SUFFICIENT CONDITIONS FOR CERTAIN STRUCTURAL PROPERTIES OF GRAPHS BASED ON WIENER-TYPE INDICES

HANYUAN DENG, MEIJUN KUANG, RENFANG WU, GUIHUA HUANG

Abstract. Let \( G = (V, E) \) be a simple connected graph with vertex set \( V \) and edge set \( E \). The Wiener-type invariants of \( G = (V, E) \) can be expressed in terms of the quantities \( W_f = \sum_{\{u, v\} \subseteq V} f(d_G(u, v)) \) for various choices of the function \( f \), where \( d_G(u, v) \) is the distance between the vertices \( u \) and \( v \) in \( G \). In this paper, we establish sufficient conditions based on Wiener-type indices under which every path of length \( r \) is contained in a Hamiltonian cycle and under which a bipartite graph on \( n + m, m > n \), vertices contains a cycle of size \( 2n \).

1. INTRODUCTION

A topological index is a numerical quantity related to a graph that is invariant under graph isomorphism. In the case when the molecular structure of a chemical compound is represented by a graph, topological indices are required to be related with some of the physicochemical, pharmacological, toxicological, or other similar properties of the underlying compound. If this is the case, then these properties can be modeled by means of topological indices. One of the most widely known topological descriptors is the Wiener index [19],

\[
W(G) = \sum_{\{u, v\} \subseteq V} d_G(u, v) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} d_G(v_i, v_j),
\]

where \( G = (V, E) \) is the graph representing the molecule under consideration, \( V = \{v_1, v_2, \cdots, v_n\} \) is its vertex set, and \( d_G(u, v) \) is the distance between vertices \( u \) and \( v \) in \( G \). More details on vertex distances and the Wiener index can be found in the reviews [5, 6, 21].

Several generalizations and modifications of the Wiener index have been put forward. Many of these Wiener-type invariants can be expressed in...
terms of the quantities

$$W_f = W_f(G) = \sum_{\{u,v\} \subseteq V} f(d_G(u, v)) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} f(d_G(v_i, v_j))$$

for various choices of the function $f$. The quantity $W_f$ is called the Wiener-type index with respect to $f$.

In particular, we observe the following: (i) if the function $f$ is $x$, then $W_f = W_x$ coincides with the ordinary Wiener index, denoted by $W(G)$; (ii) if the function $f$ is $1/x$, then $W_f = W_{1/x}$ was named the Harary index in [15], or the reciprocal Wiener index in [4], and is denoted by $H(G)$; (iii) if the function $f$ is $(x^2 + x)/2$, then $W_f = W_{x^2+x/2}$ was named the hyper-Wiener index in [17], and is denoted by $WW(G)$; and (iv), if the function $f$ is $x^\lambda$ (where $\lambda \neq 0$ is a real number), then $W_f = W_{x^\lambda}$ was named the modified Wiener index in [10], and is denoted by $W_{\lambda}(G)$. There are many papers that have studied the invariant $W_{\lambda}$; see [3, 11, 13, 14, 18] and the references cited therein for details.

In this paper we consider only simple undirected graphs—graphs that do not contain loops or multiple edges. A Hamiltonian cycle is a closed path passing through every vertex of a graph. The length of a path or a cycle in a graph is the number of its edges in the path or cycle. A graph containing a Hamiltonian cycle is said to be Hamiltonian. In fact, finding a Hamiltonian cycle is a very difficult task. It is one of the six well-known problems that constituted the class of NP-Complete problems in the initial days of the theory of computational complexity; see [8] for details. The Hamiltonicity of graphs has been studied in terms of independent sets, dominating circuits, degrees, neighborhood conditions of a graph, etc.; see [7, 12, 20, 22, 23].

In [9], Grötschel obtained a sufficient condition for the following property of a graph: given any path of length $r$, there is a cycle of length at least $m \geq r + 3$ containing this path, which implies the well-known theorem of Chvátal [2] on Hamiltonian graphs and the theorem of Pósa [16] on a graph containing cycles a certain length. In this paper, we establish sufficient conditions based on Wiener-type indices under which every path of length $r$ is contained in a Hamiltonian cycle, and conditions under which a bipartite graph on $n + m$, $m > n$, vertices contains a cycle of size $2n$.

2. Preliminaries

Before proceeding, we introduce some further notation. For a simple connected graph $G = (V, E)$, the degree of a vertex $v$ in $G$, denoted by $d_G(v)$, is the number of edges of $G$ incident with $v$, and the distance between two vertices $u$ and $v$ in $G$, denoted by $d_G(u, v)$, is the length of a shortest path connecting $u$ and $v$ in $G$. The diameter of a graph $G$, denoted by $D(G)$, is the maximum distance in $G$. The graph $K_n$ is the complete graph on $n$ vertices. Let $G$ and $H$ be two vertex-disjoint graphs. The join of $G$ and $H$, denoted by $G \vee H$, is the graph with the vertex set $V(G) \cup V(H)$ and the
edge set $E(G) \cup E(H) \cup \{uv\mid u \in V(G) \text{ and } v \in V(H)\}$. The union of $G$ and $H$, denoted by $G \cup H$, is the graph with the vertex set $V(G) \cup V(H)$ and the edge set $E(G) \cup E(H)$.

A bipartite graph with the vertex set $V \cup W$ and the edge set $E$, denoted by $G = (V,W;E)$, is one whose vertex set can be partitioned into two subsets $V$ and $W$ such that each edge has one end in $V$ and one end in $W$; such a partition $(V,W)$ is called a bipartition of the graph. A complete bipartite graph is a simple bipartite graph with bipartition $(V,W)$ in which each vertex of $V$ is joined to each vertex of $W$; if $|V| = n$ and $|W| = m$, such a graph is denoted by $K_{n,m}$.

For other notation and terminology not defined here, the readers are referred to [1].

In the following, we present two of the relevant results for a graph containing a special cycle.

**Lemma 2.1** (Theorem 8 in [9]). Let $G = (V,E)$ be a graph of order $n$, let $(d_1,d_2,\ldots,d_n)$ be the degree sequence of $G$, where $d_1 \leq d_2 \leq \cdots \leq d_n$, and let $r$ be an integer with $0 \leq r \leq n-3$. If for every integer $k$ with $r < k < (n+r)/2$, we have that $d_{n-k} \leq k$ implies that $d_{n-k} \geq n-k+r$, then for every path $Q$ of length $r$ there is a Hamiltonian cycle in $G$ which contains $Q$.

**Lemma 2.2** (Corollary 11 in [9]). Let $G = (V,W;E)$ be a bipartite graph with bipartition $(V,W)$ and degree sequence
\[(d(w_1),d(w_2),\ldots,d(w_m),d(v_1),d(v_2),\ldots,d(v_n)),\]
where $V = \{v_1,v_2,\ldots,v_n\}$, $W = \{w_1,w_2,\ldots,w_m\}$, $d(w_1) \leq \cdots \leq d(w_m)$, $d(v_1) \leq \cdots \leq d(v_n)$, and $n \leq m$. If $d(w_k) \leq k \leq n-1$ implies that $d(v_{n-k}) \geq m-k+1$, then $G$ contains a cycle of length $2n$.

3. Main Results

The following result gives a sufficient condition based on the Wiener-type index under which every path of length $r$ is contained in a Hamiltonian cycle.

**Theorem 3.1.** Let $G = (V,E)$ be a graph of order $n$, $n \geq 3$, and $0 \leq r < n-3$. If
\[W_f(G) \leq \frac{f(1)}{2}(n^2 - 3n + 2r + 4) + f(2)(n-r-2)\]
for a monotonically increasing function $f$ defined on the interval $[1,D(G)]$, or if
\[W_f(G) \geq \frac{f(1)}{2}(n^2 - 3n + 2r + 4) + f(2)(n-r-2)\]
for a monotonically decreasing function $f$ defined on the interval $[1,D(G)]$, then for each path $Q$ of length $r$ there exists a Hamiltonian cycle in $G$ which contains $Q$. 
Proof. Let $V = \{v_1, v_2, \cdots, v_n\}$ be the vertex set of $G$ and let $(d_1, d_2, \cdots, d_n)$ be the degree sequence of $G$ with $d_1 \leq d_2 \leq \cdots \leq d_n$. Assume that there is a path $Q$ of length $r$ in $G$, but that no Hamiltonian cycle contains $Q$. By Lemma 2.1, there is an integer $k$, $r < k < (n + r)/2$, such that $d_{k-r} \leq k$ and $d_{n-k} \leq n - k + r - 1$. Then

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

$$= 3k^2 - 4kr - 2nk + k + n^2 - n + 2nr + r^2 - r$$

$$= (k - r - 1)(3k - r - 2n + 4) + n^2 - 3n + 2r + 4.$$

When $n + r$ is even, we have

$$3k - r - 2n + 4 \leq \frac{3(n + r)}{2} - 3 - r - 2n + 4 = \frac{r - n + 2}{2} < 0.$$

When $n + r$ is odd, we have

$$3k - r - 2n + 4 \leq \frac{3(n + r)}{2} - \frac{3}{2} - r - 2n + 4 = \frac{r - n + 5}{2} \leq 0.$$

Thus, $\sum_{i=1}^{n} d_i \leq n^2 - 3n + 2r + 4$.

If $f$ is an monotonically increasing function defined on the interval $[1, D(G)]$, then

$$W_f(G) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} f(d_G(v_i, v_j))$$

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

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

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

$$\geq \frac{f(2)}{2} n(n - 1) - \frac{f(2) - f(1)}{2} (n^2 - 3n + 2r + 4)$$

$$= \frac{f(1)}{2} (n^2 - 3n + 2r + 4) + f(2)(n - r - 2).$$
Corollary 3.2. Let $G = (V, E)$ be a graph of order $n$, $n \geq 3$, and $0 \leq r < n - 3$. If $W(G) \leq (n^2 + n - 2r - 4)/2$, then for each path $Q$ of length $r$, there is a Hamiltonian cycle in $G$ which contains $Q$. 
Corollary 3.3. Let $G = (V, E)$ be a graph of order $n$, $n \geq 3$, and $0 \leq r < n - 3$. If $Q(G) \geq (n^2 - 2n + r + 2)/2$, then for each path $Q$ of length $r$, there is a Hamiltonian cycle in $G$ which contains $Q$.

Corollary 3.4. Let $G = (V, E)$ be a graph of order $n$, $n \geq 3$, and $0 \leq r < n - 3$. If $WW(G) \leq (n^2 + 3n - 4r - 8)/2$, then for each path $Q$ of length $r$, there is a Hamiltonian cycle in $G$ which contains $Q$.

Corollary 3.5. Let $G = (V, E)$ be a graph of order $n$, $n \geq 3$, and $0 \leq r < n - 3$. If

$$W_{\lambda}(G) \leq \frac{n^2 - 3n + 2r + 4}{2} + 2^\lambda(n - r - 2)$$

for $\lambda > 0$, or if

$$W_{\lambda}(G) \geq \frac{n^2 - 3n + 2r + 4}{2} + 2^\lambda(n - r - 2)$$

for $\lambda < 0$, then for each path $Q$ of length $r$, there is a Hamiltonian cycle in $G$ which contains $Q$.

In the following, we will establish sufficient conditions based on Wiener-type indices under which a bipartite graph contains a cycle of size $2n$.

Let $G_1 = (V, W; E)$ be the simple bipartite graph with bipartition $(V, W)$ and degree sequences $d(w_1) = 1, d(w_2) = \cdots = d(w_m) = n, d(v_1) = \cdots = d(v_{n-1}) = m - 1$, and $d(v_n) = m$. Furthermore, let $G_2 = (V, W; E)$ be the simple bipartite graph with bipartition $(V, W)$ and the degree sequences $d(w_1) = \cdots = d(w_{n-1}) = n - 1, d(w_n) = \cdots = d(w_m) = n, d(v_1) = m - n + 1, d(v_2) = \cdots = d(v_n) = m$, where $V = \{v_1, v_2, \ldots, v_n\}$ and $W = \{w_1, w_2, \ldots, w_m\}$. Note that $G_1$ and $G_2$ contain a cycle of length $2n$ if and only if $n < m$. Moreover, $G_1 \cong G_2 \cong K^*_n,n$ when $n = m$, where $K^*_n,n$ is the bipartite graph obtained from the complete bipartite graph $K_n,n$ by deleting $n - 1$ edges incident with a common vertex.

Theorem 3.6. Let $G = (V, W; E)$ be a simple bipartite graph with bipartition $(V, W)$, where $|V| = n$, $|W| = m$, and $n \leq m$. If

$$W_f(G) \leq f(1)(nm - n + 1) + \frac{f(2)}{2}(m^2 + n^2 - m - n) + f(3)(n - 1)$$

for a monotonically increasing function $f$ defined on the interval $[1, D(G)]$, or if

$$W_f(G) \geq f(1)(nm - n + 1) + \frac{f(2)}{2}(m^2 + n^2 - m - n) + f(3)(n - 1)$$

for a monotonically decreasing function $f$ defined on the interval $[1, D(G)]$, then $G$ contains a cycle of length $2n$ or $G \cong K_n^*$.n

Proof. Let $G = (V, W; E)$ be a simple bipartite graph with bipartition $(V, W)$ and degree sequences

$$(d(w_1), d(w_2), \ldots, d(w_m), d(v_1), d(v_2), \ldots, d(v_n)),$$
where \( n \leq m \), \( V = \{v_1, v_2, \ldots, v_n\} \), \( W = \{w_1, w_2, \ldots, w_m\} \), \( d(w_1) \leq \cdots \leq d(w_m) \) and \( d(v_1) \leq \cdots \leq d(v_n) \).

Suppose that \( G \) contains no cycle of length \( 2n \). By Lemma 2.2, there is an integer \( k \), \( 0 < k < n \), such that 

\[
\sum_{i=1}^{m} d(w_i) + \sum_{j=1}^{n} d(v_j) \leq k^2 + n(m - k) + (n - k)(m - k) + km
\]

\[
= 2k^2 - 2nk + 2nm
\]

\[
= 2(k - 1)(k - n + 1) - 2n + 2nm + 2
\]

\[
\leq 2nm - 2n + 2.
\]

If \( f \) is a monotonically increasing function defined on the interval \([1, D(G)]\), then:

\[
W_f(G) = \sum_{i=1}^{m} \sum_{j=1}^{n} f(d_G(w_i, v_j)) + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} f(d_G(w_i, w_j))
\]

\[
+ \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} f(d_G(v_i, v_j))
\]

\[
\geq \frac{1}{2} \left( \sum_{i=1}^{m} f(1)d(w_i) + f(3)(n - d(w_i)) \right)
\]

\[
+ \frac{1}{2} \left( \sum_{j=1}^{n} f(1)d(v_j) + f(3)(m - d(v_j)) \right)
\]

\[
+ \frac{1}{2} \left( m(m - 1)f(2) + \frac{1}{2}n(n - 1)f(2) \right)
\]

\[
= \frac{1}{2} (f(1) - f(3)) \left( \sum_{i=1}^{m} d(w_i) + \sum_{j=1}^{n} d(v_j) \right) + f(3)mn
\]

\[
+ \frac{1}{2} f(2)(m^2 + n^2 - m - n)
\]

\[
\geq \frac{1}{2} (f(1) - f(3))(2mn - 2n + 2) + f(3)mn
\]

\[
+ \frac{1}{2} f(2)(m^2 + n^2 - m - n)
\]

\[
= f(1)(nm - n + 1) + \frac{f(2)}{2}(m^2 + n^2 - m - n) + f(3)(n - 1).
\]
If $f$ is a monotonically decreasing function defined on the interval $[1, D(G)]$, then:

$$W_f(G) = \sum_{i=1}^{m} \sum_{j=1}^{n} f(d_G(w_i, v_j)) + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} f(d_G(w_i, w_j)) + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} f(d_G(v_i, v_j))$$

$$\leq \frac{1}{2} \left( \sum_{i=1}^{m} f(1)d(w_i) + f(3)(n-d(w_i)) \right)$$

$$\frac{1}{2} \left( \sum_{j=1}^{n} f(1)d(v_j) + f(3)(m-d(v_j)) \right) + \frac{1}{2} m(m-1)f(2) + \frac{1}{2} n(n-1)f(2)$$

$$= \frac{1}{2} (f(1) - f(3)) \left( \sum_{i=1}^{m} d(w_i) + \sum_{j=1}^{n} d(v_j) \right) + f(3)mn$$

$$+ \frac{1}{2} f(2)(m^2 + n^2 - m - n)$$

$$\leq \frac{1}{2} (f(1) - f(3))[2mn - 2n + 2] + f(3)mn$$

$$+ \frac{1}{2} f(2)(m^2 + n^2 - m - n)$$

$$= f(1)(nm - n + 1) + \frac{f(2)}{2} (m^2 + n^2 - m - n) + f(3)(n-1)$$

Combining these facts with our assumption, we get

$$W_f(G) = f(1)(nm - n + 1) + \frac{f(2)}{2} (m^2 + n^2 - m - n) + f(3)(n-1),$$

while all equalities above are attained. Thus, we have that

(a) the diameter of $G$ is no more than three;
(b) $d(w_1) \cdots = d(w_k) = k, d(w_{k+1}) = \cdots = d(w_m) = n, d(v_1) \cdots = d(w_{n-k}) = m - k,$ and $d(w_{n-k+1}) = \cdots = d(w_n) = m$;
(c) $k = 1$ or $k = n - 1$.

If $k = 1$, then $d(w_1) = 1, d(w_2) = \cdots = d(w_m) = n$, and $d(v_1) = \cdots = d(v_{n-1}) = m - 1, d(v_n) = m$. If $k = n - 1$, then $d(w_1) = \cdots = d(w_{n-1}) = n - 1, d(w_n) = \cdots = d(w_m) = n, d(v_1) = m - n + 1$, and $d(v_2) = \cdots = d(v_n) = m$. Both cases imply that $G \cong G_1$ and $G \cong G_2$, respectively. If $n < m$, then $G_1$ and $G_2$ contain a cycle of length $2n$. If $n = m$, then $G \cong G_1 \cong G_2 \cong K_{n,n}^*$. $\square$
From Theorem 3.6, we can get the following sufficient conditions in terms of the Wiener index $W(G)$, the Harary index $H(G)$, the hyper-Wiener index $WW(G)$ and the modified Wiener index $W_\lambda(G)$, respectively, under which a simple bipartite graph $G$ contains a cycle of length $2n$.

**Corollary 3.7.** Let $G = (V, W, E)$ be a simple bipartite graph with partition $(V, W)$, where $|V| = n$, $|W| = m$, and $n \leq m$. If

$$W(G) \leq m^2 + n^2 + nm - m + n - 2,$$

then $G$ contains a cycle of length $2n$ or $G \cong K_{n,n}^*$. 

**Corollary 3.8.** Let $G = (V, W, E)$ be a simple bipartite graph with partition $(V, W)$, where $|V| = n$, $|W| = m$ and $n \leq m$. If

$$H(G) \geq \frac{3m^2 + 3n^2 + 12nm - 3m - 11n + 8}{12},$$

then $G$ contains a cycle of length $2n$ or $G \cong K_{n,n}^*$. 

**Corollary 3.9.** Let $G = (V, W, E)$ be a simple bipartite graph with partition $(V, W)$, where $|V| = n$, $|W| = m$, and $n \leq m$. If

$$WW(G) \leq \frac{3m^2 + 3n^2 + 2mn - 3m + 7n - 10}{2},$$

then $G$ contains a cycle of length $2n$ or $G \cong K_{n,n}^*$. 

**Corollary 3.10.** Let $G = (V, W, E)$ be a simple bipartite graph with partition $(V, W)$, where $|V| = n$, $|W| = m$, and $n \leq m$. If

$$W_\lambda(G) \leq nm - n + 1 + 2^{\lambda-1}(m^2 + n^2 - m - n) + 3^\lambda(n - 1)$$

for $\lambda > 0$, or if

$$W_\lambda(G) \geq nm - n + 1 + 2^{\lambda-1}(m^2 + n^2 - m - n) + 3^\lambda(n - 1)$$

for $\lambda < 0$, then $G$ contains a cycle of length $2n$ or $G \cong K_{n,n}^*$. 

**Acknowledgments**

The authors would like to thank the referee for many helpful comments and suggestions on an earlier version of this paper.

**References**


**College of Mathematics and Computer Science, Hunan Normal University,**

**Changsha, Hunan 410081, P.R. China**

**E-mail address:** Corresponding author: hydeng@hunnu.edu.cn