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Sufficient conditions for a graph to be k-edge-hamiltonian, k-path-coverable, traceable and Hamilton-connected

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Abstract

The forgotten index of a graph is the sum of cubes of all its vertex degrees, which plays a significant role in measuring the branching of the carbon-atom skeleton. In this paper, we mainly explore sufficient conditions, in terms of the forgotten index, for a graph to be k-edge-hamiltonian, k-path-coverable, traceable and Hamilton-connected. The conditions obtained cannot be dropped.

1 Preliminaries

Throughout this paper we consider connected graphs without loops and multiple edges. Let $G = (V(G), E(G))$ be a graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. The number of edges in G that are incident to a vertex $v \in V(G)$ is said to be its degree and is denoted by $d_G(v)$. A sequence of non-negative integers $\pi = (d_1, d_2, \ldots, d_n)$ is said to be the degree sequence of G if $d_i = d_G(v_i)$ holds for any $v_i \in V(G)$, $i = 1, 2, \ldots, n$. In particular, if the vertex degrees are non-decreasing, we use $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ to denote the degree sequence for simplicity. We denote by K_n and $\overline{K}_n$ the complete graph with n vertices and its complement graph, respectively.

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As usual, a cycle (respectively, path) passing through each vertex of a graph is said to be a Hamiltonian cycle (respectively, Hamiltonian path). For a certain integer k, a connected graph G is said to be k-edge-hamiltonian if any collection of vertex-disjoint paths with at most k edges altogether belong to a hamiltonian cycle in G. A graph G is k-path-coverable if its vertex set can be covered by k or fewer vertex-disjoint paths, and we call the graph traceable if there exists a Hamiltonian path in it. A graph G is called Hamilton-connected if every two vertices in G are connected by a Hamiltonian path. In the subsequent sections, we always omit the subscript G from the notation if there is no confusion from the context. For other undefined graph-theoretic notation and terminology, the reader may refer to Bondy and Murty [8].

2 Motivation

Configuration of nodes and connections occurs in a variety of applications, which also represent organic molecules. Fortunately, graph theory has successfully provided scientists with a lot of useful tools, topological indices for instance. A topological index is a numeric quantity related to a molecule graph, which is a structural invariant and mathematically derived in an unambiguous and direct manner from the structural graph. It can be used to characterize properties of the corresponding graph. A series of topological indices, such as the Wiener index [32] and the Harary index [20, 28], have been introduced and found a large amount of useful applications. More details and information may be found in [17, 29, 30] and references therein.

It is stated that the authors in [18] proposed an approximate formula for the total π-electron energy (in short, $\mathcal{E}$). One of the main terms occurring in this expression is the first Zagreb index of the corresponding molecular graph. It is worth mentioning that this numeric quantity was precisely interpreted to be useful in measuring the extent of branching of the carbon-atom skeleton for molecules. A large number of scientists concentrated on this topological index and obtained a series of meaningful results; we encourage readers to consult [16, 22, 27] and references therein for more information. Another considerable contribution for the expression of $\mathcal{E}$ is the sum of the cubes of all vertex degrees:

$$F(G) = \sum_{u \in V} (d_G(u))^3,$$

which also plays a significant role in measuring the branching of the carbon-atom skeleton for the underlying molecule graph. The authors in the same paper call this the forgotten index of graphs. It was in 2016 that the authors in [15] investigated this graph parameter of several widely used chemical structures. We refer the interested reader to [1, 12, 14] for more information and details.

The problem of determining whether a graph keeps some property is often difficult and meaningful in graph theory. It is reported in [21] that determining whether a graph is traceable or Hamiltonian is always NP-complete. From then on, exploring such sufficient conditions for graphs, which attracts a vast number of mathematicians, became an important and meaningful aspect of graph theory. For example, the authors studied the traceability of graphs and presented a sufficient condition in terms of the Harary index; see [19]. In the same year, a similar problem was also considered in [33], and new sufficient conditions were found for a graph to be traceable in terms of the Wiener index. Subsequently, these results mentioned previously were generalized by means of other techniques; we suggest the reader consults [3, 4, 6, 7, 10, 11, 13, 25, 26, 31] for more details. To the best of our knowledge, there are few such conditions in terms of the degree-based and distance-based topological indices.

Motivated by the results in [2], in subsequent sections we attempt to explore sufficient conditions in terms of the forgotten index for graphs to be k-edge-hamiltonian, k-path-coverable, traceable and Hamilton-connected.

3 k-egde-hamiltonian graphs

We begin with an auxiliary result which will be used in later analysis.

Lemma 3.1 *([23]) Let $\pi = (d_1 \le d_2 \le \cdots \le d_n)$ be a degree sequence with $n \ge 3$ and $0 \le k \le n-3$. If*

$$d_{i-k} \le i \Rightarrow d_{n-i} \ge n-i+k \text{ for } k+1 \le i < \frac{n+k}{2},$$

then π is k-edge-hamiltonian.

Let G_1 and G_2 be two vertex-disjoint graphs, denote by $G_1 \cup G_2$ the union of these two graphs; and $G_1 \vee G_2$ the join which is obtained from the disjoint union of G_1 and G_2 by connecting each vertex in G_1 with that in G_2.

Theorem 3.2 *Let G be a connected graph of order $n \ge 9$ with $0 \le k \le n-3$.*

(1) For $k = n-4$, if

$$F(G) > \left(\frac{n-k-2}{2}\right)\left(\frac{n+k-2}{2}\right)^3 + 2\left(\frac{n+k}{2}\right)^3 + \left(\frac{n+k-2}{2}\right)(n-1)^3,$$

then G is k-edge-hamiltonian, unless $G \cong K_{n-3} \vee (K_1 \cup K_2)$.

(2) For $k = n-3$ or $k = n-5$, if

$$F(G) > \left(\frac{n-k-1}{2}\right)\left(\frac{n+k-1}{2}\right)^3 + \left(\frac{n+k-1}{2}\right)^3 + \left(\frac{n+k-1}{2}\right)(n-1)^3,$$

then G is k-edge-hamiltonian, unless $G \cong K_{n-2} \vee 2K_1$ or $G \cong K_{n-3} \vee 3K_1$.

(3) For $k \le n-6$, if

$$F(G) > (k+1)^3 + (n-k-2)(n-2)^3 + (k+1)(n-1)^3,$$

then G is k-edge-hamiltonian, unless $G \cong K_{k+1} \vee (K_1 \cup K_{n-k-2})$.

Proof. We assume that G is a graph of order $n \geq k+3$ which is not k-edge-hamiltonian. In view of Lemma 3.1, there must exist an integer i such that $d_{i-k} \leq i$ and $d_{n-i} \leq n-i+k-1$ for $k+1 \leq i \leq \frac{n+k-1}{2}$. Recall that $0 \leq k \leq n-3$, then we have

$$\begin{aligned}F(G) \leq&(i-k)i^3+(n-2i+k)(n-i+k-1)^3+i(n-1)^3\\=&3i^4-(7n+8k-6)i^3+(9n^2+(18k-15)n+9k^2-15k+6)i^2\\&-(4n^3+(15k-9)n^2+(15k^2-24k+6)n+5k^3-12k^2+9k-1)i\\&+(k+n)(k+n-1)^3.\end{aligned}$$

For simplicity, we define the following function on $[k+1, \frac{n+k-1}{2}]$:

$$\begin{aligned}\varphi_1(x)=&3x^4-(7n+8k-6)x^3+(9n^2+(18k-15)n+9k^2-15k+6)x^2\\&-(4n^3+(15k-9)n^2+(15k^2-24k+6)n+5k^3-12k^2+9k-1)x\\&+(k+n)(k+n-1)^3.\end{aligned}$$

Directly from the expression of $\varphi_1(x)$ we get

$$\begin{aligned}\varphi_1'(x)=&12x^3-3(7n+8k-6)x^2+6(3n^2+(6k-5)n+3k^2-5k+2)x\\&-(4n^3+(15k-9)n^2+(15k^2-24k+6)n+5k^3-12k^2+9k-1)\end{aligned}$$

and

$$\varphi_1''(x)=36x^2-6(7n+8k-6)x+6(3n^2+(6k-5)n+3k^2-5k+2).$$

It is routine to check that the discriminant of $\varphi_1''(x)$ is $\triangle = 36[-23n^2+(36-32k)n-8k^2+24k-12] < 0$. Hence, $\varphi_1(x)$ is a convex function on the interval $[k+1, \frac{n+k-1}{2}]$, and therefore $\varphi_1(x) \leq \max\{\varphi_1(k+1), \varphi_1(\frac{n+k-1}{2})\}$.

In the following, we need to consider two cases:

Case 1. $n+k-1$ is even.

It is routine to check that

$$\begin{aligned}\varphi_1(k+1)-\varphi_1\left(\frac{n+k-1}{2}\right)=&\frac{1}{16}k^4+\left(\frac{1}{8}n+\frac{3}{4}\right)k^3-\left(\frac{3}{8}n-\frac{27}{8}\right)k^2\\&-\left(\frac{5}{8}n^3-\frac{9}{2}n^2+\frac{81}{8}n-\frac{41}{4}\right)k\\&+\left(\frac{7}{16}n^4-\frac{39}{8}n^3+18n^2-\frac{217}{8}n+\frac{249}{16}\right).\end{aligned}$$

For convenience, we use $\rho(k)$, $k \in [0, n-3]$, to denote the right-side of the above expression. By direct calculations, we have

$$\begin{aligned}\rho'(k)=&\frac{1}{4}k^3+\left(\frac{3}{8}n+\frac{9}{4}\right)k^2-\left(\frac{3}{4}n-\frac{27}{4}\right)k\\&-\left(\frac{5}{8}n^3-\frac{9}{2}n^2+\frac{81}{8}n-\frac{41}{4}\right)\end{aligned}$$

and

$$\rho''(k) = \frac{3}{4}k^2 + \left(\frac{3}{4}n + \frac{9}{2}\right)k - \left(\frac{3}{4}n - \frac{27}{4}\right).$$

To continue the proof, we consider the following three possibilities.

Subcase 1.1. $k = n-3$ or $n-5$.

It is routine to check that $\rho(k) \le 0$, that is, $\varphi_1(x) \le \varphi_1(\frac{n+k-1}{2})$. Hence, $F(G) \le (\frac{n-k-1}{2})(\frac{n+k-1}{2})^3 + (\frac{n+k-1}{2})^3 + (\frac{n+k-1}{2})(n-1)^3$, a contradiction. As desired, G is k-edge-hamiltonian.

If $k = n-3$ or $n-5$ and $F(G) = (\frac{n-k-1}{2})(\frac{n+k-1}{2})^3 + (\frac{n+k-1}{2})^3 + (\frac{n+k-1}{2})(n-1)^3$, then all inequalities concerned previously should be equalities. Hence, $i = \frac{n+k-1}{2}$ and therefore $d_1 = d_2 = \cdots = d_{\frac{n-k-1}{2}} = \frac{n+k-1}{2}$, $d_{\frac{n-k+1}{2}} = \frac{n+k-1}{2}$ and $d_{\frac{n-k+3}{2}} = \cdots = d_n = n-1$, thus $G \cong 2K_1 \vee K_{n-2}$ (resp. $3K_1 \vee K_{n-3}$) for $k = n-3$ (resp. for $k = n-5$), which is not k-edge-hamiltonian. Hence, the conditions in Theorem 3.2 cannot be dropped.

Subcase 1.2. $1 \le k \le n-7$.

Direct calculations show that $\rho''(k) > 0$, implying that $\rho'(k)$ is an increasing function on the interval $[0, n-7]$. Thus, we have $\rho'(k) \le \rho'(n-7) = -\frac{9}{2}n^2 + \frac{51}{2}n - \frac{25}{2}n < 0$, which yields that $\rho(k)$ is decreasing for $k \in [0, n-7]$. Hence, $\rho(k) \ge \rho(n-7) = 6n^2 - 30n + 2 > 0$. As desired we confirm that $\varphi_1(k+1) - \varphi_1\left(\frac{n+k-1}{2}\right) > 0$. Hence, $F(G) \le (k+1)^3 + (n-k-2)(n-2)^3 + (k+1)(n-1)^3$, which is a contradiction. Hence, G is k-edge-hamiltonian.

Subcase 1.3. $k = 0$.

It is not difficult to find that $\rho(0) = \frac{7}{16}n^4 - \frac{39}{8}n^3 + 18n^2 - \frac{217}{8}n + \frac{249}{16} > 0$ for $n \ge 9$. Hence, $\varphi_1(k+1) - \varphi_1\left(\frac{n+k-1}{2}\right) > 0$, and consequently $F(G) \le (k+1)^3 + (n-k-2)(n-2)^3 + (k+1)(n-1)^3$, again a contradiction. Hence, G is k-edge-hamiltonian.

If $F(G) = (k+1)^3 + (n-k-2)(n-2)^3 + (k+1)(n-1)^3$, then all inequalities in previous proof should be equalities. Hence, $i = k+1$ and therefore $d_1 = k+1$, $d_2 = \cdots = d_{n-k-1} = n-2$ and $d_{n-k} = \cdots = d_n = n-1$, thus $G \cong K_{k+1} \vee (K_1 \cup K_{n-k-2})$, which is not k-edge-hamiltonian. Hence, the conditions in Theorem 3.2 cannot be dropped.

Case 2. $n+k-1$ is odd.

It routine to check that

$$\begin{aligned}\varphi_1(k+1) - \varphi_1\left(\frac{n+k-2}{2}\right) = &\frac{1}{16}k^4 + \left(\frac{1}{8}n + \frac{1}{2}\right)k^3 - \left(\frac{3}{4}n - 3\right)k^2 \\ &- \left(\frac{5}{8}n^3 - \frac{9}{2}n^2 + 12n - \frac{23}{2}\right)k \\ &+ \left(\frac{7}{16}n^4 - \frac{17}{4}n^3 + 15n^2 - \frac{47}{2}n + 14\right).\end{aligned}$$

Denote by $\varrho(k)$ the right-side of the previous expression for $k \in [0, n-4]$. By taking the first and second derivatives of $\varrho(k)$, we get

$$\begin{aligned}\varrho'(k) =& \frac{1}{4}k^3 + \left(\frac{3}{8}n + \frac{3}{2}\right)k^2 - \left(\frac{3}{2}n - 6\right)k \\ & - \left(\frac{5}{8}n^3 - \frac{9}{2}n^2 + 12n - \frac{23}{2}\right)\end{aligned}$$

and

$$\varrho''(k) = \frac{3}{4}k^2 + \left(\frac{3}{4}n + 3\right)k - \left(\frac{3}{2}n - 6\right).$$

To continue the proof, we consider the following three possibilities.

Subcase 2.1. $k = n - 4$.

It is easy to declare that $\varrho(n-4) = 0$, implying that $\varphi_1(x) \leq \varphi_1(\frac{n+k-2}{2})$. Hence, $F(G) \leq (\frac{n-k-2}{2})(\frac{n+k-2}{2})^3 + 2(\frac{n+k}{2})^3 + (\frac{n+k-2}{2})(n-1)^3$, a contradiction. Hence, G is k-edge-hamiltonian.

Furthermore, $F(G) = (n-3)^3 + 2(n-2)^3 + (n-3)(n-1)^3$ happens only if all inequalities in previous proof should be equalities. Hence, $i = \frac{n+k-2}{2} = n-3$ and therefore $d_1 = n-3$, $d_2 = d_3 = n-2$ and $d_4 = d_5 = \cdots = d_n = n-1$, thus $G \cong K_{n-3} \vee (K_1 \cup K_2)$, which is not k-edge-hamiltonian. Hence, the conditions in Theorem 3.2 cannot be dropped.

Subcase 2.2. $k \in [2, n-6]$.

The variable k assumes values between 2 and $n-6$. In that interval the function $\varrho'(k)$ monotonically increases, since $\varrho''(k) > 0$. Hence, $\varrho'(k) \leq \varrho'(n-6) = -\frac{9}{2}n^2 + \frac{51}{2}n - \frac{49}{2} < 0$ for $n \geq 5$. It immediately yields that $\varrho(k)$ is decreasing in the accordingly interval. Hence, $\varrho(k) \geq \varrho(n-6) = 6n^2 - 30n + 26 > 0$, and therefore $\varphi_1(k+1) - \varphi_1\left(\frac{n+k-2}{2}\right) > 0$. Thus, we have $F(G) \leq (k+1)^3 + (n-k-2)(n-2)^3 + (k+1)(n-1)^3$, again a contradiction. Hence, G is k-edge-hamiltonian.

Subcase 2.3. $k = 0$ or 1.

We can find that $\varrho(0) = \frac{7}{16}n^4 - \frac{17}{4}n^3 + 15n^2 - \frac{47}{2}n + 14 > 0$ and $\varrho(1) = \frac{7}{16}n^4 - \frac{39}{8}n^3 + \frac{39}{2}n^2 - \frac{289}{8}n + \frac{465}{16} > 0$ for $n \geq 5$. Therefore, $\varphi_1(k+1) - \varphi_1\left(\frac{n+k-2}{2}\right) > 0$. Thus, we have $F(G) \leq (k+1)^3 + (n-k-2)(n-2)^3 + (k+1)(n-1)^3$, which is a contradiction. Hence, G is k-edge-hamiltonian.

Furthermore, $F(G) = (k+1)^3 + (n-k-2)(n-2)^3 + (k+1)(n-1)^3$ happens only if all inequalities in previous proof should be equalities. Hence, $i = k+1$ and therefore $d_1 = k+1$, $d_2 = \cdots = d_{n-k-1} = n-2$ and $d_{n-k} = \cdots = d_n = n-1$, thus $G \cong K_{k+1} \vee (K_1 \cup K_{n-k-2})$, which is not k-edge-hamiltonian. Hence, the condition in Theorem 3.2 cannot be dropped. $\square$

4 k-path-coverable graphs

We begin with an important lemma from [9, 24] will be helpful to the proofs of the subsequent main result.

Lemma 4.1 *Let $\pi = (d_1 \le d_2 \le \cdots \le d_n)$ be a degree sequence and $k \ge 1$. If*

$$d_{i+k} \le i \Rightarrow d_{n-i} \ge n-i-k \text{ for } 1 \le i < \frac{n-k}{2},$$

then π is k-path-coverable.

Let k_1, k_2 be two non-negative real numbers in terms of n:

$$\begin{cases} k_1 = \dfrac{49n - \sqrt[3]{4m_2}}{51} - \dfrac{\sqrt[3]{2}(4n^2+324n-936)}{102\sqrt[3]{m_2}} \\ k_2 = \dfrac{49n - \sqrt[3]{4m_4}}{51} - \dfrac{\sqrt[3]{2}(4n^2+68n-1088)}{102\sqrt[3]{m_4} - \frac{4}{3}}, \end{cases}$$

where

$$\begin{cases} m_1 = 7807n^6 - 46344n^5 + 135744n^4 - 226826n^3 + 228492n^2 - 126144n + 31347 \\ m_2 = 7805n^3 - 23166n^2 + 33480n + 51\sqrt{3m_1} - 1390 \\ m_3 = 7807n^6 - 46728n^5 + 127260n^4 - 196446n^3 + 179688n^2 - 93228n + 30107 \\ m_4 = 7805n^3 - 23358n^2 + 28662n + 51\sqrt{3m_3} - 12427. \end{cases}$$

The main result is the following:

Theorem 4.2 *Let G be a connected graph of order n and $k \ge 1$.*

(1) For $k_1 \le k \le n-3$ and $n-k-1$ is even, if

$$F(G) > \left(\frac{n+k-1}{2}\right)\left(\frac{n-k-1}{2}\right)^3 + \left(\frac{n-k-1}{2}\right)^3 + \left(\frac{n-k-1}{2}\right)(n-1)^3,$$

then G is k-path-coverable, unless $G \cong K_{\frac{n-k-1}{2}} \vee (\overline{K_{\frac{n+k-1}{2}}} \cup K_1)$.

(2) For $k_2 \le k \le n-4$ and $n-k-1$ is odd, if

$$F(G) > \left(\frac{n+k-2}{2}\right)\left(\frac{n-k-2}{2}\right)^3 + 2\left(\frac{n-k}{2}\right)^3 + \left(\frac{n-k-2}{2}\right)(n-1)^3,$$

then G is k-path-coverable, unless $G \cong K_{\frac{n-k-2}{2}} \vee (\overline{K_{\frac{n+k-2}{2}}} \cup K_2)$.

(3) For $1 \le k < k_1$ and $n-k-1$ is even or $1 \le k < k_2$ and $n-k-1$ is odd, if

$$F(G) > (k+1) + (n-k-2)(n-k-2)^3 + (n-1)^3,$$

then G is k-path-coverable, unless $G \cong K_1 \vee (\overline{K_{k+1}} \cup K_{n-k-2})$.

Proof. Suppose that G is not k-path-coverable; by Lemma 4.1, there must exist an integer i such that $d_{i+k} \leq i$ and $d_{n-i} \leq n-i-k-1$ for $1 \leq i < \frac{n-k}{2}$. Thus, we have

$$\begin{aligned}F(G) \leq &(i+k)i^3 + (n-2i-k)(n-i-k-1)^3 + i(n-1)^3\\ =&3i^4 - (7n-8k-6)i^3 + [9n^2 - (18k+15)n + 9k^2 + 15k + 6]i^2\\ &-[4n^3 - (15k+9)n^2 + (15k^2+24k+6)n - (5k^3+12k^2+9k+1)]i\\ &+(k-n)(k-n+1)^3.\end{aligned}$$

For simplicity, we define the following function on $[1, \frac{n-k-1}{2}]$:

$$\begin{aligned}\varphi_2(x) =&3x^4 - (7n-8k-6)x^3 + [9n^2 - (18k+15)n + 9k^2 + 15k + 6]x^2\\ &-[4n^3 - (15k+9)n^2 + (15k^2+24k+6)n - (5k^3+12k^2+9k+1)]x\\ &+(k-n)(k-n+1)^3.\end{aligned}$$

By direct computations, we get

$$\varphi_2''(x) = 36x^2 - 6(7n-8k-6)x + 6[3n^2 - (6k+5)n + 3k^2 + 5k + 2].$$

It is not difficult to verify that $\varphi_2''(x) > 0$, implying that $\varphi_2(x)$ is a convex function on the interval $[1, \frac{n-k-1}{2}]$. Hence, $\varphi_2(x) \leq \max\{\varphi_2(1), \varphi_2(\frac{n-k-1}{2})\}$.

We need to consider the following two possibilities.

Case 1. $n-k-1$ is even.

It is routine to check that

$$\begin{aligned}\varphi_2(1) - \varphi_2\left(\frac{n-k-1}{2}\right) =&\frac{17}{16}k^4 - \left(\frac{33}{8}n - \frac{33}{4}\right)k^3 + \left(6n^2 - \frac{195}{8}n + \frac{195}{8}\right)k^2\\ &-\left(\frac{27}{8}n^3 - \frac{45}{2}n^2 + \frac{375}{8}n - \frac{131}{4}\right)k\\ &+\left(\frac{7}{16}n^4 - \frac{39}{8}n^3 + 18n^2 - \frac{217}{8}n + \frac{249}{16}\right),\end{aligned}$$

For simplicity, we use the notation $\varsigma(k)$, $k \in [1, n-3]$, to denote its right-side. Direct calculations yield that the two real roots of $\varsigma(k) = 0$ are

$$\begin{cases} k_1 = \dfrac{49n - \sqrt[3]{4m_2}}{51} - \dfrac{\sqrt[3]{2}(4n^2 + 324n - 936)}{102\sqrt[3]{m_2}} \\ k_1' = n-3, \end{cases}$$

where $m_1 = 7807n^6 - 46344n^5 + 135744n^4 - 226826n^3 + 228492n^2 - 126144n + 31347$, and $m_2 = 7805n^3 - 23166n^2 + 33480n + 51\sqrt{3m_1} - 13905$.

To complete the proof, we need to consider the following two subcases.

Subcase 1.1. $k_1 \leq k \leq n-3$.

It is not difficult to verify that $\varsigma(k) \leq 0$. Hence $\varphi_2(1) \leq \varphi_2(\frac{n-k-1}{2})$. This implies that $F(G) \leq (\frac{n+k-1}{2})(\frac{n-k-1}{2})^3 + (\frac{n-k-1}{2})^3 + (\frac{n-k-1}{2})(n-1)^3$, a contradiction. Hence, G is k-path-coverable.

Furthermore, $F(G) = (\frac{n+k-1}{2})(\frac{n-k-1}{2})^3 + (\frac{n-k-1}{2})^3 + (\frac{n-k-1}{2})(n-1)^3$ happens only if all inequalities in previous proof should be equalities. Hence, $i = \frac{n-k-1}{2}$ and therefore $d_1 = d_2 = \cdots = d_{\frac{n+k-1}{2}} = \frac{n-k-1}{2}$, $d_{\frac{n+k+1}{2}} = \frac{n-k-1}{2}$ and $d_{\frac{n+k+3}{2}} = \cdots = d_n = n-1$, thus $G \cong K_{\frac{n-k-1}{2}} \vee (\overline{K_{\frac{n+k-1}{2}}} \cup K_1)$, which is not k-path-coverable. Hence, the conditions in Theorem 4.2 cannot be dropped.

Subcase 1.2. $1 \leq k < k_1$.

Simple calculations show that $\varsigma(k) \geq 0$, implying that $\varphi_2(1) \geq \varphi_2(\frac{n-k-1}{2})$. Hence, $F(G) \leq (k+1) + (n-k-2)(n-k-2)^3 + (n-1)^3$, a contradiction. Hence, G is k-path-coverable.

If $F(G) = (k+1) + (n-k-2)(n-k-2)^3 + (n-1)^3$, then all inequalities in previous proof should be equalities. Hence, $i = 1$ and therefore $d_1 = d_2 = \cdots = d_{k+1} = 1$, $d_{k+2} = \cdots = d_{n-1} = n-k-2$ and $d_n = n-1$, thus $G \cong K_1 \vee (\overline{K_{k+1}} \cup K_{n-k-2})$, which is not k-path-coverable. Hence, the conditions in Theorem 4.2 cannot be dropped.

Case 2. $n-k-1$ is odd.

It is routine to check that

$$\begin{aligned}\varphi_2(1) - \varphi_2\left(\frac{n-k-2}{2}\right) =& \frac{17}{16}k^4 - \left(\frac{33}{8}n + \frac{17}{2}\right)k^3 + \left(6n^2 - \frac{99}{4}n + 24\right)k^2 \\ &- \left(\frac{27}{8}n^3 - \frac{45}{2}n^2 + 45n - \frac{63}{2}\right)k \\ &+ \left(\frac{7}{16}n^4 - \frac{17}{4}n^3 + 15n^2 - \frac{47}{2}n + 14\right).\end{aligned}$$

We use $\zeta(k)$ to denote the right-side of the previous expression for $k \in [0, n-4]$. It follows from direct calculations that the two real roots of $\zeta(k) = 0$ are as follows:

$$\begin{cases} k_2 = \dfrac{49n - \sqrt[3]{4m_4}}{51} - \dfrac{\sqrt[3]{2}(4n^2 + 68n - 1088)}{102\sqrt[3]{m_4} - \frac{4}{3}} \\ k_2' = n-3, \end{cases}$$

where $m_3 = 7807n^6 - 46728n^5 + 127260n^4 - 196446n^3 + 179688n^2 - 93228n + 30107$, and $m_4 = 7805n^3 - 23358n^2 + 28662n + 51\sqrt{3m_3} - 12427$.

To continue the proof, we need to consider the following possibilities.

Subcase 2.1. $k_2 \leq k \leq n-3$.

It follows that $\zeta(k) \leq 0$, and then $\varphi_2(1) \leq \varphi_2(\frac{n-k-2}{2})$. Hence

$$F(G) \leq (\frac{n+k-2}{2})(\frac{n-k-2}{2})^3 + 2(\frac{n-k}{2})^3 + (\frac{n-k-2}{2})(n-1)^3,$$

a contradiction. This implies that G is k-path-coverable.

If $F(G) = (\frac{n+k-2}{2})(\frac{n-k-2}{2})^3 + 2(\frac{n-k}{2})^3 + (\frac{n-k-2}{2})(n-1)^3$, then all inequalities in previous proof should be equalities. Hence, $i = \frac{n-k-2}{2}$ and therefore $d_1 = d_2 = \cdots = d_{\frac{n+k-2}{2}} = \frac{n-k-2}{2}$, $d_{\frac{n+k}{2}} = d_{\frac{n+k+2}{2}} = \frac{n-k}{2}$ and $d_{\frac{n+k+4}{2}} = \cdots = d_n = n-1$, thus $G \cong K_{\frac{n-k-2}{2}} \vee (\overline{K_{\frac{n+k-2}{2}}} \cup K_2)$, which is not k-path-coverable. Hence, the conditions in Theorem 4.2 cannot be dropped.

Subcase 2.2. $1 \leq k < k_2$.

Simple computations show that $\zeta(k) \geq 0$, and then $\varphi_2(1) \geq \varphi_2(\frac{n-k-2}{2})$. Hence, $F(G) \leq (k+1) + (n-k-2)(n-k-2)^3 + (n-1)^3$, a contradiction. Thus, we have G is k-path-coverable.

If $F(G) = (k+1) + (n-k-2)(n-k-2)^3 + (n-1)^3$, then all inequalities in previous proof should be equalities. Hence, $i = 1$ and therefore $d_1 = d_2 = \cdots = d_{k+1} = 1$, $d_{k+2} = \cdots = d_{n-1} = n-k-2$ and $d_n = n-1$, thus $G \cong K_1 \vee (\overline{K_{k+1}} \cup K_{n-k-2})$, which is not k-path-coverable. Hence, the conditions in Theorem 4.2 cannot be dropped. □

5 Traceable graphs

The following Lemma 5.1 will be useful for our later proof.

Lemma 5.1 *([8]) Let G be a non-trivial graph of order $n \geq 4$, with degree sequence $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$. 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.*

Now we shall state the main result:

Theorem 5.2 *Let G be a connected graph of order n and $k \geq 2$ an integer. If*

$$F(G) > n^4 - 11n^3 + 51n^2 - 105n + 82,$$

then G is traceable, unless $G \cong K_1 \vee (2K_1 \cup K_{n-3})$ or $K_2 \vee (3K_1 \cup K_2)$ or $K_2 \vee 4K_1$ or $K_3 \vee 5K_1$ or $K_4 \vee 6K_1$.

Proof. We assume that G is a graph of order $n \geq 4$ which is not traceable. It follows from Lemma 5.1 that there exist an integer $k < \frac{n+1}{2}$ such that $d_k \leq k-1$ and $d_{n-k+1} \leq n-k-1$. Recall that $k \geq 2$, then we have

$$\begin{aligned} F(G) \leq & k(k-1)^3 + (n-2k+1)(n-k-1)^3 + (k-1)(n-1)^3 \\ = & 3k^4 - (7n-2)k^3 + (9n^2-12n+6)k^2 \\ & -(4n^3-6n^2+3)k + (n^4-3n^3+3n^2-n). \end{aligned}$$

For simplicity, we define the right-side of the previous inequality to be the function $\varphi_3(k)$ on $k \in [2, \frac{n+1}{2})$, and direct calculations show the second derivative is

$$\varphi_3''(k) = 36k^2 - 6(7n-2)k + 6(3n^2 + 6(3n^2 - 4n + 2).$$

It is routine to check that the discriminant of equation $\varphi_3''(k) = 0$ is $\Delta = -828n^2 + 2448n - 1584 < 0$ for $n \geq 4$. Hence, $\varphi_3(k)$ is a convex function on the interval $[2, \frac{n+1}{2})$.

In what follows, we consider two possibilities.

Case 1. n is odd.

In this case, we have $2 \leq k \leq \frac{n-1}{2}$. It follows that $\varphi_3(k) \leq \max\{\varphi_3(2), \varphi_3(\frac{n-1}{2})\}$. Hence, we have

$$\varphi_3(2) - \varphi_3\left(\frac{n-1}{2}\right) = \frac{7}{16}n^4 - \frac{61}{8}n^3 + \frac{87}{2}n^2 - \frac{779}{8}n + \frac{1265}{16},$$

and $n_1 = 5$ and $n_2 = 8.57$ be its two real roots.

To continue the proof, we need to consider the following two subcases.

Subcase 1.1. $n = 5$ or $n \geq 9$.

It is easy to find that $\varphi_3(2) - \varphi_3\left(\frac{n-1}{2}\right) > 0$, implying that $F(G) \leq n^4 - 11n^3 + 51n^2 - 105n + 82$, a contradiction. Hence, G is traceable.

If $F(G) = n^4 - 11n^3 + 51n^2 - 105n + 82$, then all inequalities in previous proof should be equalities. Hence, $k = 2$ and therefore $d_1 = d_2 = 1$, $d_3 = \cdots = d_{n-1} = n-3$ and $d_n = n-1$, thus $G \cong K_1 \vee (2K_1 \cup K_{n-3})$, which is not traceable. This implies that our conditions in Theorem 5.2 cannot be dropped.

Subcase 1.2. $n = 7$.

By direct calculation, one can find that $\varphi_3(2) - \varphi_3\left(\frac{n-1}{2}\right) = \varphi_3(2) - \varphi_3(3) = -36 < 0$. Hence, $F(G) \leq 510$, which contradicts with the fact $F(G) > 510 > 474 = 7^4 - 11 \times 7^3 + 51 \times 7^2 - 105 \times 7 + 82$. Hence, G is traceable.

Furthermore, $F(G) = 510$ happens only if all inequalities in previous proof should be equalities. Hence, $k = 3$ and therefore $d_1 = d_2 = d_3 = 2$, $d_4 = d_5 = 3$ and $d_6 = d_7 = 6$, thus $G \cong K_2 \vee (3K_1 \cup K_2)$, which is not traceable. This implies that our conditions in Theorem 5.2 cannot be dropped.

Case 2. n is even.

In this case, we have $2 \leq k \leq \frac{n}{2}$. It follows that $\varphi_3(k) \leq \max\{\varphi_3(2), \varphi_3(\frac{n}{2})\}$. It routine to check that

$$\varphi_3(2) - \varphi_3\left(\frac{n}{2}\right) = \frac{7}{16}n^4 - \frac{33}{4}n^3 + \frac{93}{2}n^2 - \frac{205}{2}n + 82,$$

and $n_1 = 4$ and $n_2 = 10.98$ be its two real roots.

To continue the proof, we need to consider the following two subcases.

Subcase 2.1. $n = 4$ or $n \geq 12$.

It is routine to check that $\varphi_3(2) - \varphi_3\left(\frac{n}{2}\right) > 0$, implying that $F(G) \leq n^4 - 11n^3 + 51n^2 - 105n + 82$, a contradiction. Hence, G is traceable. If $n = 4$, we can deal with in a similar way, here omit the details.

If $F(G) = n^4 - 11n^3 + 51n^2 - 105n + 82$, then all the inequalities in previous proof should be equalities. Hence, $k = 2$ and therefore $d_1 = d_2 = 1$, $d_3 = \cdots = d_{n-1} = n-3$ and $d_n = n - 1$, thus $G \cong K_1 \vee (2K_1 \cup K_{n-3})$, which is not traceable. This implies that our conditions in Theorem 5.2 cannot be dropped.

Subcase 2.2. $n = 6, 8, 10$.

If $n = 6$, direct calculation shows that $\varphi_3(2) - \varphi_3\left(\frac{n}{2}\right) = \varphi_3(2) - \varphi_3(3) = -74 < 0$, implying that $F(G) \leq 282$. This contradicts to the fact $F(G) = 282 > 208 = 6^4 - 11 \times 6^3 + 51 \times 6^2 - 105 \times 6 + 82$. Hence, G is traceable.

If $F(G) = 282$, then all inequalities in previous proof should be equalities. Hence, $k = 3$ and therefore $d_1 = d_2 = d_3 = d_4 = 2$ and $d_5 = d_6 = 5$, thus $G \cong K_2 \vee 4K_1$, which is not traceable. This implies that our conditions in Theorem 5.2 cannot be dropped.

The cases for $n = 8$ and $n = 10$ could be solved in a similar way, here we omit the details. The corresponding counterexample is $K_3 \vee 5K_1$ or $K_4 \vee 6K_1$, respectively.

This completes the proof of Theorem 5.2. $\square$

6 Hamilton-connected graphs

We first introduce a result which will be used in later proofs.

Lemma 6.1 *([5]) Let $\pi = (d_1 \leq d_2 \leq \cdots \leq d_n)$ be a degree sequence with $n \geq 3$. If*

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

then G is Hamilton-connected.

We are now ready to state and prove:

Theorem 6.2 *Let G be a connected graph of order $n \geq 3$. If*

$$F(G) > n^4 - 7n^3 + 24n^2 - 38n + 30,$$

then G is Hamilton-connected, unless $G \cong K_2 \vee (K_1 \cup K_{n-3})$ or $3K_1 \vee K_3$.

Proof. We assume that G is a graph of order $n \geq 3$ which is not Hamilton-connected. It follows from Lemma 6.1 that there exist an integer $2 \leq k \leq \frac{n}{2}$ such that $d_{k-1} \leq k$ and $d_{n-k} \leq n-k$. Hence,

$$\begin{aligned} F(G) \leq &(k-1)k^3 + (n-2k+1)(n-k)^3 + k(n-1)^3 \\ = &3k^4 - (7n+2)k^3 + (9n^2+3n)k^2 \\ &-(4n^3+6n^2-3n+1)k + (n^4+n^3). \end{aligned}$$

For convenience, we use $\varphi_4(k)$ to denote a function for $k \in [2, \frac{n}{2}]$ and the second derivative is

$$\varphi_4''(k) = 36k^2 - 6(7n+2)k + 6(3n^2+n) > 0.$$

This implies that $\varphi_4(k)$ is a convex function on the interval $[2, \frac{n}{2}]$.

For simplicity, we consider the following two possibilities.

Case 1. n is odd.

In this case, we have $2 \leq k \leq \frac{n-1}{2}$. It follows that $\varphi_4(k) \leq \max\{\varphi_4(2), \varphi_4(\frac{n-1}{2})\}$. Hence, we have

$$\varphi_4(2) - \varphi_4\left(\frac{n-1}{2}\right) = \frac{7}{16}n^4 - \frac{39}{8}n^3 + \frac{39}{2}n^2 - \frac{289}{8}n + \frac{465}{16},$$

and $n_1 = 3$ and $n_2 = 5$ are its two real roots.

If $n \geq 5$, it is routine to check that $\varphi_4(2) - \varphi_4\left(\frac{n-1}{2}\right) > 0$, implying that $F(G) \leq n^4 - 7n^3 + 24n^2 - 38n + 30$, which is a contradiction. Hence, G is Hamilton-connected. If $n = 3$, we can be deal with in a similar way, here omit the details.

Furthermore, $F(G) = n^4 - 7n^3 + 24n^2 - 38n + 30$ happens only if all inequalities in previous proof should be equalities. Hence, $k = 2$ and therefore $d_1 = 2$, $d_2 = \cdots = d_{n-2} = n-2$, and $d_{n-1} = d_n = n-1$. Thus $G \cong K_2 \vee (K_1 \cup K_{n-3})$, which is not Hamilton-connected. Hence, the conditions in Theorem 6.2 cannot be dropped.

Case 2. n is even.

In this case, we have $2 \leq k \leq \frac{n}{2}$. It follows that $\varphi_4(k) \leq \max\{\varphi_4(2), \varphi_4(\frac{n}{2})\}$. Hence,

$$\varphi_4(2) - \varphi_4\left(\frac{n}{2}\right) = \frac{7}{16}n^4 - \frac{11}{2}n^3 + \frac{45}{2}n^2 - \frac{75}{2}n + 30$$

with two real roots $n_1 = 4$ and $n_2 = 6.275$. To continue the proof, we need to consider the following two subcases.

Subcase 2.1. $n = 4$ or $n \geq 8$.

It is routine to check that $\varphi_4(2) - \varphi_4\left(\frac{n}{2}\right) > 0$, implying that $F(G) \leq n^4 - 7n^3 + 24n^2 - 38n + 30$, a contradiction. Hence, G is Hamilton-connected.

If $F(G) = n^4 - 7n^3 + 24n^2 - 38n + 30$, then all inequalities in previous proof should be equalities. Hence, $k = 2$ and therefore $d_1 = 2$, $d_2 = \cdots = d_{n-2} = n - 2$, and $d_{n-1} = d_n = n - 1$. Thus $G \cong K_2 \vee (K_1 \cup K_{n-3})$, which is not Hamilton-connected. Hence, the conditions in Theorem 6.2 cannot be dropped.

Subcase 2.2. $n = 6$.

By direct calculation, one can find that $\varphi_4(2) - \varphi_4\left(\frac{n}{2}\right) = \varphi_4(2) - \varphi_4(3) = -6 < 0$. Hence, $F(G) \leq \varphi_4(3) = 456$. This contradicts with the fact $F(G) = 456 > 450 = 6^4 - 7 \times 6^3 + 24 \times 6^2 - 38 \times 6 + 30$. Hence, G is traceable.

If $F(G) = 456$, then all inequalities in previous proof should be equalities. Hence, $k = 3$ and therefore $d_1 = d_2 = d_3 = 3$, $d_4 = d_5 = d_6 = 5$, thus $G \cong 3K_1 \vee K_3$, which is not traceable. This implies that our conditions in Theorem 6.2 cannot be dropped. $\square$

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