel and the complete graph of order n respectively. A complete bipartite graph $K_{a,b}$ has $n = a + b$ vertices and $m = ab$ edges. Other undefined notation and terminology can be found in [2].

The following theorem is useful for proving our main results.

Theorem 1.1([7]) *Let G be connected graph with n vertices and m edges. If $diam(G) \leq 2$, then $W(G) = n(n-1) - m$.*

§2. Results

Theorem 2.1 *If S_n is a star graph of order n, then*

$$W(P(S_n)) = 3n^2 - 5n + 2.$$

Proof If S_n is a star graph with n vertices, m edges and $\sum\limits_{i=1}^{n} d_i^2 = (n-1)^2 + (n-1)$, then $P(S_n)$ has $n_1 = n + m = 2n - 1$ vertices and

$$m_1 = \frac{n(n-1)}{2} + \frac{1}{2}\sum_{i=1}^{n} d_i^2 = n^2 - n$$

edges.

In $P(S_n)$ distance between adjacent vertices is one and distance between nonadjacent vertices is two, therefore $diam(P(S_n)) = 2$.

By Theorem 1.1, $W(P(S_n)) = n_1(n_1 - 1) - m_1$. Hence

$$W(P(S_n)) = (2n-1)(2n-2) - n^2 + n = 3n^2 - 5n + 2. \qquad \square$$

Theorem 2.2 *If K_n is a complete graph of order n, then*

$$W(P(K_n)) = \frac{n(n^3 + n - 2)}{4}.$$

Proof If K_n is a complete graph with n vertices, m edges and $\sum\limits_{i=1}^{n} d_i^2 = n(n-1)^2$, then $P(K_n)$ has $n_1 = n + m = \frac{n^2+n}{2}$ vertices and

$$m_1 = \frac{n(n-1)}{2} + \frac{1}{2}\sum_{i=1}^{n} d_i^2 = \frac{n(n^2-n)}{2}$$

edges.

In $P(K_n)$ distance between adjacent vertices is one and distance between nonadjacent vertices is two, therefore $diam(P(K_n)) = 2$. From Theorem 1.1,

$$\begin{aligned} W(P(K_n)) &= n_1(n_1 - 1) - m_1 \\ &= \frac{n^2+n}{2}[\frac{n^2+n}{2} - 1] - \frac{n(n^2-n)}{2} = \frac{n(n^3+n-2)}{4}. \qquad \square \end{aligned}$$

Theorem 2.3 *If W_n is a wheel graph of order n, then*

$$W(P(W_n)) = 2(4n^2 - 9n + 5).$$

Proof If W_n is a wheel graph with n vertices, m edges and $\sum\limits_{i=1}^{n} d_i^2 = n^2 + 7n - 8$, then $P(W_n)$ has $n_1 = n + m = 3n - 2$ vertices and

$$m_1 = \frac{n(n-1)}{2} + \frac{1}{2}\sum_{i=1}^{n} d_i^2 = n^2 + 3n - 4$$

edges.

In $P(W_n)$ distance between adjacent vertices is one and distance between nonadjacent vertices is two, therefore $diam(P(W_n)) = 2$.

From Theorem 1.1, $W(P(W_n)) = n_1(n_1 - 1) - m_1$. Hence,

$$W(P(W_n)) = (3n-2)(3n-2-1) - (n^2 + 3n - 4) = 2(4n^2 - 9n + 5). \qquad \square$$

Theorem 2.4 *If $K_{a,b}$ is a complete bipartite graph of order $n = a + b$, then*

$$W(P(K_{a,b})) = \frac{(a+b+ab-1)(a+b+2ab)}{2}.$$

Proof If $K_{a,b}$ is a complete bipartite graph with $n = a + b$ vertices, $m = ab$ edges and

$$\sum_{i=1}^{n} d_i^2 = ab(a+b),$$

then $P(K_{a,b})$ has $n_1 = n + m = a + b + ab$ vertices and

$$m_1 = \frac{(n+m)(n+m-1)}{2} + \frac{1}{2}\sum_{i=1}^{n} d_i^2 = \frac{(a+b)(a+b+ab-1)}{2}$$

edges.

In $P(K_{a,b})$ distance between adjacent vertices is one and distance between nonadjacent vertices is two, therefore $diam(P(K_{a,b})) = 2$.

From Theorem 1.1, $W(P(K_{a,b})) = n_1(n_1 - 1) - m_1$. Therefore,

$$\begin{aligned} W(P(K_{a,b})) &= (a+b+ab)(a+b+ab-1) - \frac{(a+b)(a+b+ab-1)}{2} \\ &= \frac{(a+b+ab-1)(a+b+2ab)}{2}. \end{aligned}$$ □

Theorem 2.5 *If P_n is a path of order $n \geqslant 4$, then*

$$W(\overline{P(P_n)}) = \frac{5n^2 - 3n - 4}{2}.$$

Proof If P_n is a path with n vertices, m edges and $\sum_{i=1}^{n} d_i^2 = 4n - 6$, then $\overline{P(P_n)}$ has $n_1 = n + m = 2n - 1$ vertices and

$$m_1 = \binom{n+m}{2} - \frac{n(n-1)}{2} - \frac{1}{2}\sum_{i=1}^{n} d_i^2 = \frac{(n-1)(3n-2) - 2(2n-3)}{2}$$

edges.

In $\overline{P(P_n)}$ distance between adjacent vertices is one and distance between nonadjacent vertices is two, therefore $diam(\overline{P(P_n)}) = 2$.

From Theorem 1.1, $W(\overline{P(P_n)}) = n_1(n_1 - 1) - m_1$. So

$$W(\overline{P(P_n)}) = (2n-1)(2n-2) - \frac{(n-1)(3n-2) - 2(2n-3)}{2} = \frac{5n^2 - 3n - 4}{2}.$$ □

Theorem 2.6 *If S_n is a star of order $n \geqslant 4$, then*

$$W(\overline{P(S_n)}) = 3n(n-1).$$

Proof If S_n is a star with n vertices, m edges and $\sum\limits_{i=1}^{n} d_i^2 = (n-1)^2 + n - 1$, then $\overline{P(S_n)}$ has $n_1 = n + m = 2n - 1$ vertices and $m_1 = \binom{n+m}{2} - \frac{n(n-1)}{2} - \frac{1}{2}\sum\limits_{i=1}^{n} d_i^2 = (n-1)^2$ edges.

As $diam(\overline{P(S_n)}) = 3$. Therefore $W(\overline{P(S_n)}) = n_1(n_1 - 1) - m_1 + W_p(\overline{P(S_n)})$, where $W_p(\overline{P(S_n)})$ is Wiener polarity index of $\overline{P(S_n)}$. Hence,

$$\begin{aligned} W(\overline{P(S_n)}) &= (2n-1)(2n-2) - (n-1)^2 + m \\ &= (2n-1)(2n-2) - (n-1)^2 + n - 1 = 3n(n-1). \end{aligned}$$ □

Theorem 2.7 *If K_n is a complete graph of order $n \geqslant 4$, then*

$$W(\overline{P(K_n)}) = \frac{n(n^3 + 6n^2 - 5n - 2)}{8}.$$

Proof If K_n is a complete graph with n vertices, m edges and $\sum\limits_{i=1}^{n} d_i^2 = n(n-1)^2$, then $\overline{P(K_n)}$ has $n_1 = n + m = \frac{n^2+n}{2}$ vertices and

$$m_1 = \binom{n+m}{2} - \frac{n(n-1)}{2} - \frac{1}{2}\sum_{i=1}^{n} d_i^2 = \frac{n(n^3 - 2n^2 + 3n - 2)}{8}$$

edges.

In $\overline{P(K_n)}$ distance between adjacent vertices is one and distance between nonadjacent vertices is two, therefore $diam(\overline{P(K_n)}) = 2$. From Theorem 1.1,

$$\begin{aligned} W(\overline{P(K_n)}) &= n_1(n_1 - 1) - m_1 \\ &= \frac{n^2+n}{2}\left[\frac{n^2+n}{2} - 1\right] - \frac{n(n^3 - 2n^2 + 3n - 2)}{8} \\ &= \frac{n(n^3 + 6n^2 - 5n - 2)}{8}. \end{aligned}$$ □

Theorem 2.8 *If C_n is a cycle of order $n \geqslant 4$, then*

$$W(\overline{P(C_n)}) = \frac{n(5n+1)}{2}.$$

Proof If C_n is a cycle with n vertices, m edges and $\sum\limits_{i=1}^{n} d_i^2 = 4n$, then $\overline{P(C_n)}$ has

$n_1 = n + m = 2n$ vertices and

$$m_1 = \binom{n+m}{2} - \frac{n(n-1)}{2} - \frac{1}{2}\sum_{i=1}^{n} d_i^2 = \frac{n(3n-5)}{2}$$

edges.

In $\overline{P(C_n)}$ distance between adjacent vertices is one and distance between nonadjacent vertices is two, therefore $diam(\overline{P(C_n)}) = 2$.

From Theorem 1.1, $W(\overline{P(C_n)}) = n_1(n_1 - 1) - m_1$. So,

$$W(\overline{P(C_n)}) = 2n(2n-1) - \frac{n(3n-5)}{2} = \frac{n(5n+1)}{2}. \qquad \square$$

Theorem 2.9 *If $K_{a,b}$ is a complete bipartite graph of order $n = a + b$, then*

$$W(\overline{P(K_{a,b})}) = \frac{(a+b+ab-1)[2(a+b+ab)-ab]}{2}.$$

Proof If $K_{a,b}$ is a complete bipartite graph with $n = a + b$ vertices, $m = ab$ edges and

$$\sum_{i=1}^{n} d_i^2 = ab(a+b),$$

then $\overline{P(K_{a,b})}$ has $n_1 = n + m = a + b + ab$ vertices and

$$m_1 = \binom{n+m}{2} - \frac{(n+m)(n+m-1)}{2} - \frac{1}{2}\sum_{i=1}^{n} d_i^2 = \frac{ab(a+b+ab-1)}{2}$$

edges.

In $\overline{P(K_{a,b})}$ distance between adjacent vertices is one and distance between nonadjacent vertices is two, therefore $diam(\overline{P(K_{a,b})}) = 2$.

By Theorem 1.1,

$$\begin{aligned} W(\overline{P(K_{a,b})}) &= n_1(n_1-1) - m_1 \\ &= (a+b+ab)(a+b+ab-1) - \frac{ab(a+b+ab-1)}{2} \\ &= \frac{(a+b+ab-1)[2(a+b+ab)-ab]}{2}. \end{aligned} \qquad \square$$

Theorem 2.10 *If G is a connected graph of order n, then $W(G) < W(P(G))$.*

Proof If G is graph with n vertices and m edges then $P(G)$ is a quasi-total graph of G with $n + m$ vertices and

$$\frac{n(n-1)}{2} + \frac{1}{2}\sum_{i=1}^{n} d_i^2$$

edges.

Wiener index of graph increases when new vertices are added to the graph G. Therefore $W(G) < W(P(G))$. □

Lemma 2.11 *If G is connected graph of order n, then*

$$3n^2 - 5n + 2 \leq W(P(G)) \leq \frac{n(n^3 + n - 2)}{4},$$

and the upper bound attain if G is a complete graph and lower bound attain if G is a star graph.

Proof Let $P(G)$ is a quasi-total graph of G with $n + m$ vertices and

$$\frac{n(n-1)}{2} + \frac{1}{2}\sum_{i=1}^{n} d_i^2$$

edges.

G has maximum edges if and only if $G \cong K_n$, $P(G)$ has maximum number of vertices if and only if $G \cong K_n$.

Wiener index of a graph increases when new vertices are added to the graph and $P(K_n)$ has maximum number of vertices compared with any other $P(G)$. Therefore $W(P(G)) \leq W(P(K_n))$.

From Theorem 2.2, $W(P(K_n)) = \frac{n(n^3+n-2)}{4}$. Therefore

$$W(P(G)) \leq \frac{n(n^3 + n - 2)}{4} \tag{1}$$

with equality holds if and only if $G \cong K_n$.

For any graph G has minimum edges if and only if $G \cong T$ and $P(G)$ has minimum number of vertices if and only if $G \cong T$. Wiener index of a graph increases when new vertices are added to the graph and $P(T)$ has minimum number of vertices compared with any other $P(G)$. Therefore $W(P(T)) \leq W(P(G))$. In the case of tree $W(P(S_n)) \leq W(P(T))$. Therefore $W(P(S_n)) \leq W(P(G))$.

From Theorem 2.1, $W(P(S_n)) = 3n^2 - 5n + 2$. Hence,

$$3n^2 - 5n + 2 \leq W(P(G)) \tag{2}$$

with equality if and only if $G \cong S_n$.

From equations (1) and (2), we get that

$$3n^2 - 5n + 2 \leq W(P(G)) \leq \frac{n(n^3 + n - 2)}{4}.$$ □

Lemma 2.12 *For any connected graph G of order $n \geq 4$,*

$$\frac{5n^2 - 3n - 4}{2} \leq W(\overline{P(G)}) \leq \frac{n(n^3 + 6n^2 - 5n - 2)}{8},$$

and the upper bound attain if G is a complete graph and lower bound attain if G is a path.

Proof Let G be connected graph with $n \geq 4$ vertices and m edges. Then $P(G)$ has $n+m$ vertices and

$$\frac{n(n-1)}{2} + \frac{1}{2}\sum_{i=1}^{n} d_i^2$$

edges. $\overline{P(K_n)}$ has $n+m$ vertices and

$$\binom{n+m}{2} - (\frac{n(n-1)}{2} + \frac{1}{2}\sum_{i=1}^{n} d_i^2)$$

edges.

G has maximum edges if and only if $G \cong K_n$, $\overline{P(G)}$ has maximum number of vertices if and only if $G \cong K_n$. Wiener index of a graph increases when new vertices are added to the graph and $\overline{P(K_n)}$ has maximum number of vertices compared to any other $\overline{P(G)}$. Therefore $W(\overline{P(G)}) \leq W(\overline{P(K_n)})$. From Theorem 2.7,

$$W(\overline{P(K_n)}) = \frac{n(n^3+6n^2-5n-2)}{8}.$$

Therefore

$$W(\overline{P(G)}) \leq \frac{n(n^3+6n^2-5n-2)}{8}. \tag{3}$$

For any connected graph G with $n \geq 4$ vertices, G has minimum number of vertices if and only if $G \cong T$. Wiener index of a graph increases when new vertices are added to a graph and $\overline{P(T)}$ has minimum number of vertices compared to any other $\overline{P(G)}$. Thus, $W(\overline{P(T)}) \leq W(\overline{P(G)})$.

In case of tree $W(\overline{P(P_n)}) \leq W(\overline{P(T)})$. Therefore $W(\overline{P(P_n)}) \leq W(\overline{P(G)})$. By Theorem 2.5, $W(\overline{P(P_n)}) = \frac{5n^2-3n-4}{2}$. Therefore

$$\frac{5n^2-3n-4}{2} \leq W(\overline{P(G)}). \tag{4}$$

From equations (3) and (4), we get that

$$\frac{5n^2-3n-4}{2} \leq W(\overline{P(G)}) \leq \frac{n(n^3+6n^2-5n-2)}{8}.$$ □

The following theorem gives the Nordhaus-Gaddum type inequality for Wiener index of quasi-total graph.

Theorem 2.13 *For any graph G with $n \geq 4$,*

$$\frac{n(11n-13)}{2} \leq W(P(G)) + W(\overline{P(G)}) \leq \frac{3n(n^3+2n^2-n-2)}{8}.$$

Proof From Lemmas 2.11 and 2.12, we have

$$\begin{aligned} 3n^2-5n+2+\frac{5n^2-3n-4}{2} &\leq W(P(G))+W(\overline{P(G)}) \\ &\leq \frac{n^4+n^2-2n}{4}+\frac{n^4+6n^3-5n^2-2n}{8}. \end{aligned}$$

Thus,

$$\frac{n(11n-13)}{2} \leq W(P(G))+W(\overline{P(G)}) \leq \frac{3n(n^3+2n^2-n-2)}{8}. \qquad \square$$

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