



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

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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, $V = \{v_1, v_2, \dots, v_n\}$ 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

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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^λ (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_λ ; 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, \dots, d_n) be the degree sequence of G , where $d_1 \leq d_2 \leq \dots \leq d_n$, and let r be a integer with $0 \leq r \leq n - 3$. If for every integer k with $r < k < (n + r)/2$, we have that $d_{k-r} \leq k$ 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*

$$(d(w_1), d(w_2), \dots, d(w_m), d(v_1), d(v_2), \dots, d(v_n)),$$

where $V = \{v_1, v_2, \dots, v_n\}$, $W = \{w_1, w_2, \dots, w_m\}$, $d(w_1) \leq \dots \leq d(w_m)$, $d(v_1) \leq \dots \leq d(v_n)$, 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 $V = \{v_1, v_2, \dots, v_n\}$ be the vertex set of G and let (d_1, d_2, \dots, d_n) be the degree sequence of G with $d_1 \leq d_2 \leq \dots \leq d_n$. 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 a integer k , $r < k < (n+r)/2$, such that $d_{k-r} \leq k$ and $d_{n-k} \leq n - k + r - 1$. Then

$$\begin{aligned} \sum_{i=1}^n d_i &\leq k(k-r) + (n-k+r-1)(n-2k+r) + (n-1)k \\ &= 3k^2 - 4kr - 2nk + k + n^2 - n + 2nr + r^2 - r \\ &= (k-r-1)(3k-r-2n+4) + n^2 - 3n + 2r + 4. \end{aligned}$$

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

$$\begin{aligned} W_f(G) &= \sum_{i=1}^{n-1} \sum_{j=i+1}^n f(d_G(v_i, v_j)) \\ &\geq \frac{1}{2} \sum_{i=1}^n [f(1)d_i + f(2)(n-1-d_i)] \\ &= \frac{1}{2} \sum_{i=1}^n [(n-1)f(2) + (f(1) - f(2))d_i] \\ &= \frac{f(2)}{2}n(n-1) - \frac{f(2) - f(1)}{2} \sum_{i=1}^n d_i \\ &\geq \frac{f(2)}{2}n(n-1) - \frac{f(2) - f(1)}{2}(n^2 - 3n + 2r + 4) \\ &= \frac{f(1)}{2}(n^2 - 3n + 2r + 4) + f(2)(n-r-2). \end{aligned}$$

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

$$\begin{aligned}
W_f(G) &= \sum_{i=1}^{n-1} \sum_{j=i+1}^n f(d_G(v_i, v_j)) \\
&\leq \frac{1}{2} \sum_{i=1}^n [f(1)d_i + f(2)(n-1-d_i)] \\
&= \frac{1}{2} \sum_{i=1}^n [(n-1)f(2) + (f(1) - f(2))d_i] \\
&= \frac{f(2)}{2}n(n-1) + \frac{f(1) - f(2)}{2} \sum_{i=1}^n d_i \\
&\leq \frac{f(2)}{2}n(n-1) + \frac{f(1) - f(2)}{2}(n^2 - 3n + 2r + 4) \\
&= \frac{f(1)}{2}(n^2 - 3n + 2r + 4) + f(2)(n - r - 2).
\end{aligned}$$

Combining these facts and our assumption, we get that

$$W_f(G) = \frac{f(1)}{2}(n^2 - 3n + 2r + 4) + f(2)(n - r - 2),$$

and note that all equalities above are attained. Thus we have that:

- (a) the diameter of G is no more than two;
- (b) $d_1 = d_2 = \dots = d_{k-r} = k$, $d_{k-r+1} = \dots = d_{n-k} = n - k + r - 1$, and $d_{n-k+1} = \dots = d_n = n - 1$;
- (c) $k - r - 1 = 0$ or $3k - r - 2n + 4 = 0$.

If $k = r + 1$, then $d_1 = r + 1$, $d_2 = \dots = d_{n-r-1} = n - 2$, and $d_{n-r} = \dots = d_n = n - 1$, which implies that $G \cong (K_1 \cup K_{n-r-2}) \vee K_{r+1}$. If $3k - r - 2n + 4 = 0$, then we have $r = n - 5$ and $k = n - 3$, since $r < k < (n + r)/2$ and both r and k are integers, which implies that $G \cong \overline{K_3} \vee K_{n-3}$.

It is easy to check that both $(K_1 \cup K_{n-r-2}) \vee K_{r+1}$ and $\overline{K_3} \vee K_{n-3}$ contain any path Q of length r , and we are done. \square

Since the functions x , $1/x$, $(x^2 + x)/2$ and x^λ are monotonically increasing or decreasing on the interval $[1, D(G)]$, 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 every path of length r is contained in a Hamiltonian cycle from Theorem 3.1.

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 $H(G) \geq (n^2 - 2n + r + 2)/2$, 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 $d(w_1) = \cdots = d(w_{n-1}) = n - 1$, $d(w_n) = \cdots = d(w_m) = n$, $d(v_1) = m - n + 1$, and $d(v_2) = \cdots = d(v_n) = m$, where $V = \{v_1, v_2, \dots, v_n\}$ and $W = \{w_1, w_2, \dots, w_m\}$. 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

$$(d(w_1), d(w_2), \dots, d(w_m), d(v_1), d(v_2), \dots, d(v_n)),$$

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

Suppose that G contains no cycle of length $2n$. By Lemma 2.2, there is a integer k , $0 < k < n$, such that $d(w_k) \leq k$ and $d(v_{n-k}) \leq m - k$. Then

$$\begin{aligned} \sum_{i=1}^m d(w_i) + \sum_{j=1}^n d(v_j) &\leq k^2 + n(m - k) + (n - k)(m - k) + km \\ &= 2k^2 - 2nk + 2nm \\ &= 2(k - 1)(k - n + 1) - 2n + 2nm + 2 \\ &\leq 2nm - 2n + 2. \end{aligned}$$

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

$$\begin{aligned} W_f(G) &= \sum_{i=1}^m \sum_{j=1}^n f(d_G(w_i, v_j)) + \sum_{i=1}^{m-1} \sum_{j=i+1}^m f(d_G(w_i, w_j)) \\ &\quad + \sum_{i=1}^{n-1} \sum_{j=i+1}^n f(d_G(v_i, v_j)) \\ &\geq \frac{1}{2} \left(\sum_{i=1}^m f(1)d(w_i) + f(3)(n - d(w_i)) \right) \\ &\quad + \frac{1}{2} \left(\sum_{j=1}^n f(1)d(v_j) + f(3)(m - d(v_j)) \right) \\ &\quad + \frac{1}{2}m(m - 1)f(2) + \frac{1}{2}n(n - 1)f(2) \\ &= \frac{1}{2}(f(1) - f(3)) \left(\sum_{i=1}^m d(w_i) + \sum_{j=1}^n d(v_j) \right) + f(3)mn \\ &\quad + \frac{1}{2}f(2)(m^2 + n^2 - m - n) \\ &\geq \frac{1}{2}(f(1) - f(3))(2mn - 2n + 2) + f(3)mn \\ &\quad + \frac{1}{2}f(2)(m^2 + n^2 - m - n) \\ &= f(1)(nm - n + 1) + \frac{f(2)}{2}(m^2 + n^2 - m - n) + f(3)(n - 1). \end{aligned}$$

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

$$\begin{aligned}
W_f(G) &= \sum_{i=1}^m \sum_{j=1}^n f(d_G(w_i, v_j)) + \sum_{i=1}^{m-1} \sum_{j=i+1}^m f(d_G(w_i, w_j)) \\
&\quad + \sum_{i=1}^{n-1} \sum_{j=i+1}^n f(d_G(v_i, v_j)) \\
&\leq \frac{1}{2} \left(\sum_{i=1}^m f(1)d(w_i) + f(3)(n - d(w_i)) \right) \\
&\quad + \frac{1}{2} \left(\sum_{j=1}^n f(1)d(v_j) + f(3)(m - d(v_j)) \right) \\
&\quad + \frac{1}{2}m(m-1)f(2) + \frac{1}{2}n(n-1)f(2) \\
&= \frac{1}{2}(f(1) - f(3)) \left(\sum_{i=1}^m d(w_i) + \sum_{j=1}^n d(v_j) \right) + f(3)mn \\
&\quad + \frac{1}{2}f(2)(m^2 + n^2 - m - n) \\
&\leq \frac{1}{2}(f(1) - f(3))[2mn - 2n + 2] + f(3)mn \\
&\quad + \frac{1}{2}f(2)(m^2 + n^2 - m - n) \\
&= f(1)(nm - n + 1) + \frac{f(2)}{2}(m^2 + n^2 - m - n) + f(3)(n - 1).
\end{aligned}$$

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 bipartition (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 bipartition (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 bipartition (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 bipartition (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 $G \cong K_{n,n}^$.*

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