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Some Observations on Harary Index and Traceable Graphs*

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Abstract

A molecular graph matrix, Harary matrix, was defined in honor of Professor Frank Harary. Harary index is a graph invariant based on it. In this paper, we give sufficient conditions for a graph being traceable and Hamiltonian in terms of the Harary index of a graph and the complement of a graph, which correct and extend the result of Wang and Hua (2013) [5]. Furthermore, we also present sufficient conditions for a bipartite graph being traceable and Hamiltonian in terms of the Harary index of a bipartite graph and its quasi-complement. Finally, we give some sufficient Harary spectral conditions for a graph or a bipartite graph being traceable and Hamiltonian in terms of the Harary spectral radius of its complement or quasi-complement.

1 Introduction

All graphs considered here are finite undirected graphs without loops and multiple edges. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. For a graph, we use d_i or $d_G(v_i)$ to denote the degree of a vertex v_i in G and use $d_G(v_i, v_j)$ or d_{ij} to denote the distance between two vertices v_i and v_j in G. The union of simple graphs G and H is the graph $G \cup H$ with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$. If G and H are disjoint, we refer to their union as a disjoint union, and generally denote it by $G + H$. The disjoint union of k copies of a graph G is denoted by kG. The *join* of G and

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H, denoted by $G \vee H$, is the graph obtained from disjoint union of G and H by adding all possible edges between them. Let $\overline{G}$ denote the complement of G.

A path in a graph is called a *Hamiltonian path* if it visits every vertex precisely once. A graph containing a Hamiltonian path is said to be *traceable*. A cycle in a graph is called a *Hamiltonian cycle* if it contains all the vertices of a graph. A graph containing a Hamiltonian cycle is called a *Hamiltonian graph*.

The Harary index of a graph G, denoted by $H(G)$, has been introduced independently by Ivanciuc et.al. [6] and Plavšić et.al. [10] in 1993 for the characterization of molecular graphs. It has been named in honor of Professor Frank Harary on the occasion of his 70th birthday. The Harary index $H(G)$ is defined as the sum of reciprocals of distances between all pairs of vertices of the graph G, i.e.

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

Note that in any disconnected graph G, the distance is infinite between any two vertices from two distinct components. Therefore its reciprocal can be viewed as 0. Thus, we can define validly the Harary index of disconnected graph G as follows:

$$H(G) = \sum_{i=1}^{m} H(G_i),$$

where $G_1, G_2, \ldots, G_k$ are the components of G. We often use $\hat{D}_i(G)$ or $\hat{D}_{v_i}(G)$ to denote $\sum_{v_j \in V(G)} \frac{1}{d_G(v_i,v_j)}$, then

$$H(G) = \frac{1}{2} \sum_{v_i \in V(G)} \hat{D}_{v_i}(G) = \frac{1}{2} \sum_{i=1}^{n} \hat{D}_i(G).$$

The Harary matrix $RD(G)$ of G, which is initially called the reciprocal distance matrix and introduced by [6], is an $n \times n$ matrix whose (i,j)-entry is equal to $\frac{1}{d_{ij}}$ if $i \neq j$ and 0 otherwise. The Harary spectral radius of G is the largest eigenvalue of $RD(G)$, denoted by $\rho(G)$.

Up to now, there are many established results dealing with bounds and extremal properties of Harary index, published both in mathematical and in mathematicl chemistry literature, see [4, 8, 12–14]. In [3, 5], they presented some sufficient conditions for a graph to be traceable by using Harary index. But there is an error in its proof in [5]. Li [7] presented sufficient conditions in terms of the Harary index for a graph to be Hamiltonian or Hamilton-connected using some proof ideas in [5]. Zeng [15] give a sufficient condition, in terms of Harary index, for a connected bipartite graph to be Hamiltonian.

In this paper, we give sufficient conditions for a graph being traceable and Hamiltonian in terms of the Harary index of a graph and the complement of a graph, which correct and extend the result of Wang and Hua (2013) [5]. Furthermore, we also present sufficient conditions for a bipartite graph being traceable and Hamiltonian in terms of the Harary index of a bipartite graph and its quasi-complement. Finally, we give some sufficient Harary spectral conditions for a graph or a bipartite graph being traceable and Hamiltonian in terms of its Harary spectral radius of the complement or its quasi-complement. Our results extend and improve the results in [3, 5, 7, 15].

Note that $\delta \geq 1$ and $\delta \geq 2$ are trivial necessary conditions for a graph to be traceable and Hamiltonian, respectively. Hence we always make the assumption while finding spectral conditions for traceable and Hamiltonian graphs or bipartite graphs throughout this paper.

2 Corrigendum to Theorem 2.2 in [5]

Let $\mathbb{NP} = \{K_1 \vee (K_{n-3} + 2K_1), K_1 \vee (K_{1,3} + K_1), K_{2,4}, K_2 \vee 4K_1, K_2 \vee (3K_1 + K_2), K_1 \vee K_{2,5}, K_3 \vee 5K_1, K_2 \vee (K_{1,4} + K_1), K_4 \vee 6K_1\}$.

Lemma 2.1. ([1]) *Let G be a nontrivial graph of order n with degree sequence $(d_1, d_2, \ldots, d_n)$, where $d_1 \leq d_2 \leq \cdots \leq d_n$ and $n \geq 4$. Suppose that there is no integer $k < \frac{n+1}{2}$ such that $d_k \leq k-1$ and $d_{n-k+1} \leq n-k-1$. Then G is traceable.*

Theorem 2.2. ([5]) *Let G be a connected graph of order $n \geq 4$. If $H(G) \geq \frac{n^2-3n+5}{2}$, 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 2.2 provided a sufficient condition in terms of Harary index of a graph to be traceable. But there is an error in its proof. It should be:

Theorem 2.3. *Let G be a connected graph of order $n \geq 4$. If*

$$H(G) \geq \frac{n^2 - 3n + 5}{2},$$

then G is traceable unless $G \in \mathbb{NP}$.

Proof. Assume first that G is nontraceable connected graph with degree sequence $(d_1, d_2, \ldots, d_n)$ such that $d_1 \leq d_2 \leq \cdots \leq d_n$ and $n \geq 4$. By Lemma 2.1, there exists an integer

$k < \frac{n+1}{2}$ such that $d_k \le k-1$ and $d_{n-k+1} \le n-k-1$. Note that G is connected graph and $d_k \le k-1$, we have $k \ge 2$. Thus

$$\begin{aligned} H(G) = \tfrac{1}{2}\sum_{i=1}^{n}\hat{D}_i(G) &\le \tfrac{1}{2}\sum_{i=1}^{n}[d_i + \tfrac{1}{2}(n-1-d_i)] \\ &= \tfrac{n(n-1)}{4} + \tfrac{1}{4}\sum_{i=1}^{n} d_i \\ &\le \tfrac{n(n-1)}{4} + \tfrac{1}{4}[k(k-1)+(n-2k+1)(n-k-1)+(k-1)(n-1)] \\ &= \tfrac{n^2-3n+5}{2} - \tfrac{(k-2)(2n-3k-5)}{4}. \end{aligned}$$

Since $H(G) \ge \frac{n^2-3n+5}{2}$, we obtain that $\frac{(k-2)(2n-3k-5)}{4} \le 0$.

Case 1 : $\frac{(k-2)(2n-3k-5)}{4} = 0$, i.e. $k = 2$ or $2n-3k-5 = 0$. If $k = 2$, then G is a graph with $d_1 = d_2 = 1$, $d_3 = d_4 = \cdots = d_{n-1} = n-3$ and $d_n = n-1$, which implies $G = K_1 \vee (K_{n-3} + 2K_1)$. If $2n = 3k+5$, then $n < 13$ since $k < \frac{n+1}{2}$. Hence $n = 7, k = 3$ or $n = 10, k = 5$. The corresponding permissible graphic sequences are (2,2,2,3,3,6,6) and (4,4,4,4,4,4,9,9,9,9), which implies $G = K_2 \vee (3K_1 + K_2)$ or $G = K_4 \vee 6K_1$, respectively.

Case 2 : $\frac{(k-2)(2n-3k-5)}{4} < 0$, i.e. $k \ge 3$ and $2n-3k-5 < 0$. In this case, $n \ge 2k \ge 6$. If $n \ge 10$, then $2n-3k-5 \ge 2n - \frac{3n}{2} - 5 = \frac{n-10}{2} \ge 0$. If $n = 9$, then $k \le 4$ and $2n-3k-5 \ge 1$. If $n = 7$, then $k \le 3$, and hence, $2n-3k-5 \ge 0$. In each case, we get a contradiction.

If $n = 8$, then $k \le 4$. If $k \le 3$, then $2n-3k-5 \ge 2$, a contradiction. Now assume that $k = 4$. Then ,$d_5 \le 3$ and $17 \le m \le 18$. From the inequality $d_6 + d_7 + d_8 = 2m - \sum_{1\le i\le 5} d_i \ge 19$, we obtain $d_8 = 7$. Also note that $\sum d_i = 2m \ge 34$ and $\sum d_i$ is even. If $d_6 = d_7 = 6$ and $d_8 = 7$, then the permissible graphic sequence is (3,3,3,3,3,6,6,7), hence $G = K_1 \vee K_{2,5}$. If $d_6 = 5$ and $d_7 = d_8 = 7$, then the permissible graphic sequence is (3,3,3,3,3,5,7,7), hence $G = K_2 \vee (K_{1,3} + K_2)$. If $d_6 = 6$ and $d_7 = d_8 = 7$, then the permissible graphic sequence is (2,3,3,3,3,6,7,7), hence $G = K_2 \vee (K_{1,4} + K_1)$. If $d_6 = d_7 = d_8 = 7$, then the permissible graphic sequence is (3,3,3,3,3,7,7,7), hence $G = K_3 \vee 5K_1$.

If $n = 6$, then $k \le 3$. If $k \le 2$, then $2n-3k-5 \ge 1$, a contradiction. If $k = 3$, then $d_4 \le 2$ and $8 \le m \le 9$. From the inequality $d_5 + d_6 = 2m - \sum_{1\le i\le 4} d_i \ge 8$, we obtain $4 \le d_6 \le 5$. Also note that $\sum d_i = 2m \ge 16$ and $\sum d_i$ is even. If $d_5 = d_6 = 4$, then the permissible graphic sequence is (2,2,2,2,4,4), hence $G = K_{2,4}$. If $d_5 = 4$ and $d_6 = 5$, then the permissible graphic sequence is (1,2,2,2,4,5), hence $G = K_1 \vee (K_{1,3} + K_1)$. If $d_5 = d_6 = 5$, then the permissible graphic sequence is (2,2,2,2,5,5), hence $G = K_2 \vee 4K_1$.

Note that $G = K_2 \vee (K_{1,3} + K_2)$ is traceable and the other obtained graphs contain no Hamiltonian path. Hence $G \in \mathbb{NP}$. ■

3 Harary index on traceable and Hamiltonian graphs

Lemma 3.1. ([9]) *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 $G \in \mathbb{NP}$.*

According to Lemma 3.1, we present a simple proof of Theorem 2.3.

Proof. Suppose that G is nontraceable. Then

$$\begin{aligned} H(G) = \tfrac{1}{2}\sum_{i=1}^{n} \hat{D}_i(G) &\leq \tfrac{1}{2}\sum_{i=1}^{n}[d_i + \tfrac{1}{2}(n-1-d_i)] \\ &= \tfrac{n(n-1)}{4} + \tfrac{1}{4}\sum_{i=1}^{n} d_i \\ &= \tfrac{n(n-1)}{4} + \tfrac{1}{2}m. \end{aligned}$$

Note that $H(G) \geq \frac{n^2-3n+5}{2}$, we have

$$m \geq n^2 - 3n + 5 - \frac{n(n-1)}{2} = \binom{n-2}{2} + 2.$$

By Lemma 3.1, we obtain that $G \in \mathbb{NP}$. By a direct computation, for all $G \in \mathbb{NP}$, $H(G) \geq \frac{n^2-3n+5}{2}$. This completes the proof of Theorem 2.3. ■

Theorem 3.2. *Let G be a connected graph of order $n \geq 4$. If*

$$H(\overline{G}) \leq \frac{5n^2 - 19n + 20}{2(n-1)},$$

then G is traceable unless $G \in \{K_{1,3}, K_1 \vee (K_2 + 2K_1), K_1 \vee (K_3 + 2K_1), K_1 \vee (K_{1,3} + K_1), K_{2,4}, K_2 \vee 4K_1, K_2 \vee (3K_1 + K_2), K_1 \vee K_{2,5}, K_3 \vee 5K_1, K_2 \vee (K_{1,4} + K_1), K_4 \vee 6K_1\}$.

Proof. Suppose that G is nontraceable. Then

$$\begin{aligned} H(\overline{G}) = \tfrac{1}{2}\sum_{i=1}^{n} \hat{D}_i(\overline{G}) &\geq \tfrac{1}{2}\sum_{v\in V(G)}[d_{\overline{G}}(v) + \tfrac{1}{n-1}(n-1-d_{\overline{G}}(v))] \\ &= \tfrac{1}{2}\sum_{v\in V(G)}[1 + \tfrac{n-2}{n-1}d_{\overline{G}}(v)] \\ &= \tfrac{n}{2} + \tfrac{n-2}{2(n-1)}\sum_{v\in V(G)}(n-1-d_G(v)) \\ &= \tfrac{n(n-1)}{2} - \tfrac{n-2}{2(n-1)}\sum_{v\in V(G)} d_G(v) \\ &= \tfrac{n(n-1)}{2} - \tfrac{n-2}{n-1}m. \end{aligned}$$

Note that $H(\overline{G}) \leq \frac{5n^2-19n+20}{2(n-1)}$, we have

$$m \geq \frac{n(n-1)^2}{2(n-2)} - \frac{5n^2 - 19n + 20}{2(n-1)} = \binom{n-2}{2} + 2.$$

By Lemma 3.1, we obtain that $G \in \mathbb{NP}$. Note that $n \geq 7$,

$$H(\overline{K_1 \vee (K_{n-3} + 2K_1)}) \geq \frac{n^2 + n - 8}{4} > \frac{5n^2 - 19n + 20}{2(n-1)}.$$

So we obtain this result. ■

Let $\mathbb{NC} = \{K_2 \vee (K_{n-4} + 2K_1), K_3 \vee 4K_1, K_2 \vee (K_{1,3} + K_1), K_1 \vee K_{2,4}, K_3 \vee (K_2 + 3K_1), K_4 \vee 5K_1, K_3 \vee (K_{1,4} + K_1), K_2 \vee K_{2,5}, K_5 \vee 6K_1\}$.

Lemma 3.3. ([9]) *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 contains a Hamiltonian cycle unless $G \in \mathbb{NC}$.*

Theorem 3.4. *Let G be a graph on $n \geq 5$ vertices and m edges with $\delta \geq 2$. If*

$$H(G) \geq \frac{n^2 + 7 - 3n}{2},$$

then G is Hamiltonian unless $G \in \mathbb{NC}$.

Proof. Suppose that G is non-Hamiltonian. Then

$$\begin{aligned} H(G) = \tfrac{1}{2}\textstyle\sum_{i=1}^{n} \hat{D}_i(G) &\leq \tfrac{1}{2}\textstyle\sum_{i=1}^{n}[d_i + \tfrac{1}{2}(n-1-d_i)] \\ &= \tfrac{n(n-1)}{4} + \tfrac{1}{4}\textstyle\sum_{i=1}^{n} d_i \\ &= \tfrac{n(n-1)}{4} + \tfrac{1}{2}m. \end{aligned}$$

Note that $H(G) \geq \frac{n^2-3n+7}{2}$, we have

$$m \geq n^2 - 3n + 7 - \frac{n(n-1)}{2} = \binom{n-2}{2} + 4.$$

By Lemma 3.3, we have $G \in \mathbb{NC}$. By a direct computation, for all $G \in \mathbb{NC}$, $H(G) \geq \frac{n^2+7-3n}{2}$. This completes the proof. ■

Theorem 3.5. *Let G be a graph on $n \geq 5$ vertices and m edges with $\delta \geq 2$. If*

$$H(\overline{G}) \leq \frac{5n^2 - 23n + 28}{2(n-1)},$$

then G is Hamiltonian unless $G \in \{K_2 \vee 3K_1, K_2 \vee (K_2 + 2K_1), K_2 \vee (K_3 + 2K_1), K_3 \vee 4K_1, K_2 \vee (K_{1,3} + K_1), K_1 \vee K_{2,4}, K_3 \vee (K_2 + 3K_1), K_4 \vee 5K_1, K_3 \vee (K_{1,4} + K_1), K_2 \vee K_{2,5}, K_5 \vee 6K_1\}$.

Proof. Suppose that G is non-Hamiltonian. Then

$$\begin{aligned} H(\overline{G}) = \tfrac{1}{2}\textstyle\sum_{v\in V(G)} D_i(\overline{G}) &\geq \tfrac{1}{2}\textstyle\sum_{v\in V(G)}[d_{\overline{G}}(v) + \tfrac{1}{n-1}(n-1-d_{\overline{G}}(v))] \\ &= \tfrac{1}{2}\textstyle\sum_{v\in V(G)}[1 + \tfrac{n-2}{n-1}d_{\overline{G}}(v)] \\ &= \tfrac{n}{2} + \tfrac{n-2}{2(n-1)}\textstyle\sum_{v\in V(G)}(n-1-d_G(v)) \\ &= \tfrac{n(n-1)}{2} - \tfrac{n-2}{2(n-1)}\textstyle\sum_{v\in V(G)} d_G(v) \\ &= \tfrac{n(n-1)}{2} - \tfrac{n-2}{n-1}m. \end{aligned}$$

Since $H(\overline{G}) \leq \frac{5n^2-23n+28}{2(n-1)}$, we have

$$m \geq \frac{n(n-1)^2}{2(n-2)} - \frac{5n^2 - 23n + 28}{2(n-2)} = \binom{n-2}{2} + 4.$$

By Lemma 3.3, we obtain that $G \in \mathbb{NC}$. Note that $n \geq 8$,

$$H(\overline{K_2 \vee (K_{n-4} + 2K_1)}) \geq \frac{n^2 - n - 8}{4} > \frac{5n^2 - 23n + 28}{2(n-1)}.$$

So we obtain this theorem. ■

4 Harary index on traceable and Hamiltonian bipartite graphs

Let $G = G[X, Y]$ be a bipartite graph, where $|X| = |Y| = n \geq 2$. The bipartite graph $G^* = G^*[X, Y]$ is called the *quasi-complement* of G, which is constructed as follows: $V(G^*) = V(G)$ and $xy \in E(G^*)$ if and only if $xy \notin E(G)$ for $x \in X$, $y \in Y$.

Let $G[X, Y]$ be a traceable bipartite graph. Then $|X| = |Y|$ or $|X| = |Y| + 1$. These two types will be discussed separately.

Lemma 4.1. **([11])** *Let $G = G[X, Y]$ be a bipartite graph with $\delta \geq 1$ and m edges, where $|X| = |Y| = n \geq 3$. If $m \geq n^2 - 2n + 3$, then G is traceable.*

Theorem 4.2. *Let $G = G[X, Y]$ be a bipartite graph with $\delta \geq 1$ and m edges, where $|X| = |Y| = n \geq 3$. If*

$$H(G) \geq \frac{9n^2 - 11n + 12}{6},$$

then G is traceable.

Proof. Let G be a graph satisfying the condition in Theorem 4.2. Then

$$\begin{aligned} H(G) = \tfrac{1}{2}\textstyle\sum_{i=1}^{2n} \hat{D}_i(G) &\leq \tfrac{1}{2}\textstyle\sum_{i=1}^{2n}[d_i + \tfrac{1}{3}(n - d_i) + \tfrac{1}{2}(n-1)] \\ &= \tfrac{1}{2}\textstyle\sum_{i=1}^{2n}(\tfrac{5n-3}{6} + \tfrac{2}{3}d_i) \\ &= \tfrac{5n^2-3n}{6} + \tfrac{1}{3}\textstyle\sum_{i=1}^{2n} d_i \\ &= \tfrac{5n^2-3n}{6} + \tfrac{2}{3}m. \end{aligned}$$

Since $H(G) \geq \frac{9n^2-11n+12}{6}$, we have

$$m \geq \frac{9n^2 - 11n + 12 - 5n^2 + 3n}{6} \times \frac{3}{2} = n^2 - 2n + 3.$$

According to Lemma 4.1, then G is traceable. ■

Theorem 4.3. *Let $G = G[X, Y]$ be a bipartite graph with $\delta \geq 1$ and m edges, where $|X| = |Y| = n \geq 3$. If*

$$H(G^*) \leq \frac{12n^2 - 21n + 12}{4n - 2},$$

then G is traceable.

Proof. Let G^* be the quasi-complement of G. Then

$$\begin{aligned} H(G^*) = \tfrac{1}{2}\sum_{i=1}^{2n} \hat{D}_i(G^*) &\geq \tfrac{1}{2}\sum_{i=1}^{2n}[d_{G^*}(v_i) + \tfrac{1}{2n-1}(n - d_{G^*}(v_i)) + \tfrac{n-1}{2n-2}] \\ &= \tfrac{1}{2}\sum_{i=1}^{2n}[\tfrac{2(n-1)}{2n-1}d_{G^*}(v_i) + \tfrac{n}{2n-1} + \tfrac{1}{2}] \\ &= \tfrac{1}{2}\sum_{i=1}^{2n}[\tfrac{2(n-1)}{2n-1}d_{G^*}(v_i) + \tfrac{4n-1}{2(2n-1)}] \\ &= \tfrac{n(4n-1)}{2(2n-1)} + \tfrac{2(n-1)}{2(2n-1)}\sum_{i=1}^{2n}(n - d_G(v_i)) \\ &= \tfrac{4n^3-n}{2(2n-1)} - \tfrac{2(n-1)}{2n-1}m. \end{aligned}$$

Since $H(G^*) \leq \frac{12n^2-21n+12}{4n-2}$, we have $m \geq n^2 - 2n + 3$. ¿From Lemma 4.1, then G is traceable. ■

Let $G = K_{p,n-2} + 4e$ be a bipartite graph obtained from $K_{p,n-2}$ by adding two vertices which are adjacent to two common vertices with degree $n-2$ in $K_{p,n-2}$, respectively, where $p \geq n-1$.

Lemma 4.4. **([11])** *Let $G = G[X,Y]$ be a bipartite graph with $\delta \geq 2$ and m edges, where $|X| = |Y| = n \geq 4$. If $m \geq n^2 - 2n + 4$, then G is Hamiltonian unless $G = K_{n,n-2} + 4e$.*

Next, we consider the other type $|X| = |Y| + 1$. Let $G[X,Y]$ be a bipartite graph, where $|X| = n+1$, and $|Y| = n \geq 2$. Denote by δ_X and δ_Y the minimum degrees of vertices in X and Y, respectively. Note that $\delta_X \geq 1$ and $\delta_Y \geq 2$ are the trivial necessary conditions for G to be traceable. Let $G[X, Y+v]$ be the bipartite graph obtained from $G[X,Y]$ by adding a vertex v which is adjacent to every vertex in X. It is easy to see that $G[X,Y]$ is traceable if and only if $G[X, Y+v]$ is Hamiltonian.

Let $K_{n,n-1} + 2e$ be a graph obtained from $K_{n,n-1}$ by adding two vertices which are adjacent to a common vertex with degree $n-1$, respectively.

Theorem 4.5. *Let $G = G[X,Y]$ be a bipartite graph with $\delta_X \geq 1$ and $\delta_Y \geq 1$, where $|X| = n+1$ and $|Y| = n \geq 3$. If*

$$H(G) \geq \frac{9n^2 - 2n + 8}{6},$$

then G is traceable unless $G \in \{K_{n,n-1} + 2e, K_{n+1,n-2} + 4e\}$.

Proof. Let G be a bipartite satisfying the conditions in Theorem 4.5.

$$\begin{aligned} H(G) &= \tfrac{1}{2}\sum_{v\in V(G)} \hat{D}_v(G) \\ &\leq \tfrac{1}{2}\sum_{i=1}^{n+1}[d_i + \tfrac{1}{3}(n - d_i) + \tfrac{n}{2}] \\ &\quad + \tfrac{1}{2}\sum_{j=1}^{n}[d_j + \tfrac{1}{3}(n+1-d_j) + \tfrac{n-1}{2}] \end{aligned}$$

$$= \frac{1}{2}[\frac{5n(n+1)}{6} + \sum_{i=1}^{n+1} \frac{2d_i}{3} + \frac{n(5n-1)}{6} + \sum_{j+1}^{n} \frac{2d_j}{3}]$$
$$= \frac{5n^2+2n}{6} + \frac{1}{3}(\sum_{i=1}^{n+1} d_i + \sum_{j=1}^{n} d_j)$$
$$= \frac{5n^2+2n}{6} + \frac{2}{3}m.$$

Since $H(G) \geq \frac{9n^2-2n+8}{6}$, we have $m \geq n^2-n+2$. Note that $d(v) = n+1$ in $G[X, Y+v]$, hence

$$m(G[X, Y+v]) = m + (n+1) \geq n^2 + 3 = (n+1)^2 - 2(n+1) + 4.$$

From Lemma 4.4, we obtain that $G[X, Y+v]$ is Hamiltonian or $G[X, Y+v] = K_{n+1,n-1}+4e$. Hence $G[X, Y]$ is traceable or $G \in \{K_{n,n-1} + 2e, K_{n+1,n-2} + 4e\}$. ■

Theorem 4.6. *Let $G = G[X, Y]$ be a bipartite graph with $\delta_X \geq 1$ and $\delta_Y \geq 2$, where $|X| = n+1$ and $|Y| = n \geq 3$. If*

$$H(G^*) \leq \frac{24n^2 - 28n + 15}{4(2n-1)},$$

then G is traceable unless $G \in \{K_{3,2} + 2e, K_{4,1} + 4e, K_{4,3} + 2e, K_{5,2} + 4e, K_{5,4} + 2e, K_{6,3} + 4e, K_{6,5} + 2e, K_{7,4} + 4e\}$.

Proof. Let G^* be the quasi-complement of G. Then

$$H(G^*) = \frac{1}{2}\sum_{v\in V(G)} \hat{D}_v(G^*) \geq \frac{1}{2}\sum_{i=1}^{n+1}[d_{G^*}(v_i) + \frac{1}{2n-1}(n - d_{G^*}(v_i)) + \frac{n}{2n}]$$
$$+\frac{1}{2}\sum_{j=1}^{n}[d_{G^*}(u_j) + \frac{1}{2n-1}(n+1 - d_{G^*}(u_j)) + \frac{n-1}{2n-2}]$$
$$= \frac{1}{2}[\frac{(4n-1)(n+1)}{2(2n-1)} - \frac{2-2n}{2n-1}\sum_{i=1}^{n+1} d_{G^*}(v_i)]$$
$$+\frac{1}{2}[\frac{(4n+1)n}{2(2n-1)} - \frac{2-2n}{2n-1}\sum_{j=1}^{n} d_{G^*}(u_j)]$$
$$= \frac{8n^3+8n^2-4n-1}{4(2n-1)} - \frac{2n-2}{2(2n-1)}\sum_{i=1}^{n+1} d_G(v_i)$$
$$-\frac{2n-2}{2(2n-1)}\sum_{j=1}^{n} d_G(u_j)]$$
$$= \frac{8n^3+8n^2-4n-1}{4(2n-1)} - \frac{2n-2}{2n-1}m.$$

Since $H(G^*) \leq \frac{24n^2-28n+15}{4(2n-1)}$, we have that $m \geq n^2 - n + 2$. Note that $d(v) = n+1$ in $G[X, Y+v]$, hence

$$m(G[X, Y+v]) = m + (n+1) \geq n^2 + 3 = (n+1)^2 - 2(n+1) + 4.$$

¿From Lemma 4.4, we obtain that $G[X, Y+v]$ is Hamiltonian or $G = K_{n+1,n-1} + 4e$. Hence $G[X, Y]$ is traceable or $G \in \{K_{n,n-1} + 2e, K_{n+1,n-2} + 4e\}$. But

$$H((K_{n,n-1} + 4e)^*) = H((K_{n+1,n-2} + 4e)^*) \geq \frac{n^2 + 5n - 4}{4} > \frac{24n^2 - 28n + 15}{4(2n-1)}, n \geq 7.$$

So we have $G \in \{K_{3,2} + 2e, K_{4,1} + 4e, K_{4,3} + 2e, K_{5,2} + 4e, K_{5,4} + 2e, K_{6,3} + 4e, K_{6,5} + 2e, K_{7,4} + 4e\}$. ■

Theorem 4.7. *Let $G = G[X, Y]$ be a bipartite graph with $\delta \geq 2$ and m edges, where $|X| = |Y| = n \geq 4$. If*

$$H(G) \geq \frac{9n^2 - 11n + 16}{6},$$

then G is Hamiltonian unless $G = K_{n,n-2} + 4e$.

Proof. Assume that G is non-Hamiltonian.

$$\begin{aligned} H(G) = \tfrac{1}{2}\textstyle\sum_{i=1}^{2n} \hat{D}_i(G) &\leq \tfrac{1}{2}\textstyle\sum_{i=1}^{2n}[d_i + \tfrac{1}{3}(n - d_i) + \tfrac{1}{2}(n-1)] \\ &= \tfrac{1}{2}\textstyle\sum_{i=1}^{2n}(\tfrac{5n-3}{6} + \tfrac{2}{3}d_i) \\ &= \tfrac{5n^2-3n}{6} + \tfrac{1}{3}\textstyle\sum_{i=1}^{2n} d_i \\ &= \tfrac{5n^2-3n}{6} + \tfrac{2}{3}m. \end{aligned}$$

Note that $H(G) \geq \frac{9n^2-11n+16}{6}$, we have $m \geq n^2 - 2n + 4$. From Lemma 4.4, we obtain that $G = K_{n,n-2} + 4e$. ■

Theorem 4.8. *Let $G = G[X, Y]$ be a bipartite graph with $\delta \geq 2$ and m edges, where $|X| = |Y| = n \geq 4$. If*

$$H(G^*) \leq \frac{12n^2 - 25n + 16}{4n - 2},$$

then G is Hamiltonian unless $G \in \{K_{4,2} + 4e, K_{5,3} + 4e, K_{6,4} + 4e, K_{7,5} + 4e\}$.

Proof. Assume that G is non-Hamiltonian.

$$\begin{aligned} H(G^*) = \tfrac{1}{2}\textstyle\sum_{i=1}^{2n} \hat{D}_i(G^*) &\geq \tfrac{1}{2}\textstyle\sum_{i=1}^{2n}[d_{G^*}(v_i) + \tfrac{1}{2n-1}(n - d_{G^*}(v_i)) + \tfrac{n-1}{2n-2}] \\ &= \tfrac{1}{2}\textstyle\sum_{i=1}^{2n}[\tfrac{2(n-1)}{2n-1}d_{G^*}(v_i) + \tfrac{n}{2n-1} + \tfrac{1}{2}] \\ &= \tfrac{1}{2}\textstyle\sum_{i=1}^{2n}[\tfrac{2(n-1)}{2n-1}d_{G^*}(v_i) + \tfrac{4n-1}{2(2n-1)}] \\ &= \tfrac{n(4n-1)}{2(2n-1)} + \tfrac{2(n-1)}{2(2n-1)}\textstyle\sum_{i=1}^{2n}(n - d_G(v_i)) \\ &= \tfrac{4n^3-n}{2(2n-1)} - \tfrac{2(n-1)}{2n-1}m. \end{aligned}$$

Note that $H(G^*) \leq \frac{12n^2-25n+16}{4n-2}$, we have $m \geq n^2 - 2n + 4$. From Lemma 4.4, we obtain that $G = K_{n,n-2} + 4e$. Note that

$$H((K_{n,n-2} + 4e)^*) \geq \frac{n^2 + 3n - 8}{4} > \frac{12n^2 - 25n + 16}{4n - 2}, n \geq 8.$$

So we have $G \in \{K_{4,2} + 4e, K_{5,3} + 4e, K_{6,4} + 4e, K_{7,5} + 4e\}$. ■

5 Harary spectral radius on traceable and Hamiltonian graphs

Lemma 5.1. *Let G be a graph on n vertices. Then $\rho(G) \geq \frac{2H(G)}{n}$, and the equality holds if and only if the row sums of $RD(G)$ are all equal.*

Proof. Let $x = \frac{1}{\sqrt{n}}(1, 1, \ldots, 1)$ be a unit n-vector. Then by Raleigh principle, applied to the Harary matrix RD(G) of G, we get

$$\begin{aligned}\rho(G) &\geq \tfrac{xRD(G)x^t}{xx^t} \\ &= \tfrac{\frac{1}{\sqrt{n}}[RD_1, RD_2, \ldots, RD_n]\frac{1}{\sqrt{n}}[1,1\ldots,1]^t}{1} \\ &= \tfrac{1}{n}\sum_{1\leq i\leq n} RD_i \\ &= \tfrac{2H(G)}{n}.\end{aligned}$$

Now suppose each row of $RD(G)$ sums to a constant, say k and $2H(G) = nk$. Then by the Theorem of Frobenius [2], k is simple and greatest eigenvalue of $RD(G)$. Thus $\rho(G) = k = \frac{nk}{n} = \frac{2H(G)}{n}$ and hence equality holds.

Conversely if equality holds, then x is the eigenvector corresponding to $\rho(G)$ and hence $xRD(G) = \rho(G)x$. So the row sums of $RD(G)$ are all equal. The proof is completed. ■

Theorem 5.2. *Let G be a connected graph of order $n \geq 4$. If*

$$\rho(\overline{G}) \leq \frac{5n^2 - 19n + 20}{n(n-1)},$$

then G is traceable unless $G = K_{1,3}$.

G	$\overline{G}$	$\rho(\overline{G})$	$\frac{5n^2-19n+20}{n(n-1)}$
$K_{1,3}$	$K_3 \cup K_1$	2	2
$K_1 \vee (K_{n-3} + 2K_1)$	$(K_2 \vee (n-3)K_1) \cup K_1$	$\frac{n-2+\sqrt{n^2+20n-60}}{4}$	$\frac{5n^2-9n+20}{n(n-1)}$
$K_1 \vee (K_{1,3} + K_1)$	$(K_1 \vee (K_3 + K_1)) \cup K_1$	3.4575	2.8667
$K_{2,4}$	$K_2 \cup K_4$	3	2.8667
$K_2 \vee 4K_1$	$K_4 \cup 2K_1$	3	2.8667
$K_2 \vee (3K_1 + K_2)$	$(K_3 \vee 2K_1) \cup 2K_1$	3.8117	3.1429
$K_1 \vee K_{2,5}$	$K_2 \cup K_5 \cup K_1$	4	3.3571
$K_3 \vee 5K_1$	$K_5 \vee 3K_1$	4	3.3571
$K_2 \vee (K_{1,4} + K_1)$	$(K_1 \vee (K_4 + K_1)) \cup 2K_1$	4.4115	3.3571
$K_4 \vee 6K_1$	$K_6 \cup 4K_1$	5	3.6667

Table 1: The harary spectral radius of complements of graphs

Proof. Suppose that G is nontraceable. From Lemma 5.1, we have

$$\rho(\overline{G}) \geq \frac{2H(\overline{G})}{n} \geq (n-1) - \frac{2(n-2)m}{n(n-1)}.$$

Since $\rho(\overline{G}) \leq \frac{5n^2-19n+20}{n(n-1)}$, we have $m \geq \binom{n-2}{2} + 2$. According to Lemma 3.1, we have $G \in \mathbb{NP}$. By a direct computation, we have the above Table 1. ¿From Table 1, we obtain the result. ■

Theorem 5.3. *Let G be a graph on $n \geq 5$ vertices and m edges with $\delta \geq 2$. If*

$$\rho(\overline{G}) \leq \frac{5n^2 - 23n + 28}{n(n-1)},$$

then G is Hamiltonian.

G	$\overline{G}$	$\rho(\overline{G})$	$\frac{5n^2-23n+28}{n(n-1)}$
$K_2 \vee (K_{n-4} + 2K_1)$	$(K_2 \vee (n-4)K_1) \cup 2K_1$	$\frac{n-3+\sqrt{n^2+18n-79}}{4}$	$\frac{5n^2-23n+28}{n(n-1)}$
$K_3 \vee (4K_1)$	$K_4 \cup 3K_1$	3	2.6667
$K_2 \vee (K_{1,3} + K_1)$	$(K_1 \vee (K_3 + K_1)) \cup 2K_1$	3.4575	2.6667
$K_1 \vee K_{2,4}$	$K_4 \cup K_2 \cup K_1$	3	2.6667
$K_3 \vee (K_2 + 3K_1)$	$(K_3 \vee 2K_1) \cup 3K_1$	3.8117	2.9286
$K_4 \vee 5K_1$	$K_5 \cup 4K_1$	4	3.1389
$K_3 \vee (K_{1,4} + K_1)$	$(K_1 \vee (K_4 + K_1)) \cup 3K_1$	4.4115	3.1389
$K_2 \vee K_{2,5}$	$K_5 \cup K_2 \cup 2K_1$	4	3.1389
$K_5 \vee 6K_1$	$K_6 \cup 5K_1$	5	3.4545

Table 2: The harary spectral radius of complements of graphs

Proof. Suppose that G is non-Hamiltonian. From Lemma 5.1, we have

$$\rho(\overline{G}) \geq \frac{2H(\overline{G})}{n} \geq (n-1) - \frac{2(n-2)m}{n(n-1)}.$$

Since $\rho(\overline{G}) \leq \frac{5n^2-23n+28}{n(n-1)}$, we have $m \geq \binom{n-2}{2} + 4$. According to Lemma 3.3, we obtain $G \in \mathbb{NC}$. By a direct computation, we have the following Table 2. From Table 2, we complete the proof. ■

6 Harary spectral radius on traceable and Hamiltonian biparatite graphs

Theorem 6.1. *Let $G = G[X, Y]$ be a bipartite graph with $\delta \geq 1$ and m edges, where $|X| = |Y| = n \geq 3$. If*

$$\rho(G^*) \leq \frac{12n^2 - 21n + 12}{4n^2 - 2n},$$

then G is traceable.

Proof. According to Lemma 5.1, we have

$$\rho(G^*) \geq \frac{2H(G^*)}{2n} \geq \frac{1}{n}[\frac{4n^3 - n}{2(2n-1)} - \frac{2(n-1)}{2n-1}m].$$

Note that $\rho(G^*) \leq \frac{12n^2-21n+12}{4n^2-2n}$, we have $m \geq n^2 - 2n + 3$. By Lemma 4.1, then G is traceable. ■

Theorem 6.2. *Let $G = G[X, Y]$ be a bipartite graph with $\delta_X \geq 1$ and $\delta_Y \geq 2$, where $|X| = n + 1$ and $|Y| = n \geq 3$. If*

$$\rho(G^*[X, Y]) \leq \frac{24n^2 - 28n + 15}{8n^2 - 2},$$

then G is traceable.

Proof. According to Lemma 5.1, we have

$$\rho(G^*) \geq \frac{2H(G^*)}{2n+1} \geq \frac{2}{2n+1}[\frac{8n^3 + 8n^2 - 4n - 1}{4(2n-1)} - \frac{2(n-1)}{2n-1}m].$$

Note that $\rho(G^*[X, Y]) \leq \frac{24n^2-28n+15}{8n^2-2}$, we have $m \geq n^2 - n + 2$. Note that $d(v) = n + 1$ in $G[X, Y + v]$, hence

$$m(G[X, Y + v]) = m + (n + 1) \geq n^2 + 3 = (n + 1)^2 - 2(n + 1) + 4.$$

From Lemma 4.4, $G = G[X, Y + v]$ is Hamiltonian unless $G = K_{n+1,n-1} + 4e$. Hence $G = G[X, Y]$ is traceable unless $G \in \{K_{n,n-1} + 2e, K_{n+1,n-2} + 4e\}$. Note that

$$\rho((K_{n,n-1} + 2e)^*) = \frac{n-1+\sqrt{n^2+26n-23}}{4} > \frac{24n^2-28n+15}{8n^2-2},\ n \geq 3.$$

$$\rho((K_{n+1,n-2} + 4e)^*) = \frac{n-1+\sqrt{n^2+26n-23}}{4} > \frac{24n^2-28n+15}{8n^2-2},\ n \geq 3.$$

The proof is completed. ■

Theorem 6.3. *Let $G = G[X, Y]$ be a bipartite graph with $\delta \geq 2$, where $|X| = |Y| = n \geq 4$. If*

$$\rho(G^*) \leq \frac{12n^2 - 25n + 16}{4n^2 - 2n},$$

then G is Hamiltonian.

Proof. According to Lemma 5.1, we have

$$\rho(G^*) \geq \frac{2H(G^*)}{2n} \geq \frac{1}{n}[\frac{4n^3 - n}{2(2n-1)} - \frac{2(n-1)}{2n-1}m].$$

Note that $\rho(G^*) \leq \frac{12n^2-25n+16}{4n^2-2n}$, we have $m \geq n^2 - 2n + 4$. By Lemma 4.4, we obtain that $G = K_{n,n-2} + 4e$. Note that

$$\rho((K_{n,n-2} + 4e)^*) = \frac{n - 2 + \sqrt{n^2 + 24n - 48}}{4} > \frac{12n^2 - 25n + 16}{4n^2 - 2n}, n \geq 4.$$

The proof is completed. ■

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