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The Topological Indices And Some Hamiltonian Properties Of Graphs*

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Abstract

In this paper, we present sufficient conditions for a graph to be Hamiltonian or traceable in light of topological indices of the forgotten topology index and the reciprocal Randić 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 $d(v)$ denote the degree of a vertex v in G. The minimum degree vertices of G is denoted by $\delta(G)$. 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. 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 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. For two disjoint graphs G and H, the join of G and H is denoted by $G \vee H$. Given a graph G, a subset S of $V(G)$ is said to be an independent set of G if the subgraph $G[S]$, induced by S, is a graph with $|S|$ isolated vertices. As usual, K_n denotes the complete graph on n vertices.

Graph theory has provided chemists with a variety of useful tools such as topological indices. For instance, topological indices have been used to give a high degree of predictability of pharmaceutical properties. One of the most important topological indices is the Randić index. The Randić index

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}},$$

of a graph G was introduced by the chemist Milan Randić under the name of branching index [13]. Gutman et al. [4] introduced a variant of the Randić index which was named as the reciprocal Randić index. The exact definition of the reciprocal Randić index for a graph G is as follows

$$RR(G) = \sum_{uv \in E(G)} \sqrt{d(u)d(v)}.$$

The reciprocal Rand´c index is useful for predicting the normal boiling point of isomeric octanes. See references [2, 7, 8, 12, 14, 15] for more information on topological indices.

In 2015, Furtula and Gutman [3] named the sum of cubes of vertex degrees of a graph G as the forgotten topological index, and denoted it by $F(G)$. In other words, the forgotten topological index is defined as follows

$$F = F(G) = \sum_{uv \in E} [d(u)^2 + d(v)^2] = \sum_{v \in V} d(v)^3.$$

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The forgotten topological index was employed in the formulas for total π-electron energy in [5], as a measure of branching extent of the carbon-atom skeleton of the underlying molecule.

The problem of deciding whether a given graph possesses certain properties is often difficult. For example, determining whether a given graph is Hamiltonian or traceable is NP-complete [6]. Thus, finding sufficient conditions for those graphical properties becomes meaningful in graph theory.

In this paper, we aim at obtaining sufficient conditions based upon the forgotten topology index and the reciprocal Randić index for the Hamiltonian and traceable graphs. Below are some results in this research area which have been obtained. Using the first Zagreb index, Li and Taylor [9] presented sufficient conditions for Hamiltonian properties of graphs. Using the hyper-Zagreb index, Li [10] gave sufficient conditions for Hamiltonian properties of graphs, Li [9] presented sufficient condition for Hamiltonian properties of graphs by using the Harary index of a graph. Using the first Zagreb index, An et al. [1] presented sufficient conditions for k-connectivity, β-deficiency and k-Hamiltonicity of graphs.

Main Results

In this section, we present sufficient conditions in terms of the forgotten topology index and the reciprocal Randić index conditions for the Hamiltonian and traceable graphs.

We begin with the forgotten topology index and the reciprocal Randić index conditions for the Hamiltonian graphs.

Theorem 1 *Let G be a k-connected $(k \geq 2)$ graph of order n.*

1) If

$$F(G) \geq (n-k-1)\left(n^3 + n^2(k-2) - n\left(2k^2+4k-1\right) + k^3 + 3k^2 + 3k\right),$$

then G is Hamiltonian or $K_k \vee K_{k+1}^c$.

2) If

$$RR(G) \geq (n-k-1)\left((k+1)\sqrt{(n-k-1)(n-1)} + \frac{(n-k-2)(n-1)}{2}\right),$$

then G is Hamiltonian or $K_k \vee K_{k+1}^c$.

Proof. Let G be a graph satisfying the conditions in Theorem 1. Suppose that G is not Hamiltonian. Then G is not a complete graph. We further have that $n \geq 2k+1$ otherwise $2\delta \geq 2k \geq n$ and G is Hamiltonian which is a contradiction. Since $k \geq 2$, G contains a cycle. Choose a longest cycle C in G and give an orientation on C, since G is not Hamiltonian, there exists a vertex $x_0 \in V(G) - V(C)$. By Menger's theorem, we can find $s(s \geq k)$ pairwise disjoint (except for x_0) paths $P_1, P_2, \ldots, P_s$ between x_0 and $V(C)$. Let u_i be the end vertex of P_i on C, where $1 \leq i \leq s$. We use u_i^+ to denote the successor of u_i along with the orientation of C, where $1 \leq i \leq s$. Then $S := \{x_0, u_1^+, u_2^+, \ldots, u_s^+\}$ is independent otherwise G would have cycles which are longer than C. Assuming that $T := V(G) - S = \{v_1, v_2, \ldots, v_r\}$, we have

$$|T| = r = n - |S| = n - (k+1) \geq k.$$

Now we prove the first statement. By the definition of the forgotten topology index, we have

$$\begin{aligned}
F(G) &= \sum_{v \in V(G)} d^3(v) \\
&= d^3(x_0) + d^3(u_1^+) + \cdots + d^3(u_k^+) + d^3(v_1) + d^3(v_2) + \cdots + d^3(v_r) \\
&\leq (k+1)r^3 + r(n-1)^3 \\
&= (k+1)(n-k-1)^3 + (n-k-1)(n-1)^3 \\
&= (n-k-1)\left(n^3 + n^2(k-2) - n\left(2k^2+4k-1\right) + k^3 + 3k^2 + 3k\right).
\end{aligned}$$

Thus

$$F(G) = (n-k-1)\left(n^3 + n^2(k-2) - n\left(2k^2+4k-1\right) + k^3 + 3k^2 + 3k\right).$$

It follows that

$$d(x_0) = d(u_1^+) = \cdots = d(u_k^+)) = r = n-(k+1)$$

and

$$d(v_1) = \cdots = d(v_r) = d(v_{n-(k+1)}) = n-1.$$

If $r = n-(k+1) \geq (k+1)$, then one can easily see that G is Hamiltonian, a contradiction. Thus, $r \leq k$. Hence, $r = k$ and G is $K_k \vee K_{k+1}^c$. This completes the proof of the first part in Theorem 1.

For proof of the second statement, by the definition of the reciprocal Randić index, we have

$$\begin{aligned}
RR(G) &= \sum_{uv\in E}\sqrt{d(u)d(v)} \\
&= \sum_{u\in S, v\in T, uv\in E}\sqrt{d(u)d(v)} + \sum_{u\in T, v\in T, uv\in E}\sqrt{d(u)d(v)} \\
&\leq \sum_{u\in S, v\in T}\sqrt{d(u)d(v)} + \sum_{u\in T, v\in T, u\neq v}\sqrt{d(u)d(v)} \\
&\leq r(k+1)\sqrt{r(n-1)} + \frac{r(r-1)(n-1)}{2} \\
&= (n-k-1)(k+1)\sqrt{(n-k-1)(n-1)} + \frac{(n-k-1)(n-k-2)(n-1)}{2} \\
&= (n-k-1)\left((k+1)\sqrt{(n-k-1)(n-1)} + \frac{(n-k-2)(n-1)}{2}\right).
\end{aligned}$$

Thus

$$RR(G) = (n-k-1)\left((k+1)\sqrt{(n-k-1)(n-1)} + \frac{(n-k-2)(n-1)}{2}\right).$$

It follows that

$$d(x_0) = d(u_1^+) = \cdots = d(u_k^+)) = r = n-(k+1)$$

and

$$d(v_1) = \cdots = d(v_r) = d(v_{n-(k+1)}) = n-1.$$

If $r = n-(k+1) \geq (k+1)$, then one can easily see that G is Hamiltonian, which is a contradiction. Thus, $r \leq k$. Hence, $r = k$ and G is $K_k \vee K_{k+1}^c$. This completes the proof of the second part in Theorem 1. ■

Next, we present the forgotten topology index and the reciprocal Randić index conditions for the traceable graphs.

Theorem 2 *Let G be a k-connected $(k \geq 1)$ graph of order n.*

1) If

$$F(G) \geq (n-k-2)\left(n^3 + n^2(k-1) - n\left(2k^2-8k-5\right) + k^3 + 6k^2 + 14k + 7\right),$$

then G is traceable or $K_k \vee K_{k+2}^c$.

2) If

$$RR(G) \geq (n-k-2)\left((k+2)\sqrt{(n-k-2)(n-1)} + \frac{(n-k-3)(n-1)}{2}\right),$$

then G is traceable or $K_k \vee K_{k+2}^c$.

Proof. Let G be a graph satisfying the conditions in Theorem 2. Suppose that G is not traceable. Then G is not a complete graph. We further have that $n \geq 2k+2$ otherwise $2\delta \geq 2k \geq n-1$ and G is traceable. Choose a longest path P in G and give an orientation on P. Let y and z be the two end vertices of P. Since G is not traceable, there exists a vertex $x_0 \in V(G) \setminus V(P)$. By Menger's theorem, we can find $s (s \geq k)$ pairwise disjoint (except for x_0) paths $P_1, P_2, \ldots, P_s$ between x_0 and $V(P)$. Let u_i be the end vertex of P_i on P, where $1 \leq i \leq s$. Since P is a longest path in G, $u_i \notin \{y, z\}$, for each $i \in \{1, \ldots, s\}$, otherwise G would have paths which are longer than P. We use u_i^+ to denote the successor of u_i along the orientation of P, where $1 \leq i \leq s$. Then $S := \{x_0, y, u_1^+, u_2^+, \ldots, u_s^+\}$ is independent otherwise G would have paths which are longer than P. For convenience, assume that $T := V(G) - S = \{v_1, v_2, \ldots, v_r\}$. Thus

$$|T| = r = n - |S| = n - (k+2) \geq k.$$

Now we prove the first statement. By the definition of the forgotten index, we have

$$\begin{aligned}
F(G) &= \sum_{v \in V(G)} d^3(v) \\
&= d^3(x_0) + d^3(y) + d^3(u_1^+) + \cdots + d^3(u_k^+) + d^3(v_1) + d^3(v_2) + \cdots + d^3(v_r) \\
&\leq (k+2)r^3 + r(n-1)^3 \\
&= (k+2)(n-k-2)^3 + (n-k-2)(n-1)^3 \\
&= (n-k-2)\left(n^3 + n^2(k-1) - n\left(2k^2 - 8k - 5\right) + k^3 + 6k^2 + 14k + 7\right).
\end{aligned}$$

Thus

$$F(G) = (n-k-2)\left(n^3 + n^2(k-1) - n\left(2k^2 - 8k - 5\right) + k^3 + 6k^2 + 14k + 7\right).$$

It follows that

$$d(x_0) = d(y) = d(u_1^+) = \cdots = d(u_k^+)) = r = n - (k+2)$$

and

$$d(v_1) = \cdots = d(v_r) = d(v_{n-(k+2)}) = n - 1.$$

If $r = n-(k+2) \geq (k+2)$, then one can easily see that G is traceable, a contradiction. Thus, $r \leq k$. Hence, $r = k$ and G is $K_k \vee K_{k+2}^c$. This completes the proof of the first part in Theorem 2.

For proof of the second statement, by the definition of the reciprocal Randić index, we have

$$\begin{aligned}
RR(G) &= \sum_{uv \in E} \sqrt{d(u)d(v)} \\
&= \sum_{u \in S, v \in T, uv \in E} \sqrt{d(u)d(v)} + \sum_{u \in T, v \in T, uv \in E} \sqrt{d(u)d(v)} \\
&\leq \sum_{u \in S, v \in T} \sqrt{d(u)d(v)} + \sum_{u \in T, v \in T, u \neq v} \sqrt{d(u)d(v)} \\
&\leq r(k+2)\sqrt{r(n-1)} + \frac{r(r-1)(n-1)}{2} \\
&= (n-k-2)(k+2)\sqrt{(n-k-1)(n-1)} + \frac{(n-k-1)(n-k-2)(n-1)}{2} \\
&= (n-k-2)\left((k+2)\sqrt{(n-k-2)(n-1)} + \frac{(n-k-3)(n-1)}{2}\right).
\end{aligned}$$

Thus

$$RR(G) = (n-k-2)\left((k+2)\sqrt{(n-k-2)(n-1)} + \frac{(n-k-3)(n-1)}{2}\right).$$

This implies that

$$d(x_0) = d(y) = d(u_1^+) = \cdots = d(u_k^+)) = r = n - (k+2)$$

and

$$d(v_1) = \cdots = d(v_r) = d(v_{n-(k+2)}) = n - 1.$$

If $r = n - (k + 2) \geq (k + 2)$, then it is easy to check that G is is traceable, a contradiction. Thus, $r \leq k$. Hence, $r = k$ and G is $K_k \vee K_{k+2}^c$. This completes the proof of the second part in Theorem 2. ■

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