

Wiener Index, Harary Index and Hamiltonicity of Graphs

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Abstract

In this paper, we prove tight sufficient conditions for traceability and Hamiltonicity of connected graphs with given minimum degree, in terms of Wiener index and Harary index. We also prove some result on Hamiltonicity of balanced bipartite graphs in the similar fashion. In two recent papers [9,10], Liu et al. corrected some previous work on traceability of connected graphs in terms of Wiener index and Harary index, respectively, such as [5,18]. We generalize these results and give short and unified proofs. All results in this paper are best possible.

1 Introduction

Let G be a graph. For two vertices u, v of G , the *distance* between u and v in G , denoted by $d_G(u, v)$, is the length of a shortest path from u to v in G . We denote by $diam(G)$ the diameter of G , and denote by $\delta(G)$ the minimum degree of G . For two graphs G and H , we denote the *union* of G and H by $G + H$, and the *join* of G and H by $G \vee H$. A graph is called *Hamiltonian* (*traceable*) if there is a cycle (path) including all vertices in it. A bipartite graph is called *balanced* if its each partition set has the same number of vertices. For terminology and notation not defined here, we refer the reader to West [16].

Our main purpose of this paper is to give tight sufficient conditions for Hamiltonicity and traceability of connected graphs and of connected balanced bipartite graphs with given

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minimum degree, in terms of Wiener index and Harary index, respectively. Furthermore, our work not only gives short and unified proofs of previous work due to Hua and Wang [5], and Yang [18], but also generalizes all these theorems. Our main tools come from Ning and Ge [13], and Li and Ning [7], respectively.

Recall that the *Wiener index* of a connected graph G , denote by $W(G)$, is defined to be the sum of distances between every pair of vertices in G . That is,

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

The Harary index is also a useful topological index in chemical graph theory and has received much attention during the past decades. This index has been introduced in 1993 by Plavšić et al. [15] and by Ivanciue et al. [6], independently. For a connected graph G , the *Harary index* of G , denoted by $H(G)$, is defined as

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

These two indices have found many applications in chemistry and there are lots of papers dealing with these two indices, see surveys [11, 17].

In this paper, we mainly consider the following two problems related to Wiener index, Harary index and Hamiltonian properties of graphs, which are motivated by the main problems studied in [7]. The main results in this paper are solutions to the following two problems.

Problem 1. Among all non-Hamiltonian graphs (non-traceable graphs) G of order n with $\delta(G) \geq k$, determine the values of $\min W(G)$ and $\max H(G)$, respectively.

Problem 2. Among all non-Hamiltonian balanced bipartite graphs G of order $2n$ with $\delta(G) \geq k$, determine the values of $\min W(G)$ and $\max H(G)$, respectively.

We organize this paper as follows. In Section 2, we give some notes on an old theorem about Hamilton cycles due to Erdős and its generalizations. As shown by Liu et al. [9, 10], there are some errors in proofs of some previous work on traceability of connected graphs, in terms of Wiener index and Harary index. We remark that these theorems can be unified in a short proof (by using the generalizations of Erdős' theorem). In Section 3, we prove the correct form and also prove a similar result on Hamilton cycles in connected graphs. In Sections 4 and 5, by imposing the minimum degree of graphs, we generalize the above

results to connected graphs and to connected balanced bipartite graphs, respectively. In the last section, we give some ideas on traceability of connected balanced and nearly-balanced bipartite graphs with given minimum degree, still in terms of these two indices.

2 Erdős' theorem on Hamilton cycles, its refinements and some notes

To find tight edge conditions for Hamilton cycles in graphs is a standard topic in graph theory. In 1962, Erdős [4] proved the following theorem, which generalized Ore's theorem [14] by introducing the minimum degree of a graph as a new parameter.

Theorem 2.1 (Main Theorem in [4]). *Let G be a graph of order n . If $\delta(G) \geq k$, where $1 \leq k \leq (n-1)/2$, and*

$$e(G) > \max \left\{ \binom{n-k}{2} + k^2, \binom{\lceil (n+1)/2 \rceil}{2} + \left\lfloor \frac{n-1}{2} \right\rfloor^2 \right\},$$

then G is Hamiltonian.

The original Erdős' theorem has the following concise form, which is listed as an exercise in West [16].

Theorem 2.2 (Exercise 7.2.28 in [16]). *Let G be a graph of order $n \geq 6k$ with $\delta(G) \geq k \geq 1$. If*

$$e(G) > \binom{n-k}{2} + k^2$$

then G is Hamiltonian.

When $k = 1$, a refinement of Erdős' theorem can date back to Ore [14], and was also given by Bondy [2]. (See also Exercise 28 on Page 126 of Bollobás' book [1]). When $k = 2$, Ning and Ge [13] further proved the following refined theorem.

Lemma 2.1 (Lemma 2 in [13]). *Let G be a graph on $n \geq 5$ vertices and m edges with $\delta \geq 2$. If $m \geq \binom{n-2}{2} + 4$, then G is Hamiltonian unless $G \in \mathcal{G}_1 = \{K_2 \vee (K_{n-4} + 2K_1), K_3 \vee 4K_1, K_2 \vee (K_{1,3} + K_1), K_1 \vee K_{2,4}, K_3 \vee (K_2 + 3K_1), K_4 \vee 5K_1, K_3 \vee (K_{1,4} + K_1), K_2 \vee K_{2,5}, K_5 \vee 6K_1\}$.*

As a corollary, Ning and Ge [13] also proved the following theorem on traceability of connected graphs.

Lemma 2.2 (Lemma 4 in [13]). *Let G be a graph on $n \geq 4$ vertices and m edges with $\delta \geq 1$. If $m \geq \binom{n-2}{2} + 2$, then G is traceable unless $G \in \mathcal{G}_2 = \{K_1 \vee (K_{n-3} + 2K_1), K_2 \vee 4K_1, K_1 \vee (K_{1,3} + K_1), K_{2,4}, K_2 \vee (3K_1 + K_2), K_3 \vee 5K_1, K_2 \vee (K_{1,4} + K_1), K_1 \vee K_{2,5}, K_4 \vee 6K_1\}$.*

Here, we would like to comment on some previous work on Wiener index, Harary index and traceability of connected graphs. Hua and Wang [5] gave a sufficient condition for traceability of connected graphs in terms of Harary index. While in [18], Yang gave a similar sufficient condition for traceability of connected graphs in terms of Wiener index. However, as shown by Liu et al., there are some errors in all the proofs. In two papers [9, 10], Liu et al. have corrected the proof of Hua and Wang’s result and Yang’s result, respectively. We point out that the proofs of Hua–Wang’s result and Yang’s result can be unified by using Lemma 2.2 (together with some facts). Furthermore, we will give a short and unified proof in the next section. All results in this paper are given in the similar fashion.

3 Corrected and unified forms of Hua–Wang’s theorem and Yang’s theorem

In this section, we first prove a result on Hamiltonicity of connected graphs with $\delta(G) \geq 2$, in terms of Wiener index and Harary index.

In order to state our results, we introduce some notation in [7]. We define: for $1 \leq k \leq (n-1)/2$, $L_n^k = K_1 \vee (K_k + K_{n-k-1})$ and $N_n^k = K_k \vee (K_{n-2k} + kK_1)$. Note that $L_n^1 = N_n^1$. We denote by \underline{L}_n^k and \underline{N}_n^k the graphs obtained from L_{n+1}^{k+1} and N_{n+1}^{k+1} , respectively, by deleting one vertex of degree n , i.e., for $0 \leq k \leq n/2 - 1$,

$$\underline{L}_n^k = K_{k+1} + K_{n-k-1} \text{ and } \underline{N}_n^k = K_k \vee (K_{n-2k-1} + (k+1)K_1).$$

The next fact is useful. Since its proof is simple, we omit the proof.

Fact 1. *Let G be a connected graph on n vertices. Then there holds:*

- (i) $W(G) + e(G) \geq n(n-1)$, where the equality holds if and only if $\text{diam}(G) \leq 2$;
- (ii) $e(G) \geq 2H(G) - \binom{n}{2}$, where the equality holds if and only if $\text{diam}(G) \leq 2$.

Theorem 3.1. *Let G be a connected graph of order $n \geq 5$, where $\delta(G) \geq 2$. If $W(G) \leq W(N_n^2)$ or $H(G) \geq H(N_n^2)$, then G is Hamiltonian unless $G \in \mathcal{G}_1$.*

Proof. Since $\text{diam}(N_n^2) = 2$, by Fact 1, we obtain that $W(N_n^2) = n(n-1) - e(N_n^2)$ and $H(N_n^2) = \frac{1}{2}(e(N_n^2) + \binom{n}{2})$.

If $W(G) \leq W(N_n^2)$, then by Fact 1(i), we have $e(G) \geq n(n-1) - W(G) \geq e(N_n^2) = \binom{n-2}{2} + 4$. If $H(G) \geq H(N_n^2)$, then by Fact 1(ii), we have $e(G) \geq 2H(G) - \binom{n}{2} \geq 2H(N_n^2) - \binom{n}{2} = e(N_n^2) = \binom{n-2}{2} + 4$.

By Lemma 2.1, G is Hamiltonian unless $G \in \mathcal{G}_1$. Furthermore, for every graph $G' \in \mathcal{G}_1$, since $\text{diam}(G') = 2$, by Fact 1, we have $W(G') = n(n-1) - e(G') = n(n-1) - e(N_n^2) = W(N_n^2)$ and $H(G') = \frac{1}{2}(e(G') + \binom{n}{2}) = \frac{1}{2}(e(N_n^2) + \binom{n}{2}) = H(N_n^2)$, where $n = |G'|$. This completes the proof. ■

The second purpose of this section is to show that, some previous work [5, 18] on Wiener index, Harary index, and the traceability of connected graphs can be deduced directly from some structural lemma due to the second author and Ge [13]. And these results can be proved by a unified and short proof.

We firstly list some theorems due to Hua and Wang [5], and due to Yang [18], respectively.

Theorem 3.2 (Theorem 2.2 in [5]). *Let G be a connected graph of order $n \geq 4$. If $H(G) \geq \frac{1}{2}n^2 - \frac{3}{2}n + \frac{5}{2}$, then G is traceable, unless $G \in \{K_1 \vee (K_{n-3} + 2K_1), K_2 \vee (3K_1 + K_2), K_4 \vee 6K_1\}$.*

Theorem 3.3 (Theorem 2.2 in [18]). *Let G be a connected graph of order $n \geq 4$. If $W(G) \leq \frac{(n+5)(n-2)}{2}$, then G is traceable, unless $G \in \{K_1 \vee (K_{n-3} + 2K_1), K_2 \vee (3K_1 + K_2), K_4 \vee 6K_1\}$.*

Notice that $\underline{N}_n^1 = K_1 \vee (K_{n-3} + 2K_1)$, $H(\underline{N}_n^1) = \frac{1}{2}n^2 - \frac{3}{2}n + \frac{5}{2}$, and $W(\underline{N}_n^1) = \frac{(n+5)(n-2)}{2}$. In fact, the corrected forms of Theorems 3.2 and 3.3 include six more extremal graphs, as shown by Liu et al. [9, 10]. In the following, we write the clear form of Liu et al.'s theorems, and give a unified and short proof, similar as the proof of Theorem 3.1.

Theorem 3.4 (Theorem 2.2 in [9] and Theorem 2.3 in [10]). *Let G be a connected graph of order $n \geq 4$. If $W(G) \leq W(\underline{N}_n^1)$ or $H(G) \geq H(\underline{N}_n^1)$, then G is traceable unless $G \in \mathcal{G}_2$.*

Proof. Since $\text{diam}(\underline{N}_n^1) = 2$, by Fact 1, we obtain $W(\underline{N}_n^1) = n(n-1) - e(\underline{N}_n^1)$ and $H(\underline{N}_n^1) = \frac{1}{2}(e(\underline{N}_n^1) + \binom{n}{2})$.

If $W(G) \leq W(\underline{N}_n^1)$, then by Fact 1 (i), we have $e(G) \geq n(n-1) - W(G) \geq n(n-1) - W(\underline{N}_n^1) = e(\underline{N}_n^1) = \binom{n-2}{2} + 2$. If $H(G) \geq H(\underline{N}_n^1)$, then by Fact 1 (ii), we have

$e(G) \geq 2H(G) - \binom{n}{2} \geq 2H(\underline{N}_n^1) - \binom{n}{2} = e(\underline{N}_n^1) = \binom{n-2}{2} + 2$. By Lemma 2.2, G is traceable unless $G \in \mathcal{G}_2$.

Furthermore, for every graph $G' \in \mathcal{G}_1$, since $\text{diam}(G') = 2$, by Fact 1, we have $W(G') = n(n-1) - e(G') = n(n-1) - e(\underline{N}_n^1) = W(\underline{N}_n^1)$ and $H(G') = \frac{1}{2}(e(G') + \binom{n}{2}) = \frac{1}{2}(e(\underline{N}_n^1) + \binom{n}{2}) = H(\underline{N}_n^1)$, where $n = |G'|$. This completes the proof. ■

4 Wiener index, Harary index and Hamiltonicity of connected graphs

In this section, we will prove sharp results on traceability and Hamiltonicity of connected graphs with given minimum degree, in terms of Wiener index and Harary index. Our proofs depend on a structural result due to Li and Ning [7], which refines a theorem of Erdős [4].

To prove spectral analogs of Erdős' theorem, Li and Ning [7] proved the following refined form of the concise Erdős' theorem.

Lemma 4.1 (Lemma 2 in [7]). *Let G be a graph of order $n \geq 6k + 5$, where $k \geq 1$. If $\delta(G) \geq k$ and*

$$e(G) > \binom{n-k-1}{2} + (k+1)^2,$$

then G is Hamiltonian unless $G \subseteq L_n^k$ or N_n^k .

Lemma 4.2 (Lemma 3 in [7]). *Let G be a graph of order $n \geq 6k + 10$, where $k \geq 0$. If $\delta(G) \geq k$ and*

$$e(G) > \binom{n-k-2}{2} + (k+1)(k+2),$$

then G is traceable unless $G \subseteq L_n^k$ or N_n^k .

Next, we give solutions to Problem 1 (when n is sufficiently large), whose proofs depend on the above structural lemmas.

Theorem 4.1. *Let G be a connected graph of order $n \geq 6k + 5$, where $\delta(G) \geq k \geq 1$. If $W(G) \leq W(N_n^k)$ or $H(G) \geq H(N_n^k)$, then G is Hamiltonian unless $G = N_n^k$.*

Proof. Since $\text{diam}(N_n^k) = \text{diam}(L_n^k) = 2$, by Fact 1, we obtain that $W(G') = n(n-1) - e(G')$ and $H(G') = \frac{1}{2}(e(G') + \binom{n}{2})$, if $G' \in \{N_n^k, L_n^k\}$.

If $W(G) \leq W(N_n^k)$, then by Fact 1 (i), we have $e(G) \geq n(n-1) - W(N_n^k) \geq n(n-1) - (n(n-1) - e(N_n^k)) = e(N_n^k) = \binom{n-k}{2} + k^2 > \binom{n-k-1}{2} + (k+1)^2$ when $n > 3k + 2$.

If $H(G) \geq H(N_n^k)$, then by Fact 1 (ii), we also have $e(G) \geq 2H(N_n^k) - \binom{n}{2} = e(N_n^k) = \binom{n-k}{2} + k^2 > \binom{n-k-1}{2} + (k+1)^2$ when $n > 3k+2$. By Lemma 4.1, G is Hamiltonian unless $G \subseteq L_n^k$ or N_n^k .

If $G \not\subseteq N_n^k$, then $W(G) > W(N_n^k)$ and $H(G) < H(N_n^k)$, a contradiction. Recall that $e(N_n^k) = \binom{n-k}{2} + k^2$ and $e(L_n^k) = \binom{n-k}{2} + \frac{(k+1)k}{2}$. Thus $e(N_n^k) > e(L_n^k)$ when $k \geq 2$ and $e(N_n^k) = e(L_n^k)$ when $k = 1$. Hence $W(L_n^k) > W(N_n^k)$ when $k \geq 2$ and $W(L_n^1) = W(N_n^1)$; $H(L_n^k) < H(N_n^k)$ when $k \geq 2$ and $H(L_n^1) = H(N_n^1)$. So, if $G \subseteq L_n^k$ and $k \geq 2$, then $W(G) \geq W(L_n^k) > W(N_n^k)$ and $H(G) \leq H(L_n^k) < H(N_n^k)$, a contradiction. It follows $G = N_n^k$ when $k \geq 2$ or $k = 1$ (in this case, $G = L_n^1 = N_n^1$). This completes the proof. ■

Theorem 4.2. *Let G be a connected graph of order $n \geq 6k + 10$, where $\delta(G) \geq k \geq 1$. If $W(G) \leq W(\underline{N}_n^k)$ or $H(G) \geq H(\underline{N}_n^k)$, then G is traceable unless $G = \underline{N}_n^k$.*

Proof. Since $\text{diam}(\underline{N}_n^k) = 2$, by Fact 1, we obtain that $W(G') = n(n-1) - e(G')$ and $H(G') = \frac{1}{2}(e(G') + \binom{n}{2})$, if $G' = \underline{N}_n^k$.

If $W(G) \leq W(\underline{N}_n^k)$, by Fact 1 (i), we have $e(G) \geq n(n-1) - W(\underline{N}_n^k) = n(n-1) - (n(n-1) - e(\underline{N}_n^k)) = e(\underline{N}_n^k) = \binom{n-k-1}{2} + k(k+1) > \binom{n-k-2}{2} + (k+1)(k+2)$ when $n > 3k+4$. If $H(G) \geq H(\underline{N}_n^k)$, by Fact 1 (ii), we also have $e(G) \geq 2H(\underline{N}_n^k) - \binom{n}{2} = e(\underline{N}_n^k) = \binom{n-k-1}{2} + k(k+1) > \binom{n-k-2}{2} + (k+1)(k+2)$ when $n > 3k+4$. By Lemma 4.2, G is traceable unless $G \subseteq \underline{L}_n^k$ or \underline{N}_n^k . Since G is connected, we have $G \subseteq \underline{N}_n^k$.

If $G \not\subseteq \underline{N}_n^k$, then $W(G) > W(\underline{N}_n^k)$ and $H(G) < H(\underline{N}_n^k)$, a contradiction. Thus, $G = \underline{N}_n^k$. This completes the proof. ■

5 Wiener index, Harary index and Hamiltonicity of connected balanced bipartite graphs

In this section, we will prove sharp results on Hamiltonicity of connected balanced bipartite graphs with given minimum degree, in terms of Wiener index and Harary index. Our proofs depend on the following structural result due to Li and Ning, which refines a theorem of Moon and Moser [12].

Lemma 5.1 (Lemma 5 in [7]). *Let G be a balanced bipartite graph of order $2n$. If $\delta(G) \geq k \geq 1$, $n \geq 2k + 1$ and*

$$e(G) > n(n-k-1) + (k+1)^2,$$

then G is Hamiltonian unless $G \subseteq B_n^k$.

In the above theorem, we define B_n^k ($1 \leq k \leq n/2$) as the graph obtained from $K_{n,n}$ by deleting all edges in its one subgraph $K_{n-k,k}$. Note that $e(B_n^k) = n(n-k) + k^2$ and B_n^k is not Hamiltonian.

The following useful fact is simple, and we omit the proof.

Fact 2. *Let G be a connected balanced bipartite graph of order $2n$. Then there holds:*

- (i) $e(G) + 3(n^2 - e(G)) + 4\binom{n}{2} \leq W(G)$, where the equality holds if and only if for any two vertices x, y , if x, y are in different partition sets then $d(x, y) \leq 3$, and if x, y are in the same partition set then $d(x, y) = 2$;
- (ii) $e(G) + \frac{1}{3}(n^2 - e(G)) + \binom{n}{2} \geq H(G)$, where the equality holds if and only if for any two vertices x, y , if x, y are in different partition sets then $d(x, y) \leq 3$, and if x, y are in the same partition set then $d(x, y) = 2$.

The following theorem gives a solution to Problem 2.

Theorem 5.1. *Let G be a connected balanced bipartite graph of order $2n$, where $n \geq 2k+2$ and $\delta(G) \geq k \geq 1$. If $W(G) \leq W(B_n^k)$ or $H(G) \geq H(B_n^k)$, then G is Hamiltonian unless $G = B_n^k$.*

Proof. By Fact 2, we have $W(B_n^k) = 5n^2 - 2n - 2e(B_n^k)$ and $H(B_n^k) = e(B_n^k) + 3(n^2 - e(B_n^k)) + \binom{n}{2}$. If $W(G) \leq W(B_n^k)$, then $e(G) \geq \frac{1}{2}(5n^2 - 2n - W(G)) \geq \frac{1}{2}(5n^2 - 2n - W(B_n^k)) = e(B_n^k)$. If $H(G) \geq H(B_n^k)$, then $e(G) \geq e(B_n^k)$. When $n \geq 2k+2$, $e(B_n^k) = n(n-k) + k^2 > n(n-k-1) + (k+1)^2$. By Lemma 5.1, G is Hamiltonian unless $G \subseteq B_n^k$. If $G \subsetneq B_n^k$, then $W(G) > W(B_n^k)$, a contradiction. This completes the proof. ■

Since the bound in Theorem 5.1 is tight, some previous work (see Theorem 2.2 in [19]) in this direction is a direct corollary.

6 Concluding remarks

One may ask to study the traceability of connected bipartite graphs with given minimum degree. We know such a graph should be balanced or nearly-balanced. Recently, Li and Ning [8] studied spectral conditions for traceability of bipartite graphs with given minimum degree. The study of traceability of bipartite graphs in terms of Wiener index

and Harary index is very similar to the ones in [8]. Some structural theorems developed in [8] about traceability of connected balanced and nearly-balanced bipartite graphs will play the central roles in proofs of these results. We omit the details and refer them to the interested reader.

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