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SOME TOPOLOGICAL INDICES AND GRAPH PROPERTIES

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ABSTRACT. In this paper, by using the degree sequences of graphs, we present sufficient conditions for a graph to be Hamiltonian, traceable, Hamilton-connected or k-connected in light of numerous topological indices such as the eccentric connectivity index, the eccentric distance sum, the connective eccentricity index.

1. Introduction

Let G be a connected graph with vertex set V(G) and edge set E(G) such that |V| = n and |E| = m. Let d(v) be the degree of a vertex v in G. Let d(u, v) be the distance between two vertices u and v in G, that is, the length of the shortest path connecting u and v in G. The eccentricity $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex. Let K_n, S_n, P_n be a complete graph, a star and a path on v vertices, respectively.

A cycle C in a graph G is called a Hamiltonian cycle of G if C contains all the vertices of G. A graph G is called Hamiltonian if G has a Hamiltonian cycle. A path P in a graph G is called a Hamiltonian path of G if P contains all the vertices of G. A graph G is called traceable if G has a Hamiltonian path. A graph G is called Hamilton-connected if for each pair of vertices in G there is a Hamiltonian path between them. A graph G is said to be k-connected (or k-vertex connected) if there does not exist a set of K 1 vertices whose removal disconnects the graph. If G and G are two vertex-disjoint graphs, we use $G \vee H$ to denote the join of G and G.

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The topological indices are widely used in organic chemistry and have been found to be useful in chemical documentation, isomer discrimination, structure-property relationships, structure-activity (SAR) relationships and pharmaceutical drug design [14, 23]. In past decades, plenty of mathematical properties of numerous topological indices are reported such as the the matching energy [5, 6], Randić index [24] and the Balaban index [7].

For a connected graph G, its Wiener index, denoted by W(G), is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v) = \frac{1}{2} \sum_{v \in V(G)} D(v).$$

Here $D(v) = \sum_{u \in V(G)} d_G(u, v)$. It can be easily verified that $D(v) \geq d(v) + 2(n - 1 - d(v))$. The Wiener index and its modifications are well studied in the past years, see [9, 17, 21, 19, 20].

The eccentric connectivity index (ECI) [22] of a connected graph G, denoted by $\xi^c(G)$, is defined as

$$\xi^{c}(G) = \sum_{v \in V(G)} \varepsilon(v)d(v).$$

The eccentric distance sum (EDS) [11] of a connected graph G is defined as

$$\xi^d(G) = \sum_{v \in V(G)} \varepsilon(v) \cdot D(v).$$

The connective eccentricity index (CEI) [10] of a connected graph G is defined as

$$\xi^{ce}(G) = \sum_{v \in V(G)} \frac{d(v)}{\varepsilon(v)}.$$

The above three topological indices involving eccentricities are widely studied from mathematical view, see [13, 18, 26, 27, 28].

In [25], Yang presented a sufficient condition for a graph to be traceable by using Wiener index. In [12], Hua and Wang presented a sufficient condition for a graph to be traceable by using Harary index. Li [15, 16] presented sufficient conditions in terms of the Harary index and Wiener index for a graph to be Hamiltonian or Hamilton-connected using some proof ideas in [25].

In this paper, as a continuance of the above results, we further study the conditions for a graph to be Hamiltonian, traceable, Hamilton-connected or k-connected in light of numerous topological indices such as the ECI, EDS and CEI.

2. Preliminaries

We first present some lemmas that will be used later.

Lemma 2.1. [8] Let G be a graph of order $n \geq 3$ with degree sequence $d_1 \leq d_2 \leq \cdots \leq d_n$. If $d_k \leq k < \frac{n}{2} \Rightarrow d_{n-k} \geq n-k$, then G is Hamiltonian.

Lemma 2.2. [1] Let G be a nontrivial graph of order $n \ge 4$ with degree sequence $d_1 \le d_2 \le \cdots \le d_n$. If $d_k + 1 \le k < \frac{n+1}{2} \Rightarrow d_{n-k+1} \le n-k-1$, then G is traceable.

Lemma 2.3. [3] Let G be a graph of order $n \geq 4$ with degree sequence $d_1 \leq d_2 \leq \cdots \leq d_n$. 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 G is k-connected.

Lemma 2.4. [2] Let G be a graph of order $n \geq 4$ with degree sequence $d_1 \leq d_2 \leq \cdots \leq d_n$. If $2 \leq k \leq \frac{n}{2}, d_{k-1} \leq k \Rightarrow d_{n-k} \geq n-k+1$, then G is Hamilton-connected.

Lemma 2.5. [2, Page 210, Corollary 5] Let G = (X, Y; E) be a bipartite graph such that $X = \{x_1, x_2, ..., x_n\}$, $Y = \{y_1, y_2, ..., y_n\}$, $n \ge 2$, and $d(x_1) \le d(x_2) \le ... \le d(x_n)$, $d(y_1) \le d(y_2) \le ... \le d(y_n)$. If $d(x_k) \le k < n \Rightarrow d(y_{n-k}) \ge n - k + 1$, then G is Hamiltonian.

Lemma 2.6. [4] Let G be a 2-connected graph of order $n \geq 12$. If $m \geq {n-2 \choose 2} + 4$, then G is Hamiltonian or $G = K_2 \vee ((2K_1) \cup K_{n-4})$.

Lemma 2.7. [4] Let G be a 3-connected graph of order $n \ge 18$. If $m \ge {n-3 \choose 2} + 9$, then G is Hamiltonian or $G = K_3 \lor ((3K_1) \cup K_{n-6})$.

Lemma 2.8. [4] Let G be a k-connected graph of order n. If $m \ge {n \choose 2} - (k+1)(n-k-1)/2 + 1$, then G is Hamiltonian.

3. Main Results

Theorem 3.1. Let G be a connected graph of order $n \geq 6$.

- (1) If $\xi^{c}(G) \ge n^{3} 3n^{2} + 4n \frac{4m^{2}}{n} > 0$, then G is Hamiltonian.
- (2) If $\xi^d(G) \leq \frac{1}{n(n-1)}(n^2 + n 4)^2$, then G is Hamiltonian.
- (3) If $\xi^{ce}(G) \ge (n-1)\frac{n^2-3n+5}{n}$, then G is Hamiltonian.

Proof. Suppose that G is not Hamiltonian, then from Lemma 2.1, there exists an integer $1 \le k \le \frac{n-1}{2}$ such that $d_k \le k$ and $d_{n-k} \le n-k-1$.

(1) We consider $\xi^c(G)$. Since $\varepsilon(v) \leq n - d(v)$, from the definition, we have

$$\xi^{c}(G) = \sum_{v \in V(G)} \varepsilon(v) d(v) \leq \sum_{v \in V(G)} (n - d(v)) d(v)$$

$$= n \left(\sum_{v \in V(G)} d(v) \right) - \sum_{v \in V(G)} d^{2}(v)$$

$$\leq n \left(\sum_{v \in V(G)} d(v) \right) - \frac{1}{n} \left(\sum_{v \in V(G)} d(v) \right)^{2}$$

$$= n \left(\sum_{v \in V(G)} d(v) \right) - \frac{4m^{2}}{n}$$

$$\leq n \left[k^{2} + (n - 2k)(n - k - 1) + k(n - 1) \right] - \frac{4m^{2}}{n}$$

$$= n^{2}(n - 1) + n \left[3k^{2} - (2n - 1)k \right] - \frac{4m^{2}}{n}.$$

Suppose $f(x) = 3x^2 - (2n-1)x$ with $1 \le x \le \frac{1}{2}(n-1)$. It is easy to see that $f_{\max}(x) = \max\{f(1), f(\frac{1}{2}(n-1))\}$. As f(1) = 4-2n, $f(\frac{1}{2}(n-1)) = \frac{1}{4}(1-n^2)$, $f(\frac{n-1}{2})-f(1) = -\frac{1}{4}(n-5)(n-3) < 0$, so we have $f_{\max}(x) = f(1)$. Thus, $\xi^c(G) \le n^2(n-1) + n(4-2n) - \frac{4m^2}{n} = n^3 - 3n^2 + 4n - \frac{4m^2}{n}$, so we get the result.

If $\xi^c(G) = n^3 - 3n^2 + 4n - \frac{4m^2}{n}$, then all the inequalities in the proof should be equalities, so k = 1, and hence $d_1 = 1$, $d_2 = d_3 = \cdots = d_{n-1} = n-2$, $d_n = n-1$. Thus $G = K_1 \vee (K_1 \cup K_{n-2})$, which is not Hamiltonian as stated in [1]. But this graph dose not satisfy $\sum_{v \in V(G)} d^2(v) = \frac{1}{n} \left(\sum_{v \in V(G)} d(v)\right)^2$, thus the equality can not hold.

(2) We consider $\xi^d(G)$. Since $\varepsilon(v) \geq \frac{D(v)}{n-1}$, $D(v) \geq d(v) + 2(n-1-d(v))$, from the definition, we have

$$\xi^{d}(G) = \sum_{v \in V(G)} \varepsilon(v) \cdot D(v) \ge \sum_{v \in V(G)} \frac{D(v)}{n-1} \cdot D(v)$$

$$= \frac{1}{n-1} \sum_{v \in V(G)} (D(v))^{2}$$

$$\ge \frac{1}{n-1} \sum_{v \in V(G)} \left[4(n-1)^{2} - 4(n-1)d(v) + (d(v))^{2} \right]$$

$$= 4n(n-1) - 4 \sum_{v \in V(G)} d(v) + \frac{1}{n-1} \sum_{v \in V(G)} (d(v))^{2}$$

$$\ge 4n(n-1) - 4 \sum_{v \in V(G)} d(v) + \frac{1}{n-1} \cdot \frac{1}{n} \left(\sum_{v \in V(G)} d(v) \right)^{2}$$

$$= \frac{1}{n(n-1)} \left[\left(\sum_{v \in V(G)} d(v) - 2n(n-1) \right)^{2} - 4n(n-1) \sum_{v \in V(G)} d(v) + 4n^{2}(n-1)^{2} \right]$$

$$= \frac{1}{n(n-1)} \left[\sum_{v \in V(G)} d(v) - 2n(n-1) \right]^{2}.$$

As $\sum_{v \in V(G)} d(v) < 2n(n-1)$, we have

$$\xi^{d}(G) \geq \frac{1}{n(n-1)} \left[k^{2} + (n-2k)(n-k-1) + k(n-1) - 2n(n-1) \right]^{2}$$

$$= \frac{1}{n(n-1)} \left\{ 2n(n-1) - \left[k^{2} + (n-2k)(n-k-1) + k(n-1) \right] \right\}^{2}$$

$$= \frac{1}{n(n-1)} \left[-3k^{2} + (2n-1)k + n^{2} - n \right]^{2}.$$

Suppose $f(x) = -3x^2 + (2n-1)x + n^2 - n$ with $1 \le x \le \frac{1}{2}(n-1)$. As $f(1) = n^2 + n - 4$, $f(\frac{n-1}{2}) = \frac{1}{4}(n-1)(5n+1)$, $f(\frac{n-1}{2}) - f(1) = \frac{1}{4}(n-3)(n-5) > 0$, so we have $f_{\min}(x) = \min\{f(1), f(\frac{1}{2}(n-1))\} = f(1)$. Thus $\xi^d(G) \ge \frac{1}{n(n-1)}(n^2 + n - 4)^2$, and we get the result.

If $\xi^d(G) = \frac{1}{n(n-1)}(n^2 + n - 4)^2$, then k = 1, the remaining is as in the previous proof.

(3) We consider $\xi^{ce}(G)$. From the definition, we have

$$\xi^{ce}(G) = \sum_{v \in V(G)} \frac{d(v)}{\varepsilon(v)}$$

$$\leq \sum_{v \in V(G)} \frac{n-1}{D(v)} \cdot d(v)$$

$$\leq (n-1) \sum_{v \in V(G)} \frac{d(v)}{2(n-1) - d(v)}.$$

Suppose $f(x) = \frac{x}{2(n-1)-x}$, then we have $f'(x) = \frac{2(n-1)}{[2(n-1)-x]^2} > 0$, and thus f(x) is strictly increasing, therefore

$$\xi^{ce}(G) \leq (n-1) \left[\frac{k^2}{2(n-1)-k} + \frac{(n-2k)(n-k-1)}{2(n-1)-(n-k-1)} + \frac{k(n-1)}{2(n-1)-(n-1)} \right]$$

$$= (n-1) \left[\frac{k^2}{2n-k-2} + \frac{(n-2k)(n-k-1)}{n+k-1} + k \right].$$

Since $1 \le k \le \frac{n-1}{2}$, then $2n-k-2-(n+k-1)=n-2k-1 \ge 0$, so $\frac{k^2}{2n-k-2} \le \frac{k^2}{n+k-1}$. Further, $\frac{(n-2k)(n-k-1)}{n+k-1} = \frac{(n-2k)(n+k-1-2k)}{n+k-1} = n-2k-\frac{2k(n-2k)}{n+k-1}$. Therefore,

$$\begin{split} \xi^{ce}(G) & \leq (n-1) \left[\frac{k^2}{n+k-1} - \frac{2k(n-2k)}{n+k-1} - k + n \right] \\ & = (n-1) \left[\frac{k^2 - 2k(n-2k)}{n+k-1} - k + n \right] \\ & = (n-1) \left\{ \frac{k \left[4k - (3n-1) \right]}{n+k-1} + n \right\}. \end{split}$$

Suppose $f(x) = \frac{x[4x-(3n-1)]}{n+x-1}$ with $1 \le x \le \frac{1}{2}(n-1)$. As $f(1) = \frac{5-3n}{n}$, $f(\frac{n-1}{2}) = -\frac{1}{3}(n+1)$, $f(\frac{n-1}{2}) - f(1) = -\frac{1}{3n}(n-3)(n-5) < 0$, so we have $f_{\max}(x) = \max\{f(1), f(\frac{1}{2}(n-1))\} = f(1)$. Thus $\xi^{ce}(G) \le (n-1)\frac{n^2-3n+5}{n}$, and we get the result.

If $\xi^{ce}(G) = (n-1)\frac{n^2-3n+5}{n}$, then all the inequalities in the proof should be equalities, so k=1, and hence $d_1=1$, $d_2=d_3=\cdots=d_{n-1}=n-2$, $d_n=n-1$. Thus $G=K_1\vee (K_1\cup K_{n-2})$, which is not Hamiltonian as stated in [1].

On the other hand, $\varepsilon(v) \geq \frac{D(v)}{n-1}$, with equality if and only if d(v,u) (for fixed $v \in V(G)$) is a constant for all $u \in V(G)$ with $v \neq u$. Thus, $G = K_1 \vee (K_1 \cup K_{n-2})$ can not satisfy it, the equality can not hold.

Theorem 3.2. Let G be a connected graph of order $n \ge 11$.

- (1) If $\xi^{c}(G) \ge n^{3} 5n^{2} + 10n \frac{4m^{2}}{n} > 0$, then G is traceable.
- (2) If $\xi^d(G) \leq \frac{1}{n(n-1)}(n^2 + 3n 10)^2$, then G is traceable.
- (3) If $\xi^{ce}(G) \ge (n-1) \frac{n^2 5n + 12}{n+1}$, then G is traceable.

Proof. Suppose that G is not traceable, then by Lemma 2.2, there is an integer $k \leq \frac{n}{2}$ such that $d_k \leq k-1$ and $d_{n-k+1} \leq n-k-1$. Since G is connected and $d_k \leq k-1$, we have $k \geq 2$.

(1) We consider $\xi^c(G)$. As in Theorem 3.1, we have

$$\xi^{c}(G) \leq n \left(\sum_{v \in V(G)} d(v) \right) - \frac{4m^{2}}{n}$$

$$\leq n \left[k(k-1) + (n-2k+1)(n-k-1) + (k-1)(n-1) \right] - \frac{4m^{2}}{n}$$

$$= n^{2}(n-1) - \frac{4m^{2}}{n} + n \left[3k^{2} - (2n+1)k \right].$$

Suppose $f(x) = 3x^2 - (2n+1)x$ with $2 \le x \le \frac{n}{2}$. As f(2) = 10 - 4n, $f(\frac{n}{2}) = -\frac{1}{4}n(n+2)$, $f(\frac{n}{2}) - f(2) = -\frac{1}{4}(n-10)(n-4) < 0$, so we have $f_{\max}(x) = \max\{f(2), f(\frac{n}{2})\} = f(2)$. Thus $\xi^c(G) \le n^2(n-1) - \frac{4m^2}{n} + n(10-4n) = n^3 - 5n^2 + 10n - \frac{4m^2}{n}$, so we get the result.

If $\xi^c(G) = n^3 - 5n^2 + 10n - \frac{4m^2}{n}$, then k = 2, and hence $d_1 = d_2 = 1$, $d_3 = \cdots = d_{n-1} = n - 3$, $d_n = n - 1$. Thus $G = K_1 \vee (K_{n-3} \cup 2K_1)$, which is not traceable. But this graph does not satisfy $\sum_{v \in V(G)} d^2(v) = \frac{1}{n} \left(\sum_{v \in V(G)} d(v)\right)^2$, thus the equality can not hold.

(2) We consider $\xi^d(G)$, as in Theorem 3.1, we have

$$\xi^d(G) \geq \frac{1}{n(n-1)} \left[\sum_{v \in V(G)} d(v) - 2n(n-1) \right]^2.$$

Since $2n(n-1) - \sum_{v \in V(G)} d(v) > 0$, we have

$$\xi^{d}(G) \geq \frac{1}{n(n-1)} \left[k(k-1) + (n-2k+1)(n-k-1) + (k-1)(n-1) - 2n(n-1) \right]^{2}$$

$$= \frac{1}{n(n-1)} \left\{ 2n(n-1) - \left[k(k-1) + (n-2k+1)(n-k-1) + (k-1)(n-1) \right] \right\}^{2}$$

$$= \frac{1}{n(n-1)} \left[-3k^{2} + (2n+1)k + n(n-1) \right]^{2}.$$

Suppose $f(x) = -3x^2 + (2n+1)x + n^2 - n$ with $2 \le x \le \frac{n}{2}$. As $f(2) = n^2 + 3n - 10$, $f(\frac{n}{2}) = \frac{1}{4}n(5n-2)$, $f(\frac{n}{2}) - f(2) = \frac{1}{4}(n-4)(n-10) \ge 0$, so we have $f_{\min}(x) = \min\{f(2), f(\frac{n}{2})\} = f(2)$. Thus $\xi^d(G) \ge \frac{1}{n(n-1)}(n^2 + 3n - 10)^2$, so we get the result.

If $\xi^d(G) = \frac{1}{n(n-1)}(n^2 + 3n - 10)^2$, then k = 2, the remaining is as in the previous proof.

(3) We consider $\xi^{ce}(G)$. As in Theorem 3.1,

$$\xi^{ce}(G) \le (n-1) \sum_{v \in V(G)} \frac{d(v)}{2(n-1) - d(v)}.$$

Suppose $f(x) = \frac{x}{2(n-1)-x}$, then $f'(x) = \frac{2(n-1)}{[2(n-1)-x]^2} > 0$, so

$$\xi^{ce}(G) \leq (n-1) \left[\frac{k(k-1)}{2(n-1) - (k-1)} + \frac{(n-2k+1)(n-k-1)}{2(n-1) - (n-k-1)} + \frac{(k-1)(n-1)}{2(n-1) - (n-1)} \right]$$

$$= (n-1) \left[\frac{k(k-1)}{2n-k-1} + \frac{(n-2k+1)(n-k-1)}{n+k-1} + k-1 \right].$$

Since $2 \le k \le \frac{n}{2}$, then $2n-k-1-(n+k-1) = n-2k \ge 0$. As $\frac{(n-2k+1)(n-k-1)}{n+k-1} = \frac{(n-2k+1)(n+k-1-2k)}{n+k-1} = \frac{(n-2k+1)(n-k-1)}{n+k-1} = \frac{(n-2k+1)(n-k-1)}{$ $n-2k+1-\frac{2k(n-2k+1)}{n+k-1}$, therefore,

$$\xi^{ce}(G) \leq (n-1) \left[\frac{k(k-1)}{n+k-1} - \frac{2k(n-2k+1)}{n+k-1} - k + n \right]$$

$$= (n-1) \left[\frac{k(k-1) - 2k(n-2k+1)}{n+k-1} - k + n \right]$$

$$= (n-1) \left\{ \frac{k[4k - (3n+2)]}{n+k-1} + n \right\}.$$

Suppose $f(x) = \frac{x[4x - (3n+2)]}{n+x-1}$ with $2 \le x \le \frac{n}{2}$. It is easy to see that $f_{\max}(x) = \max\{f(2), f(\frac{n}{2})\}$. As $f(2) = \frac{6(2-n)}{n+1}$, $f(\frac{n}{2}) = -\frac{n(n+2)}{3n-2}$, $f(\frac{n}{2}) - f(2) = -\frac{(n-4)(n^2 - 11n + 6)}{(3n-2)(n+1)} < 0$, so we have $f_{\max}(x) = f(2)$. Thus $\xi^{ce}(G) \leq (n-1)\frac{n^2-5n+12}{n+1}$, so we get the result. If $\xi^{ce}(G) = (n-1)\frac{n^2-5n+12}{n+1}$, then k=2, and hence $d_1 = d_2 = 1$, $d_3 = \cdots = d_{n-1} = n-3$,

 $d_n = n - 1$. Thus $G = K_1 \vee (K_{n-3} \cup 2K_1)$, which is not traceable.

On the other hand, $\varepsilon(v) \geq \frac{D(v)}{n-1}$, with equality if and only if d(v,u) (for fixed $v \in V(G)$) is a constant for all $u \in V(G)$ with $v \neq u$. But $G = K_1 \vee (K_{n-3} \cup 2K_1)$ can not satisfy it, and the equality case can not occur.

Theorem 3.3. Let G be a connected graph of order $n \geq 2$.

- (1) If $\xi^{c}(G) \geq n^{3} 3n^{2} + 2kn \frac{4m^{2}}{n} > 0$, then G is k-connected.
- (2) If $\xi^d(G) \leq \frac{1}{n(n-1)}(n^2 + n 2k)^2$, then G is k-connected. (3) If $\xi^{ce}(G) \geq (n-1)(\frac{3k-3n-1}{n} + n)$, then G is k-connected.

Proof. Suppose that G is not k-connected, then from Lemma 2.3, there exists an integer $1 \le i \le \frac{n-k+1}{2}$ such that $d_i \leq i + k - 2$ and $d_{n-k+1} \leq n - i - 1$. Obviously, $1 \leq k \leq n - 1$.

(1) We consider $\xi^c(G)$, as in Theorem 3.1, we have

$$\xi^{c}(G) \leq n \left(\sum_{v \in V(G)} d(v) \right) - \frac{4m^{2}}{n}$$

$$\leq n \left[i(i+k-2) + (n-k-i+1)(n-i-1) + (k-1)(n-1) \right] - \frac{4m^{2}}{n}$$

$$= n^{2}(n-1) - \frac{4m^{2}}{n} + 2n \left[i^{2} - (n-k+1)i \right].$$

Suppose $f(x) = x^2 - (n-k+1)x$ with $1 \le x \le \frac{n-k+1}{2}$, then $f(x) \le f(1) = k-n$. Thus $\xi^{c}(G) \le n^{2}(n-1) - \frac{4m^{2}}{n} + 2n(k-n) = n^{3} - 3n^{2} + 2kn - \frac{4m^{2}}{n}$, so we get the result.

If $\xi^c(G) = n^3 - 3n^2 + 2kn - \frac{4m^2}{n}$, then all the inequalities in the proof should be equalities, so i = 1, $d_1 = k-1, d_2 = \cdots = d_{n-k+1} = n-2, d_{n-k+2} = \cdots = d_n = n-1.$ Thus $G = (K_1 \cup K_{n-k}) \vee K_{k-1}$, which is not k-connected. But it can not satisfy $\sum_{v \in V(G)} d^2(v) = \frac{1}{n} \left(\sum_{v \in V(G)} d(v) \right)^2$, thus the equality can not hold.

(2) We consider $\xi^d(G)$. As in Theorem 3.1,

$$\xi^d(G) \ge \frac{1}{n(n-1)} \left[\sum_{v \in V(G)} d(v) - 2n(n-1) \right]^2.$$

Since $2n(n-1) - \sum_{v \in V(G)} d(v) > 0$, then

$$\xi^{d}(G) \geq \frac{1}{n(n-1)} \left[i(i+k-2) + (n-k-i+1)(n-i-1) + (k-1)(n-1) - 2n(n-1) \right]^{2}$$

$$= \frac{1}{n(n-1)} \left\{ 2n(n-1) - \left[i(i+k-2) + (n-k-i+1)(n-i-1) + (k-1)(n-1) \right] \right\}^{2}$$

$$= \frac{1}{n(n-1)} \left[-2i^{2} - 2i(-1+k-n) + n(n-1) \right]^{2}.$$

Suppose $f(x) = -2x^2 - 2x(-1 + k - n) + n(n - 1)$ with $1 \le x \le \frac{n - k + 1}{2}$, $f(1) \le f(x) \le f(\frac{n - k + 1}{2})$, f(1) = n(n + 1) - 2k. Thus $\xi^d(G) \ge \frac{1}{n(n - 1)}(n(n + 1) - 2k)^2$, so we get the result.

If $\xi^d(G) = \frac{1}{n(n-1)}(n^2 + n - 2k)^2$, then all the inequalities in the proof should be equalities, so i = 1, the remaining is as in the previous proof.

(3) We consider $\xi^{ce}(G)$, as in Theorem 3.1, we have

$$\xi^{ce}(G) \le (n-1) \sum_{v \in V(G)} \frac{d(v)}{2(n-1) - d(v)}.$$

Suppose $f(x) = \frac{x}{2(n-1)-x}$, $f'(x) = \frac{2(n-1)}{[2(n-1)-x]^2} > 0$, so

$$\begin{split} \xi^{ce}(G) & \leq (n-1) \Big[\frac{i(i+k-2)}{2(n-1)-(i+k-2)} + \frac{(n-k-i+1)(n-i-1)}{2(n-1)-(n-i-1)} \\ & + \frac{(k-1)(n-1)}{2(n-1)-(n-1)} \Big] \\ & = (n-1) \left[\frac{i(i+k-2)}{2n-k-i} + \frac{(n-k-i+1)(n-i-1)}{n+i-1} + k - 1 \right]. \end{split}$$

Since $1 \le i \le \frac{n-k+1}{2}$, then $2n-k-i-(n+i-1)=n-k-2i+1 \ge 0$. Further, $\frac{(n-k-i+1)(n-i-1)}{n+i-1} = \frac{(n-k-i+1)(n+i-1-2i)}{n+i-1} = n-k-i+1 - \frac{2i(n-k-i+1)}{n+i-1}$.

Therefore,

$$\begin{split} \xi^{ce}(G) & \leq (n-1) \left[\frac{i(i+k-2)}{n+i-1} - \frac{2i(n-k-i+1)}{n+i-1} - i + n \right] \\ & = (n-1) \left[\frac{i(i+k-2) - 2i(n-k-i+1)}{n+i-1} - i + n \right] \\ & = (n-1) \left[\frac{i(2i+3k-3n-3)}{n+i-1} + n \right]. \end{split}$$

Suppose $f(x) = \frac{x(2x+3k-3n-3)}{n+x-1}$ with $1 \le x \le \frac{n-k+1}{2}$, we can easily compute that $f_{\max}(x) = f(1) = \frac{3k-3n-1}{n}$. Thus $\xi^{ce}(G) \le (n-1)(\frac{3k-3n-1}{n}+n)$, so we get the result.

If $\xi^{ce}(G) = (n-1)(\frac{3k-3n-1}{n}+n)$, then $i=1, d_1=k-1, d_2=\cdots=d_{n-k+1}=n-2, d_{n-k+2}=\cdots=d_n=n-1$. Thus $G=(K_1\cup K_{n-k})\vee K_{k-1}$, which is not k-connected.

On the other hand, $\varepsilon(v) \geq \frac{D(v)}{n-1}$, with equality if and only if d(v,u) (for fixed $v \in V(G)$) is a constant for all $u \in V(G)$ with $v \neq u$. But $G = (K_1 \cup K_{n-k}) \vee K_{k-1}$ can not satisfy it, the equality can not hold.

Theorem 3.4. Let G be a connected graph of order $n \geq 7$.

- (1) If $\xi^c(G) \ge n^3 3n^2 + 6n \frac{4m^2}{n} > 0$, then G is Hamilton-connected.
- (2) If $\xi^d(G) \leq \frac{1}{n(n-1)}(n^2+n-6)^2$, then G is Hamilton-connected.
- (3) If $\xi^{ce}(G) \geq (n-1)(\frac{8}{n}+n-3)$, then G is Hamilton-connected.

Proof. Suppose that G is not Hamilton-connected, then from Lemma 2.4, there exists an integer $2 \le k \le \frac{n}{2}$ such that $d_{k-1} \le k$ and $d_{n-k} \le n-k$.

(1) We consider $\xi^c(G)$, as in Theorem 3.1, we have

$$\xi^{c}(G) \leq n \left(\sum_{v \in V(G)} d(v) \right) - \frac{4m^{2}}{n}$$

$$\leq n \left[(k-1)k + (n-2k+1)(n-k) + k(n-1) \right] - \frac{4m^{2}}{n}$$

$$= n^{2}(n+1) - \frac{4m^{2}}{n} + n \left[3k^{2} - (2n+3)k \right].$$

Suppose $f(x) = 3x^2 - (2n+3)x$ with $2 \le x \le \frac{n}{2}$. As f(2) = 6 - 4n, $f(\frac{n}{2}) = -\frac{1}{4}n(n+6)$, $f(\frac{n}{2}) - f(2) = -\frac{1}{4}(n-6)(n-4) < 0$, so we have $f_{\max}(x) = \max\{f(2), f(\frac{n}{2})\} = f(2)$. Thus, $\xi^c(G) \le n^2(n+1) - \frac{4m^2}{n} + n(6-4n) = n^3 - 3n^2 + 6n - \frac{4m^2}{n}$, so we get the result.

If $\xi^{c}(G) = n^{3} - 3n^{2} + 6n - \frac{4m^{2}}{n}$, then k = 2, $d_{1} = 2$, $d_{2} = d_{3} = \cdots = d_{n-2} = n-2$, $d_{n-1} = d_{n} = n-1$. Thus $G = K_{2} \vee (K_{1} \cup K_{n-3})$, which is not Hamilton-connected. But it can not satisfy $\sum_{v \in V(G)} d^{2}(v) = \frac{1}{n} \left(\sum_{v \in V(G)} d(v)\right)^{2}$, thus the equality can not hold.

(2) We consider $\xi^d(G)$, as in Theorem 3.1, we have

$$\xi^d(G) \ge \frac{1}{n(n-1)} \left[\sum_{v \in V(G)} d(v) - 2n(n-1) \right]^2.$$

Since $2n(n-1) - \sum_{v \in V(G)} d(v) > 0$, then

$$\xi^{d}(G) \geq \frac{1}{n(n-1)} \left[k(k-1) + (n-2k+1)(n-k) + k(n-1) - 2n(n-1) \right]^{2}$$

$$= \frac{1}{n(n-1)} \left\{ 2n(n-1) - \left[k(k-1) + (n-2k+1)(n-k) + k(n-1) \right] \right\}^{2}$$

$$= \frac{1}{n(n-1)} \left[-3k^{2} + (2n+3)k + n(n-3) \right]^{2}.$$

Suppose $f(x) = -3x^2 + (2n+3)x + n(n-3)$ with $2 \le x \le \frac{n}{2}$. As $f(2) = n^2 + n - 6$, $f(\frac{n}{2}) = \frac{1}{4}n(5n-6)$, $f(\frac{n}{2}) - f(2) = \frac{1}{4}(n-4)(n-6) > 0$, so we have $f_{\min}(x) = \min\{f(2), f(\frac{n}{2})\} = f(2)$. Thus $\xi^d(G) \ge \frac{1}{n(n-1)}(n^2 + n - 6)^2$, so we get the result.

If $\xi^d(G) = \frac{1}{n(n-1)}(n^2 + n - 6)^2$, then k = 2, the remaining is as in the previous proof.

(3) We consider $\xi^{ce}(G)$, as in Theorem 3.1, we have

$$\xi^{ce}(G) \le (n-1) \sum_{v \in V(G)} \frac{d(v)}{2(n-1) - d(v)}.$$

Suppose $f(x) = \frac{x}{2(n-1)-x}$, $f'(x) = \frac{2(n-1)}{[2(n-1)-x]^2} > 0$, so

$$\begin{split} \xi^{ce}(G) & \leq & (n-1) \left[\frac{k(k-1)}{2(n-1)-k} + \frac{(n-2k+1)(n-k)}{2(n-1)-(n-k)} + \frac{k(n-1)}{2(n-1)-(n-1)} \right] \\ & = & (n-1) \left[\frac{k(k-1)}{2n-k-2} + \frac{(n-2k+1)(n-k)}{n+k-2} + k \right]. \end{split}$$

Since $2 \le k \le \frac{n}{2}$, then $2n - k - 2 - (n + k - 2) = n - 2k \ge 0$. Further, $\frac{(n-2k+1)(n-k)}{n+k-2} = \frac{(n-2k+1)(n+k-2-2k+2)}{n+k-2} = n - 2k + 1 - \frac{(2k-2)(n-2k+1)}{n+k-2}$.

Therefore,

$$\begin{split} \xi^{ce}(G) & \leq (n-1) \left[\frac{k(k-1)}{n+k-2} - \frac{(2k-2)(n-2k+1)}{n+k-2} - k+n+1 \right] \\ & = (n-1) \left[\frac{k(k-1) - (2k-2)(n-2k+1)}{n+k-2} - k+n+1 \right] \\ & = (n-1) \left\{ \frac{4k^2 - (3n+5)k + 2n+2}{n+k-2} + n+1 \right\}. \end{split}$$

Suppose $f(x) = \frac{4x^2 - (3n+5)x + 2n+2}{n+x-2}$ with $2 \le x \le \frac{n}{2}$. As $f(\frac{n}{2}) = -\frac{n^2 + n - 4}{3n-4}$, $f(2) = \frac{8}{n} - 4$, $f(\frac{n}{2}) - f(2) = -\frac{(n-4)(n^2 - 7n + 8)}{n(3n-4)} < 0$. So we have $f_{\max}(x) = \max\{f(2), f(\frac{n}{2})\} = f(2)$. Thus $\xi^{ce}(G) \le (n-1)[f(2) + n + 1] = (n-1)(\frac{8}{n} + n - 3)$, so we get the result.

If $\xi^{ce}(G) = (n-1)(\frac{8}{n} + n - 3)$, then k = 2, $d_1 = 2$, $d_2 = d_3 = \cdots = d_{n-2} = n-2$, $d_{n-1} = d_n = n-1$. Thus $G = K_2 \vee (K_1 \cup K_{n-3})$, which is not Hamilton-connected.

On the other hand, $\varepsilon(v) \geq \frac{D(v)}{n-1}$, with equality if and only if d(v,u) (for fixed $v \in V(G)$) is a constant for all $u \in V(G)$ with $v \neq u$. Thus, $G = K_2 \vee (K_1 \cup K_{n-3})$ can not satisfy it, the equality can not hold.

Theorem 3.5. Let G = (X, Y; E) be a connected bipartite graph with $X = \{x_1, x_2, \dots, x_n\}$, $Y = \{y_1, y_2, \dots, y_n\}$, and $n \ge 2$. Then we have:

- (1) If $\xi^d(G) \leq \frac{1}{n(n-1)}(n^2 + 2n 4)^2 + \frac{n(5n-2)^2}{n-1}$, then G is Hamiltonian.
- (2) If $\xi^{ce}(G) \ge (n-1) \left[\frac{1}{6} (n^2 2n + 2) + \frac{n^2}{3n-2} \right]$, then G is Hamiltonian.

Proof. Suppose that G is not Hamiltonian, then from Lemma 2.5, there exists an integer k < n such that $d(x_k) \le k$ and $d(y_{n-k}) \le n - k$. Let $N(x_1) := \{z_1, z_2, \dots z_s\}$ be the neighbors of x_1 , where $s = d(x_1)$. Then $d(x_1, z_i) = 1$ for each $z_i \in N(x_1)$, $d(x_1, x_i) \ge 2$ for each x_i with $2 \le i \le n$, and $d(x_1, y_i) \ge 3$ for each $y_i \in Y - N(x_1)$.

(1) We consider $\xi^d(G)$. First, we have

$$D(x_1) \ge d(x_1) + 2(n-1) + 3(n - d(x_1)) = 5n - 2 - 2d(x_1).$$

Similarly, for each i with $2 \le i \le n$ and each j with $1 \le j \le n$,

$$D(x_i) \ge d(x_i) + 2(n-1) + 3(n - d(x_i)) = 5n - 2 - 2d(x_i).$$

$$D(y_j) \ge d(y_j) + 2(n-1) + 3(n - d(y_j)) = 5n - 2 - 2d(y_j).$$

Therefore, we have

$$\xi^{d}(G) = \sum_{v \in V(G)} \varepsilon(v) \cdot D(v) \ge \sum_{v \in V(G)} \frac{D(v)}{n-1} \cdot D(v) = \frac{1}{n-1} \sum_{v \in V(G)} (D(v))^{2}$$

$$= \frac{1}{n-1} \left[\sum_{x_{i} \in X} (D(v_{i})^{2}) + \sum_{y_{j} \in Y} (D(v_{j})^{2}) \right]$$

$$\ge \frac{1}{n-1} \left\{ \sum_{x_{i} \in X} \left[(5n-2)^{2} - 4(5n-2)d(x_{i}) + 4(d(x_{i}))^{2} \right] + \sum_{y_{j} \in Y} \left[(5n-2)^{2} - 4(5n-2)d(y_{j}) + 4(d(y_{j}))^{2} \right] \right\}$$

$$= \frac{1}{n-1} \left[2n(5n-2)^{2} - 4(5n-2) \sum_{v \in V(G)} d(v) + 4 \sum_{v \in V(G)} (d(v))^{2} \right]$$

$$\ge \frac{1}{n-1} \left[2n(5n-2)^{2} - 4(5n-2) \sum_{v \in V(G)} d(v) + \frac{4}{n} (\sum_{v \in V(G)} d(v))^{2} \right]$$

$$= \frac{1}{n(n-1)} \left[2n^{2}(5n-2)^{2} - 4n(5n-2) \sum_{v \in V(G)} d(v) + 4 (\sum_{v \in V(G)} d(v))^{2} \right]$$

$$= \frac{1}{n(n-1)} \left[n(5n-2) - 2 \sum_{v \in V(G)} d(v) \right]^{2} + \frac{n(5n-2)^{2}}{n-1}.$$

Since

$$2\sum_{v \in V(G)} d(v) \leq 2\left[k^2 + (n-k)n + (n-k)^2 + kn\right]$$

$$< 2\left[kn + (n-k)n + (n-k)n + kn\right]$$

$$= 4n^2 \leq n(5n-2),$$

it follows that

$$\xi^{d}(G) \geq \frac{1}{n(n-1)} \left[n(5n-2) - 2(k^{2} + (n-k)n + (n-k)^{2} + nk) \right]^{2} + \frac{n(5n-2)^{2}}{n-1}$$
$$= \frac{1}{n(n-1)} \left[-4k^{2} + 4nk + n(n-2) \right]^{2} + \frac{n(5n-2)^{2}}{n-1}.$$

Suppose $f(x) = -4x^2 + 4nx + n(n-2)$ with $1 \le x \le n-1$. It is easy to see that $f_{\min}(x) = \min\{f(1), f(n-1)\}$. As f(1) = f(n-1), $f_{\min}(x) = f(1) = n^2 + 2n - 4$, thus $\xi^d(G) \ge \frac{1}{n(n-1)}(n^2 + 2n - 4)^2 + \frac{n(5n-2)^2}{n-1}$.

If $\xi^d(G) = \frac{1}{n(n-1)}(n^2 + 2n - 4)^2 + \frac{n(5n-2)^2}{n-1}$, then k = 1, $d(x_1) = 1$, $d(x_2) = \cdots = d(x_n) = n$, $d(y_1) = d(y_2) = \cdots = d(y_{n-1}) = n - 1$, $d(y_n) = n$. Thus $G = K_{n,n} - K_{1,n-1}$, which is not Hamiltonian. On the other hand, $\varepsilon(v) \geq \frac{D(v)}{n-1}$, with equality if and only if d(v, u) (for fixed $v \in V(G)$) is a constant for all $u \in V(G)$ with $v \neq u$. However, $G = K_{n,n} - K_{1,n-1}$ can not satisfy it, the equality can not hold.

(2) We consider $\xi^{ce}(G)$.

$$D(x_1) \ge d(x_1) + 2(n-1) + 3(n - d(x_1)) = 5n - 2 - 2d(x_1).$$

Similarly, for each i with $2 \le i \le n$ and each j with $1 \le j \le n$,

$$D(x_i) \ge d(x_i) + 2(n-1) + 3(n - d(x_i)) = 5n - 2 - 2d(x_i).$$

$$D(y_j) \ge d(y_j) + 2(n-1) + 3(n - d(y_j)) = 5n - 2 - 2d(y_j).$$

Therefore,

$$\xi^{ce}(G) = \sum_{v \in V(G)} \frac{d(v)}{\varepsilon(v)}$$

$$\leq \sum_{x_i \in X} \frac{n-1}{D(x_i)} \cdot d(x_i) + \sum_{y_j \in X} \frac{n-1}{D(y_j)} \cdot d(y_j)$$

$$\leq (n-1) \left[\sum_{x_i \in X} \frac{d(x_i)}{5n-2-2d(x_i)} + \sum_{y_j \in X} \frac{d(y_j)}{5n-2-2d(y_j)} \right].$$

Suppose $f(x) = \frac{x}{5n-2-2x}$, then we have $f'(x) = \frac{5n-2}{(5n-2-2x)^2} > 0$, so

$$\begin{split} \xi^{ce}(G) & \leq & (n-1) \left[\frac{k^2}{5n-2-2k} + \frac{(n-k)n}{5n-2-2n} + \frac{(n-k)^2}{5n-2-2(n-k)} + \frac{kn}{5n-2-2n} \right] \\ & = & (n-1) \left[\frac{k^2}{5n-2-2k} + \frac{(n-k)^2}{3n+2k-2} + \frac{n^2}{3n-2} \right]. \end{split}$$

Since $1 \le k \le n-1$, then,

$$\xi^{ce}(G) \leq (n-1) \left[\frac{k^2}{5(k+1) - 2 - 2k} + \frac{(n-k)^2}{3(k+1) + 2k - 2} + \frac{n^2}{3n - 2} \right]$$

$$= (n-1) \left[\frac{k^2}{3k+3} + \frac{(n-k)^2}{5k+1} + \frac{n^2}{3n-2} \right]$$

$$\leq (n-1) \left[\frac{k^2}{3k+3} + \frac{(n-k)^2}{3k+3} + \frac{n^2}{3n-2} \right]$$

$$= (n-1) \left[\frac{k^2 + (n-k)^2}{3k+3} + \frac{n^2}{3n-2} \right].$$

Suppose $f(x) = \frac{x^2 + (n-x)^2}{3x+3}$ with $1 \le x \le (n-1)$. It is easy to see that $f_{\max}(x) = \max\{f(1), f(n-1)\}$. As $f(n-1) = \frac{1}{3n}(n^2 - 2n + 2)$, $f(1) = \frac{1}{6}(n^2 - 2n + 2)$, $f(n-1) - f(1) = -\frac{(n-2)(n^2 - 2n + 2)}{6n} < 0$, so we have $f_{\max}(x) = f(1)$.

If $\xi^{ce}(G)=(n-1)\left[\frac{1}{6}(n^2-2n+2)+\frac{n^2}{3n-2}\right]$, then k=1, the remaining is as in the previous proof.

Theorem 3.6. Let G be a 2-connected graph of order $n \ge 12$. If $\xi^d(G) \le \frac{1}{n(n-1)} \left[n^2 + 3n - 12 \right]^2$, then G is Hamiltonian.

Proof. Suppose that G is not Hamiltonian and G is not $K_2 \vee (2K_1 \cup K_{n-4})$, then from Lemma 2.6, we have that $m \leq \binom{n-2}{2} + 3$. As in Theorem 3.1,

$$\xi^d(G) \ge \frac{1}{n(n-1)} \left[\sum_{v \in V(G)} d(v) - 2n(n-1) \right]^2.$$

Since $2n(n-1) - \sum_{v \in V(G)} d(v) > 0$, then

$$\xi^d(G) \ge \frac{1}{n(n-1)} [2n(n-1) - 2m]^2$$

 $\ge \frac{1}{n(n-1)} [n^2 + 3n - 12]^2.$

On the other hand, $\varepsilon(v) \geq \frac{D(v)}{n-1}$, with equality if and only if d(v, u) (for fixed $v \in V(G)$) is a constant for all $u \in V(G)$ with $v \neq u$. Thus, $K_2 \vee (2K_1 \cup K_{n-4})$ can not satisfy it, the equality can not hold. \square

Theorem 3.7. Let G be a 3-connected graph of order $n \ge 18$. If $\xi^d(G) \le \frac{1}{n(n-1)} \left[n^2 + 5n - 28 \right]^2$, then G is Hamiltonian.

Proof. Suppose that G is not Hamiltonian and G is not $K_3 \vee (3K_1 \cup K_{n-6})$. Then from Lemma 2.7, we have that $m \leq {n-3 \choose 2} + 8$. Therefore,

$$\xi^{d}(G) \geq \frac{1}{n(n-1)} \left[\sum_{v \in V(G)} d(v) - 2n(n-1) \right]^{2}$$

$$\geq \frac{1}{n(n-1)} \left[2n(n-1) - 2m \right]^{2}$$

$$\geq \frac{1}{n(n-1)} \left[n^{2} + 5n - 28 \right]^{2}.$$

On the other hand, $\varepsilon(v) \geq \frac{D(v)}{n-1}$, with equality if and only if d(v,u) (for fixed $v \in V(G)$) is a constant for all $u \in V(G)$ with $v \neq u$. Thus, $K_3 \vee (3K_1 \cup K_{n-6})$ can not satisfy it, the equality can not hold. \square

Theorem 3.8. Let G be a k-connected graph of order $n \geq 18$. If

$$\xi^d(G) \le \frac{1}{n(n-1)} \left[n(n-1) + (k+1)(n-k-1) \right]^2,$$

then G is Hamiltonian.

Proof. Suppose that G is not Hamiltonian, then from Lemma 2.8, we have that $m \leq {n \choose 2} - (k+1)(n-k-1)/2$. Therefore,

$$\xi^{d}(G) \geq \frac{1}{n(n-1)} \left[\sum_{v \in V(G)} d(v) - 2n(n-1) \right]^{2}$$

$$= \frac{1}{n(n-1)} \left[2n(n-1) - 2m \right]^{2}$$

$$\geq \frac{1}{n(n-1)} \left[n(n-1) + (k+1)(n-k-1) \right]^{2},$$

which is a contradiction. This completes the proof.

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