On Degree-Distance index of a graph

Shivaswamy[1,*], P M Siddaraju[2] and Nanjundaswamy M[3]

Department of Mathematics, BMSCE, Bengaluru 560019, Karnataka, India

[2]*Department of Mathematics*

Government First Grade College for Women, Chamarajanagara-571313

Karnataka, INDIA.

[3]*Department of Mathematics*

Government first grade college for women

Byrapura, T Narasipur taluk, Mysore district - 571124

Karnataka, INDIA.

Abstract

In this article, we give sufficient conditions for the Hamiltonian and graphical properties of graphs in the terms of degree-distance index. The degree distance index of the graph is defined as the $S(G) = \sum_{u,v \in V(G)} (d(u) + d(v))d_G(u, v)$ where $d(u)$ is the degree of the vertex in a graph and $d_G(u, v)$ is the distance between the vertices u and v in the graph G.

Keyword: Degree distance index, Topological index, Hamiltonian Properties.

1 Introduction

In this paper, we are concerned with a topological invariant of a molecular graph called the Degree distance index. Let G be a connected graph of order n and size m. Let $V(G)$ be the vertex set of G. We use $d_G(u,v)$ to denote the distance between vertices u and v of the graph G, and d(u) is used to denote the degree of the vertex u of the graph. Let K_n denote the complete graph on n vertices. Then the Degree distance index (or degree distance) of G is defined as:

$$S(G) = \sum_{u,v \in V(G)} (d(u)+d(v))d_G(u,v) = \frac{1}{2}\sum_{u \in V(G)}\sum_{v \in V(G)} (d(u)+d(v))d_G(u,v)$$

Dobrynin and Kochetova [10] and Gutman [11] independently studied the degree distance sum of a graph. The same was studied by Tomescu [22], Tomescu [22] and Bucicovschi and Cioab [7]. A related concept studied earlier for the chemical applications called " Molecular topological index " MTI by H. P. Schultz in 1989 is defined as follows [19]: Let G be a graph with labeled vertices $v_1, v_2, ..., v_n$. Then

$$MTI(G) = \sum_{i=1}^{n} [v(A+D)]_i$$

where A and D are adjacency and distance matrices of G and $v = (d(v_1), d(v_2), ..., d(v_n))$.It can be easily seen from [11] that $MTI(G) = M_1(G) + S(G)$, where $M_1(G)$ is first Zagrab index and $S(G)$ is degree distance index.

A connected graph is said to be traceable (or Hamiltonian) if it has a Hamiltonian path (or cycle). A path (or cycle) is said to be a Hamiltonian path (or cycle) if it traverses through all vertices exactly once. A graph is said to be Hamiltonian-connected if it has a Hamiltonian path between every pair of vertices. A graph is said to be k- connected if it remains connected by removing fewer than k vertices. A graph on n vertices is k-edge Hamiltonian if every path of length not exceeding k, $1 \leq k \leq n-2$, is contained in a Hamiltonian cycle. The graph G is called k-path coverable if $V(G)$ can be covered by k or fewer than k vertex disjoint paths, obviously 1-path coverable is traceable. For a graph G, if $G[V\ X]$ is Hamiltonian for all $|X| \leq k$, , we call G to be k-Hamiltonian. In particular, 0-Hamiltonian is same as Hamiltonian. For other undefined graph-theoretic notations and terminology, the reader may refer to [6].

The problem of finding a Hamiltonian cycle is NP-complete as reported in [14]. In 2013, Yang [23] studied the Hamiltonian path in terms of the Wiener index and extended it to the Hamiltonian graph [18]. In the same year, Hua [12] discussed sufficient conditions for traceability in terms of the Harary index. Further, sufficient conditions for k-connected, β- deficient, and Hamiltonian cycle in terms of the first Zagreb index are studied in [2]. Also, An [3] studied graph properties based on reciprocal degree distance and An [1] discussed sufficient conditions for Hamiltonian-connectedness in terms of the first Zagreb index and reciprocal distance. In [20], the author(s) described sufficient conditions for k-edge Hamiltonian, k-path coverable, traceable, and Hamilton-connected graphs in terms of the forgotten index. In [13], author(s) studied sufficient conditions for Hamiltonicity with respect to the Wiener index, hyper-Wiener index, and Harary index. The Hamiltonian and graphical properties in terms of the eccentricity-based topological index are studied in [17, 24].

In this article, we explore sufficient conditions for the Hamiltonian path, Hamiltonian cycle, Hamiltonian-connected, and k-connected graphs in terms of the Degree distance index. The paper is organized as follows: In Section 2, we give some useful propositions which are needed in subsequent sections. In Section 3, we present the results and proofs of this paper.

2 Preliminaries

In this section, we will introduce four-degree conditions. In the following propositions, we suppose that the graph satisfies the degree sequence $\pi = (d_1 \leq d_2 \leq .... \leq d_n)$ condition.

Proposition1. [9] Let G be a graph of order $n \geq 3$ having degree sequence π. If

$$d_i \leq i - 1 \leq \frac{1}{2}(n-1) \Rightarrow d_{n-i} \geq n - i - 1$$

then G is traceable.

Proposition2. [9] Let G be a graph of order $n \geq 3$ having degree sequence π. If

$$d_i \leq i < \frac{n}{2} \Rightarrow d_{n-i} \geq n - i$$

then G is Hamiltonian.

Proposition3. [8] Let G be a graph of order $n \geq 3$ having degree sequence π. If

$$d_{i-1} \leq i \Rightarrow d_{n-i} \geq n - i + 1, for 2 \leq i \leq \frac{n}{2}$$

then G is Hamiltonian connected.

Proposition4. . [4] Let G be a graph of order $n \geq 4$ having degree sequence π. 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.

Proposition 5. [15] Let G be a graph with degree sequence π and $n \geq 3$ and $0 \leq k \leq n - 3$. If

$$d_{i-k} \leq i \Rightarrow d_{n-i} \geq n - i + k, for k + 1 \leq i \leq \frac{n + k}{2}$$

then π is k-edge Hamiltonian.

Proposition 6. [9] Let G be graph with degree sequence π and $0 \leq k \leq n - 3$. If

$$d_i \leq i + k \Rightarrow d_{n-i-k} \geq n - i, for 1 \leq i \leq \frac{1}{2}(n - k)$$

then G is k- Hamiltonian.

Proposition 7. [5, 16] If $k \geq 1$ and the degree sequence π of G satisfies

$$d_{i+k} \leq i \rightarrow d_{n-i} \geq n - i - k, for 1 \leq i \leq \frac{1}{2}(n - k)$$

then G is k-path coverable.

Define a graph G_4as follows: A graph whose set of vertices has partition $A \bigcup B \bigcup C \bigcup D$ such that $|A| = |C| = k$ and $|B| = |D| = m - k$ and and whose edges connect each vertex

$u \in A \bigcup B$ to each vertex $v \in C \bigcup D$ except when $u \in A$ and $v \in D$.

Proposition8. [9]Let G be a bipartite graph with vertices $(u_1, u_2, ..., u_n)$ and $(v_1, v_2, ..., v_n)$ such that $d(u_1) \leq d(u_2) \leq .... \leq d(u_n)$ and $d(v_1) \leq d(v_2) \leq .... \leq d(v_n)$ and

$$d(u_k) \leq k < n \rightarrow d(v_{n-k}) \geq n - k + 1$$

Then G is either Hamiltonian or G_4.

3 Degree distance index and Hamiltonicity

This section gives sufficient conditions for a graph to be traceable, Hamiltonian, Hamiltonian-connected, k-connected graphs, k-path coverable, k-Hamiltonian,k-edge Hamiltonian in terms of Degree distance index. Further, we give sufficient condition for bipartite graph to be Hamiltonian in terms of Degree distance index.

Let G be a connected graph, and $S(G)$ denotes the Degree distance index of G:For a vertex v of G,define $D(v) = \sum_{u \in G} d_G(v, u)$ and $D'(v) = d(v)D(v)$. Then

$$\begin{aligned} S(G) &= \sum_{v \in G} D'(v) \\ &= \sum_{v \in G} d(v)D(v) \end{aligned}$$

$$\leq \sum_{v \in G} d(v)[d(v) + (n - 1 - d(v))(n - 1 - d(v))] \quad (1)$$

$$= (n-1)^2 \sum_{v \in G} d(v) - (2n - 3) \sum_{v \in G} (d(v))^2 + \sum_{v \in G} (d(v))^3$$

We now have the following:

Theorem 1. Let G be a connected graph of order $n \geq 5$ and size m. If

$$S(G) \geq 2n^4 - 12n^3 + 27n^2 - 27n + 10 - \frac{(2n-3)}{n}4m^2$$

then G is traceable.

Proof. Suppose that G is not traceable, then by Proposition 1 and Equation1, the Degree distance index of G:

$$\begin{aligned}
S(G) &\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - (2n-3)\sum_{v\in G}(d(v))^2 \\
&\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - \frac{(2n-3)}{n}\left(\sum_{v\in G} d(v)\right)^2 \\
&\leq (n-1)^2[k(k-1) + (n-2k+1)(n-k-1) + (k-1)(n-1)] \\
&+ [k(k-1)^3 + (n-2k+1)(n-k-1)^3 + (k-1)(n-1)^3]\frac{(2n-3)}{n}4m^2 \\
&= (n-1)^2[3k^2 - (2n+1)k + n^2 - n] + [3k^4 - (7n-2)k^3 + (9n^2 - 12n + 6)k^2 \\
&- (4n^3 - 4n^2 + 3)k + n^4 - 3n^3 + 3n^2 - n] - \frac{(2n-3)}{n}4m^2 \\
&= 3k^4 - (7n-2)k^3 + (12n^2 - 18n + 9)k^2 - (6n^3 - 9n^2 + 4)k \\
&+ 2n^4 - 6n^3 + 6n^2 - 2n - \frac{(2n-3)}{n}4m^2 \\
&= 2n^4 - 12n^3 + 27n^2 - 27n + 10 - \frac{(2n-3)}{n}4m^2 \\
&+ (k-1)[3k^3 - (7n-5)k^2 + (12n^2 - 25n + 14)k - 6n^3 + 21n^2 - 25n + 10]
\end{aligned}$$

Combining with the condition of the Theorem 1, we know that $(k-1)[3k^3-(7n-5)k^2+(12n^2-25n+14)k-6n^3+21n^2-25n+10] \geq 0$. Since G is connected and $k \geq d_k+1 \geq 2$. Let $q(x) = 3x^3 - (7n-5)k^2 + (12n^2 - 25n + 14)x - 6n^3 + 21n^2 - 25n + 10$. Since k is an integer we have $2 \leq k \leq \frac{n+1}{2}$ is equivalent to $k \leq \frac{n}{2}$. So what follows we assume that $k \leq \frac{n}{2}$

The first derivative of $q(x)$ is $q'(x) = 9x^2 - 2(7n-5)x + (12n^2 - 25n + 14)$ and the discriminant $\Delta$of $q'(x) = 0$ is $\Delta = 4(7n-5)^2 - 36(12n^2 - 25n + 14) = -4(59n^2 - 155n + 101) < 0 \forall n \geq 2$. Therefore $q'(x) > 0$ and $q(x)$ is strictly increasing in the interval of $[2, \frac{n}{2}]$. Hence $max(q(x))$ is obtained at the right endpoint of the interval $[2, \frac{n}{2}]$.We consider the parity of n. If n is even then

$$max(q(x)) = q(\frac{n}{2}) = -\frac{1}{8}n(n(11n-78)+144)+10 < 0, \forall n \geq 5.$$

If n is odd then

$$max(q(x)) = q(\frac{n-1}{2}) = -\frac{1}{8}(n-1)(n(11n-38)+31) < 0, \forall n \geq 3.$$

Therefore $max(q(x)) < 0 \forall n \geq 5$. Then $S(G) \leq 2n^4 - 12n^3 + 27n^2 - 27n + 10 - \frac{(2n-3)}{n}4m^2$. Thus proof is coplete □

Theorem 2. Let G be a connected graph of order $n \geq 12$ and size m. If

$$S(G) \geq 2n^4 - 18n^3 + 82n^2 - 162n + 136 - \frac{(2n-3)}{n}4m^2$$

then G is Hamiltonian.

Proof. Suppose that G is not Hamiltonian, then by Proposition 2 and Equation 1, the Degree distance index of G:

$$\begin{aligned}
S(G) &\leq (n-1)^2 \sum_{v \in G} d(v) + \sum_{v \in G} (d(v))^3 - (2n-3) \sum_{v \in G} (d(v))^2 \\
&\leq (n-1)^2 \sum_{v \in G} d(v) + \sum_{v \in G} (d(v))^3 - \frac{(2n-3)}{n} (\sum_{v \in G} (d(v))^2 \\
&\leq (n-1)^2 [k^2 + (n-2k)(n-k-1) + k(n-1)] \\
&+ [k^4 + (n-2k)(n-k-1)^3 + k(n-1)^3] \frac{(2n-3)}{n} 4m^2 \\
&= (n-1)^2 [3k^2 - (2n-1)k + n^2 - n] + [3k^4 - (7n-6)k^3 + (9n^2 - 15n + 6)k^2 \\
&- (4n^3 - 9n^2 + 6n - 1)k + n^4 - 3n^3 + 3n^2 - n] - \frac{(2n-3)}{n} 4m^2 \\
&= 3k^4 - (7n-6)k^3 + (12n^2 - 21n + 9)k^2 - (6n^3 - 14n^2 + 10n - 2)k \\
&+ 2n^4 - 6n^3 + 6n^2 - 2n - \frac{(2n-3)}{n} 4m^2 \\
&= 2n^4 - 18n^3 + 82n^2 - 162n + 136 - \frac{(2n-3)}{n} 4m^2 \\
&+ (k-2)[3k^3 - (7n-12)k^2 + (12n^2 - 35n + 33)k - 6n^3 + 38n^2 - 80n + 68]
\end{aligned}$$

Combining with the condition of the Theorem 2, we know that $(k-2)[3k^3-(7n-12)k^2+(12n^2-35n+33)k-6n^3+38n^2-80n+68] \geq 0$. Since $2 \leq k < \frac{n}{2}$ is equivalent to $k \leq \frac{1}{2}(n-1)$. So what follows, we suppose $k \leq \frac{1}{2}(n-1)$. Let $q(x) = 3x^3-(7n-12)x^2+(12n^2-35n+33)x-6n^3+38n^2-80n+68$ where $2 \leq x \leq \frac{1}{2}(n-1)$. We divide the proof into following two parts.

Case1:$(k-2)q(x) = 0$, we have $k = 2$ or $q(x) = 0$, It is easy to see that $q'(x) = 9x^2-2(7n-12)x+(12n^2-35n+33)$ and the discriminant Δ of the equation $q'(x) = 0$ is $\Delta = 4(7n-12)^2-36(12n^2-35n+33) = -4(59n^2-147n+153) < 0 \forall n \geq 1$. Therefore $q'(x) > 0$ and q(x) is strictly increasing in the interval $2 \leq x < \frac{1}{2}(n-1)$. Then max(q(x)) is in the right endpoints of the domain of interval$[2, \frac{1}{2}(n-1)]$. Since k is an integer, we need to consider the parity of n. If n is even then $max(q(x)) = q(\frac{1}{2}(n-2))$. By a simple calculation, we have

$$q(\frac{1}{2}(n-2)) = -\frac{1}{8}n(n-4)(11n-86)+44 < 0, \forall n \geq 9$$

If n is odd, then $max(q(x)) = q(\frac{1}{2}(n-1))$. By a simple calculation, we have

$$q(\frac{1}{2}(n-1)) = \frac{1}{8}[-11n^3+159n^2-421n+433] < 0, \forall n \geq 12$$

In both the cases $q(x) < 0$. From the above analysis, we can see that $q(x) \neq 0$ for $2 \leq x \leq \frac{1}{2}(n-1)$ and $n \geq 12$. Hence we only need to consider the case $k = 2$. If $k = 2$ then $S(G) \leq 2n^4-18n^3+82n^2-162n+136-\frac{(2n-3)}{n}4m^2$. If equality holds then $d_1 = d_2 = 2, d_3 = ... = d_{n-2} = n-3, d_{n-1} = d_n = n-1$, which implies $G = K_2 \vee (2K_1+K_{n-4})$. But in this case the equality $\sum_{v \in V(G)} d(v)^2 = \frac{1}{n}\left(\sum_{v \in (V(G))} d(v)\right)^2$ does not holds.

Case 2: $(k-2)q(x) > 0$. In this case $k \geq 3$ and $q(x) = 3x^3-(7n-12)x^2+(12n^2-35n+33)x-6n^3+38n^2-80n+68 > 0$. By **case 1**, we know that $q(x)$ is strictly increasing and $max(q(x)) < 0$. Therefore for $3 \leq x \leq \frac{1}{2}(n-1)$, we have $3x^3-(7n-12)x^2+(12n^2-35n+33)x-6n^3+38n^2-80n+68 < 0$.A contradiction. Thus proof is complete. □

Theorem 3. Let G be a connected graph of order $n \geq 13$ and size m. If

$$S(G) \geq 2n^4-18n^3+92n^2-194n+204-(2n-3)\frac{4m^2}{n}$$

then G is Hamiltonian-connected.

Proof. Let G is non-Hamiltonian connected graph, then by Proposition 3 and Equation 1, the Degree distance index of G:

$$\begin{aligned}
S(G) &\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - (2n-3)\sum_{v\in G}(d(v))^2 \\
&\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - \frac{(2n-3)}{n}\left(\sum_{v\in G}(d(v)\right)^2 \\
&\leq (n-1)^2[k(k-1)+(n-2k+1)(n-k)+k(n-1)] - (2n-3)\frac{4m^2}{n} \\
&+ [k^3(k-1)+(n-2k+1)(n-k)^3+k(n-1)^3] \\
&= 3k^4-(7n+2)k^3+(12n^2-3n+3)k^2-(6n^3+5n^2-7n+4)k+2n^4-n^2+n \\
&- (2n-3)\frac{4m^2}{n} \\
&= 2n^4-18n^3+92n^2-194n+204-(2n-3)\frac{4m^2}{n} \\
&+ (k-3)[3k^3-(7n-7)k^2+(12n^2-24n+24)k-6n^3+31n^2-65n+68]
\end{aligned}$$

According to the condition of the Theorem 3, we have $(k-3)[3k^3-(7n-7)k^2+(12n^2-24n+24)k-6n^3+31n^2-65n+68] \geq 0$. Note that $k \geq d_{k-1} \geq \delta(G) \geq 3$. Let $q(x) = 3x^3-(7n-7)x^2+(12n^2-24n+24)x-6n^3+31n^2-65n+68$ with $3 \leq x \leq \frac{n}{2}$. We divide the proof into following two parts.

Case1:$(k-3)q(x) = 0$, then $k = 3$ or $q(x) = 0$, The first derivative of $q(x)$ is $q'(x) = 9x^2-2(7n-7)x+(12n^2-24n+24)$ and the discriminant Δ of the equation $q'(x) = 0$ is $\Delta = 4[(7n-7)^2-9(12n^2-24n+24) = -4(59n^2-118n+167) < 0\forall n \geq 2$. Therefore $q'(x) > 0$ and q(x) is strictly increasing in the interval $[3, \frac{\pi}{2}]$. Then $max(q(x))$ is obtained in the right end point of the interval $max(q(x)) = q(\frac{n}{2})$. By a simple calculation, we have

$$q(\frac{n}{2}) = -\frac{1}{8}n(n(11n-166)+424)+68 < 0, \forall n \geq 13$$

When n is odd, then $max(q(x)) = q(\frac{n-1}{2})$. By a simple calculation, we have

$$q(\frac{n-1}{2}) = \frac{1}{8}[-11n^3 + 137n^2 - 361n + 459] < 0, \forall n \geq 10$$

In both the cases $q(x) < 0 \forall n \geq 13$. By the above discussion, $f(x) \neq 0$ for $n \geq 13$. Hence we need to consider the case $k = 3$.We have $S(G) \geq 2n^4 - 18n^3 + 92n^2 - 194n + 204 - (2n-3)\frac{4m^2}{n}$. and $d_1 = d_2 = 3, d_3 = ... = d_{n-3} = n-3$ and $d_{n-1} = d_n = n-1$. Hence the graph is $G = K_3 \bigvee (2K_1 + K_{n-5})$. But in this case the equality $\sum_{v \in V(G)} d(v)^2 = \frac{1}{n}\bigg(\sum_{v \in (V(G))} d(v)\bigg)^2$ does not holds.

Case 2: $k \geq 4$. We have $3k^3 - (7n-7)k^2 + (12n^2 - 24n + 24)k - 6n^3 + 31n^2 - 65n + 68 \geq 0$. By **case 1** we have $3k^3 - (7n-7)k^2 + (12n^2 - 24n + 24)k - 6n^3 + 31n^2 - 65n + 68 < 0$ in the interval $[3, \frac{\pi}{2}]$.A contradiction. This completes the proof.

Theorem 4. Let G be a connected graph of order n, size m and $1 \leq k \leq n-1$. If

$$S(G) > k^3 + 3k^2 + (5n^2 + 7n + 12)k + 2n^4 - 12n^3 + 22n^2 - 18n - (2n-3)\frac{4m^2}{n}$$

then G is k-connected.

Proof. Let G is not k-connected graph, then by Proposition 4 and Equation 1, the Degree distance index of G:

$$\begin{aligned}
S(G) &\leq (n-1)^2 \sum_{v \in G} d(v) + \sum_{v \in G} (d(v))^3 - (2n-3) \sum_{v \in G} (d(v))^2 \\
&\leq (n-1)^2 \sum_{v \in G} d(v) + \sum_{v \in G} (d(v))^3 - \frac{(2n-3)}{n}\bigg(\sum_{v \in G}(d(v)\bigg)^2 \\
&\leq (n-1)^2[i(i+k-2) + (n-i-k+1)(n-i-1) + (k-1(n-1))] - (2n-3)\frac{4m^2}{n} \\
&+ [i(i+k-2)^3 + (n-i-k+1)(n-i-1)^3 + (k-1)(n-1)^3] \\
&= 2i^4 - (4n-4k+4)i^3 + (3k^2 - (3n+9)k + 8n^2 - 10n + 14)i^2 \\
&+ (k^3 - 6k^2 + (5n^2 + 10n + 17)k - 6n^3 + 8n^2 - 2n - 12)i + 2n^4 - 6n^3 + 6n^2 - 2n \\
&- (2n-3)\frac{4m^2}{n}
\end{aligned}$$

Let $q(x) = 2x^4 - (4n-4k+4)x^3 + (3k^2 - (3n+9)k + 8n^2 - 10n + 14)x^2 + (k^3 - 6k^2 +$

$(5n^2+10n+17)k-6n^3+8n^2-2n-12)x+2n^4-6n^3+6n^2-2n$ with $1 \leq x \leq \frac{n-k+1}{2}$. Then the first and second derivatives of $q(x)$ are

$$\begin{aligned} q'(x) &= 8x^3-3(4n-4k+4)x^2+2(3k^2-(3n+9)k+8n^2-10n+14)x \\ &+ (k^3-6k^2+(5n^2+10n+17)k-6n^3+8n^2-2n+12) \end{aligned}$$

and

$$q^{"}(x) = 24x^2-6(4n-4k+4)x+2(3k^2-(3n+9)k+8n^2-10n+14)$$

the discriminant Δ of the equation $q^{"}(x)=0$ is $\Delta = 36(4n-4k+4)^2-192(3k^2-(3n+9)k+8n^2-10n+14) = 192(-5n^2-(3k-16)n+3k-11) < 0, \forall n \geq 2$, and $1 \leq k \leq n-1$. Hence $q^{"}(x) > 0$ and $q(x)$ is convex function in the interval $[1, \frac{n-k+1}{2}]$ and $q(x) \in [q(1), q(\frac{n-k+1}{2})]$, By direct calculations we have

$$q(1) = k^3-3k^2+(5n^2+7n+12)k+2n^4-12n^3+22n^2-18n$$

and

$$\begin{aligned} q(\frac{n-k+1}{2}) &= \frac{1}{8}[-k^4-(2n-10)k^3-(4n^2+60n+40)k^2+(18n^3+42n^2+94n+54)k \\ &+ 5n^4-40n^3+58n^2-48n-23] \end{aligned}$$

Consider the difference
$q(1)-q(\frac{n-k+1}{2}) = \frac{1}{8}[k^4+(2n-2)k^3+(4n^2+60n+16)k^2-(18n^3+2n^2+38n-42)k+11n^4-56n^3+118n^2-96n+23]$. Let $r(x) = x^4+(2n-2)x^3+(4n^2+60n+16)x^2-(18n^3+2n^2+38n-42)x+11n^4-56n^3+118n^2-96n+23$ with $1 \leq x \leq n-1$. The first and second derivatives of $r(x)$ are

$$r'(x) \quad = \quad 4x^3 + 3(2n-2)x^2 + 2(4n^2 + 60n + 16)x - (18n^3 + 2n^2 + 38n - 42)$$

and

$$r''(x) \quad = \quad 12x^2 + 6(2n-2)x + 2(4n^2 + 60n + 16)$$

the discriminant Δ of the equation is $\Delta = 36(2n-2)^2 - 96(4n^2+60n+16) = -48(5n^2 + 126n + 29) < 0, \forall n \geq 1$. Hence the function $r(x)$ is convex in the interval of $[1, n-1]$. By direct calculation, we have $r(1) = (n-2)(11n^3 - 52n^2 + 16n - 40) > 0, \forall n \geq 5$ and $r(n-1) = 0$. Therefore $r(1) - r(n-1) > 0, \forall n \geq 5$.This implies that $r(x) > 0$ and hence $q(1) - q(\frac{n-k+1}{2}) > 0, \forall n \geq 5$. We conclude that $q(x) \leq q(1)$ and $S(G) \leq k^3 - 3k^2 + (5n^2 + 7n + 12)k + 2n^4 - 12n^3 + 22n^2 - 18n - (2n-3)\frac{4m^2}{n}$ This completes the proof.

Theorem 5. Let G be a connected graph of order n, size m and k be a positive integer such that $0 \leq k \leq n-3$. If

$$S(G) \quad > \quad k^3 + 13k^2 + (5n^2 - 13n + 22)k + 2n^4 - 12n^3 + 32n^2 - 40n + 20 - (2n-3)\frac{4m^2}{n}$$

then G is k-edge Hamiltonian.

Proof. Suppose that G is not k-edge Hamiltonian then by Proposition 5 and Equation 1. the Degree distance index of G:

$$
\begin{aligned}
S(G) &\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - (2n-3)\sum_{v\in G}(d(v))^2 \\
&\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - \frac{(2n-3)}{n}\left(\sum_{v\in G}(d(v)\right)^2 \\
&\leq (n-1)^2[i(i-k)+(n-2i+k)(n-i+k-1)+i(n-1)] \\
&+ [(i-k)i^3+(n-2i+k)(n-i+k-1)^3+i(n-1)^3] - (2n-3)\frac{4m^2}{n} \\
&= 3i^4-(7n+8k-6)i^3+(12n^2+18nk+9k^2-15k-21n+9)i^2 \\
&+ (-5k^3-19n^2k-6n^3-15nk^2+32nk+14n^2+12k^2-3k-10n+2)i+2n^4-6n^3+6n^2 \\
&- 2n+k^4+4nk^3+7n^2k^2+6n^3k-3k^3-11nk^2-14n^2k+4k^2+10nk-2k-(2n-3)\frac{4m^2}{n}
\end{aligned}
$$

Let $q(x) = 3x^4-(7n+8k-6)x^3+(12n^2+18nk+9k^2-15k-21n+9)x^2+(-5k^3-19n^2k-6n^3-15nk^2+32nk+14n^2+12k^2-3k-10n+2)x$ with $k+1\leq x\leq \frac{n+k}{2}$. The first and second derivatives of $q(x)$ are

$$
\begin{aligned}
q'(x) &= 12x^3-3(7n+8k-6)x^2+2(12n^2+18nk+9k^2-15k-21n+9)x \\
&+ (-5k^3-19n^2k-6n^3-15nk^2+32nk+14n^2+12k^2-3k-10n+2)
\end{aligned}
$$

and

$$
q^{"}(x) = 36x^2-6(7n+8k-6)x+2(12n^2+18nk+9k^2-15k-21n+9)
$$

the discriminant Δ of the equation $q^{"}(x)=0$ is $\Delta = 36[(7n+8k-6)^2-8(12n^2+18nk+9k^2-15k-21n+9)] = 36(-8k^2-32nk-47n^2+24k+84n-36) < 0$ for $n\geq 2$. Therefore $q^{"}(x)>0$ in the interval $[k+1,\frac{n+k}{2}]$ hence function is convex. $q(x)\in[k+1,\frac{n+k}{2}]$ and $max(q(x))\in[q(k+1),q(\frac{n+k}{2})]$. By simple calculation, we have

$$
q(k+1) = -(k+1)(k^3+(4n-5)k^2+(7n^2-15n-4)k+6n^3-26n^2+38n-20)
$$

$$q(\frac{n+k}{2}) \;=\; -\frac{1}{16}(n+k)(17k^3+(49n-48)k^2+(67n^2-136n-12)k+11n^3-40n^2+44n-16)$$

Consider the difference

$$\begin{aligned}
q(k+1)-q(\frac{n+k}{2}) &= -(k+1)(k^3+(4n-5)k^2+(7n^2-15n-4)k+6n^3-26n^2+38n-20)\\
&+ \frac{n+k}{2}(17k^3+(49n-48)k^2+(67n^2-136n-12)k\\
&+ 11n^3-40n^2+44n-16)\\
&= \frac{1}{2}[15k^4+(58n-60)k^3+(102n^2-162n+6)k^2\\
&+ (66n^3-138n^2-14n+32)k+11n^4-52n^3+96n^2-92n+20]\\
&\geq 252k^4+1100k^3+1600k^2+798k+95(n\geq k+3)\\
&> 0, fork \geq 1
\end{aligned}$$

Hence $q(k+1)-q(\frac{n+k}{2})>0, q(k+1)\geq q(\frac{n+k}{2}).max(q(x))=q(k+1)$. Then $S(G)\leq -(k+1)(k^3+(4n-5)k^2+(7n^2-15n-4)k+6n^3-26n^2+38n-20)+2n^4-6n^3+6n^2-2n+k^4+4nk^3+7n^2k^2+6n^3k-3k^3-11nk^2-14n^2k+4k^2+10nk-2k-(2n-3)=k^3+13k^2+(5n^2-13n+22)k+2n^4-12n^3+32n^2-40n+20-(2n-3)\frac{4m^2}{n}$. This proves the theorem. □

Theorem 6. Let G be a connected graph of order n, size m and k be a positive integer such that $0\leq k\leq n-3$. If

$$S(G) \;>\; k^3+3k^2-(5n^2-13n+12)k+2n^4-12n^3+32n^2-40n+20$$

then G is k-edge Hamiltonian.

Proof. Suppose that G is not k- Hamiltonian then by Proposition 6 and Equation 1. the Degree distance index of G:

$$\begin{aligned}
S(G) &\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - (2n-3)\sum_{v\in G}(d(v))^2 \\
&\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - \frac{(2n-3)}{n}\left(\sum_{v\in G}(d(v)\right)^2 \\
&\leq (n-1)^2[i(i+k)+(n-2i-k)(n-i-1)+(i+k)(n-1)] \\
&+ [i(i+k)^3+(n-2i-k)(n-i-1)^3+(i+k)(n-1)^3]-(2n-3)\frac{4m^2}{n} \\
&= 3i^4-(7n-4k-6)i^3+(12n^2-3nk+3k^2+3k-21n+9)i^2 \\
&+ (k^3+5n^2k-6n^3-10nk+14n^2+5k-10n+2)i+2n^4 \\
&- 6n^3+6n^2-2n-(2n-3)\frac{4m^2}{n}
\end{aligned}$$

Let $q(x) = 3x^4-(7n-4k-6)x^3+(12n^2-3nk+3k^2+3k-21n+9)x^2+(k^3+5n^2k-6n^3-10nk+14n^2+5k-10n+2)x+2n^4-6n^3+6n^2-2n$ with $1 \leq x \leq \frac{n-k}{2}$. Since x is an integer,we suppose $1 \leq x \leq \frac{n-k-1}{2}$ The first and second derivatives of $q(x)$ are

$$\begin{aligned}
q'(x) &= 12x^3-3(7n-4k-6)x^2+2(12n^2-3nk+3k^2+3k-21n+9)x \\
&+ (k^3+5n^2k-6n^3-10nk+14n^2+5k-10n+2)
\end{aligned}$$

and

$$q^{"}(x) = 36x^2-6(7n-4k-6)x+2(12n^2-3nk+3k^2+3k-21n+9)$$

the discriminant Δ of the equation $q^{"}(x)=0$ is $\Delta = 36[(7n-4k-6)^2-8(12n^2-3nk+3k^2+3k-21n+9)] = 36(-47k^2-32nk+84n-8k^2+24k-36) < 0$ for $1 \leq k \leq n-3, n \geq 1$. Therefore $q^{"}(x) > 0$ for the interval $[1, \frac{n-k-1}{2}]$ and hence $q(x)$ is convex function in the interval $[1, \frac{n-k-1}{2}]$ and $max(q(x)) \in [q(1), q(\frac{n-k-1}{2})]$. By direct calculation, we have

$$q(1) = k^3+3k^2-(5n^2-13n+12)k+2n^4-12n^3+32n^2-40n+20$$

and

$$q(\frac{n-k-1}{2}) = -\frac{1}{16}(n-k-1)[k^3+(n-3)k^2+(n-1)(3n-7)k-(n-1)^2(21n-11)]$$

consider the equation $q(1)-q(\frac{n-k-1}{2}) = \frac{1}{16}(k^4+(2n+12)k^3+(4n^2-14n+58)k^2-(18n^3+40n^2-182n+188)k+11n^4-118n^3+416n^2-586n+309] > 0$ This implies that $q(1) > q(\frac{n-k-1}{2})$ Hence $max(q(x)) = q(1).S(G) \leq k^3+3k^2-(5n^2-13n+12)k+2n^4-12n^3+32n^2-40n+20-(2n-3)\frac{4m^2}{n}$. The proof is completed. □

Theorem 7. Let G be a connected graph of order n, size m and k be a positive integer. If

$$\begin{aligned} S(G) &> k^4-(4n-8)k^3+(7n^2-26n+25)k^2-(6n^3-33n^2+60n-38)k \\ &+ 2n^4-12n^3+32n^2-40n+20-\frac{(2n-3)}{n}4m^2 \end{aligned}$$

then G is k-path Coverable.

Proof. Suppose that G is not k- path Coverable then by Proposition 7 and Equation 1. the Degree distance index of G:

$$\begin{aligned} S(G) &\leq (n-1)^2\sum_{v\in G} d(v)+\sum_{v\in G}(d(v))^3-(2n-3)\sum_{v\in G}(d(v))^2 \\ &\leq (n-1)^2\sum_{v\in G} d(v)+\sum_{v\in G}(d(v))^3-\frac{(2n-3)}{n}\left(\sum_{v\in G}(d(v)\right)^2 \\ &\leq (n-1)^2[i(i+k)+(n-2i-k)(n-i-k-1)+i(n-1)] \\ &+ [(i+k)i^3+(n-2i-k)(n-i-k-1)^3+i(n-1)^3]-\frac{(2n-3)}{n}4m^2 \\ &= 3i^4-(8k-7n+6)i^3+(9k^2-18kn+12n^2+15k-21n+9)i^2 \\ &+ (5k^3-15nk^2+19n^k-6n^3+12k^2-32kn+14n^2+13k-10n+2)i \\ &+ k^4-(4n-3)k^3+(7n^2-11n+4)k^2-(6n^3-14n^2+10n-2)k+2n^4 \\ &- 6n^3+6n^2-2n-\frac{(2n-3)}{n}4m^2 \end{aligned}$$

Let $q(x) = 3x^4-(8k-7n+6)x^3+(9k^2-18kn+12n^2+15k-21n+9)x^2+(5k^3-15nk^2+$

$19n^2k - 6n^3 + 12k^2 - 32kn + 14n^2 + 13k - 10n + 2)x$ with $1 \leq x \leq \frac{n-k-1}{2}$. Since x is an integer,we want to calculate $max(q(x))$ in the interval $[1, \frac{n-k-1}{2}]$ The first and second derivatives of $q(x)$ are

$$\begin{aligned} q'(x) &= 12x^3 + 3(8k - 7n + 6)x^2 + 2(9k^2 - 18kn + 12n^2 + 15k - 21n + 9)x \\ &+ (5k^3 - 15nk^2 + 19n^2k - 6n^3 + 12k^2 - 32nk + 14n^2 + 13k - 10n + 2) \end{aligned}$$

and

$$q^{"}(x) = 36x^2 + 6(8k - 7n + 6)x + 2(9k^2 - 18nk + 12n^2 + 15k - 21n + 9)$$

the discriminant Δ of the equation $q^{"}(x) = 0$ is $\Delta = 36[(8k - 7n + 6)^2 - 8(9k^2 - 18kn + 12n^2 + 15k - 21n + 9)] = -47n^2 - 8k^2 + 32kn - 24k + 84n - 36) < 0, \forall n \geq 1, k \geq 1$. Therefore $q^{"}(x) > 0$ hence $q(x)$ is convex in the interval $[1, q(\frac{n-k-1}{2})]$. Hence $max(q(x)) \in [q(1), q(\frac{n-k-1}{2})]$. By simple calculation, we have

$$q(1) = 5k^3 - 3(5n - 7)k^2 + (19n^2 - 50n + 36)k - 6n^3 + 26n^2 - 38n + 20$$

and

$$\begin{aligned} q(\frac{n-k-1}{2}) &= \frac{1}{16}(n - k - 1)[17k^3 + (49n - 35)k^2 + (n - 1)(67n - 39)k - 11n^3 \\ &+ 32n^2 + 11n - 11] \end{aligned}$$

the difference equation

$$\begin{aligned} q(1) - q(\frac{n-k-1}{2}) &= \frac{1}{16}(17k^3 - (66n - 132)k^3 + (116n^2 - 430n + 410)k^2 \\ &- (78n^3 - 510n^2 + 934n - 604)k + 11n^4 - 140n^3 + 438n^2 - 586n + 309] \\ &\geq 3k^3 + 2k^2 + k + 2(n \geq k + 1) \\ &> 0, \forall k \geq 1 \end{aligned}$$

Hence $max(q(x)) = q(1)$ then $S(G) \leq k^4 - (4n-8)k^3 + (7n^2 - 26n + 25)k^2 - (6n^3 - 33n^2 + 60n - 38)k + 2n^4 - 12n^3 + 32n^2 - 40n + 20 - 4m^2\frac{(2n-3)}{n}$. The proof is completed. □

Theorem 8. Let G be a bipartite graph of order $2n$, size m and $n \geq 2$. If

$$S(G) \quad > \quad 4(2n^4 - 5n^3 + 6n^2 - 4n + 1) - \frac{(2n-3)}{n}4m^2$$

then G is Hamiltonian.

Proof. Suppose that G is not Hamiltonian, then by Proposition 8 and Equation 1. the Degree distance index of G:

$$\begin{aligned}
S(G) &\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - (2n-3)\sum_{v\in G}(d(v))^2 \\
&\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - \frac{(2n-3)}{n}\big(\sum_{v\in G}(d(v)\big)^2 \\
&\leq (n-1)^2[ii + (n-i)n + (n-i)(n-i) + in] \\
&+ [ii^3 + (n-i)n^3 + (n-i)(n-i)^3 + in^3]\frac{(2n-3)}{n}4m^2 \\
&= 2i^4 - 4ni^3 + (8n^2 - 4n + 2)i^2 - (6n^3 - 4n^2 + 2n)i \\
&+ 4n^4 - 4n^3 + 2n^2 - \frac{(2n-3)}{n}4m^2
\end{aligned}$$

Let $q(x) = 2x^4 - 4nx^3 + (8n^2 - 4n + 2)x^2 - (6n^3 - 4n^2 + 2n) + 4n^4 - 4n^3 + 2n^2$ with $1 \leq x \leq n$. Since x is an integer,we want to calculate $max(q(x))$ in the interval $[1, n-1]$ The first and second derivatives of $q(x)$ are

$$q'(x) \quad = \quad 8x^3 - 12nx^2 + 2(8n^2 - 4n + 2)x - (6n^3 - 4n^2 + 2n)$$

and

$$q^{"}(x) \quad = \quad 24x^2 - 24nx + 2(8n^3 - 4n + 2)$$

the discriminant Δ of the equation $q^{"}(x) = 0$ is $\Delta = 576n^2 - 192(8n^2 - 4n + 2) =$

$-192(5n^2-4n+2) < 0, \forall n \geq 2$. Therefore $q^{"}(x) > 0$ hence $q(x)$ is convex in the interval $[1, n-1]$. $max(q(x)) \in [q(1), q(n-1)]$. By simple calculation, we have

$$q(1) = 4(2n^4 - 5n^3 + 6n^2 - 4n + 1)$$

and

$$q(n-1) = 4(2n^4 - 5n^3 + 6n^2 - 4n + 1)$$

the difference equation $q(1) - q(n-1) = max(q(x))$in $[1, n-1]$. We have $max(q(x)) = q(1)$. Therefore, $S(G) \leq 4(2n^4 - 5n^3 + 6n^2 - 4n + 1) - \frac{4m^2}{n}$. The theorem is proved. □

References

[1] M. An, The first Zagreb index,reciprocal degree distance and Hamiltonian-connectedness of graphs Inform. Process. Lett.176(2022) pp 5.

[2] M.An and K.Ch. Das, First Zagreb Index,k-Connectivity,$\beta Deficiency$ and k-Hamiltonicity of Graphs MATCH Commun. Math. Comput. Chem. 80 (2018) 141-151.

[3] M. An,Y. Zhang,K. Ch. Das and L/ Xiong, Reciprocal degree distance and graph properties Discrete Applied Math. 258(2019) 1-7.

[4] J. A. Bondy, Properties of graphs with constraints on degree Studia Sci. Math. Hungar. 4 (1969) 473-475.

[5] J. A. Bondy and V. Chvátal, A Method in Graph Theory Discrete Math. 15 (1976) 111-135.

[6] J. A. Bondy and U. S. R. Murty, Graph Theory with Application, Springer Publishing Company first ed. (2008).

[7] O. Bucicovschi and S. M. Cioaba, The minimum degree distance of graphs of given order and size Discrete Appl. Math. 156 (2008) 3518-3521.

[8] G. Chartrand , S. F. Kapoor and H. V. Kronk, A Generalization of Hamiltonian-connected Graphs J. de Mathématiques Pures et Appliquées, 48 (1969) 109-116.

[9] V. Chvátal, On Hamilton's Ideals J. Comb. Theory Series B 12(2) (1972) 163-168.

[10] A. A. Dobrynin and A. A. Kochetova, Degree distance of a graph: a degree analogue of the Wiener index J. Chem. Inf. Comput. Sci. 34 (1994) 1082-1086.

[11] I. Gutman, Selected properties of the Degree distance molecular topological index J. Chem. Inf. Comput. Sci. 34 (1994) 1087-1089.

[12] H. Hua and M. Wang, On Harary index and traceable graphs MATCH Commun. Math. Comput. Chem. 70 (2013) 297-300.

[13] G. Jiang, L. Ren, and G. Yu, Sufficient Conditions for Hamiltonicity of Graphs with Respect to Wiener Index, Hyper-Wiener Index, and Harary Index J. Chem. 2019 pp 9.

[14] R. M. Karp, Reducibility among Combinatorial Problems. in: R. E. Miller, J. W. Thatcher, J. D. Bohlinger, (Eds.) Complexity of Computer Computations. The IBM Research Symposia Series. Springer, Boston, MA. 2009 pp. 85-103.

[15] H. V. Kronk, A note on k-path hamiltonian graphs J. Combin. Theory 7 (1969) 104-106.

[16] L. Lesniak, On n-hamiltonian graphs Discrete Math. 14 (1976) 165-169.

[17] Y. Li and Q. Zhu, On sufficient topological indices conditions for properties of graphs J. Comb. Optim. 41 (2021) 487-503.

[18] Y. Li and Q. Zhu, On sufficient topological indices conditions for properties of graphs J. Comb. Optim. 41 (2021) 487-503.

[19] H. P. Schultz, Topological organic chemistry. 1. Graph theory and topological indices of alkanes J. Chem. Inf. Comput. Sci. 29 (1989) 227-228.

[20] G. Su, Z. Li, and H. Shi, Sufficient conditions for a graph to be k-edge-hamiltonian, k-path coverable, traceable and Hamilton-connected Australas. J. Combin. Th. 77 (2020) 269-284.

[21] A. I. Tomescu, Unicyclic and bicyclic graphs having minimum degree distance Discrete Appl. Math. 156 (2008) 125-130.

[22] I. Tomescu, Some extremal properties of the degree distance of a graph Discrete Appl. Math. 98 (1999) 159-163.

[23] L. Yang, Wiener Index and Traceable Graphs Bull. Aust. Math. Soc. 88 (2013) 380-383.

[24] X. Zhu, L. Feng, M. Liu, W. Liu and Y. Hu, Some topological indices and graphical properties Transactions on Combinatorics 6(4) (2017) 51-65.