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THE WIENER NUMBER OF POWERS OF THE MYCIELSKIAN

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Abstract

The Wiener number of a graph G is defined as $\frac{1}{2}\sum_{u,v\in V(G)} d(u,v)$, d the distance function on G. The Wiener number has important applications in chemistry. We determine a formula for the Wiener number of an important graph family, namely, the Mycielskians $\mu(G)$ of graphs G. Using this, we show that for $k \geq 1$, $W(\mu(S_n^k)) \leq W(\mu(T_n^k)) \leq W(\mu(P_n^k))$, where S_n, T_n and P_n denote a star, a general tree and a path on n vertices respectively. We also obtain Nordhaus-Gaddum type inequality for the Wiener number of $\mu(G^k)$.

Keywords: Wiener number, Mycielskian, powers of a graph.

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1. Introduction

Let G be a simple connected undirected graph with vertex set $V(G)$ and edge set $E(G)$. Then G is of order $|V(G)|$ and size $|E(G)|$. Given two distinct vertices u, v of G, let $d(u,v)$ denote the distance between u and v (= number of edges in a shortest path between u and v in G). The Wiener number (also called Wiener index) $W(G)$ of the graph G is defined by

$$W(G) = \frac{1}{2}\sum_{a,b\in V(G)} d(a,\, b) = \sum_{i=1}^{D} ip(i,\, G),$$

where $p(i, G)$ denotes the number of pairs of vertices which are at distance i in G, and D is the diameter of G. The Wiener number is one of the oldest molecular-graph based structure-descriptors, first proposed by the American chemist Harold Wiener [13] as an aid to determine the boiling point of paraffins. Some of the recent articles in this topic are ([1, 2, 3, 4, 5, 7] and [14]).

In a search for triangle-free graphs with arbitrarily large chromatic numbers, Mycielski [11] developed an interesting graph transformation as follows. For a graph $G = (V, E)$, the Mycielskian of G is the graph $\mu(G)$ with vertex set $V \cup V' \cup \{u\}$, where $V' = \{x' : x \in V\}$ and is disjoint from V, and edge set $E \cup \{xy' : xy \in E\} \cup \{y'u : y' \in V'\}$. The vertex x' is called the twin of the vertex x (and x the twin of x') and the vertex u is the root of $\mu(G)$. In recent times, there has been an increasing interest in the study of Mycielskians, especially, in the study of their circular chromatic numbers (see, for instance, [9, 6, 8] and [10]).

Let H be a spanning connected subgraph of a (connected) graph G. Then for any pair of vertices u, v of G, $d_G(u, v) \leq d_H(u, v)$. The k-th power of a graph G, denoted by G^k, is the graph with the same vertex set as G and in which two vertices are adjacent if and only if their distance in G is at most k. Clearly, $G^1 = G$.

The complement $\overline{G}$ of a graph G is the graph with the same vertex set as G and in which two verties u, v are adjacent if and only if u, v are non-adjacent in G. In 1956, Nordhaus and Gaddum [12] gave bounds for the sum of the chromatic number $\chi(G)$ of a graph G and its complement $\overline{G}$ as follows,

Theorem 1.1. *For a graph G of order n, $2\sqrt{n} \leq \chi(G) + \chi(\overline{G}) \leq n + 1$.*

Zhang and Wu [15] presented the corresponding Nordhaus-Gaddum (in short NG) type inequality for the Wiener number as:

Theorem 1.2. *Let G be a connected graph of order $n \geq 5$ with connected complement $\overline{G}$. Then $3\binom{n}{2} \leq W(G) + W(\overline{G}) \leq \frac{n^3+3n^2+2n-6}{6}$.*

The bounds in Theorem 1.2 are sharp.

2. Wiener Number of the Mycielskian of a Graph

We start this section by obtaining a formula for the Wiener number of the Mycielskian of a graph.

Theorem 2.1. *The Wiener number of the Mycielskian of a connected graph G of order n and size m is given by $W(\mu(G)) = 6n^2 - n - 7m - 4p(2,G) - p(3,G)$.*

Proof. By definition,

$$W(\mu(G)) = \frac{1}{2} \sum_{a,b \in V(\mu(G))} d(a,\, b).$$

Hence
$$\begin{aligned} W(\mu(G)) &= \sum_{\substack{a=u,\\ b' \in V'}} d(a,\, b') + \sum_{\substack{a=u,\\ b \in V}} d(a,\, b) + \frac{1}{2} \sum_{a',b' \in V'} d(a',\, b') \\ &\quad + \frac{1}{2} \sum_{a,b \in V} d(a,\, b) + \sum_{\substack{a \in V,\\ b' \in V'}} d(a,\, b') \\ &= \sum\nolimits_1 + \sum\nolimits_2 + \sum\nolimits_3 + \sum\nolimits_4 + \sum\nolimits_5 \text{ (say).} \end{aligned}$$

One can observe that, $\sum_1 = n$, $\sum_2 = 2n$, $\sum_3 = 2\binom{n}{2}$. As distance between any pair of vertices in V is atmost 4 in $\mu(G)$, $\sum_4 = \sum_{i=1}^{3} ip(i,\, G) + 4\big[\binom{n}{2} - \sum_{i=1}^{3} p(i,G)\big]$. Now the maximum distance from any vertex in V to any vertex in V' is 3. Note that if $ab \in E$, then $ab', ba' \in E(\mu(G))$, that is, each edge of G will contribute two edges between V and V'. Also for every $a \in V$, $d(a,a') = 2$, and for every $a, b \in V$ such that $d(a,b) = 2$, we have $d(a,b') = d(b,a') = 2$. Thus $\sum_5 = 2n + 2\sum_{i=1}^{2} ip(i,\, G) + 3\big[n^2 - n - 2\sum_{i=1}^{2} p(i,G)\big]$ and therefore, $W(\mu(G)) = 6n^2 - n - 7m - 4p(2,G) - p(3,G)$. ■

This formula comes in handy when finding the Wiener number of $\mu(G)$ for which $p(2,G)$ and $p(3,G)$ are known even if the diameter of G is very large.

In [1], X. An et al. have shown that $W(S_n^k) \leq W(T_n^k) \leq W(P_n^k)$, $k \geq 1$ where S_n, P_n and T_n denotes a star, a path and a tree other than a star and a path on n vertices. The formula mentioned in Theorem 2.1 helps us in proving that $W(\mu(S_n^k)) \leq W(\mu(T_n^k)) \leq W(\mu(P_n^k))$ for any $k \geq 1$. However, this cannot be deduced from X. An's result mentioned above. In fact, there are graphs G and H with same order and size such that $W(G) > W(H)$ and $W(\mu(G)) < W(\mu(H))$. For example, let G be C_6 with a pendant edge attached at a pair of opposite vertices and H be C_7 with a single pendant edge, then $W(G) = 62$ and $W(H) = 61$ while $W(\mu(G)) = 273$ and $W(\mu(H)) = 275$.

Theorem 2.2. $W(\mu(S_n^k)) \leq W(\mu(T_n^k)) \leq W(\mu(P_n^k))$, $k \geq 1$.

Proof. By virtue of Theorem 2.1, the result in Theorem 2.2 is equivalent to $A = 7p(1, S_n^k) + 4p(2, S_n^k) + p(3, S_n^k) \geq B = 7p(1, T_n^k) + 4p(2, T_n^k) + p(3, T_n^k) \geq C = 7p(1, P_n^k) + 4p(2, P_n^k) + p(3, P_n^k)$.

We first prove that $A \geq B$. If $k \geq 2$, then $S_n^k = K_n$ which implies that $p(1, S_n^k) = \binom{n}{2} \geq \sum_{i=1}^{3} p(i, T_n^k)$ and this inequality implies $A \geq B$ (as $7 > 4 > 1$). If $k = 1$, then $diam(S_n) = 2$ and $D = diam(T_n) \geq 2$. This gives, $p(2, S_n) = \sum_{i=2}^{D} p(i, T_n)$, and therefore $7p(1, S_n) + 4p(2, S_n) \geq 7p(1, T_n) + 4p(2, T_n) + p(3, T_n)$. Once again, $A \geq B$.

Next we prove that $B \geq C$ by induction on n. $B \geq C$ is obvious for $n \leq 4$. Let T_n be a tree of order $n \geq 5$ and let $P_n = vv_1 \cdots v_{n-1}$ be a path of order n. Let $P = uu_1 \ldots u_d$ be a longest path of T_n ($d < n - 1$). u is then a pendant vertex of T_n and $T_n - \{u\}$ is a tree of order $n - 1$. By induction hypothesis, $B \geq C$ for $T_n - \{u\}$ and $P_n - \{v\}$. Let $p(a, i, G)$ denote the number of vertices in G that are at distance i from a. Clearly, $p(i, T_n^k) = p(i, T_n^k - \{u\}) + p(u, i, T_n^k)$. So it is enough to prove that $7p(u, 1, T_n^k) + 4p(u, 2, T_n^k) + p(u, 3, T_n^k) \geq 7p(v, 1, P_n^k) + 4p(v, 2, P_n^k) + p(v, 3, P_n^k)$.

We know that $p(v, i, P_n^k) \leq k$ for each $i = 1$ to $D = diam(P_n^k)$. If there are k vertices of P^k in T_n^k adjacent to u, then $p(u, 1, T_n^k) \geq p(v, 1, P_n^k)$. If not, u will be a universal vertex of T_n^k (that is, a vertex adjacent to all the other vertices of T_n^k). Thus in any case, $p(u, 1, T_n^k) \geq p(v, 1, P_n^k)$.

If $p(u, 2, T_n^k) < p(v, 2, P_n^k) \leq k$, then $diam(T_n^k) \leq 2$ (This is because if $diam(T_n^k) > 2$, then along the longest path in T_n^k, there will be k vertices which would be at distance 2 from u which is a contradiction). This gives $p(u, 1, T_n^k) + p(u, 2, T_n^k) = (n - 1) \geq p(v, 1, P_n^k) + p(v, 2, P_n^k) + p(v, 3, P_n^k)$, and as $7 > 4 > 1$, $7p(u, 1, T_n^k) + 4p(u, 2, T_n^k) \geq 7p(v, 1, P_n^k) + 4p(v, 2, P_n^k) + p(v, 3, P_n^k)$.

Next if, $p(u, 2, T_n^k) \geq p(v, 2, P_n^k)$ and $p(u, 3, T_n^k) \geq p(v, 3, P_n^k)$ then clearly, $B \geq C$. Otherwise, $diam(T_n^k) \leq 3$, (Same argument as above) which shows that $p(u, 1, T_n^k) + p(u, 2, T_n^k) + p(u, 3, T_n^k) = (n - 1) \geq p(v, 1, P_n^k) + p(v, 2, P_n^k) + p(v, 3, P_n^k)$ and hence $7p(u, 1, T_n^k) + 4p(u, 2, T_n^k) + p(u, 3, T_n^k) \geq 7p(v, 1, P_n^k) + 4p(v, 2, P_n^k) + p(v, 3, P_n^k)$. ■

It can easily be seen from the proof of Theorem 2.2 that when $k = 1$, we have strict inequality for $n \geq 5$.

Corollary 2.3. *If G is a connected graph of order n, then $W(\mu(G^k)) \leq W(\mu(P_n^k))$.*

Proof. Let T be a spanning tree of G. In view of Theorem 2.2, it suffices to prove that $W(\mu(G^k)) \leq W(\mu(T^k))$. Any pair of vertices of T^k at distance i will be at distance at most i in G^k. Therefore, $7p(1, G^k) + 4p(2, G^k) + p(3, G^k) \geq 7p(1, T^k) + 4p(2, T^k) + p(3, T^k)$. Thus $W(\mu(G^k)) \leq W(\mu(P_n^k))$. ■

3. NG Type Results for the Wiener Number of Mycielski Graphs and Their Powers

When G (of order n and size m) has no isolated vertices, $\mu(G)$ is connected while $\overline{\mu(G)}$ is connected always. It is easy to see that the diameter of $\overline{\mu(G)}$ is 2 and one can establish that $W(\overline{\mu(G)}) = 2n^2 + 2n + 3m$.

This shows that $W(\mu(G)) + W(\overline{\mu(G)}) = 8n^2 + n - 4m - 4p(2, G) - p(3, G)$.

As in the proof of Theorem 2.2, one can prove the following.

Theorem 3.1. $W(\mu(S_n^k)) + W(\overline{\mu(S_n^k)}) \leq W(\mu(T_n^k)) + W(\overline{\mu(T_n^k)}) \leq W(\mu(P_n^k)) + W(\overline{\mu(P_n^k)})$ *for any $k \geq 1$.*

Now $W(\mu(G)) + W(\overline{\mu(G)})$ is maximum, when $4m + 4p(2, G) + p(3, G)$ is least. As $W(P_n^k) = \sum_{i=1}^{n-1} \lceil \frac{i}{k} \rceil (n-i)$ (see [1]), $p(i, P_n^k) = \sum_{j=1}^{k} \{n - (k(i-1)+j)\}$ for $i < D$, the diameter of P_n^k and thus we see that $4m + 4p(2, P_n^k) + p(3, P_n^k)$ is least when $k = 1$. From the proof of Corollary 2.3, $W(\mu(G^k)) + W(\overline{\mu(G^k)}) \leq W(\mu(T^k)) + W(\overline{\mu(T^k)})$ where T is a spanning tree of G. Hence, for $n \geq 3$, we have $W(\mu(G^k)) + W(\overline{\mu(G^k)}) \leq W(\mu(P_n^k)) + W(\overline{\mu(P_n^k)}) \leq W(\mu(P_n)) + W(\overline{\mu(P_n)}) = 8n^2 - 8n + 15$. $W(\mu(G)) + W(\overline{\mu(G})$ is minimum for graphs with diameter at most two and for these graphs $W(\mu(G)) + W(\overline{\mu(G)}) = 8n^2 + n - 4\binom{n}{2} = 6n^2 + 3n$, and therefore, $6n^2 + 3n \leq W(\mu(G^k)) + W(\overline{\mu(G^k)}) \leq 8n^2 - 8n + 15$. Zhang and Wu [15] presented the NG type inequality for the Wiener number as given in Theorem 1.2. In our case, for Mycielski graphs $|V(\mu(G))| = 2n + 1$. Thus the corresponding inequality of Zhang and Wu [15] for graphs of order $2n + 1$ is given by $6n^2 + 3n \leq W(G) + W(\overline{G}) \leq \frac{8n^3+24n^2+22n}{6}$. We can easily see that our bound for $W(\mu(G^k)) + W(\overline{\mu(G^k)})$ is better than the bound of Zhang and Wu for $\mu(G^k)$ as $\frac{8n^3+24n^2+22n}{6} - (8n^2 - 8n + 15) > 0$, $n \geq 3$.

In a similar way, we might be tempted to obtain the NG type inequalities for the following sums:

(i) $W(\mu(G)^k) + W(\overline{\mu(G)^k})$,

(ii) $W(\mu(G)^k) + W(\overline{\mu(G)}^k)$,

(iii) $W(\mu(G^k)) + W(\mu(\overline{G^k}))$,

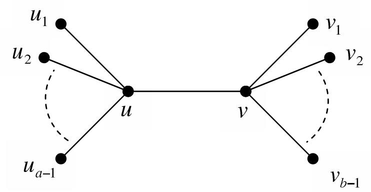
(iv) $W(\mu(G^k)) + W(\mu(\overline{G}^k))$.

Of these four, (i), (ii) and (iii) are uninteresting as $\overline{G^k}$ is disconnected in most of the choices for G while $\overline{\mu(G)^k}$ $(k \geq 2)$ is always disconnected (as u becomes a universal vertex in $(\mu(G))^k$) and diameter of $\mu(G)$ and $\overline{\mu(G)}$ are 4 and 2 respectively. Thus NG type inequality seems interesting only for (iv). For this, we need the following lemma due to Zhang and Wu [15].

Lemma 3.2. *Let G be a connected graph with connected complement. Then*

(1) *if $diam(G) > 3$, then $diam(\overline{G}) = 2$,*

(2) *if $diam(G) = 3$, then $\overline{G}$ has a spanning subgraph which is a double star (see Figure 3.1).*



$S_{a,b}$

Figure 3.1

Let G be a graph of order $n \geq 5$ with connected complement $\overline{G}$. If $diam(\overline{G})$ $= 2$, we can observe the following.

(i) $p(2, \overline{G}) = p(1, G)$.

(ii) $W(\mu(\overline{G})) = 6n^2 - n - 7\left(\binom{n}{2} - p(2, \overline{G})\right) - 4p(2, \overline{G}) = \frac{5}{2}n^2 + \frac{5}{2}n + 3p(1, G)$.

(iii) $W(\mu(G)) + W(\mu(\overline{G})) = \frac{17}{2}n^2 + \frac{3}{2}n - 4p(1, G) - 4p(2, G) - p(3, G)$. (3.1)

For $k \geq 2$, $\overline{G}^k = \overline{P_n}^k = K_n$ which implies that $\mu(\overline{G}^k) = \mu(\overline{P_n}^k)$. Therefore, by virtue of Corollary 2.3, we get that $W(\mu(G^k)) + W(\mu(\overline{G}^k) \leq W(\mu(P_n^k)) +$

$W(\mu(\overline{P_n}^k))$ for $k \geq 2$. The above inequality also holds for $k = 1$. This could be seen by arguments similar to those given in the proof of Theorem 2.2 and Corollary 2.3. Thus we have,

Theorem 3.3. *Let G be a connected graph of order $n \geq 5$ with connected complement $\overline{G}$. If $diam(\overline{G}) = 2$, then $W(\mu(G^k)) + W(\mu(\overline{G}^k)) \leq W(\mu(P_n^k)) + W(\mu(\overline{P_n}^k))$.*

Lemma 3.4. *Let G be a connected graph of order $n \geq 5$ with connected complement $\overline{G}$. Then $W(\mu(G^2)) + W(\mu(\overline{G}^2)) \leq W(\mu(P_n^2)) + W(\mu(\overline{P_n}^2))$.*

Proof. As $diam(\overline{P_n} = 2)$, by using Theorem 2.1,

$$\begin{aligned} W(\mu(\overline{P_n}^2)) &= 6n^2 - n - 7p(1, \overline{P_n}^2) \\ &= 6n^2 - n - 7\tbinom{n}{2} = \tfrac{5}{2}n^2 + \tfrac{5}{2}n. \\ \text{For } n = 5,\ W(\mu(P_5^2)) &= 6.25 - 5 - 7(4+3) - 4(2+1) = 84. \\ \text{For } n \geq 6,\ W(\mu(P_n^2)) &= 6n^2 - n - 7p(1, P_n^2) - 4p(2, P_n^2) - p(3, P_n^2) \\ &= 6n^2 - n - 14n + 21 - 8n + 28 - 2n + 11 \\ &= 6n^2 - 25n + 60. \end{aligned}$$

Hence, $W(\mu(P_5^2)) + W(\mu(\overline{P_5}^2)) = 159$, and

$$W(\mu(P_n^2)) + W(\mu(\overline{P_n}^2)) = \frac{17}{2}n^2 - \frac{45}{2}n + 60, \text{for } n \geq 6. \tag{3.2}$$

By virtue of Theorem 3.3, it is enough to consider the case when, $diam(G) = diam(\overline{G}) = 3$. For these G and $\overline{G}$, $p(1, G) = p(2, \overline{G}) + p(3, \overline{G})$, $p(1, \overline{G}) = p(2, G) + p(3, G)$ and $p(1, G) + p(1, \overline{G}) = \binom{n}{2}$. Now by Theorem 2.1,

$$\begin{aligned} W(\mu(G^2)) &= 6n^2 - n - 7p(1, G^2) - 4p(2, G^2) \\ &= 6n^2 - n - 7(p(1, G) + p(2, G)) - 4p(3, G) \\ &= 6n^2 - n - 7p(1, G) - 7(p(1, \overline{G}) - p(3, G)) - 4p(3, G) \\ &= 6n^2 - n - 7\tbinom{n}{2} + 3p(3, G). \end{aligned}$$

Thus, $W(\mu(G^2)) + W(\mu(\overline{G}^2)) = 12n^2 - 2n - 7n^2 + 7n + 3(p(3,G) + p(3,\overline{G}))$,

$$W(\mu(G^2)) + W(\mu(\overline{G}^2)) = 5n^2 + 5n + 3(p(3,G) + p(3,\overline{G})). \tag{3.3}$$

As $diam(G) = diam(\overline{G}) = 3$, by Lemma 3.2 each of G and $\overline{G}$ contains a double star, say, S_{a_1,b_1} and S_{a_2,b_2} (see Figure 3.1) as spanning subgraphs of G and $\overline{G}$ respectively. Hence $p(3,G) \le (a_1 - 1)(b_1 - 1) = a_1b_1 - n + 1$ and $p(3,\overline{G}) \le (a_2 - 1)(b_2 - 1) = a_2b_2 - n + 1$. Also, $a_ib_i \le \lfloor \frac{n^2}{4} \rfloor$ for $i = 1, 2$. Thus,

$$W(\mu(G^2)) + W(\mu(\overline{G}^2)) \le 5n^2 - n + 6\lfloor \frac{n^2}{4} \rfloor + 6. \tag{3.4}$$

It can be seen that $5n^2 - n + 6\lfloor \frac{n^2}{4} \rfloor + 6 < \frac{17}{2}n^2 - \frac{45}{2}n + 60$, for $n \ge 7$. We now consider the remaining cases, namely 5 and 6 separately.

Case (i). $n = 5$.
When $n = 5$, by equations (3.2) and (3.3), $W(\mu(G^2)) + W(\mu(\overline{G}^2)) = 125 + 25 + 3(p(3,G) + p(3,\overline{G})) \le 162$ and we have already seen that, $W(\mu(P_5^2)) + W(\mu(\overline{P_5}^2)) = 159$. We show that $W(\mu(G^2)) + W(\mu(\overline{G}^2)) \le 159$. Suppose $W(\mu(G^2)) + W(\mu(\overline{G}^2)) = 160$, then $p(3,G) + p(3,\overline{G}) = \frac{10}{3}$, which is a contradiction. Similarly, we will have a contradiction when $W(\mu(G^2)) + W(\mu(\overline{G}^2)) = 161$. Finally, if $W(\mu(G^2)) + W(\mu(\overline{G}^2)) = 162$; then, $p(3,G) + p(3,\overline{G}) = \frac{12}{3} = 4$. Since $n = 5$ and $diam(G) = diam(\overline{G}) = 3$, $p(3,G)$ and $p(3,\overline{G})$ cannot be greater than 2 and therefore $p(3,G) = p(3,\overline{G}) = 2$. There are only two graphs G of order 5 (see Figure 3.2) with the property that $n = 5$, $p(3,G) = 2$. But for these two graphs $p(3,\overline{G}) = 0$ which is a contradiction.

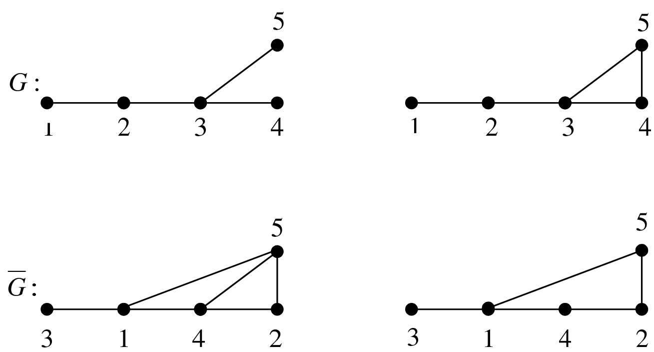


Fig 3.2

Case (ii). $n = 6$.
Here $W(\mu(G^2)) + W(\mu(\overline{G}^2)) = 210 + 3(p(3,G) + p(3,\overline{G})) \leq 234$ and $W(\mu(P_5^2)) + W(\mu(\overline{P_5}^2)) = 231$. Proving $W(\mu(G^2)) + W(\mu(\overline{G}^2)) \leq 231$ is similar to case(i). In this case the graphs with the required property are as shown in Figure 3.3.

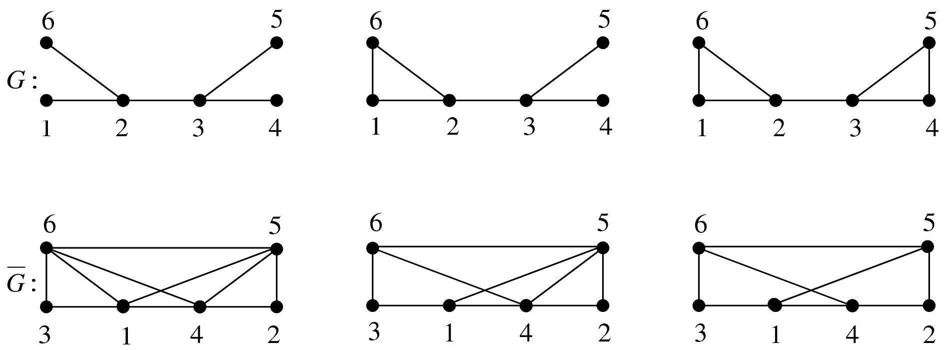


Fig 3.3

■

We now give the result for a general k.

Theorem 3.5. *Let G be a connected graph of order $n \geq 5$ with connected complement $\overline{G}$. Then for any $k \geq 1$, $5n^2 + 5n \leq W(\mu(G^k)) + W(\mu(\overline{G}^k)) \leq W(\mu(P_n^k)) + W(\mu(\overline{P_n}^k)) \leq W(\mu(P_n)) + W(\mu(\overline{P_n})) = \frac{17}{2}n^2 - \frac{15}{2}n + 15$.*

Proof. $W(\mu(G^k)) + W(\mu(\overline{G}^k))$ is minimum when G^k and $\overline{G}^k$ are complete. Thus $5n^2 + 5n \leq W(\mu(G^k)) + W(\mu(\overline{G}^k))$. By equation 3.1 and arguments similar to that in Theorem 2.2, $W(\mu(G)) + W(\mu(\overline{G})) \leq W(\mu(P_n)) + W(\mu(\overline{P_n}))$. By virtue of Theorem 3.3 and Lemma 3.4, the only case left out for the upper bound to be true is when $diam(G) = diam(\overline{G}) = 3$ and $k \geq 3$. In this case, $G^k = \overline{G}^k = K_n$ and we see that $W(\mu(G^k))$ is minimum for $G^k = K_n$ and therefore $W(\mu(G^k)) + W(\mu(\overline{G}^k)) \leq W(\mu(P_n^k)) + W(\mu(\overline{P_n}^k)) \leq W(\mu(P_n)) + W(\mu(\overline{P_n})) = \frac{17}{2}n^2 - \frac{15}{2}n + 15$ (by using equation 3.1). ■

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