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The structure of graphs with extremal hyper-Wiener index

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Abstract. The hyper-Wiener index of a graph G is defined as $WW(G) = \frac{1}{2}\sum\limits_{\{u,v\}\subseteq V(G)}(d_G^2(u,v) + d_G(u,v))$, where $d_G(u,v)$ denotes the distance between u and v in G. In this paper, we determine the maximum hyper-Wiener index of 2-connected graphs and 2-edge-connected graphs, which extends the result of Plesnik [On the sum of all distances in a graph or digraph, J. Graph Theory 8 (1984) 1-21]. Then based on the above results, we characterize the first two maximum graphs among the graphs with two vertices of odd degree, the minimum graphs among the graphs with $2k$ $(0 \leq k \leq \lfloor \frac{n}{2} \rfloor)$ vertices of odd degree, which extends the result of Hou, Chen and Zhang [Hyper-Wiener index of Eulerian graphs, Appl. Math. J. Chin. Univ. 31 (2016) 248-252].

1. Introduction

The Wiener index is one of the oldest and most studied topological index from application and theoretical viewpoints. As an extension of the Wiener index, the hyper-Wiener index is also an important topological index.

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of vertex u in graph G, denoted by $d_G(u)$, is the number of edges incident to u. A pendent vertex is a vertex with degree one. If a path $v_1v_2\cdots v_k$ is an induced sub-path of G with $d_G(v_1) \geq 3$, $d_G(v_2) = d_G(v_3) = \cdots = d_G(v_{k-1}) = 2$ and $d_G(v_k) = 1$, then we call $v_1v_2\cdots v_k$ is a pendent path of G.

The distance $d_G(u,v)$ between vertices u and v is the length of the shortest path between vertices u and v in G. Let $ecc_G(u) = \max\{d_G(u,v)|v \in V(G)\}$ be the eccentricity of vertex u in G. The Wiener index of a graph G is defined as [31]

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

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and the hyper-Wiener index of G is defined as [16, 26]

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (d_G^2(u,v) + d_G(u,v)).$$

One can refer to [1, 3–6, 8, 10–14, 17, 20, 21, 24, 25, 28, 30, 33, 34] for the mathematical properties of the hyper-Wiener index and its applications in chemistry.

Let $D_G(u) = \sum\limits_{v \in V(G)} d_G(u,v)$ and $DD_G(u) = \sum\limits_{v \in V(G)} d_G^2(u,v)$. Then hyper-Wiener index can also be written as $WW(G) = \frac{1}{4} \sum\limits_{u \in V(G)} (DD_G(u) + D_G(u))$.

We call a vertex u of a connected graph G with at least three vertices the cut-vertex if $G-u$ is disconnected. A block of a graph G is the maximal connected subgraph of G that has no cut-vertex [2]. An endblock of a graph G is a block of G that contains only one cut-vertex of G. If v is a cut-vertex of G and H is a component of $G - v$, then $G[V(H) \cup \{v\}]$ is called a branch of G at v. A graph is called k-vertex-connected (k-connected for short) if the graph is still connected whenever fewer than k vertices are removed. Similarly, a graph is called k-edge-connected if the graph is still connected whenever fewer than k edges are removed.

Let $\mathcal{G}(n, 2k)$ be the set of the connected graphs with n vertices and $2k$ vertices of odd degree. If $k = 0$, then $\mathcal{G}(n, 0)$ denotes the set of Eulerian graphs with n vertices. The research of extremal graph with given the number of vertices of even/odd degree can be found in [7, 18, 19, 22, 27, 29]. We use $|U|$ to denote the cardinality of the set U. We denote C_n, P_n, and K_n, the cycle, path, and complete graph of order n, respectively. In this paper, all notations and terminologies used but not defined can refer to Bondy and Murty [2].

The remainder of this paper is organized as follows. In Section 2, we determine the maximum hyper-Wiener index among 2-connected graphs and 2-edge-connected graphs. In Section 3, we determine the first two maximum graphs among $\mathcal{G}(n, 2)$ with respect to the hyper-Wiener index, and in Section 4, we determine the minimum graphs among $\mathcal{G}(n, 2k)$ for $0 \le k \le \lfloor \frac{n}{2} \rfloor$. In Section 5, we conclude this paper and propose an open problem.

2. The maximum values of 2-(edge)-connected graphs

In this section, we give some sharp upper bounds about the hyper-Wiener index among 2-connected graphs and 2-edge-connected graphs. Firstly, we give a sharp upper bound for $DD_G(v)$, where G is a 2-connected graph.

Lemma 2.1. [23] *Let G be a 2-connected graph with $|V(G)| = n$. For any vertex $v \in V(G)$, we have $D_G(v) \le \lfloor \frac{1}{4} n^2 \rfloor$. Moreover, the equality holds for all vertices of G if and only if $G \cong C_n$.*

Lemma 2.2. *Let G be a 2-connected graph with $|V(G)| = n$. Suppose that $v \in V(G)$, $ecc_G(v) = k$ and $W_i = \{x | d(v,x) = i\}$, $w_i = |W_i|$ for $0 \le i \le k$. Then*
(1) $w_i \ge 2$ for $1 \le i \le k-1$;
(2) $k \le \lfloor \frac{n}{2} \rfloor$.

Proof. On the contrary, we suppose that there exists $1 \le i \le k-1$ such that $w_i = 1$. All paths from any $v (\in W_0)$ to any $x \in W_j$ for $i+1 \le j \le k$ must through some vertex $y_i \in W_i$. Then the unique vertex in W_i is a cut vertex, which is a contradiction since G is a 2-connected graph.

By $w_0 = 1$, $w_k \ge 1$, and the result of (1), we have $n = \sum\limits_{i=0}^{k} w_i \ge 1 + 2(k-1) + 1 = 2k$, thus $k \le \lfloor \frac{n}{2} \rfloor$. □

Lemma 2.3. *Let G be a 2-connected graph with $|V(G)| = n$. For any vertex $v \in V(G)$, we have*

$$DD_G(v) \le \begin{cases} \frac{1}{12} n(n^2+2), & if\ n \text{ is even;} \\ \frac{1}{12} n(n^2-1), & if\ n \text{ is odd.} \end{cases}$$

Moreover, the equalities hold for all vertices of G if and only if $G \cong C_n$.

Proof. Let $v \in V(G)$, $ecc_G(v) = k$ and $W_i = \{x|d(v,x) = i\}$, $w_i = |W_i|$ for $0 \le i \le k$. Clearly, $w_0 = 1$, $w_k \ge 1$, and by Lemma 2.2, we have $w_i \ge 2$ for $1 \le i \le k-1$ and $k \le \lfloor \frac{n}{2} \rfloor$. Since $\sum_{i=0}^{k} w_i = n$ and $DD_G(v) = 1^2w_1 + 2^2w_2 + \cdots + k^2w_k$, we have

$$\begin{aligned} DD_G(v) &= 1^2w_1 + 2^2w_2 + \cdots + k^2w_k \\ &\le (1^2 + 2^2 + \cdots + (k-1)^2) \times 2 + k^2(n - 1 - 2(k-1)) \\ &= \frac{1}{3}k(k-1)(2k-1) + k^2(n - 2k + 1) \\ &\triangleq \xi_k. \end{aligned}$$

Therefore $\xi'_k = -4k^2 + 2kn + \frac{1}{3} > 0$ for $k \le \lfloor \frac{n}{2} \rfloor$. Thus

$$DD_G(v) \le \begin{cases} \xi_{\frac{n}{2}} = \frac{1}{12}n(n^2+2), \ if\ n\ is\ even; \\ \xi_{\frac{n-1}{2}} = \frac{1}{12}n(n^2-1), \ if\ n\ is\ odd. \end{cases}$$

If the equality holds, then $d(v) = 2$ for any vertex $v \in V(G)$. Thus these upper bounds are achieved for all $v \in V(G)$ if and only if $G \cong C_n$. □

Lemma 2.4. [23] *Let G be a 2-connected graph with $|V(G)| = n$. Then $W(G) \le \frac{1}{2}n\lfloor \frac{1}{4}n^2 \rfloor$, with equality if and only if $G \cong C_n$.*

By Lemmas 2.1 and 2.3, we have

Lemma 2.5. *Let G be a 2-connected graph with $|V(G)| = n$. Then*

$$WW(G) \le \begin{cases} \frac{1}{48}n^2(n+1)(n+2), \ if\ n\ is\ even; \\ \frac{1}{48}n(n+1)(n-1)(n+3), \ if\ n\ is\ odd, \end{cases}$$

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

For 2-edge-connected graph G, the following results are useful.

Lemma 2.6. [23] *Let G be a 2-edge-connected graph with $|V(G)| = n$. For any vertex $v \in V(G)$, we have $ecc_G(v) \le \lfloor \frac{1}{3}(2n-2) \rfloor$, and the equality can be achieved.*

Lemma 2.7. [23] *Let G be a 2-edge-connected graph with $|V(G)| = n$. For any vertex $v \in V(G)$, we have $D_G(v) \le \lfloor \frac{1}{3}(n^2 - n) \rfloor$, and the equality can be achieved.*

Theorem 2.8. *Let G be a 2-edge-connected graph with $|V(G)| = n$. For any vertex $v \in V(G)$, we have $DD_G(v) \le \frac{2}{27}(n-1)^2(2n+1)$, and the equality can be achieved.*

Proof. Suppose that G is a 2-edge-connected graph and we make a mathematical induction on the number of blocks.

Case 1. G is a block.

Since G is a block, G is a 2-connected graph. By Lemma 2.3, if n is even, then $DD_G(v) \le \frac{1}{12}n(n^2+2) \le \frac{2}{27}(n-1)^2(2n+1)$ for $n \ge 4$; if n is odd, then $DD_G(v) \le \frac{1}{12}n(n^2-1) \le \frac{2}{27}(n-1)^2(2n+1)$ for $n \ge 3$.

Case 2. G has at least two blocks.

Let G_1 be an endblock of G, G_2 be the union of other blocks such that $V(G_1) \cap V(G_2) = \{u\}$. For convenience, we let $V_i = V(G_i)$, $n_i = |V_i|$ for $i = 1, 2$. Then $n_1 + n_2 - 1 = n$.

Subcase 2.1. $v \in V(G_1)$.

By the definition of $DD_G(v)$, Lemmas 2.3, 2.6, 2.7 and the induction hypothesis, we have

$$\begin{aligned}
DD_G(v) &= \sum_{x\in V_1} d_G^2(v,x) + \sum_{x\in V_2\setminus\{u\}} d_G^2(v,x) \\
&= \sum_{x\in V_1} d_G^2(v,x) + \sum_{x\in V_2\setminus\{u\}} (d_G(v,u)+d_G(u,x))^2 \\
&= DD_{G_1}(v) + \sum_{x\in V_2\setminus\{u\}} d_G^2(v,u) + \sum_{x\in V_2\setminus\{u\}} d_G^2(u,x) + 2\sum_{x\in V_2\setminus\{u\}} d_G(v,u)\cdot d_G(u,x) \\
&\le DD_{G_1}(v) + (n_2-1)(ecc_{G_1}(v))^2 + DD_{G_2}(u) + 2ecc_{G_1}(v)\cdot D_{G_2}(u) \\
&\le \frac{1}{12}n_1(n_1^2+2) + (n_2-1)\left(\frac{1}{3}(2n_1-2)\right)^2 + \frac{2}{27}(n_2-1)^2(2n_2+1) \\
&\quad +2\left(\frac{1}{3}(2n_1-2)\right)\left(\frac{1}{3}(n_2^2-n_2)\right) \\
&= \frac{1}{12}n_1(n_1^2+2) + \frac{4}{9}(n-n_1)(n_1-1)^2 + \frac{2}{27}(n-n_1)^2(2n-2n_1+3) \\
&\quad +\frac{4}{9}(n_1-1)(n-n_1)(n-n_1+1).
\end{aligned}$$

If $n_1 \ge 4$, we have $\frac{2}{27}(n-1)^2(2n+1) - DD_G(v) \ge \frac{7}{108}n_1^3 - \frac{2}{9}n_1^2 - \frac{1}{6}n_1 + \frac{2}{27} \ge 0$.
If $n_1 = 3$, then $DD_{G_1}(v) \le \frac{1}{12}n_1(n_1^2-1) = 2$, we can similarly prove that $\frac{2}{27}(n-1)^2(2n+1) - DD_G(v) > 0$.
Subcase 2.2. $v \in V(G_2)$.
By the definition of $DD_G(v)$, Lemmas 2.3, 2.6, 2.7 and the induction hypothesis, we have

$$\begin{aligned}
DD_G(v) &= \sum_{x\in V_2} d_G^2(v,x) + \sum_{x\in V_1\setminus\{u\}} d_G^2(v,x) \\
&= \sum_{x\in V_2} d_G^2(v,x) + \sum_{x\in V_1\setminus\{u\}} (d_G(v,u)+d_G(u,x))^2 \\
&= DD_{G_2}(v) + \sum_{x\in V_1\setminus\{u\}} d_G^2(v,u) + \sum_{x\in V_1\setminus\{u\}} d_G^2(u,x) + 2\sum_{x\in V_1\setminus\{u\}} d_G(v,u)\cdot d_G(u,x) \\
&\le DD_{G_2}(v) + (n_1-1)(ecc_{G_2}(v))^2 + DD_{G_1}(u) + 2ecc_{G_2}(v)\cdot D_{G_1}(u) \\
&\le \frac{2}{27}(n_2-1)^2(2n_2+1) + (n_1-1)\left(\frac{1}{3}(2n_2-2)\right)^2 + \frac{1}{12}n_1(n_1^2+2) \\
&\quad +2\left(\frac{1}{3}(2n_2-2)\right)\left(\frac{1}{3}(n_1^2-n_1)\right) \\
&= \frac{2}{27}(n-n_1)^2(2n-2n_1+3) + \frac{4}{9}(n_1-1)(n-n_1)^2 + \frac{1}{12}n_1(n_1^2+2) \\
&\quad +\frac{4}{9}(n-n_1)(n_1^2-n_1).
\end{aligned}$$

If $n_1 \ge 4$, we have $\frac{2}{27}(n-1)^2(2n+1) - DD_G(v) \ge \frac{7}{108}n_1^3 - \frac{2}{9}n_1^2 - \frac{1}{6}n_1 + \frac{2}{27} \ge 0$.
If $n_1 = 3$, then $DD_{G_1}(u) \le \frac{1}{12}n_1(n_1^2-1) = 2$, we can similarly prove that $\frac{2}{27}(n-1)^2(2n+1) - DD_G(v) > 0$.
Combining the above arguments, we complete the proof. □

Theorem 2.9. *Let G be a 2-edge-connected graph with $|V(G)| = n$. Then*

$$WW(G) \le \begin{cases} \frac{1}{48}n^2(n+1)(n+2), & if\ n\ is\ even; \\ \frac{1}{48}n(n+1)(n-1)(n+3), & if\ n\ is\ odd, \end{cases}$$

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

Proof. We can verify the conclusion directly for $n \le 5$. Next we only consider $n \ge 6$. We make a mathematical induction on the number of blocks.

Case 1. G is a block.

Since G is a block, then G is a 2-connected graph. By Lemma 2.5, the conclusion holds.

Case 2. G has at least two blocks.

Let G_1 be an endblock of G, G_2 be the union of other blocks such that $V(G_1) \cap V(G_2) = \{u\}$. For convenience, we let $V_i = V(G_i)$, $n_i = |V_i|$ for $i = 1, 2$. Then $n_1 + n_2 - 1 = n$. We choose the G_1 such that $n_1 \le \frac{1}{2}(n+1)$. For convenience, we let $\phi(x, y) = d_G(x, y) + d_G^2(x, y)$.

Subcase 2.1. n_1 is even.

By the definition of $DD_G(v)$, $WW(G)$, Lemmas 2.1, 2.3, 2.5, 2.7, Theorem 2.8 and the induction hypothesis, we have $WW(G_1) \le \frac{n_1^2}{48}(n_1+1)(n_1+2)$ and

$$\begin{aligned}
2WW(G) &= \sum_{\substack{x\in V_1\\ y\in V_1}} \phi(x,y) + \sum_{\substack{x\in V_2\\ y\in V_2}} \phi(x,y) + \sum_{\substack{x\in V_1\setminus\{u\}\\ y\in V_2\setminus\{u\}}} \phi(x,y)\\
&= 2WW(G_1) + 2WW(G_2) + \sum_{x\in V_1\setminus\{u\}} \sum_{y\in V_2\setminus\{u\}} \phi(x,y)\\
&= 2WW(G_1) + 2WW(G_2) + \sum_{x\in V_1\setminus\{u\}} ((n_2-1)\phi(x,u) + D_{G_2}(u) + DD_{G_2}(u)\\
&\quad +2d(x,u)\cdot D_{G_2}(u))\\
&= 2WW(G_1) + 2WW(G_2) + (n_2-1)(D_{G_1}(u) + DD_{G_1}(u))\\
&\quad +(n_1-1)(D_{G_2}(u) + DD_{G_2}(u)) + 2D_{G_1}(u)\cdot D_{G_2}(u)\\
&\le \frac{n_1^2}{24}(n_1+1)(n_1+2) + \frac{n_2^2}{24}(n_2+1)(n_2+2) + (n_2-1)(\frac{n_1^2}{4} + \frac{n_1}{12}(n_1^2+2))\\
&\quad +(n_1-1)(\frac{1}{3}(n_2^2-n_2) + \frac{2}{27}(n_2-1)^2(2n_2+1)) + 2\cdot\frac{1}{4}n_1^2\cdot\frac{1}{3}(n_2^2-n_2)\\
&= \frac{n_1^2}{24}(n_1+1)(n_1+2) + \frac{1}{24}(n-n_1+1)^2(n-n_1+2)(n-n_1+3)\\
&\quad +(n-n_1)(\frac{1}{4}n_1^2 + \frac{1}{12}n_1(n_1^2+2)) + \frac{1}{3}(n_1-1)(n-n_1)(n-n_1+1)\\
&\quad +\frac{2}{27}(n-n_1)^2(n_1-1)(2n-2n_1+3) + \frac{1}{6}n_1^2(n-n_1)(n-n_1+1).
\end{aligned}$$

Thus $2WW(C_n) - 2WW(G) \ge \frac{1}{24}n(n+1)(n-1)(n+3) - 2WW(G) \ge \frac{1}{54}n^3n_1 - \frac{1}{54}n^3 + \frac{1}{36}n^2n_1^2 - \frac{1}{8}n^2n_1 - \frac{7}{36}n^2 - \frac{1}{36}nn_1^3 + \frac{19}{72}nn_1^2 - \frac{7}{36}nn_1 - \frac{1}{2}n - \frac{1}{54}n_1^4 - \frac{13}{108}n_1^3 + \frac{19}{72}n_1^2 + \frac{3}{8}n_1 - \frac{1}{4} \triangleq f_{n_1}$.

Clearly, we have $f'_{n_1} = \frac{1}{216}(4n^3 + 3n^2(4n_1-9) - 6n(3n_1^2 - 19n_1 + 7) - 16n_1^3 - 78n_1^2 + 114n_1 + 81)$, and $f''_{n_1} = \frac{1}{216}(12n^2 - 36nn_1 + 114n - 48n_1^2 - 156n_1 + 114)$.

Since $4 \le n_1 \le \frac{n+1}{2}$, and the two roots of $f''_{n_1} = 0$ are $x_1 = \frac{1}{8}(\sqrt{25n^2+230n+321} - 3n - 13)$ and $x_2 = \frac{1}{8}(-\sqrt{25n^2+230n+321} - 3n - 13)$, then $f'_{n_1} \ge \min\{f'_4, f'_{\frac{n+1}{2}}\} > 0$. Thus $f_{n_1} \ge f_4 = \frac{1}{18}n^3 - \frac{1}{4}n^2 + \frac{7}{6}n - \frac{251}{36} > 0$ for $n \ge 6$.

Subcase 2.2. n_1 is odd.

Since $WW(G_1) \le \frac{1}{48}n_1(n_1+1)(n_1-1)(n_1+3)$, similarly we have $2WW(C_n) - 2WW(G) \ge \frac{1}{24}n(n+1)(n-1)(n+3) - 2WW(G) \ge \frac{1}{54}n^3n_1 - \frac{1}{54}n^3 + \frac{1}{36}n^2n_1^2 - \frac{1}{8}n^2n_1 - \frac{7}{36}n^2 - \frac{1}{36}nn_1^3 + \frac{19}{72}nn_1^2 - \frac{7}{36}nn_1 - \frac{1}{2}n - \frac{1}{54}n_1^4 - \frac{13}{108}n_1^3 + \frac{7}{18}n_1^2 + \frac{1}{2}n_1 - \frac{1}{4} \triangleq g_{n_1}$.

Clearly, we have $g'_{n_1} = \frac{1}{216}(4n^3 + 3n^2(4n_1-9) - 6n(3n_1^2 - 19n_1 + 7) - 16n_1^3 - 78n_1^2 + 168n_1 + 108)$, and $g''_{n_1} = \frac{1}{216}(12n^2 - 36nn_1 + 114n - 48n_1^2 - 156n_1 + 168)$.

Since $3 \le n_1 \le \frac{n+1}{2}$, and the two roots of $g''_{n_1} = 0$ are $x_1 = \frac{1}{8}(\sqrt{25n^2+230n+393} - 3n - 13)$ and $x_2 = \frac{1}{8}(-\sqrt{25n^2+230n+393} - 3n - 13)$, then $g'_{n_1} \ge \min\{g'_3, g'_{\frac{n+1}{2}}\} > 0$. Thus $g_{n_1} \ge f_3 = \frac{1}{27}n^3 - \frac{23}{72}n^2 + \frac{13}{24}n > 0$ for $n \ge 7$.

If $n = 6$, in this case, $n_1 = 3$. It is easy to calculate the hyper-Wiener index of these graphs are less than the hyper-Wiener index of C_6.

Combining the above arguments, we complete the proof. □

It is clear that the results of Lemmas 2.3, 2.5 and Theorems 2.8, 2.9 generalize the results of [23] about the Wiener index.

3. The maximum graphs with given number of vertices of odd degree

Recall that $\mathcal{G}(n, 2k)$ denotes the set of the connected graphs with n vertices and $2k$ vertices of odd degree. For $k = 0$, Hou et al. [15] determined the maximum graphs among $\mathcal{G}(n, 0)$ (i.e. Eulerian graph) with respect to the hyper-Wiener index is C_n. For the continue, we consider the situation of $k = 1$, and we determine the first two maximum graphs among $\mathcal{G}(n, 2)$ with respect to the hyper-Wiener index.

Lemma 3.1. [15] *Let G and $G - uv$ be connected graphs where $uv \in E(G)$, then $WW(G) < WW(G - uv)$.*

Lemma 3.2. [12] *If T is a tree of order n, then $WW(S_n) \leq WW(T) \leq WW(P_n)$.*

By Lemmas 3.1 and 3.2, we know P_n has the maximum hyper-Wiener index among connected graphs with n vertices. Since $P_n \in \mathcal{G}(n, 2)$, we have the following result.

Proposition 3.3. *Let $G \in \mathcal{G}(n, 2)$. Then $WW(G) \leq WW(P_n) = \frac{1}{24}n(n-1)(n+1)(n+2)$, with equality if and only if $G \cong P_n$.*

Let $H_{n,a}$ be the graph of order n obtained from C_a and P_{n-a} by adding one edge between one vertex of C_a and one pendent vertex of P_{n-a}.

Lemma 3.4. (Lemma 2.4 of[9]) *Let $a \geq 4$, F be a connected graph with $|V(F)| \geq 2$. Suppose G_1 is the graph obtained from F and C_a by identifying a vertex $v(\in V(F))$ and one vertex of C_a; G_2 is the graph obtained from F and $H_{a,3}$ by identifying the same vertex $v(\in V(F))$ and the pendent vertex of $H_{a,3}$. Then we have $WW(G_1) < WW(G_2)$.*

Lemma 3.5. *Let $3 \leq a \leq n-1$. Then $WW(H_{n,a}) \leq WW(H_{n,3}) = \frac{1}{24}(n^4 + 2n^3 - 13n^2 + 10n + 24)$, with equality if and only if $a = 3$.*

Proof. Let $F = P_{n-a+1}$ and v be a pendent vertex of F. By Lemma 3.4, we have $WW(H_{n,a}) \leq WW(H_{n,3}) = \frac{1}{24}(n^4 + 2n^3 - 13n^2 + 10n + 24)$, with equality if and only if $a = 3$. □

Lemma 3.6. [27] *Let G be a connected graph with $|V(G)| = n$, $v \in V(G)$ and $d_G(v) = t$. Then $D_G(v) \leq \frac{1}{2}(n-2)(n-3) + 2$ for $3 \leq t \leq n-1$.*

Lemma 3.7. *Let G be a connected graph with $|V(G)| = n$, $v \in V(G)$ and $d_G(v) = t$. Then $DD_G(v) \leq \frac{1}{6}(n-3)(n-2)(2n-5) + 2$ for $3 \leq t \leq n-1$.*

Proof. If $d_G(v) = t$, then $DD_G(v) \leq 1^2 \times t + 2^2 + 3^2 + \cdots + (n-t)^2 = \frac{1}{6}(n-t)(n-t+1)(2n-2t+1) + t - 1 \leq \frac{1}{6}(n-3)(n-2)(2n-5) + 2$ for $3 \leq t \leq n-1$. □

Similar to the proof of Lemmas 3.6 and 3.7 and $1 \leq d_G(v) \leq n-1$, we have

Lemma 3.8. *Let G be a connected graph with $|V(G)| = n$ and $v \in V(G)$. Then $D_G(v) \leq \frac{1}{2}n(n-1)$, $DD_G(v) \leq \frac{1}{6}n(n-1)(2n-1)$, with equality if and only if $G \cong P_n$ and v is a terminal vertex.*

Lemma 3.9. (Lemma 2.3 of[9]) *Let G be a connected graph with a cut-vertex v such that G_1 and G_2 are two connected subgraphs of G having v as the only common vertex and $G_1 \cup G_2 = G$. Let $n_i = |V(G_i)|$ for $i = 1, 2$. Then*

$$\begin{aligned} WW(G) &= WW(G_1) + WW(G_2) + \frac{1}{2}(n_1 - 1)(D_{G_2}(v) + DD_{G_2}(v)) \\ &\quad + \frac{1}{2}(n_2 - 1)(D_{G_1}(v) + DD_{G_1}(v)) + D_{G_1}(v)D_{G_2}(v). \end{aligned}$$

Lemma 3.10. *Let G be a graph of order n with no isolated vertices. If G has exactly two vertices with odd degree and $G \ncong P_n$, then G contain at least one cycle.*

Proof. By Handshaking Lemma, we have $2m(G) = \sum_{v \in V(G)} d_G(v) \geq 1 + 1 + 2(n-2) = 2(n-1)$. Then $m \geq n-1$. If $m = n-1$, then the degree sequence of G is $1, 1, 2, 2, \cdots, 2$, it implies $G \cong P_n$, a contradiction. Thus $m \geq n$ and G contains at least one cycle. □

Lemma 3.11. *Let $G \in \mathcal{G}(n, 2)$, x, y be the unique two vertices of odd degree in G with $d_G(x) = 1$ and $d_G(y) \geq 3$. Then $WW(G) \leq WW(H_{n,3})$, with equality if and only if $G \cong H_{n,3}$.*

Proof. The assertion can be verified directly for $n = 4, 5$. We suppose the assertion holds for the graphs with the number of vertices less than n, then we prove the assertion holds for the graphs with the number of vertices equal to n.

Since x, y are the unique two vertices of odd degree of G with $d_G(x) = 1$ and $d_G(y) \geq 3$, then G has a pendent path P. Without loss of generality, we suppose $P = vx_1x_2 \cdots x_{b-2}x$ with $d_G(v) \geq 3$ and $d_G(x) = 1$. Let $P_1 = P \setminus \{v\}$, $K = G \setminus P_1$, $|V(K)| = a$. Then $a + b - 1 = n$.

By Lemma 3.9, we have

$$\begin{aligned} WW(G) &= WW(K) + WW(P) + \frac{1}{2}(a-1)(D_P(v) + DD_P(v)) \\ &\quad + \frac{1}{2}(b-1)(D_K(v) + DD_K(v)) + D_K(v)D_P(v). \end{aligned}$$

Let $H^*_{n,4}$ be the simple connected graph obtained from $H_{n,4}$ by adding an edge between one vertex of degree three and one vertex of degree two.

If $a = 3$ or 4, then G contains at least one cycle by Lemma 3.10. Thus $G \cong H_{n,3}$ if $a = 3$ and $G \in \{H_{n,4}, H^*_{n,4}\}$ if $a = 4$. By Lemmas 3.1 and 3.5, we have $WW(H^*_{n,4}) < WW(H_{n,4}) < WW(H_{n,3})$. Thus the conclusion holds.

Next, we consider the case of $5 \leq a \leq n-1$.

Case 1. There is no cut-edge in K.

In this case, K is a 2-edge-connected graph. By Lemma 2.7, Theorems 2.8 and 2.9, we have $WW(K) \leq \frac{1}{48}a^2(a+1)(a+2)$, $WW(P) = \frac{1}{24}b(b-1)(b+1)(b+2)$, $D_P(v) = \frac{1}{2}b(b-1)$, $DD_P(v) = \frac{1}{6}b(b-1)(2b-1)$, $D_K(v) \leq \frac{1}{3}a(a-1)$, $DD_K(v) \leq \frac{2}{27}(a-1)^2(2a+1)$. By $a + b - 1 = n$, we have

$$\begin{aligned} WW(G) &\leq \frac{1}{48}a^2(a+1)(a+2) + \frac{1}{24}b(b-1)(b+1)(b+2) + \frac{1}{6}b(a-1)(b-1)(b+1) \\ &\quad + \frac{1}{54}(b-1)(9a(a-1) + 2(a-1)^2(2a+1)) + \frac{1}{6}ab(a-1)(b-1) \\ &= \frac{1}{48}a^2(a+1)(a+2) + \frac{1}{24}(n-a)(n-a+1)(n-a+2)(n-a+3) \\ &\quad + \frac{1}{6}(a-1)(n-a)(n-a+1)(n+2) \\ &\quad + \frac{1}{54}(n-a)(9a(a-1) + 2(a-1)^2(2a+1)). \end{aligned} \tag{1}$$

Since $WW(H_{n,3}) = \frac{1}{24}(n^4 + 2n^3 - 13n^2 + 10n + 24)$, then

$$\begin{aligned} WW(H_{n,3}) - WW(G) &\geq \frac{n^2a^2}{12} - \frac{n^2a}{12} - \frac{n^2}{2} - \frac{2na^3}{27} + \frac{7na^2}{36} - \frac{na}{12} + \frac{25n}{54} \\ &\quad + \frac{5a^4}{432} - \frac{13a^3}{144} - \frac{5a}{108} + 1 \triangleq \varphi_a, \end{aligned}$$

and $\varphi'_a = \frac{1}{432}(36n^2(2a-1) - 12n(8a^2 - 14a + 3) + 20a^3 - 117a^2 - 20)$, $\varphi''_a = \frac{1}{432}(60a^2 - 192na - 234a + 72n^2 + 168n)$.

The two roots of $\varphi''_a = 0$ are $\theta_1 = \frac{1}{20}(-\sqrt{544n^2 + 1376n + 1521} + 32n + 39)$, $\theta_2 = \frac{1}{20}(\sqrt{544n^2 + 1376n + 1521} + 32n + 39)$ with $0 < \theta_1 < n-1 < \theta_2$.

If $n \geq 11$, then $5 \leq \theta_1 < n-1 < \theta_2$, and $\varphi''_5 > 0$, $\varphi''_{n-1} < 0$; if $6 \leq n \leq 10$, then $0 < \theta_1 < 5 < n-1 < \theta_2$ and $\varphi''_5 < 0$, $\varphi''_{n-1} < 0$. Thus if $n \geq 11$, then φ'_a is monotonically increasing in $[5, \theta_1]$ and monotonically decreasing in $[\theta_1, n-1]$. If $n \leq 10$, then φ'_a is monotonically decreasing in $[5, n-1]$.

Since the monotonicity of the function φ'_a and $\varphi'_5 > 0$ for $n \geq 6$, we know φ_a monotonically decreasing in $[5, n-1]$ or φ_a first monotonically increasing and then monotonically decreasing in $[5, n-1]$. Then $\varphi_a \geq \min\{\varphi_5, \varphi_{n-1}\}$ for $5 \leq a \leq n-1$. Since $\varphi_5 > 0$ and $\varphi_{n-1} > 0$ for $n \geq 5$, then $\varphi_a > 0$ for $5 \leq a \leq n-1$. Thus the conclusion holds.

Case 2. There exists at least one cut-edge in K.

In this case, v is not a vertex of odd degree of G. Without loss of generality, we let uw be a cut-edge which is the farthest from v and $d_G(u, v) > d_G(w, v)$. It is easy to know that another odd degree vertex except vertex x is in H, where H is the union of branches of $G \setminus \{uw\}$ containing u, then H is a 2-edge-connected graph.

Let $F = G \setminus (H \setminus \{u\})$ and $|V(H)| = p$, $|V(F)| = q$. Then $p + q - 1 = n$. By Lemma 3.9, we have

$$\begin{aligned} WW(G) = {} & WW(H) + WW(F) + \frac{1}{2}(p-1)(D_F(u) + DD_F(u)) \\ & + \frac{1}{2}(q-1)(D_H(u) + DD_H(u)) + D_F(u)D_H(u). \end{aligned} \tag{2}$$

We first prove the following claim.

Claim. $WW(F) < WW(H_{q,3})$.

Let $F = F_1 \cup P$ and $F_1 \cap P = \{v\}$. Then F_1 has exactly two vertices u and v with odd degree, and $d_{F_1}(u) = 1$, $d_{F_1}(v) \geq 3$. Let $|V(F_1)| = r$. Then $r + b - 1 = q$, and we have

$$\begin{aligned} WW(F) &= WW(F_1) + WW(P) + \frac{1}{2}(r-1)(D_P(v) + DD_P(v)) \\ &\quad + \frac{1}{2}(b-1)(D_{F_1}(v) + DD_{F_1}(v)) + D_{F_1}(v)D_P(v). \end{aligned}$$

Since P is a path with b vertices and v is the terminal vertex of P, then $WW(P) = \frac{1}{24}b(b-1)(b+1)(b+2)$, $D_P(v) = \frac{1}{2}b(b-1)$, $DD_P(v) = \frac{1}{6}b(b-1)(2b-1)$.

By Lemma 3.5 and the induction hypothesis, we have $WW(F_1) \leq WW(H_{r,3}) = \frac{1}{24}(r^4 + 2r^3 - 13r^2 + 10r + 24)$,

Since $d_{F_1}(v) \geq 3$, then by Lemmas 3.6 and 3.7, we have $D_{F_1}(v) \leq \frac{1}{2}(r-2)(r-3) + 2$, $DD_{F_1}(v) \leq \frac{1}{6}(r-2)(r-3)(2r-5) + 2$. Then by $b + r - 1 = q$, we have

$$\begin{aligned} WW(F) &\leq \frac{1}{24}(r^4 + 2r^3 - 13r^2 + 10r + 24) + \frac{1}{24}b(b-1)(b+1)(b+2) \\ &\quad + \frac{1}{6}b(r-1)(b-1)(b+1) + \frac{1}{6}(b-1)(r-1)(r-2)(r-3) + 2(b-1) \\ &\quad + \frac{1}{4}b(b-1)((r-2)(r-3) + 4) \\ &= \frac{1}{24}(r^4 + 2r^3 - 13r^2 + 10r + 24) + \frac{1}{24}(q-r+1)(q-r)(q-r+2)(q+3r-1) \\ &\quad + \frac{1}{6}(q-r)(r-1)(r-2)(r-3) + 2(q-r) + \frac{1}{4}(q-r)(q-r+1)(r^2 - 5r + 10). \end{aligned}$$

Since $WW(H_{q,3}) = \frac{1}{24}(q^4 + 2q^3 - 13q^2 + 10q + 24)$, then

$$WW(H_{q,3}) - WW(F) \geq q^2 r - 3q^2 - qr^2 + 4qr - 3q - r^2 + 3r \triangleq \psi_r.$$

By $d_{F_1}(v) \geq 3$ and $r + b - 1 = q$, we have $4 \leq r < q$. Since $\psi_4 = \psi_{q-1} = (q-4)(q+1) > 0$ for $q \geq 5$, then $WW(F) < WW(H_{q,3})$. The claim holds.

By Theorems 2.8, 2.9 and the above claim, we have $WW(H) \leq \frac{1}{48}p^2(p+1)(p+2)$, $WW(F) < WW(H_{q,3}) = \frac{1}{24}(q^4 + 2q^3 - 13q^2 + 10q + 24)$. By Lemma 2.7 and Theorem 2.8, we have $D_H(u) \leq \frac{1}{3}p(p-1)$, $DD_H(u) \leq$

$\frac{2}{27}(p-1)^2(2p+1)$. By Lemma 3.8, we have $D_F(u) \leq \frac{1}{2}q(q-1)$, $DD_F(u) \leq \frac{1}{6}q(q-1)(2q-1)$. Then by $p+q-1=n$ and equation (2), we have

$$\begin{aligned} WW(G) &< \frac{1}{48}p^2(p+1)(p+2) + \frac{1}{24}(q^4+2q^3-13q^2+10q+24) + \frac{1}{6}q(p-1)(q^2-1) \\ &\quad + \frac{1}{2}(q-1)(\frac{1}{3}p(p-1) + \frac{2}{27}(p-1)^2(2p+1)) + \frac{1}{6}pq(p-1)(q-1) \\ &= \frac{1}{48}p^2(p+1)(p+2) + \frac{1}{24}((n-p+1)^4 + 2(n-p+1)^3 - 13(n-p+1)^2 \\ &\quad + 10(n-p+1) + 24) + \frac{1}{6}(p-1)(n-p+1)(n-p)(n+2) \\ &\quad + \frac{1}{54}(n-p)(9p(p-1) + 2(p-1)^2(2p+1)). \end{aligned} \tag{3}$$

Comparing with the result of equation (1), we let $a = p$ in equation (1), then (1) − (3) $= \frac{1}{2}(n^2 - 2np + n + p^2 - p - 2) \geq 0$ for $p \leq n-1$. Thus we have $WW(G) < WW(H_{n,3})$. This completes the proof. □

Lemma 3.12. *Let $G \in \mathcal{G}(n,2)$, $G \not\cong P_n$, and x, y be the unique two vertices of odd degree in G with $d_G(x) = d_G(y) = 1$. Then $WW(G) < WW(H_{n,3})$.*

Proof. Since x, y are the unique two vertices of odd degree in G and $d_G(x) = d_G(y) = 1$, then G has a pendent path, say $P = vx_1x_2\cdots v_{b-2}x$ where $d_G(v)(\geq 3)$ is even and $d_G(x) = 1$. Let $P_1 = P \setminus \{v\}$, $K = G \setminus P_1$ and $|V(K)| = a$. Then $a+b-1 = n$. Clearly, $K \in \mathcal{G}(a,2)$ and v, y are the unique two vertices of odd degree in K with $d_K(v) \geq 3$, $d_K(y) = 1$.

By Lemma 3.11, we have $WW(K) \leq WW(H_{a,3}) = \frac{1}{24}(a^4 + 2a^3 - 13a^2 + 10a + 24)$. We also know that $WW(P) = \frac{1}{24}b(b-1)(b+1)(b+2)$, $D_P(v) = \frac{1}{2}b(b-1)$, $DD_P(v_1) = \frac{1}{6}b(b-1)(2b-1)$.

Since $d_K(v) \geq 3$ and Lemmas 3.6, 3.7, we have $D_K(v) \leq \frac{1}{2}(a-2)(a-3)+2$, $DD_K(v) \leq \frac{1}{6}(a-2)(a-3)(2a-5)+2$. Thus by $a+b-1=n$ and Lemma 3.9, we have

$$\begin{aligned} WW(G) &= WW(K) + WW(P) + \frac{1}{2}(a-1)(D_P(v) + DD_P(v)) \\ &\quad + \frac{1}{2}(b-1)(D_K(v) + DD_K(v)) + D_K(v)D_P(v) \\ &\leq \frac{1}{24}(a^4 + 2a^3 - 13a^2 + 10a + 24) + \frac{1}{24}b(b-1)(b+1)(b+2) \\ &\quad + \frac{1}{6}b(a-1)(b-1)(b+1) + \frac{1}{2}(b-1)(\frac{1}{3}(a-1)(a-2)(a-3) + 4) \\ &\quad + \frac{1}{4}b(b-1)((a-2)(a-3) + 4) \\ &= \frac{1}{24}(a^4 + 2a^3 - 13a^2 + 10a + 24) \\ &\quad + \frac{1}{24}(n-a)(n-a+1)(n-a+2)(n+3a-1) \\ &\quad + \frac{1}{2}(n-a)(\frac{1}{3}(a-1)(a-2)(a-3) + 4) \\ &\quad + \frac{1}{4}(n-a)(n-a+1)((a-2)(a-3) + 4). \end{aligned}$$

Since $WW(H_{n,3}) = \frac{1}{24}(n^4 + 2n^3 - 13n^2 + 10n + 24)$, then

$$WW(H_{n,3}) - WW(G) \geq n^2a - 3n^2 - na^2 + 4na - 3n - a^2 + 3a \triangleq h_a.$$

By $d_K(v) \geq 3$ and $a+b-1 = q$, we have $4 \leq a \leq n-1$. Since $h_4 = h_{q-1} = (n-4)(n+1) > 0$ for $n \geq 5$, then $WW(G) < WW(H_{n,3})$, and we complete the proof. □

Lemma 3.13. *Let $G \in \mathcal{G}(n,2)$, and x, y be the unique two vertices of odd degree in G, with $d_G(x) \geq 3$, $d_G(y) \geq 3$. Then $WW(G) < WW(H_{n,3})$.*

Proof. The assertion can be verified directly for $n = 4, 5$. We suppose the assertion holds for the graphs with the number of vertices less than n, then we prove the assertion holds for the graphs with the number of vertices equal to n.

Case 1. There is no cut-edge in G.

Then G is a 2-edge-connected graph and $G \ncong C_n$. Then we have $WW(G) < WW(C_n) = \frac{1}{48}n^2(n+1)(n+2)$.

$$\begin{aligned} WW(H_{n,3}) - WW(G) &> WW(H_{n,3}) - WW(C_n) \\ &= \frac{1}{24}(n^4 + 2n^3 - 13n^2 + 10n + 24) - \frac{1}{48}n^2(n+1)(n+2) \\ &= \frac{n^4}{48} + \frac{n^3}{48} - \frac{7n^2}{72} + \frac{5n}{12} + 1 > 0 \text{ for } n \geq 5. \end{aligned}$$

Case 2. There exists at least one cut-edge in G.

Without loss of generality, we let uw be one of end-cut edge and H the block of $G \setminus \{uw\}$ containing u. Let $K = G \setminus (H \setminus \{u\})$ and $|V(H)| = a$, $|V(K)| = b$. Then $a + b - 1 = n$. By Lemma 3.9, we have

$$\begin{aligned} WW(G) &= WW(H) + WW(K) + \frac{1}{2}(a-1)(D_K(u) + DD_K(u)) \\ &\quad + \frac{1}{2}(b-1)(D_H(u) + DD_H(u)) + D_H(u)D_K(u). \end{aligned}$$

If $a = 3$ or 4, then H is a 2-connected graph. By Lemmas 2.1, 2.3 and 2.5, we have $WW(H) \leq WW(C_a)$, $D_H(u) \leq D_{C_a}(u)$, $DD_H(u) \leq DD_{C_a}(u)$. By Lemma 3.1 and the induction hypothesis, we have $WW(K) \leq WW(H_{b,3}) < WW(P_b)$. By Lemma 3.8, we have $D_K(u) \leq D_{P_b}(u)$, $DD_K(u) \leq DD_{P_b}(u)$. Thus $WW(G) < WW(H_{n,a}) \leq WW(H_{n,3})$.

If $a \geq 5$, the H is a 2-edge-connected graph, thus $WW(H) \leq \frac{1}{48}a^2(a+1)(a+2)$. Since there are two vertices with odd degree in K, say u and x, and $d_K(u) = 1$, $d_K(x) \geq 3$. By Lemma 3.11, we have $WW(K) \leq WW(H_{b,3}) = \frac{1}{24}(b^4 + 2b^3 - 13b^2 + 10b + 24) < \frac{1}{24}b(b-1)(b+1)(b+2) = WW(P_b)$. By Lemma 2.7 and Theorem 2.8, we have $D_H(u) \leq \frac{1}{3}a(a-1)$, $DD_H(u) \leq \frac{2}{27}(a-1)^2(2a+1)$. By Lemma 3.8, we have $D_K(u) \leq \frac{1}{2}b(b-1)$, $DD_K(u) \leq \frac{1}{6}b(b-1)(2b-1)$. The same calculation as **Case 1** of Lemma 3.11, we have $WW(G) < WW(H_{n,3})$.

This completes the proof. □

By Lemmas 3.11, 3.12 and 3.13, we determine the second maximum graph among $\mathcal{G}(n,2)$ with respect to hyper-Wiener index.

Theorem 3.14. *Let $G \in \mathcal{G}(n,2)$ and $G \ncong P_n$. Then*

$$WW(G) \leq WW(H_{n,3}),$$

with equality if and only if $G \cong H_{n,3}$.

4. The minimum graphs with given number of vertices of odd degree

Recall that $\mathcal{G}(n,2k)$ denotes the set of connected graphs with n vertices and $2k$ vertices of odd degree. Let M_l be the set of matching with l independent edges in K_n. Then $K_n \setminus M_l \in \mathcal{G}(n,2k)$, where $l = k$ if n is odd, $l = \frac{n}{2} - k$ if n is even. In this section, we determine the minimum graphs among $\mathcal{G}(n,2k)$ for any $0 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

Theorem 4.1. *Let $G \in \mathcal{G}(n,2k)$. Then*

$$WW(G) \geq WW(K_n \setminus M_l),$$

where $l = \begin{cases} k, & if\ n \text{ is odd} \\ \frac{n}{2} - k, & if\ n \text{ is even} \end{cases}$*, with equality if and only if $G \cong K_n \setminus M_l$.*

Proof. Suppose that $G \in \mathcal{G}(n, 2k)$, $V(G) = \{u_1, u_2, \cdots, u_n\}$, and $u_1, u_2, \cdots, u_{2k}$ are the vertices with odd degree.

Case 1. n is even.

For $1 \le i \le 2k$, we have $d_G(u_i) \le n-1$ and

$$D_G(u_i) + DD_G(u_i) \ge (\underbrace{1+1+\cdots+1}_{n-1}) + (\underbrace{1^2+1^2+\cdots+1^2}_{n-1}) = 2n-2.$$

For $2k+1 \le i \le n$, we have $d_G(u_i) \le n-2$ and

$$D_G(u_i) + DD_G(u_i) \ge (2 + \underbrace{1+1+\cdots+1}_{n-2}) + (2^2 + \underbrace{1^2+1^2+\cdots+1^2}_{n-2}) = 2n+2.$$

Thus

$$\begin{aligned} WW(G) &= \frac{1}{4}\sum_{v\in V(G)}(D_G(v) + DD_G(v)) \\ &\ge \frac{1}{4}(2k(2n-2) + (n-2k)(2n+2)) \\ &= \frac{1}{2}(n^2+n-4k), \end{aligned}$$

with equality if and only if $d_G(u_i) = n-1$ for $i \in \{1, 2, \cdots, 2k\}$ and $d_G(u_i) = n-2$ for $i \in \{2k+1, 2k+2, \cdots, n\}$, i.e., $G \cong K_n \setminus M_{\frac{n}{2}-k}$.

Case 2. n is odd.

For $1 \le i \le 2k$, we have $d_G(u_i) \le n-2$ and

$$D_G(u_i) + DD_G(u_i) \ge (2 + \underbrace{1+1+\cdots+1}_{n-2}) + (2^2 + \underbrace{1^2+1^2+\cdots+1^2}_{n-2}) = 2n+2.$$

For $2k+1 \le i \le n$, we have $d_G(u_i) \le n-1$ and

$$D_G(u_i) + DD_G(u_i) \ge (\underbrace{1+1+\cdots+1}_{n-1}) + (\underbrace{1^2+1^2+\cdots+1^2}_{n-1}) = 2n-2.$$

Thus

$$\begin{aligned} WW(G) &= \frac{1}{4}\sum_{v\in V(G)}(D_G(v) + DD_G(v)) \\ &\ge \frac{1}{4}(2k(2n+2) + (n-2k)(2n-2)) \\ &= \frac{1}{2}(n^2-n+4k), \end{aligned}$$

with equality if and only if $d_G(u_i) = n-2$ for $i \in \{1, 2, \cdots, 2k\}$ and $d_G(u_i) = n-1$ for $i \in \{2k+1, 2k+2, \cdots, n\}$, i.e., $G \cong K_n \setminus M_k$. □

Let $k = 0$, we have the following result by Theorem 4.1.

Corollary 4.2. [15] *Let $G \in \mathcal{G}(n, 0)$. Then*

$$WW(G) \ge WW(K_n \setminus M_l),$$

where $l = \begin{cases} 0, & if\ n\ is\ odd \\ \frac{n}{2}, & if\ n\ is\ even \end{cases}$*, with equality if and only if $G \cong K_n \setminus M_l$.*

5. Conclusions

In this paper, we determine the maximum hyper-Wiener index of 2-connected graphs and 2-edge-connected graphs, which extends the result of Plesnik [On the sum of all distances in a graph or digraph, J. Graph Theory 8 (1984) 1-21]. Then based on the above results, we characterize the first two maximum graphs among the graphs with two vertices of odd degree, the minimum graphs among the graphs with $2k$ $(0 \leq k \leq \lfloor \frac{n}{2} \rfloor)$ vertices of odd degree, which extends the result of Hou, Chen and Zhang [Hyper-Wiener index of Eulerian graphs, Appl. Math. J. Chin. Univ. 31 (2016) 248-252]. The problem of characterizing the maximum graphs among the graphs with given $2k(2 \leq k \leq \lfloor \frac{n}{2} \rfloor)$ vertices of odd degree is still open.

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