Filomat 32:2 (2018), 489–502
https://doi.org/10.2298/FIL1802489Z

Published by Faculty of Sciences and Mathematics,
University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

Wiener-type Invariants on Graph Properties

Qiannan Zhou[a], Ligong Wang[a], Yong Lu[a]

[a] *Department of Applied Mathematics, School of Science, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, P.R. China*

Abstract. The Wiener-type invariants of a simple connected graph $G = (V(G), E(G))$ can be expressed in terms of the quantities $W_f = \sum_{\{u,v\}\subseteq V(G)} f(d_G(u, v))$ for various choices of the function $f(x)$, where $d_G(u, v)$ is the distance between vertices u and v in G. In this paper, we mainly give some sufficient conditions for a connected graph to be k-connected, β-deficient, k-hamiltonian, k-edge-hamiltonian, k-path-coverable or satisfy $\alpha(G) \leq k$.

1. Introduction

Throughout this paper, we only consider graphs which are simple, undirected and finite. We refer the reader to [3] for terminologies and notations not defined here. Let G denote a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. Let $d_i = d_{v_i} = d_G(v_i)$ denote the degree of v_i. Denote by $(d_1, d_2, \ldots, d_n)$ the degree sequence of the graph G, where $d_1 \leq d_2 \leq \cdots \leq d_n$. Let G and H be two disjoint graphs. The disjoint union of G and H, denoted by $G + H$, is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$. The disjoint union of k graphs G is denoted by kG. The join of G and H, denoted by $G \vee H$, is the graph obtained from disjoint union of G and H by adding edges joining every vertex of G to every vertex of H. The complement $\overline{G}$ of G is the graph on $V(G)$ with edge set $[V]^2 \setminus E(G)$.

In theoretical chemistry, molecular structure descriptors, also called topological indices, are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds. For $v_i, v_j \in V(G)$, let $d_G(v_i, v_j)$ denote the distance between v_i and v_j. The *Wiener index* $W(G)$ of a connected graph G is defined by

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

In 1947, the Wiener index was introduced by Wiener [29], who used it for modeling the shape of organic molecules and for calculating several of their physico-chemical properties. More details on vertex distances and Wiener index can be found in [8, 9, 16, 28, 29].

In 1993, for the characterization of molecular graphs, Ivanciuc et al. [14] and Plavšić et al. [26] independently introduced the *Harary index* $H(G)$ of a graph G. It has been named in honor of Professor

2010 *Mathematics Subject Classification*. Primary 05C50; Secondary 05C40, 05C07
Keywords. Wiener-type index, degree sequence, graph properties.
Received: 05 January 2016; Accepted: 24 October 2017
Communicated by Paola Bonacini
Corresponding author: Ligong Wang
Research supported by the National Natural Science Foundation of China (No. 11171273).
Email addresses: qnzhoumath@163.com (Qiannan Zhou), lgwangmath@163.com (Ligong Wang), luyong.gougou@163.com (Yong Lu)

Frank Harary on the occasion of his 70th birthday. The definition of Harary index is as follows:

$$H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d_G(u,v)}.$$

More details on Harary index can be found in [6, 25, 30, 32, 34].

Some generalizations and modifications of the Wiener index were proposed. Many of these Wiener-type invariants can be expressed in terms of the quantities

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

for various choices of the function $f(x)$. We know that when $f(x) = x$, W_x is the Wiener index; when $f(x) = \frac{1}{x}$, $W_{\frac{1}{x}}$ is the Harary index; when $f(x) = \frac{x^2+x}{2}$, $W_{\frac{x^2+x}{2}}$ is called the *hyper-Wiener index* [27], which is denoted by WW; when $f(x) = x^\lambda$, where $\lambda \neq 0$ is a real number, W_{x^λ} is called the *modified Wiener index* [11], which is denoted by W_λ. More details on Wiener-type invariants can be found in [7, 12, 15].

In recent years, some sufficient conditions in terms of Wiener index and Harary index are given for a graph to be Hamiltonian, traceable or have other graph properties. More details can be found in [10, 13, 21–24, 31, 33]. In 2016, Kuang et al. [18] gave some sufficient conditions on Wiener-type invariants for a graph to be Hamiltonian or traceable, for a connected bipartite graph to be Hamiltonian which included some previous results.

In this paper, we mainly give some sufficient conditions in terms of Wiener-type invariants for some graph properties. In Section 2, we will give some graph notations and useful lemmas. In Section 3, we will present some sufficient conditions for a connected graph to be k-connected, β-deficient, k-hamiltonian, k-edge-hamiltonian and k-path-coverable, respectively, in terms of Wiener-type index.

2. Some definitions and lemmas

First, we give some notations of graphs used in this paper.

A connected graph G is called to be *k-connected* (or k-vertex connected) if it has more than k vertices and remains connected whenever fewer than k vertices are removed.

The *deficiency* def(G) of a graph G is the number of vertices unmatched under a maximum matching in G. In particular, G has a 1-factor if and only if def(G)=0. If def$(G)\leq \beta$, then we call G *β-deficient*.

A cycle is called a *Hamilton cycle* if it contains every vertex of a graph. The graph is said to be *Hamiltonian* if it has a Hamilton cycle. A graph is *k-hamiltonian* if for all $|X| \leq k$, the subgraph induced by $V(G)\backslash X$ is Hamiltonian. Thus 0-hamilotnian is the same as Hamiltonian.

A graph G is *k-edge-hamiltonian* if any collection of vertex-disjoint paths with at most k edges altogether belong to a Hamilton cycle in G.

A path is called a *Hamilton path* if it contains every vertex of a graph. The graph is said to be *traceable* if it has a Hamilton path. More generally, G is *k-path-coverable* if $V(G)$ can be covered by k or fewer vertex-disjoint paths. In particular, 1-path-coverable is the same as traceable.

A subset S of $V(G)$ is called an *independent set* of G if no two vertices of S are adjacent in G. The number of vertices in a maximum independent set of G is called the *independence number* of G and is denoted by $\alpha(G)$.

An integer sequence $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ is called *graphical* if there exists a graph G having π as its vertex degree sequence, in that case, G is called a *realization* of π. If P is a graph property, such as hamiltonian or k-connected, we call a graphical sequence π *forcibly P* if every realization of π has property P. Historically, the vertex degrees of a graph have been used to provide sufficient conditions for the graph to have certain properties, such as hamiltonicity or k-connectedness.

Next, we give some useful lemmas.

Lemma 2.1. *([2]) Let G be a graph of order $n \geq 4$ with degree sequence $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$. If*

$$d_i \leq i + k - 2 \Rightarrow d_{n-k+1} \geq n - i, for\ 1 \leq i \leq \frac{1}{2}(n - k + 1),$$

then π is forcibly k-connected.

Lemma 2.2. *([19]) Let $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ be a graphical sequence and let $0 \leq \beta \leq n$ with $n \equiv \beta (mod\ 2)$. If*

$$d_{i+1} \leq i - \beta \Rightarrow d_{n+\beta-i} \geq n - i - 1, for\ 1 \leq i \leq \frac{1}{2}(n + \beta - 2),$$

then π is forcibly β-deficient.

Lemma 2.3. *([4]) Let $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ be a graphical sequence and $0 \leq k \leq n - 3$. If*

$$d_i \leq i + k \Rightarrow d_{n-i-k} \geq n - i, for\ 1 \leq i < \frac{1}{2}(n - k),$$

then π is forcibly k-hamiltonian.

Lemma 2.4. *([17]) Let $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ be a graphical sequence and $0 \leq k \leq n - 3$. If*

$$d_{i-k} \leq i \Rightarrow d_{n-i} \geq n - i + k, for\ k + 1 \leq i < \frac{1}{2}(n + k),$$

then π is forcibly k-edge-hamiltonian.

Lemma 2.5. *([5, 20]) Let $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ be a graphical sequence and $k \geq 1$. If*

$$d_{i+k} \leq i \Rightarrow d_{n-i} \geq n - i - k, for\ 1 \leq i < \frac{1}{2}(n - k),$$

then π is forcibly k-path-coverable.

Lemma 2.6. *([1]) Let $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ be a graphical sequence and $k \geq 1$. If*

$$d_{k+1} \geq n - k,$$

then π is forcibly $\alpha(G) \leq k$.

3. Main Results

Theorem 3.1. *Let G be a connected graph of order $n \geq k + 1$. If*

$$W_f(G) \leq \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n - k[f(2) - f(1)],$$

for a monotonically increasing function $f(x)$ on $x \in [1, n - 1]$, or

$$W_f(G) \geq \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n + k[f(1) - f(2)],$$

for a monotonically decreasing function $f(x)$ on $x \in [1, n - 1]$, then G is k-connected unless $G = K_{k-1} \vee (K_1 + K_{n-k})$.

Proof. Assume that G is not k-connected and has degree sequence $(d_1, d_2, \ldots, d_n)$, where $d_1 \leq d_2 \leq \cdots \leq d_n$. By Lemma 2.1, there is an integer $1 \leq i \leq \dfrac{n-k+1}{2}$ such that $d_i \leq i+k-2$ and $d_{n-k+1} \leq n-i-1$. Obviously, $1 \leq k \leq n-1$. Note that G is connected. If $f(x)$ is a monotonically increasing function for $x \in [1, n-1]$, then

$$\begin{aligned}
W_f(G) &= \frac{1}{2}\sum_{s=1}^{n}\sum_{t=1}^{n} f(d_G(v_s, v_t)) \\
&\geq \frac{1}{2}\sum_{s=1}^{n}[f(1)d_s + f(2)(n-1-d_s)] \\
&= \frac{1}{2}\sum_{s=1}^{n}[(n-1)f(2) - (f(2)-f(1))d_s] \\
&= \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}\sum_{s=1}^{n} d_s \\
&= \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}\Big(\sum_{s=1}^{i} d_s + \sum_{s=i+1}^{n-k+1} d_s + \sum_{s=n-k+2}^{n} d_s\Big) \\
&\geq \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}[i(i+k-2) + (n-k-i+1)(n-i-1) + (k-1)(n-1)] \\
&= \frac{1}{2}n(n-1)f(2) - [f(2)-f(1)]\Big[\frac{n^2-3n}{2} - (i-1)(n-i-k) + k\Big] \\
&= \frac{f(1)}{2}n^2 + \Big[f(2) - \frac{3}{2}f(1)\Big]n - k[f(2)-f(1)] + [f(2)-f(1)](i-1)(n-i-k).
\end{aligned}$$

Similarly, if $f(x)$ is a monotonically decreasing function for $x \in [1, n-1]$, then

$$W_f(G) \leq \frac{f(1)}{2}n^2 + \Big[f(2) - \frac{3}{2}f(1)\Big]n + k[f(1)-f(2)] - [f(1)-f(2)](i-1)(n-i-k).$$

If $f(x)$ is a monotonically increasing function on $[1, n-1]$, by the condition of Theorem 3.1, we have $(i-1)(n-i-k) \leq 0$. Then we discuss the following two cases.

Case 1. Assume that $(i-1)(n-i-k) = 0$. In this case, we get $W_f(G) = \dfrac{f(1)}{2}n^2 + [f(2) - \dfrac{3}{2}f(1)]n - k[f(2)-f(1)]$. So all the inequalities in the above arguments should be equalities. Thus, we have (a) the diameter of G is no more than two; (b) $d_1 = \cdots = d_i = i+k-2$, $d_{i+1} = \cdots = d_{n-k+1} = n-i-1$ and $d_{n-k+2} = \cdots = d_n = n-1$; and (c) $i = 1$ or $n = i+k$.

If $i = 1$, then $d_1 = k-1$, $d_2 = \cdots = d_{n-k+1} = n-2$, $d_{n-k+2} = \cdots = d_n = n-1$. It implies that $G = K_{k-1} \vee (K_1 + K_{n-k})$, which is not k-connected as stated in [1]. If $n = i+k$, since $i \leq \dfrac{n-k+1}{2}$ and $n \geq k+1$, then $n = k+1$. Thus $1 \leq i \leq \frac{n-k+1}{2} = 1$, then $i = 1$. This case is the same as we discussed above.

Case 2. We assume $i \geq 2$ and $n-i-k < 0$. Note that $i \leq \frac{n-k+1}{2}$, hence $0 \leq i-1 \leq n-i-k$, a contradiction. If $f(x)$ is a monotonically decreasing function on $[1, n-1]$, we can prove the result by a similar method. The proof is complete. □

From Theorem 3.1, the previous work (see Theorem 3.1 in [10]) is a direct corollary when $f(x) = x, \frac{1}{x}$. Moreover, when $f(x) = \frac{x^2+x}{2}, x^\lambda$ in Theorem 3.1, we have the following corollaries.

Corollary 3.2. *Let G be a connected graph of order $n \geq k+1$. If its hyper-Wiener index*

$$WW(G) \leq \frac{1}{2}n^2 + \frac{3}{2}n - 2k,$$

then G is k-connected unless $G = K_{k-1} \vee (K_1 + K_{n-k})$.

Corollary 3.3. *Let G be a connected graph of order* $n \geq k+1$. *If its modified Wiener index*

$$W_\lambda(G) \leq \frac{1}{2}n^2 + (2^\lambda - \frac{3}{2})n - k(2^\lambda - 1),$$

for $\lambda > 0$, *or*

$$W_\lambda(G) \geq \frac{1}{2}n^2 + (2^\lambda - \frac{3}{2})n + k(1 - 2^\lambda),$$

for $\lambda < 0$, *then G is k-connected unless* $G = K_{k-1} \vee (K_1 + K_{n-k})$.

Theorem 3.4. *Let G be a connected graph of order* $n \geq 10$ *with* $n \equiv \beta$ *(mod 2) and* $0 \leq \beta \leq n$. *If*

$$W_f(G) \leq \frac{f(1)}{2}n^2 + [2f(2) - \frac{5}{2}f(1)]n + (2\beta - 5)[f(2) - f(1)],$$

for a monotonically increasing function $f(x)$ *on* $x \in [1, n-1]$, *or*

$$W_f(G) \geq \frac{f(1)}{2}n^2 + [2f(2) - \frac{5}{2}f(1)]n - (2\beta - 5)[f(1) - f(2)],$$

for a monotonically decreasing function $f(x)$ *on* $x \in [1, n-1]$, *then G is* β*-deficient unless* $G \in \{K_1 \vee (2K_1 + K_{n-3}), K_4 \vee 6K_1\}$.

Proof. Suppose that G is not β-deficient and has degree sequence $(d_1, d_2, \ldots, d_n)$, where $d_1 \leq d_2 \leq \cdots \leq d_n$. By Lemma 2.2, there is an integer $1 \leq i \leq \frac{1}{2}(n + \beta - 2)$ such that $d_{i+1} \leq i - \beta$ and $d_{n+\beta-i} \leq n - i - 2$. Note that G is connected. If $f(x)$ is a monotonically increasing function for $x \in [1, n-1]$, as the proof of Theorem 3.1, then we have

$$\begin{aligned}
W_f(G) &\geq \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}\sum_{s=1}^{n} d_s \\
&= \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}(\sum_{s=1}^{i+1} d_s + \sum_{s=i+2}^{n+\beta-i} d_s + \sum_{s=n+\beta-i+1}^{n} d_s) \\
&\geq \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}[(i+1)(i-\beta) + (n+\beta-2i-1)(n-i-2) + (i-\beta)(n-1)] \\
&= \frac{1}{2}n(n-1)f(2) - [f(2)-f(1)][\frac{n^2-5n+10}{2} - (i-1)(n - \frac{3}{2}i + \beta - 4) - 2\beta] \\
&= \frac{f(1)}{2}n^2 + [2f(2) - \frac{5}{2}f(1)]n + (2\beta-5)[f(2)-f(1)] + [f(2)-f(1)](i-1)(n - \frac{3}{2}i + \beta - 4).
\end{aligned}$$

Similarly, if $f(x)$ is a monotonically decreasing function for $x \in [1, n-1]$, then

$$W_f(G) \leq \frac{f(1)}{2}n^2 + [2f(2) - \frac{5}{2}f(1)]n - (2\beta-5)[f(1)-f(2)] - [f(1)-f(2)](i-1)(n - \frac{3}{2}i + \beta - 4).$$

If $f(x)$ is a monotonically increasing function on $[1, n-1]$, by the condition of Theorem 3.4, we have $(i-1)(n - \frac{3}{2}i + \beta - 4) \leq 0$. Then we discuss the following two cases.

Case 1. Assume $(i-1)(n - \frac{3}{2}i + \beta - 4) = 0$. In this case, we get $W_f(G) = \frac{f(1)}{2}n^2 + [2f(2) - \frac{5}{2}f(1)]n + (2\beta - 5)[f(2) - f(1)]$. So all the inequalities in the above arguments should be equalities. Thus, we have

(a) the diameter of G is no more than two; (b) $d_1 = \cdots = d_{i+1} = i - \beta$, $d_{i+2} = \cdots = d_{n+\beta-i} = n - i - 2$ and $d_{n+\beta-i+1} = \cdots = d_n = n - 1$; and (c) $i = 1$ or $n = \frac{3}{2}i - \beta + 4$.

If $i = 1$, then $d_1 = d_2 = 1 - \beta$, so $\beta = 0$, otherwise v_1 and v_2 are two isolated vertices and G is disconnected. Then $d_1 = d_2 = 1$, $d_3 = \cdots = d_{n-1} = n - 3$, $d_n = n - 1$. It implies that $G = K_1 \vee (2K_1 + K_{n-3})$, which is not β-deficient as stated in [1]. If $n = \frac{3}{2}i - \beta + 4$, since $i \leq \frac{1}{2}(n + \beta - 2)$, $n \geq 10$, then $n = 10$, $\beta = 0$ and $i = 4$. The corresponding graphic sequences is $(4, 4, 4, 4, 4, 4, 9, 9, 9, 9)$, which implies $G = K_4 \vee 6K_1$.

Case 2. We assume $i \geq 2$ and $n - \frac{3}{2}i + \beta - 4 < 0$. Since $i \leq \frac{1}{2}(n + \beta - 2)$ and $n \geq 10$, $n - \frac{3}{2}i + \beta - 4 \geq \frac{n}{4} + \frac{\beta}{4} - \frac{5}{2} \geq 0$, a contradiction.

If $f(x)$ is a monotonically decreasing function on $[1, n - 1]$, we can prove the result by a similar method. The proof is complete. □

From Theorem 3.4, the previous work (see Theorem 3.2 in [10]) is a direct corollary when $f(x) = x, \frac{1}{x}$. Moreover, when $f(x) = \frac{x^2 + x}{2}, x^\lambda$ in Theorem 3.4, we have the following corollaries.

Corollary 3.5. *Let G be a connected graph of order $n \geq 10$ with $n \equiv \beta (mod\ 2)$ and $0 \leq \beta \leq n$. If its hyper-Wiener index*

$$WW(G) \leq \frac{1}{2}n^2 + \frac{7}{2}n + 4\beta - 10,$$

then G is β-deficient unless $G \in \{K_1 \vee (2K_1 + K_{n-3}), K_4 \vee 6K_1\}$.

Corollary 3.6. *Let G be a connected graph of order $n \geq 10$ with $n \equiv \beta (mod\ 2)$ and $0 \leq \beta \leq n$. If its modified Wiener index*

$$W_\lambda(G) \leq \frac{1}{2}n^2 + (2^{\lambda+1} - \frac{5}{2})n + (2\beta - 5)(2^\lambda - 1),$$

for $\lambda > 0$, or

$$W_\lambda(G) \geq \frac{1}{2}n^2 + (2^{\lambda+1} - \frac{5}{2})n - (2\beta - 5)(1 - 2^\lambda),$$

for $\lambda < 0$, then G is β-deficient unless $G \in \{K_1 \vee (2K_1 + K_{n-3}), K_4 \vee 6K_1\}$.

Theorem 3.7. *Let G be a connected graph of order $n \geq 3$ and $0 \leq k \leq n - 3$. If*

$$W_f(G) \leq \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n - (k + 2)[f(2) - f(1)],$$

for a monotonically increasing function $f(x)$ on $x \in [1, n - 1]$, or

$$W_f(G) \geq \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n + (k + 2)[f(1) - f(2)],$$

for a monotonically decreasing function $f(x)$ on $x \in [1, n - 1]$, then G is k-hamiltonian unless $G \in \{K_{k+1} \vee (K_1 + K_{n-k-2}), 3K_1 \vee K_{k+2}\ (n = k + 5)\}$.

Proof. Suppose that G is not k-hamiltonian and has degree sequence $(d_1, d_2, \ldots, d_n)$, where $d_1 \leq d_2 \leq \cdots \leq d_n$. By Lemma 2.3, there exists an integer k, such that $d_i \leq i + k$ and $d_{n-i-k} \leq n - i - 1$. Note that G is connected. If $f(x)$ is a monotonically increasing function for $x \in [1, n - 1]$, as the proof of Theorem 3.1, then we have

$$\begin{aligned}
W_f(G) &\geq \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}\sum_{s=1}^{n} d_s \\
&= \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}\Big(\sum_{s=1}^{i} d_s + \sum_{s=i+1}^{n-i-k} d_s + \sum_{s=n-i-k+1}^{n} d_s\Big) \\
&\geq \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}[i(i+k) + (n-2i-k)(n-i-1) + (i+k)(n-1)] \\
&= \frac{1}{2}n(n-1)f(2) - [f(2)-f(1)][\frac{n^2-3n}{2} - (i-1)(n-\frac{3}{2}i-k-2) + k + 2] \\
&= \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n - (k+2)[f(2)-f(1)] + [f(2)-f(1)](i-1)(n-\frac{3}{2}i-k-2).
\end{aligned}$$

Similarly, if $f(x)$ is a monotonically decreasing function for $x \in [1, n-1]$, then

$$W_f(G) \leq \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n + (k+2)[f(1)-f(2)] - [f(1)-f(2)](i-1)(n-\frac{3}{2}i-k-2).$$

If $f(x)$ is a monotonically increasing function on $[1, n-1]$, by the condition of Theorem 3.7, we have $(i-1)(n-\frac{3}{2}i-k-2) \leq 0$. Then we discuss the following two cases.

Case 1. Assume that $(i-1)(n-\frac{3}{2}i-k-2) = 0$. In this case, we get $W_f(G) = \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n - (k+2)[f(2)-f(1)]$. So all the inequalities in the above arguments should be equalities. Thus, we have (a) the diameter of G is no more than two; (b) $d_1 = \cdots = d_i = i+k$, $d_{i+1} = \cdots = d_{n-i-k} = n-i-1$ and $d_{n-i-k+1} = \cdots = d_n = n-1$; and (c) $i = 1$ or $n = \frac{3}{2}i + k + 2$.

Subcase 1.1. If $i = 1$, then $d_1 = k+1$, $d_2 = \cdots = d_{n-k-1} = n-2$, $d_{n-k} = \cdots = d_n = n-1$. It implies that $G = K_{k+1} \vee (K_1 + K_{n-k-2})$.

Subcase 1.2. If $n = \frac{3}{2}i + k + 2$, since $i < \frac{1}{2}(n-k)$, then $n < k+8$, i.e., $n \leq k+7$. Note that $n \geq k+3$. Then $n = k+5$, $i = 2$. Thus $d_1 = d_2 = k+2$, $d_3 = n-3 = k+2$, $d_4 = \cdots = d_n = n-1 = k+4$, which implies $G = K_{k+2} \vee 3K_1$.

Case 2. We assume $i \geq 2$ and $n - \frac{3}{2}i - k - 2 < 0$. Since $i < \frac{1}{2}(n-k)$, then $n - \frac{3}{2}i - k - 2 > n - \frac{3}{2}\cdot\frac{1}{2}(n-k) - k - 2 = \frac{n}{4} - \frac{k}{4} - 2$. When $n \leq k+7$, if $n = k+3$ or $n = k+4$, then $i = 1$, a contradiction. If $n = k+5$, $i = 2$, then the case has been discussed in Subcase 1.2. If $n = k+6$, $i = 2$, then $n - \frac{3}{2}i - k - 2 = k+6-3-k-2 = 1 > 0$, a contradiction. If $n = k+7$, $i = 2$, then $n - \frac{3}{2}i - k - 2 = k+7-3-k-2 = 2 > 0$, a contradiction. If $n = k+7$, $i = 3$, then $n - \frac{3}{2}i - k - 2 = k + 7 - \frac{9}{2} - k - 2 = \frac{1}{2} > 0$, a contradiction. When $n \geq k+8$, then $n - \frac{3}{2}i - k - 2 > \frac{n}{4} - \frac{k}{4} - 2 \geq 0$, a contradiction.

If $f(x)$ is a monotonically decreasing function on $[1, n-1]$, we can prove the result by a similar method. The proof is complete. □

By Theorem 3.7, when $f(x) = x, \frac{1}{x}, \frac{x^2+x}{2}, x^\lambda$, we have the following corollaries.

Corollary 3.8. *Let G be a connected graph of order $n \geq 3$ and $0 \leq k \leq n-3$. If its Wiener index*

$$W(G) \leq \frac{1}{2}n^2 + \frac{1}{2}n - k - 2,$$

then G is k-hamiltonian unless $G \in \{K_{k+1} \vee (K_1 + K_{n-k-2}), 3K_1 \vee K_{k+2}\ (n = k+5)\}$.

Corollary 3.9. *Let G be a connected graph of order $n \geq 3$ and $0 \leq k \leq n-3$. If its Harary index*

$$H(G) \geq \frac{1}{2}n^2 - n + \frac{1}{2}(k+2),$$

then G is k-hamiltonian unless $G \in \{K_{k+1} \vee (K_1 + K_{n-k-2}), 3K_1 \vee K_{k+2}\ (n = k+5)\}$.

Corollary 3.10. *Let G be a connected graph of order $n \geq 3$ and $0 \leq k \leq n-3$. If its hyper-Wiener index*

$$WW(G) \leq \frac{1}{2}n^2 + \frac{3}{2}n - 2(k+2),$$

then G is k-hamiltonian unless $G \in \{K_{k+1} \vee (K_1 + K_{n-k-2}), 3K_1 \vee K_{k+2}\ (n = k+5)\}$.

Corollary 3.11. *Let G be a connected graph of order $n \geq 3$ and $0 \leq k \leq n-3$. If its modified Wiener index*

$$W_f(G) \leq \frac{1}{2}n^2 + (2^\lambda - \frac{3}{2})n - (2^\lambda - 1)(k+2),$$

for $\lambda > 0$, or

$$W_f(G) \geq \frac{1}{2}n^2 + (2^\lambda - \frac{3}{2})n + (1 - 2^\lambda)(k+2),$$

for $\lambda < 0$, then G is k-hamiltonian unless $G \in \{K_{k+1} \vee (K_1 + K_{n-k-2}), 3K_1 \vee K_{k+2}\ (n = k+5)\}$.

Theorem 3.12. *Let G be a connected graph of order $n \geq 8$ and $0 \leq k \leq n-3$. If*

$$W_f(G) \leq \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n - (nk + \frac{1}{2}k^2 - \frac{5}{2}k + 2)[f(2) - f(1)],$$

for a monotonically increasing function $f(x)$ on $x \in [1, n-1]$, or

$$W_f(G) \geq \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n + (nk + \frac{1}{2}k^2 - \frac{5}{2}k + 2)[f(1) - f(2)],$$

for a monotonically decreasing function $f(x)$ on $x \in [1, n-1]$, then G is k-edge-hamiltonian unless $G = K_1 \vee (K_1 + K_{n-2})$.

Proof. Suppose that G is not k-edge-hamiltonian and has degree sequence $(d_1, d_2, \ldots, d_n)$, where $d_1 \leq d_2 \leq \cdots \leq d_n$. By Lemma 2.4, there exists an integer $k+1 \leq i < \frac{1}{2}(n+k)$, such that $d_{i-k} \leq i$ and $d_{n-i} \leq n-i+k-1$. Note that G is connected. If $f(x)$ is a monotonically increasing function for $x \in [1, n-1]$, as the proof of Theorem 3.1, we have

$$\begin{aligned}
W_f(G) &\geq \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}\sum_{s=1}^{n} d_s \\
&= \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}(\sum_{s=1}^{i-k} d_s + \sum_{s=i-k+1}^{n-i} d_s + \sum_{s=n-i+1}^{n} d_s) \\
&\geq \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}[(i-k)i + (n-2i+k)(n-i+k-1) + i(n-1)] \\
&= \frac{1}{2}n(n-1)f(2) - [f(2)-f(1)][\frac{n^2-3n}{2} - (i-1)(n - \frac{3}{2}i + 2k - 2) \\
&\quad + nk + \frac{1}{2}k^2 - \frac{5}{2}k + 2] \\
&= \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n - (nk + \frac{1}{2}k^2 - \frac{5}{2}k + 2)[f(2) - f(1)] \\
&\quad + [f(2) - f(1)](i-1)(n - \frac{3}{2}i + 2k - 2).
\end{aligned}$$

Similarly, if $f(x)$ is a monotonically decreasing function for $x \in [1, n-1]$, then

$$W_f(G) \leq \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n + (nk + \frac{1}{2}k^2 - \frac{5}{2}k + 2)[f(1) - f(2)] \\ - [f(1) - f(2)](i-1)(n - \frac{3}{2}i + 2k - 2).$$

If $f(x)$ is a monotonically increasing function on $[1, n-1]$, by the condition of Theorem 3.12, we have $(i-1)(n - \frac{3}{2}i + 2k - 2) \leq 0$. Then we discuss the following two cases.

Case 1. Assume that $(i-1)(n - \frac{3}{2}i + 2k - 2) = 0$. In this case, we get $W_f(G) = \frac{f(1)}{2}n^2 + [f(2) - \frac{3}{2}f(1)]n - (nk + \frac{1}{2}k^2 - \frac{5}{2}k + 2)[f(2) - f(1)]$. So all the inequalities in the above arguments should be equalities. Thus we have (a) the diameter of G is no more than two; (b) $d_1 = \cdots = d_{i-k} = i$, $d_{i-k+1} = \cdots = d_{n-i} = n - i + k - 1$, $d_{n-i+1} = \cdots = d_n = n - 1$; and (c) $i = 1$ or $n = \frac{3}{2}i - 2k + 2$.

Subcase 1.1. If $i = 1$, since $k + 1 \leq i$, then $k = 0$. Hence $d_1 = 1$, $d_2 = \cdots = d_{n-1} = n - 2$, $d_n = n - 1$, which implies $G = K_1 \vee (K_1 + K_{n-2})$.

Subcase 1.2. If $n = \frac{3}{2}i - 2k + 2$, since $i < \frac{1}{2}(n + k)$, then $k + 3 \leq n < -5k + 8$. Hence $k = 0$, $n = 5$, $i = 2$, which is a contradiction to $n \geq 8$.

Case 2. We assume $i \geq 2$ and $n - \frac{3}{2}i + 2k - 2 < 0$. Since $i < \frac{1}{2}(n + k)$, $n \geq k + 3$, $n - \frac{3}{2}i + 2k - 2 > n - \frac{3}{2} \cdot \frac{1}{2}(n + k) + 2k - 2 = \frac{n}{4} + \frac{5}{4}k - 2 \geq \frac{6k - 5}{4}$. If $k \geq 1$, then $n - \frac{3}{2}i + 2k - 2 > 0$, a contradiction. If $k = 0$, then $i < \frac{n}{2}$, $n - \frac{3}{2}i - 2 > n - \frac{3}{2} \cdot \frac{n}{2} - 2 = \frac{n}{4} - 2 \geq 0$, a contradiction. Combining with the discussion of Case 1, we can get the conclusion.

If $f(x)$ is a monotonically decreasing function on $[1, n-1]$, we can prove the result by a similar method. The proof is complete. □

By Theorem 3.12, when $f(x) = x, \frac{1}{x}, \frac{x^2 + x}{2}, x^\lambda$, we have the following corollaries.

Corollary 3.13. *Let G be a connected graph of order $n \geq 8$ and $0 \leq k \leq n - 3$. If its Wiener index*

$$W(G) \leq \frac{1}{2}n^2 + \frac{1}{2}n - (nk + \frac{1}{2}k^2 - \frac{5}{2}k + 2),$$

then G is k-edge-hamiltonian unless $G = K_1 \vee (K_1 + K_{n-2})$.

Corollary 3.14. *Let G be a connected graph of order $n \geq 8$ and $0 \leq k \leq n - 3$. If its Harary index*

$$H(G) \geq \frac{1}{2}n^2 - n + \frac{1}{2}(nk + \frac{1}{2}k^2 - \frac{5}{2}k + 2),$$

then G is k-edge-hamiltonian unless $G = K_1 \vee (K_1 + K_{n-2})$.

Corollary 3.15. *Let G be a connected graph of order $n \geq 8$ and $0 \leq k \leq n - 3$. If its hyper-Wiener index*

$$WW(G) \leq \frac{1}{2}n^2 + \frac{3}{2}n - 2(nk + \frac{1}{2}k^2 - \frac{5}{2}k + 2),$$

then G is k-edge-hamiltonian unless $G = K_1 \vee (K_1 + K_{n-2})$.

Corollary 3.16. *Let G be a connected graph of order $n \geq 8$ and $0 \leq k \leq n-3$. If its modified Wiener index*

$$W_f(G) \leq \frac{1}{2}n^2 + (2^\lambda - \frac{3}{2})n - (2^\lambda - 1)(nk + \frac{1}{2}k^2 - \frac{5}{2}k + 2),$$

for $\lambda > 0$, or

$$W_f(G) \geq \frac{1}{2}n^2 + (2^\lambda - \frac{3}{2})n + (1 - 2^\lambda)(nk + \frac{1}{2}k^2 - \frac{5}{2}k + 2),$$

for $\lambda < 0$, then G is k-edge-hamiltonian unless $G = K_1 \vee (K_1 + K_{n-2})$.

Theorem 3.17. *Let G be a connected graph of order $n \geq 4$, $k \geq 1$.*

(1) If $f(x)$ is a monotonically increasing function $f(x)$ on $x \in [1, n-1]$, then we have the following results.

(i) For $k = n-3$ or $k < \frac{n-2}{5}$ and $n-k-1$ is odd, or $k < \frac{n-5}{5}$ and $n-k-1$ is even, if $W_f(G) \leq \frac{f(1)}{2}(n^2-n) - \frac{f(2)-f(1)}{2}(k^2-2nk-2n+5k+4)$, then G is k-path-coverable unless $G = K_1 \vee (\overline{K_{k+1}} + K_{n-k-2})$.

(ii) For $\frac{n-2}{5} \leq k \leq n-4$ and $n-k-1$ is odd, if $W_f(G) \leq \frac{f(2)+3f(1)}{8}n^2 + \frac{f(2)-3f(1)}{4}n + \frac{f(2)-f(1)}{2}[\frac{1}{4}k^2 + \frac{1}{2}nk + \frac{1}{2}k - 2]$, then G is k-path-coverable unless $G = K_{\frac{n-k-2}{2}} \vee (\overline{K_{\frac{n+k-2}{2}}} + K_2)$.

(iii) For $\frac{n-5}{5} \leq k \leq n-3$ and $n-k-1$ is even, if $W_f(G) \leq \frac{f(2)+3f(1)}{8}n^2 - \frac{f(1)}{2}n + \frac{f(2)-f(1)}{8}[k^2+2nk-1]$, then G is k-path-coverable unless $G = K_{\frac{n-k-1}{2}} \vee (\overline{K_{\frac{n+k-1}{2}}} + K_1)$.

(2) If $f(x)$ is a monotonically decreasing function $f(x)$ on $x \in [1, n-1]$, then we have the following results.

(i) For $k = n-3$ or $k < \frac{n-2}{5}$ and $n-k-1$ is odd, or $k < \frac{n-5}{5}$ and $n-k-1$ is even, if $W_f(G) \geq \frac{f(1)}{2}(n^2-n) - \frac{f(2)-f(1)}{2}(k^2-2nk-2n+5k+4)$, then G is k-path-coverable unless $G = K_1 \vee (\overline{K_{k+1}} + K_{n-k-2})$.

(ii) For $\frac{n-2}{5} \leq k \leq n-4$ and $n-k-1$ is odd, if $W_f(G) \geq \frac{f(2)+3f(1)}{8}n^2 + \frac{f(2)-3f(1)}{4}n + \frac{f(2)-f(1)}{2}[\frac{1}{4}k^2 + \frac{1}{2}nk + \frac{1}{2}k - 2]$, then G is k-path-coverable unless $G = K_{\frac{n-k-2}{2}} \vee (\overline{K_{\frac{n+k-2}{2}}} + K_2)$.

(iii) For $\frac{n-5}{5} \leq k \leq n-3$ and $n-k-1$ is even, if $W_f(G) \geq \frac{f(2)+3f(1)}{8}n^2 - \frac{f(1)}{2}n + \frac{f(2)-f(1)}{8}[k^2+2nk-1]$, then G is k-path-coverable unless $G = K_{\frac{n-k-1}{2}} \vee (\overline{K_{\frac{n+k-1}{2}}} + K_1)$.

Proof. By refining the technique of Feng et al. [10], we have the following proof. Assume that G is not k-path-coverable and has degree sequence $(d_1, d_2, \ldots, d_n)$, where $d_1 \leq d_2 \leq \cdots \leq d_n$. By Lemma 2.5, there is an integer $1 \leq i \leq \frac{1}{2}(n-k-1)$ such that $d_{i+k} \leq i$ and $d_{n-i} \leq n-i-k-1$. Note that G is connected. If $f(x)$ is a monotonically increasing function for $x \in [1, n-1]$, as in the proof of Theorem 3.1, we have

$$\begin{aligned}
W_f(G) &\geq \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}\sum_{s=1}^{n} d_s \\
&= \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}(\sum_{s=1}^{i+k} d_s + \sum_{s=i+k+1}^{n-i} d_{n-i} + \sum_{s=n-i+1}^{n} d_s) \\
&\geq \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}[(i+k)i + (n-2i-k)(n-i-k-1) + i(n-1)] \\
&= \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}(n-k)(n-k-1) - \frac{f(2)-f(1)}{2}[3i^2 - (2n-4k-1)i].
\end{aligned}$$

Similarly, if $f(x)$ is a monotonically decreasing function for $x \in [1, n-1]$, then

$$W_f(G) \leq \frac{1}{2}n(n-1)f(2) + \frac{f(1)-f(2)}{2}(n-k)(n-k-1) + \frac{f(1)-f(2)}{2}[3i^2 - (2n-4k-1)i].$$

If $f(x)$ is a monotonically increasing function on $[1, n-1]$, then we have the following discussion.

Suppose $g(x) = 3x^2 - (2n-4k-1)x$ with $1 \leq x \leq \frac{1}{2}(n-k-1)$. Since $n-k \geq 2i+1 \geq 3$, $1 \leq k \leq n-3$. Because x is an integer, then we have to consider $n-k-1$ is odd or even.

Case 1. If $n-k-1$ is odd, then $1 \leq x \leq \frac{1}{2}(n-k-2)$. So, $g(1) = -2n+4k+4$, $g(\frac{1}{2}(n-k-2)) = (-\frac{1}{4}n + \frac{5}{4}k - 1)(n-k-2)$, $g(\frac{1}{2}(n-k-2)) - g(1) = -\frac{1}{4}(n-k-4)(n-5k-2)$. Then we consider the following three subcases.

Subcase 1.1. If $k = n-3$, then $n-k-4 = -1 < 0$, $n-5k-2 = -4n+13 < 0$. Hence $g(\frac{1}{2}(n-k-2)) < g(1)$, $g_{max}(x) = g(1)$. Thus,

$$\begin{aligned} W_f(G) &\geq \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}(n-k)(n-k-1) - \frac{f(2)-f(1)}{2}(4+4k-2n) \\ &= \frac{f(1)}{2}(n^2-n) - \frac{f(2)-f(1)}{2}(k^2 - 2nk - 2n + 5k + 4). \end{aligned}$$

So we get the result. If $W_f(G) = \frac{f(1)}{2}(n^2-n) - \frac{f(2)-f(1)}{2}(k^2 - 2nk - 2n + 5k + 4)$, then $i = 1$, and hence $d_1 = \cdots = d_{k+1} = 1$, $d_{k+2} = \cdots = d_{n-1} = n-k-2$, $d_n = n-1$, which implies $G = K_1 \vee (\overline{K_{k+1}} + K_{n-k-2})$.

Subcase 1.2. If $\frac{n-2}{5} \leq k \leq n-4$, then $n-k-4 > 0$, $n-5k-2 < 0$. Hence $g(\frac{1}{2}(n-k-2)) > g(1)$, $g_{max}(x) = g(\frac{1}{2}(n-k-2))$. Thus,

$$\begin{aligned} W_f(G) &= \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}(n-k)(n-k-1) \\ &\quad - \frac{f(2)-f(1)}{2}(-\frac{1}{4}n + \frac{5}{4}k - 1)(n-k-2) \\ &= \frac{f(2)+3f(1)}{8}n^2 + \frac{f(2)-3f(1)}{4}n + \frac{f(2)-f(1)}{2}[\frac{1}{4}k^2 + \frac{1}{2}nk + \frac{1}{2}k - 2]. \end{aligned}$$

So we get the result. If $W_f(G) = \frac{f(2)+3f(1)}{8}n^2 + \frac{f(2)-3f(1)}{4}n + \frac{f(2)-f(1)}{2}[\frac{1}{4}k^2 + \frac{1}{2}nk + \frac{1}{2}k - 2]$, then $i = \frac{1}{2}(n-k-2)$, and hence $d_1 = d_2 = \cdots = d_{\frac{n+k-2}{2}} = \frac{n-k-2}{2}$, $d_{\frac{n+k}{2}} = d_{\frac{n+k+2}{2}} = \frac{n-k}{2}$, $d_{\frac{n+k+4}{2}} = \cdots = d_n = n-1$, which implies $G = K_{\frac{n-k-2}{2}} \vee (\overline{K_{\frac{n+k-2}{2}}} + K_2)$.

Subcase 1.3. If $k < \frac{n-2}{5}$, then $n-k-4 > 0$, $n-5k-2 > 0$. Then $g(\frac{1}{2}(n-k-2)) < g(1)$, $g_{max}(x) = g(1)$. This case is the same as proved in Subcase 1.1. We omit the details.

Case 2. If $n-k-1$ is even, then $1 \leq x \leq \frac{1}{2}(n-k-1)$. So $f(1) = -2n+4k+4$, $f(\frac{1}{2}(n-k-1)) = -\frac{1}{4}(n-k-1)(n-5k+1)$, $f(\frac{1}{2}(n-k-1)) - f(1) = -\frac{1}{4}(n-k-3)(n-5k-5)$. Then we consider the following two subcases.

Subcase 2.1. If $\frac{n-5}{5} \le k \le n-3$, then $n-k-3 > 0$, $n-5k-5 < 0$. Hence $g(\frac{1}{2}(n-k-1)) > g(1)$, $g_{max}(x) = g(\frac{n-k-1}{2})$. Thus,

$$\begin{aligned} W_f(G) &= \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}(n-k)(n-k-1) \\ &\quad - \frac{f(2)-f(1)}{2}[-\frac{1}{4}(n-k-1)(n-5k+1)] \\ &= \frac{f(2)+3f(1)}{8}n^2 - \frac{f(1)}{2}n + \frac{f(2)-f(1)}{8}[k^2+2nk-1]. \end{aligned}$$

So we get the result. If $W_f(G) = \frac{f(2)+3f(1)}{8}n^2 - \frac{f(1)}{2}n + \frac{f(2)-f(1)}{8}[k^2+2nk-1]$, then $i = \frac{1}{2}(n-k-1)$, and hence $d_1 = d_2 = \cdots = d_{\frac{n+k-1}{2}} = \frac{n-k-1}{2}$, $d_{\frac{n+k+1}{2}} = \frac{n-k-1}{2}$, $d_{\frac{n+k+3}{2}} = \cdots = d_n = n-1$. Thus, $G = K_{\frac{n-k-1}{2}} \vee (\overline{K_{\frac{n+k-1}{2}}} + K_1)$.

Subcase 2.2. If $k < \frac{n-5}{5}$, then $n-k-3 > 0$, $n-5k-5 > 0$. Hence $g(\frac{1}{2}(n-k-1)) < g(1)$, $g_{max} = g(1)$. This case is the same as proved in Subcase 1.1. We omit the details.

If $f(x)$ is a monotonically decreasing function on $[1, n-1]$, we can prove the result by a similar method. The proof is complete. □

From Theorem 3.17, the previous work (see Theorem 3.4 in [10]) is a direct corollary when $f(x) = x, \frac{1}{x}$. Moreover, when $f(x) = \frac{x^2+x}{2}, x^\lambda$ in Theorem 3.17, we have the following corollaries.

Corollary 3.18. *Let G be a connected graph of order* $n \ge 4$, $k \ge 1$.

(1) *For* $k = n-3$ *or* $k < \frac{n-2}{5}$ *and* $n-k-1$ *is odd, or* $k < \frac{n-5}{5}$ *and* $n-k-1$ *is even, if its hyper-Wiener index* $WW(G) \le \frac{1}{2}(n^2-n) - (k^2-2nk-2n+5k+4)$, *then G is k-path-coverable unless* $G = K_1 \vee (\overline{K_{k+1}} + K_{n-k-2})$.

(2) *For* $\frac{n-2}{5} \le k \le n-4$ *and* $n-k-1$ *is odd, if its hyper-Wiener index* $WW(G) \le \frac{3}{4}n^2 + \frac{1}{4}k^2 + \frac{1}{2}nk + \frac{1}{2}k - 2$, *then G is k-path-coverable unless* $G = K_{\frac{n-k-2}{2}} \vee (\overline{K_{\frac{n+k-2}{2}}} + K_2)$.

(3) *For* $\frac{n-5}{5} \le k \le n-3$ *and* $n-k-1$ *is even, if its hyper-Wiener index* $WW(G) \le \frac{3}{4}n^2 - \frac{1}{2}n + \frac{1}{4}[k^2+2nk-1]$, *then G is k-path-coverable unless* $G = K_{\frac{n-k-1}{2}} \vee (\overline{K_{\frac{n+k-1}{2}}} + K_1)$.

Corollary 3.19. *Let G be a connected graph of order* $n \ge 4$, $k \ge 1$.

(1) *If* $\lambda > 0$, *then we have the following results.*

  (i) *For* $k = n-3$ *or* $k < \frac{n-2}{5}$ *and* $n-k-1$ *is odd, or* $k < \frac{n-5}{5}$ *and* $n-k-1$ *is even, if its modified Wiener index* $W_\lambda(G) \le \frac{1}{2}(n^2-n) - \frac{2^\lambda-1}{2}(k^2-2nk-2n+5k+4)$, *then G is k-path-coverable unless* $G = K_1 \vee (\overline{K_{k+1}} + K_{n-k-2})$.

  (ii) *For* $\frac{n-2}{5} \le k \le n-4$ *and* $n-k-1$ *is odd, if its modified Wiener index* $W_\lambda(G) \le \frac{2^\lambda+3}{8}n^2 + \frac{2^\lambda-3}{4}n + \frac{2^\lambda-1}{2}(\frac{1}{4}k^2 + \frac{1}{2}nk + \frac{1}{2}k - 2)$, *then G is k-path-coverable unless* $G = K_{\frac{n-k-2}{2}} \vee (\overline{K_{\frac{n+k-2}{2}}} + K_2)$.

  (iii) *For* $\frac{n-5}{5} \le k \le n-3$ *and* $n-k-1$ *is even, if its modified Wiener index* $W_\lambda(G) \le \frac{2^\lambda+3}{8}n^2 - \frac{1}{2}n + \frac{2^\lambda-1}{8}(k^2+2nk-1)$, *then G is k-path-coverable unless* $G = K_{\frac{n-k-1}{2}} \vee (\overline{K_{\frac{n+k-1}{2}}} + K_1)$.

(2) *If* $\lambda < 0$, *then we have the following results.*

  (i) *For* $k = n-3$ *or* $k < \frac{n-2}{5}$ *and* $n-k-1$ *is odd, or* $k < \frac{n-5}{5}$ *and* $n-k-1$ *is even, if its modified Wiener index* $W_\lambda(G) \ge \frac{1}{2}(n^2-n) - \frac{2^\lambda-1}{2}(k^2-2nk-2n+5k+4)$, *then G is k-path-coverable unless* $G = K_1 \vee (\overline{K_{k+1}} + K_{n-k-2})$.

(ii) For $\frac{n-2}{5} \le k \le n-4$ *and* $n-k-1$ *is odd, if its modified Wiener index* $W_\lambda(G) \ge \frac{2^\lambda+3}{8}n^2 + \frac{2^\lambda-3}{4}n + \frac{2^\lambda-1}{2}(\frac{1}{4}k^2 + \frac{1}{2}nk + \frac{1}{2}k - 2)$*, then G is k-path-coverable unless* $G = K_{\frac{n-k-2}{2}} \vee (\overline{K_{\frac{n+k-2}{2}}} + K_2)$.

(iii) For $\frac{n-5}{5} \le k \le n-3$ *and* $n-k-1$ *is even, if its modified Wiener index* $W_\lambda(G) \ge \frac{2^\lambda+3}{8}n^2 - \frac{1}{2}n + \frac{2^\lambda-1}{8}(k^2+2nk-1)$*, then G is k-path-coverable unless* $G = K_{\frac{n-k-1}{2}} \vee (\overline{K_{\frac{n+k-1}{2}}} + K_1)$.

Theorem 3.20. *Let G be a connected graph of order n and* $\alpha(G)$ *be its independent number. If*

$$W_f(G) \le \frac{f(1)}{2}(n^2-n) + \frac{f(2)-f(1)}{2}(k^2+k),$$

for a monotonically increasing function $f(x)$ *on* $x \in [1, n-1]$*, or*

$$W_f(G) \ge \frac{f(1)}{2}(n^2-n) - \frac{f(1)-f(2)}{2}(k^2+k),$$

for a monotonically decreasing function $f(x)$ *on* $x \in [1, n-1]$*, then G satisfies* $\alpha(G) \le k$ *unless* $G = \overline{K_{k+1}} \vee K_{n-k-1}$.

Proof. Suppose that G does not satisfy $\alpha(G) \le k$ and has degree sequence $(d_1, d_2, \ldots, d_n)$, where $d_1 \le d_2 \le \cdots \le d_n$. By Lemma 2.6, we have $d_{k+1} \le n-k-1$. Note that G is connected. If $f(x)$ is a monotonically increasing function for $x \in [1, n-1]$, as the proof of Theorem 3.1, we have

$$\begin{aligned} W_f(G) &\ge \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}\sum_{s=1}^{n} d_s \\ &= \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}(\sum_{s=1}^{k+1} d_s + \sum_{s=k+2}^{n} d_s) \\ &\ge \frac{1}{2}n(n-1)f(2) - \frac{f(2)-f(1)}{2}[(k+1)(n-k-1) + (n-k-1)(n-1)] \\ &= \frac{f(1)}{2}(n^2-n) + \frac{f(2)-f(1)}{2}(k^2+k). \end{aligned}$$

Similarly, if $f(x)$ is a monotonically decreasing function for $x \in [1, n-1]$, then

$$W_f(G) \le \frac{f(1)}{2}(n^2-n) - \frac{f(1)-f(2)}{2}(k^2+k).$$

If $f(x)$ is a monotonically increasing function on $[1, n-1]$, we can get a contradiction. If $W_f(G) = \frac{f(1)}{2}(n^2-n) + \frac{f(2)-f(1)}{2}(k^2+k)$, then all the inequalities in the above arguments should be equalities. Thus, we have (a) the diameter of G is no more than two; (b) $d_1 = \cdots = d_{k+1} = n-k-1$, $d_{k+2} = \cdots = d_n = n-1$. It implies that $G = \overline{K_{k+1}} \vee K_{n-k-1}$, which does not satisfy $\alpha(G) \le k$.

If $f(x)$ is a monotonically decreasing function on $[1, n-1]$, we can prove the result by a similar method. The proof is complete. □

From Theorem 3.20, the previous work (see Theorem 3.6 in [10]) is a direct corollary when $f(x) = x, \frac{1}{x}$. Moreover, when $f(x) = \frac{x^2+x}{2}, x^\lambda$ in Theorem 3.20, we have the following corollaries.

Corollary 3.21. *Let G be a connected graph of order n,* $\alpha(G)$ *be its independent number. If its hyper-Wiener index*

$$WW(G) \le \frac{1}{2}(n^2-n) + k^2 + k,$$

then G satisfies $\alpha(G) \le k$ *unless* $G = \overline{K_{k+1}} \vee K_{n-k-1}$.

Corollary 3.22. *Let G be a connected graph of order n, $\alpha(G)$ be its independent number. If its modified Wiener index*

$$W_\lambda(G) \le \frac{1}{2}(n^2 - n) + \frac{2^\lambda - 1}{2}(k^2 + k),$$

for $\lambda > 0$, or

$$W_\lambda(G) \ge \frac{1}{2}(n^2 - n) - \frac{1 - 2^\lambda}{2}(k^2 + k),$$

for $\lambda < 0$, then G satisfies $\alpha(G) \le k$ unless $G = \overline{K_{k+1}} \vee K_{n-k-1}$.

Acknowledgements

The authors thank to Professor Lihua Feng for giving them the preprints of [10]. The authors are also grateful to the referees for their valuable comments, corrections and suggestions which led to considerable improvements in presentation.

References

[1] D. Bauer, H.J. Broersma, J. van den Heuvel, N. Kahl, A. Nevo, E. Schmeichel, D.R. Woodall, M. Yatauro, Best monotone degree conditions for graph properties: a survey, Graphs Combin. 31 (2015) 1–22.
[2] J.A. Bondy, Properties of graphs with constraints on degree, Studia Sci. Math. Hunger, 4 (1969) 473–475.
[3] J.A. Bondy, U.S.R. Murty, Graph Theory, Grad. Texts in Math, vol. 244, Springer, New York, 2008.
[4] V. Chvátal, On Hamiltons ideals, J. Combin. Theory Ser. B, 12 (1972) 163–168.
[5] J.A. Bondy, V. Chvátal, A method in graph theory, Discrete Math. 15 (1976) 111-135.
[6] K.C. Das, B. Zhou, N. Trinajstić, Bounds on Harary index, J. Math. Chem. 46 (2009) 1369–1376.
[7] M.V. Diudea, I. Gutman, Wiener-type topological indices, Croatica Chemica Acta, 71 (1998) 21–52.
[8] A.A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, Acta Appl. Math., 66 (2001) 211–249.
[9] A.A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002) 247–924.
[10] L. H. Feng, X. M. Zhu, W. J. Liu, Wiener index, Harary index and graph properties, Discrete Appl. Math. 223 (2017) 72–83.
[11] I. Gutman, A property of the Wiener number and its modidications, Indian J. Chem. 36A (1997) 128–132.
[12] A. Hamzeh, S. Hossein-Zadeh, A.R. Ashrafi, Extremal graphs under Wiener-type invariants, MATCH Commun. Math. Comput. Chem. 69 (2013) 47–54.
[13] H.B. Hua, M.L. Wang, On Harary index and traceable graphs, MATCH Commun. Math. Comput. Chem. 70 (2013) 297–300.
[14] O. Ivanciuc, T.S. Balaban, A.T. Balaban, Reciprocal distance matrix, related local vertex invariants and topolgical indices, J. Math. Chem. 12 (1993) 309–318.
[15] S. Klavšić, I. Gutman, Relation between Wiener-type topological indices of benzenoid molecules, Chem. Phys. Lett. 373 (2003) 328–332.
[16] M. Knor, R. Škrekovski, A. Tepeh, Mathematical aspects of Wiener index, Ars Math. Contemp., 11 (2016) 327–352.
[17] H.V. Kronk, A note on k-path hamiltonian graphs, J. Combin. Theory, 7 (1969) 104–106.
[18] M.J. Kuang, G.H. Huang, H.Y. Deng, Some sufficient conditions for Hamiltonian property in terms of Wiener-type invariants, Proceedings Mathematical Sciences, 126 (2016) 1–9.
[19] M. Las Vergnas, Problémes de Couplages et Problémes Hamiltoniens en Théorie des Graphes, PhD Thesis, Université Paris VIPierre et Marie Curie, 1972.
[20] L. Lesniak, On n-hamiltonian graphs, Discrete Math. 14 (1976) 165–169.
[21] R. Li, Harary index and some Hamiltonian properties of graphs, AKCE International Journal of Graphs and Computing, 12 (2015) 64–69.
[22] R. Li, Wiener index and some Hamiltonian properties of graphs, International Journal of Mathematics and Soft Computing, 5 (2015) 11–16.
[23] R.F. Liu, X. Du, H.C. Jia, Some observations on Harary index and traceable graphs, MATCH Commun. Math. Comput. Chem. 77 (2017) 195–208.
[24] R.F. Liu, X. Du, H.C. Jia, Wiener index on traceable and Hamiltonian graphs. Bull. Aust. Math. Soc. 94 (2016) 362–372.
[25] B. Lučić, A. Miličević, N. Trinajstić, Harary index-twelve years later, Croat. Chem. Acta. 75 (2002) 847–868.
[26] D. Plavšić, S. Nikolić, Z. Mihalić, On the Harary index for the characterization of chemical graphs, J. Math. Chem. 12 (1993) 235–250.
[27] M. Randić, Novel molecular descriptor for structure-property studies, Chem. Phys. Lett. 211 (1993) 478–483.
[28] R. Todeschini, V. Consonni, Handbook of Molecular Descriptpors, (2000) (Weinheim: Wiley VCH).
[29] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69 (1947) 17–20.
[30] K.X. Xu, N. Trinajstić, Hyper-Wiener indices and Harary indices of graphs with cut edges, Util. Math. 84 (2011) 153–163.
[31] L.H. Yang, Wiener index and traceable graphs, Bulletin of the Australian Mathematical Society, 88 (2013) 380–383.
[32] G.H. Yu, L.H. Feng, On the maximal Harary index of a class of bicyclic graphs, Util. Math. 82 (2010) 285–292.
[33] T. Zeng, Harary index and Hamiltonian property of graphs, MATCH Commun. Math. Comput. Chem. 70 (2013) 645–649.
[34] B. Zhou, X. Cai, N. Trinajstić, On the Harary index, J. Math. Chem. 44 (2008) 611–618.