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ON HYPER-ZAGREB INDEX CONDITIONS FOR HAMILTONICITY OF GRAPHS

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Abstract. During the last decade, several research groups have published results on sufficient conditions for the hamiltonicity of graphs by using some topological indices. We mainly study hyper-Zagreb index and some hamiltonian properties. We give some sufficient conditions for graphs to be traceable, hamiltonian or Hamilton-connected in terms of their hyper-Zagreb indices. In addition, we also use the hyper-Zagreb index of the complement of a graph to present a sufficient condition for it to be Hamilton-connected.

Keywords: hyper-Zagreb index; hamiltonian; sufficient condition

MSC 2020: 05C45, 05C07

1. INTRODUCTION

Over the past decades, topological indices have attracted much attention. These indices are from the field of chemical graph theory. A topological index is regarded as a molecular descriptor to be calculated based on the molecular graph of a chemical compound. Further, many topological indices have been used to characterize the topology of a graph, and they are widely known as graph invariants.

Since topological indices are concise and useful for characterizing the structure of a graph, many graph theorists began to use them to establish sufficient conditions for graphs to posses hamiltonian properties. Wiener index and Harary index have been widely used to study hamiltonian properties, see [6], [10], [11], [14], [15], [22].

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In this paper, we study the relation between hyper-Zagreb index and some hamiltonian properties of graphs including traceability, hamiltonicity and Hamiltonconnectivity. A graph is called *traceable* if it contains a Hamilton path, *hamiltonian* if it contains a Hamilton cycle and *Hamilton-connected* if every two vertices are connected by a Hamilton path. Let G = (V(G), E(G)) be a graph with vertex set V(G) and edge set E(G). The complement of G is denoted by \overline{G} . Denote by m(G) = |E(G)| the number of edges of G. For $u \in V(G)$, we use $d_G(u)$ to denote the degree of u. If there is no confusion, we will omit the subscript G. The Zagreb indices have been introduced by Gutman and Trinajestić a few decades ago, see [9]. They are defined as

$$M_1 = \sum_{u \in V(G)} (d(u))^2, \quad M_2 = \sum_{uv \in E(G)} d(u)d(v),$$

which are called the *first Zagreb index* and the *second Zagreb index*, respectively. More background and results about these two Zagreb indices can be found in [8], [18], [19], [20]. The hyper-Zagreb index of G was introduced by Shirdel et al. in [17] and is defined as

$$HM(G) = \sum_{uv \in E(G)} (d(u) + d(v))^2.$$

Some recent results about hyper-Zagreb index can be seen in [5], [7], [16].

Li in [13] presented several sufficient conditions for graphs to be traceable or hamiltonian with respect to the hyper-Zagreb index of the complement of the graph. Motivated by this, we aim to give sufficient conditions on hyper-Zagreb index for graphs to possess some hamiltonian properties including traceability, hamiltonicity and Hamilton-connectivity. As a supplement, we will also give a sufficient condition for graphs to be Hamilton-connected in terms of the hyper-Zagreb index of the complement of the graph. Throughout the paper, we consider simple and undirected graphs only. Unless otherwise stated, we use the terminology and notation described in [3].

2. Preliminaries

In this section, we first recall three degree sequence results on hamiltonian properties of graphs. Here, the degrees of the *n* vertices of a graph *G* are ordered in a nondecreasing way as a degree sequence (d_1, d_2, \ldots, d_n) . We start this section by introducing a degree sequence result for traceable graphs.

Lemma 2.1 ([3]). Let G be a graph with degree sequence (d_1, d_2, \ldots, d_n) , where $d_1 \leq d_2 \leq \ldots \leq d_n$ and $n \geq 4$. Suppose that there is no integer $k < \frac{1}{2}(n+1)$ such that $d_k \leq k-1$ and $d_{n-k+1} \leq n-k-1$. Then G is traceable.

The next result is a well-known degree sequence on hamiltonicity that dates back to the 1970s.

Lemma 2.2 ([4]). Let G be a graph with degree sequence (d_1, d_2, \ldots, d_n) , where $d_1 \leq d_2 \leq \ldots \leq d_n$ and $n \geq 3$. If there is no integer $k < \frac{1}{2}n$ such that $d_k \leq k$ and $d_{n-k} \leq n-k-1$, then G contains a Hamilton cycle.

The third degree sequence result is on Hamilton-connected graphs.

Lemma 2.3 ([1], Theorem 12, page 218, [12], Lemma 3). Let G be a graph of order $n \ge 3$ with degree sequence (d_1, d_2, \ldots, d_n) , where $d_1 \le d_2 \le \ldots \le d_n$. If there is no integer $2 \le k \le \frac{1}{2}n$ such that $d_{k-1} \le k$ and $d_{n-k} \le n-k$, then G is Hamilton-connected.

In the proofs of our main results, we need the following result which is due to Bondy and Chvátal, see [2]. It deals with the closure $cl_{n+1}(G)$ obtained from a graph G by recursively adding edges between nonadjacent pairs of vertices with degree sum at least n + 1, until no such pair remains in the resulting graph.

Lemma 2.4 ([2]). A graph G is Hamilton-connected if and only if $cl_{n+1}(G)$ is Hamilton-connected.

The last lemma we need is a sufficient condition for graphs to be Hamiltonconnected in terms of the edge number of the graph.

Lemma 2.5 ([21]). Let G be a connected graph on $n \ge 6$ vertices and m edges with minimum degree $\delta(G) \ge 3$. If $m(G) \ge \binom{n-2}{2} + 6$, then G is Hamiltonconnected unless $G \in \mathcal{NP} = \{K_3 \lor (K_{n-5} + 2K_1), K_6 \lor 6K_1, K_4 \lor (K_2 + 3K_1), K_5 \lor 5K_1, K_4 \lor (K_{1,4} + K_1), K_4 \lor (K_{1,3} + K_2), K_3 \lor K_{2,5}, K_4 \lor 4K_1, K_3 \lor (K_1 + K_{1,3}), K_3 \lor (K_{1,2} + K_2), K_2 \lor K_{2,4}\}.$

3. Sufficient conditions on HM(G)

In this section, we mainly use the hyper-Zagreb index of G to give sufficient conditions for G to be traceable, hamiltonian and Hamilton-connected, respectively. We will show our main results, each followed by its proof. Before giving our theorems, we first introduce an upper bound for hyper-Zagreb index of graphs, which is the basis of the proofs of our main results. By the definition of hyper-Zagreb index, we have

(1)

$$HM(G) = \sum_{uv \in E(G)} (d(u) + d(v))^{2}$$

$$= \sum_{uv \in E(G)} (d^{2}(u) + d^{2}(v) + 2d(u)d(v))$$

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

$$\leq \sum_{u \in V(G)} d^{3}(u) + \sum_{uv \in E(G)} (d^{2}(u) + d^{2}(v))$$

$$= \sum_{u \in V(G)} d^{3}(u) + \sum_{u \in V(G)} d^{3}(u)$$

$$= 2\sum_{u \in V(G)} d^{3}(u).$$

The first result is for traceable graphs.

Theorem 3.1. Let G be a connected graph of order $n \ge 5$. If

$$HM(G) \ge 2n^4 - 14n^3 + 36n^2 - 40n + 16,$$

then G is traceable.

Proof. Suppose G is not traceable and has degree sequence $d_1 \leq d_2 \leq \ldots \leq d_n$. Then by Lemma 2.1, there is an integer $k < \frac{1}{2}(n+1)$ such that $d_k \leq k-1$ and $d_{n-k+1} \leq n-k-1$. Hence, by (1), we have

$$\begin{split} HM(G) &\leqslant 2\sum_{i=1}^n d_i^3 = 2 \bigg(\sum_{i=1}^k d_i^3 + \sum_{i=k+1}^{n-k+1} d_i^3 + \sum_{i=n-k+2}^n d_i^3 \bigg) \\ &\leqslant 2[k(k-1)^3 + (n-2k+1)(n-k-1)^3 + (k-1)(n-1)^3] \\ &= 2n^4 - 14n^3 + 36n^2 - 40n + 16 + (k-1)[6k^3 - (14n-10)k^2 + (18n^2 - 38n + 22)k - 8n^3 + 30n^2 - 38n + 16]. \end{split}$$

Due to the condition of Theorem 3.1, we get that $(k-1)[6k^3 - (14n-10)k^2 + (18n^2 - 38n+22)k - 8n^3 + 30n^2 - 38n+16] \ge 0$. Note that G is connected. We have $k \ge d_k + 1 \ge 2$. Hence, $6k^3 - (14n-10)k^2 + (18n^2 - 38n+22)k - 8n^3 + 30n^2 - 38n+16 \ge 0$. Since k is an integer, $k < \frac{1}{2}(n+1)$ is equivalent to $k \le \frac{1}{2}n$. In the following proof, we always assume that $k \le \frac{1}{2}n$.

Let $f(x) = 6x^3 - (14n - 10)x^2 + (18n^2 - 38n + 22)x - 8n^3 + 30n^2 - 38n + 16$, where $2 \le x \le \frac{1}{2}n$. It is easy to calculate that $f'(x) = 18x^2 - (28n - 20)x + 18n^2 - 38n + 22$ and the discriminant of equation f'(x) = 0 is $\Delta = -16(32n^2 - 101n + 74) < 0$ for

 $n \ge 1$. Hence, f'(x) > 0 for $2 \le x \le \frac{1}{2}n$. Then f(x) is a strictly monotonically increasing function on the interval $[2, \frac{1}{2}n]$. And $f_{\max}(x)$ is obtained by the right endpoint of the domain of f(x). Since k is an integer, we need to discuss the parity of n. When n is even, then

$$f_{\max}(x) = f\left(\frac{n}{2}\right) = -\frac{7}{4}n^3 + \frac{27}{2}n^2 - 27n + 16.$$

But $f(\frac{1}{2}n) < 0$ for $n \ge 5$, which implies f(x) < 0 for $2 \le x \le \frac{1}{2}n$, a contradiction. When n is odd, then

$$f_{\max}(x) = f\left(\frac{n-1}{2}\right) = -\frac{7}{4}n^3 + \frac{37}{4}n^2 - \frac{57}{4}n + \frac{27}{4}.$$

But $f(\frac{1}{2}(n-1)) < 0$ for $n \ge 4$, which implies f(x) < 0 for $2 \le x \le \frac{1}{2}n$, a contradiction.

This completes the proof.

Next, we present and prove the result which gives sufficient condition on hyper-Zagreb index of a graph G for G to be hamiltonian.

Theorem 3.2. Let G be a connected graph of order $n \ge 12$ with minimum degree $\delta(G) \ge 2$. If

$$HM(G) \ge 2n^4 - 22n^3 + 114n^2 - 258n + 244,$$

then G is hamiltonian.

Proof. Suppose G is not hamiltonian and has degree sequence $d_1 \leq d_2 \leq \ldots \leq d_n$. Then by Lemma 2.2, we obtain that there exists an integer $k < \frac{1}{2}n$ such that $d_k \leq k$ and $d_{n-k} \leq n-k-1$. Hence, by (1), we have

(2)
$$HM(G) \leq 2\sum_{i=1}^{n} d_i^3$$

 $= 2\left(\sum_{i=1}^{k} d_i^3 + \sum_{i=k+1}^{n-k} d_i^3 + \sum_{i=n-k+1}^{n} d_i^3\right)$
 $\leq 2[k \cdot k^3 + (n-2k)(n-k-1)^3 + k(n-1)^3]$
(3) $= 2n^4 - 22n^3 + 114n^2 - 258n + 244 + (k-2)[6k^3 - (14n-24)k^2 + (18n^2 - 58n + 60)k - 8n^3 + 54n^2 - 128n + 122].$

Combining with the condition of Theorem 3.2, we know that $(k-2)[6k^3 - (14n-24)k^2 + (18n^2 - 58n + 60)k - 8n^3 + 54n^2 - 128n + 122] \ge 0$. Since k is

 \square

an integer, $k < \frac{1}{2}n$ is equivalent to $k \leq \frac{1}{2}(n-1)$. In the following proof, we always suppose $k \leq \frac{1}{2}(n-1)$. Note that $k \geq d_k \geq \delta(G) \geq 2$. Let $f(x) = 6x^3 - (14n - 24)x^2 + (18n^2 - 58n + 60)x - 8n^3 + 54n^2 - 128n + 122$, where $2 \leq x \leq \frac{1}{2}(n-1)$. We divide the following proof into two cases.

Case 1: (k-2)f(x) = 0. In this case, we have k = 2 or f(x) = 0. It is easy to get $f'(x) = 18x^2 - (28n - 48)x + 18n^2 - 58n + 60$ and the discriminant of equation f'(x) = 0 is $\Delta = -16(32n^2 - 93n + 126) < 0$ for $n \ge 1$. Therefore, f'(x) > 0 for $2 \le x \le \frac{1}{2}(n-1)$ and f(x) is strictly monotonically increasing on the interval $[2, \frac{1}{2}(n-1)]$. Then $f_{\max}(x)$ is obtained by the right endpoints of the domain of f(x). Since k is an integer, we need to consider the parity of n. If n is even, then $f_{\max}(x) = f(\frac{1}{2}(n-2))$. By a simple calculation, we have

$$f\left(\frac{n-2}{2}\right) = -\frac{7}{4}n^3 + \frac{45}{2}n^2 - 69n + 80.$$

But $f(\frac{1}{2}(n-2)) < 0$ when $n \ge 10$, which implies f(x) < 0. If n is odd, then $f_{\max}(x) = f(\frac{1}{2}(n-1))$. By a simple calculation, we get

$$f\left(\frac{n-1}{2}\right) = -\frac{7}{4}n^3 + \frac{107}{4}n^2 - \frac{329}{4}n + \frac{389}{4}.$$

But $f(\frac{1}{2}(n-1)) < 0$ when $n \ge 12$, which implies f(x) < 0.

By the above analyses we can see that $f(x) \neq 0$ for $1 \leq x \leq \frac{1}{2}(n-1)$ and $n \geq 12$. Hence, we only need to consider the case k = 2. If k = 2, we have $HM(G) = 2n^4 - 22n^3 + 114n^2 - 258n + 244$ and inequalities (2) and (3) both should be equalities. If (3) is an equality, then $d_1 = d_2 = 2$, $d_3 = \ldots = d_{n-2} = n-3$ and $d_{n-1} = d_n = n-1$, which implies $G = K_2 \vee (K_{n-4} + 2K_1)$. But this graph does not satisfy $2\sum_{uv \in E(G)} d_u d_v = \sum_{uv \in E(G)} (d_u^2 + d_v^2)$, which yields that (2) can not be an equality, a contradiction.

Case 2: (k-2)f(x) > 0. In this case, we have $k \ge 3$ and $6k^3 - (14n - 24)k^2 + (18n^2 - 58n + 60)k - 8n^3 + 54n^2 - 128n + 122 > 0$. By the proof of Case 1, we know that f(x) is strictly monotonically increasing and $f_{\max}(x) < 0$. So for $3 \le k \le 2/(n-1)$, we still have $6k^3 - (14n - 24)k^2 + (18n^2 - 58n + 60)k - 8n^3 + 54n^2 - 128n + 122 < 0$, a contradiction.

This completes the proof.

At the end of this section, we use the hyper-Zagreb index of a graph G to give a sufficient condition for G to be Hamilton-connected. **Theorem 3.3.** Let G be a connected graph of order $n \ge 13$ with minimum degree $\delta(G) \ge 3$. If

$$HM(G) \ge 2n^4 - 22n^3 + 126n^2 - 306n + 372,$$

then G is Hamilton-connected.

Proof. Suppose G is not Hamilton-connected and has degree sequence $d_1 \leq d_2 \leq \ldots \leq d_n$. Then by Lemma 2.3, there exists an integer $2 \leq k \leq \frac{1}{2}n$ such that $d_{k-1} \leq k$ and $d_{n-k} \leq n-k$. Hence, by (1) we have

$$(4) \quad HM(G) \leq 2\sum_{i=1}^{n} d_i^3$$

$$= 2\left(\sum_{i=1}^{k-1} d_i^3 + \sum_{i=k}^{n-k} d_i^3 + \sum_{i=n-k+1}^{n} d_i^3\right)$$

$$\leq 2[(k-1) \cdot k^3 + (n-2k+1)(n-k)^3 + k(n-1)^3]$$

$$(5) \quad = 2n^4 - 22n^3 + 126n^2 - 306n + 372 + (k-3)[6k^3 - (14n-14)k^2 + (18n^2 - 36n + 42)k - 8n^3 + 42n^2 - 102n + 124].$$

Combining with the condition of Theorem 3.3, we have $(k-3)[6k^3 - (14n - 14)k^2 + (18n^2 - 36n + 42)k - 8n^3 + 42n^2 - 102n + 124] \ge 0$. Note that $k \ge d_{k-1} \ge \delta(G) \ge 3$. Let $f(x) = 6x^3 - (14n - 14)x^2 + (18n^2 - 36n + 42)x - 8n^3 + 42n^2 - 102n + 124$, where $3 \le x \le \frac{1}{2}n$. We divide the following proof into two cases.

Case 1: k = 3 or f(x) = 0. It is easy to obtain that $f'(x) = 18x^2 - (28n - 28)x + 18n^2 - 36n + 42$ and the discriminant of equation f'(x) = 0 is $\Delta = -64(8n^2 - 16n + 35) < 0$ for $n \ge 1$. Hence, f'(x) > 0 for $3 \le x \le \frac{1}{2}n$, and f(x) is a strictly monotonically increasing function on the interval $[3, \frac{1}{2}n]$. Then $f_{\max}(x)$ is obtained by the right endpoint of the domain of f(x). Since k is an integer, we need to discuss the parity of n. When n is even, then $f_{\max}(x) = f(\frac{1}{2}n)$. By a simple calculation, we have

$$f\left(\frac{n}{2}\right) = -\frac{7}{4}n^3 + \frac{55}{2}n^2 - 81n + 124.$$

But $f(\frac{1}{2}n) < 0$ when $n \ge 13$, which implies f(x) < 0. When n is odd, then $f_{\max}(x) = f(\frac{1}{2}(n-1))$. By a simple calculation, we have

$$f\left(\frac{n-1}{2}\right) = -\frac{7}{4}n^3 + \frac{93}{4}n^2 - \frac{285}{4}n + \frac{423}{4}.$$

But $f(\frac{1}{2}(n-1)) < 0$ when $n \ge 10$, which implies f(x) < 0.

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By the above analyses we can see that $f(x) \neq 0$ for $3 \leq x \leq \frac{1}{2}n$ and $n \geq 13$. Hence, we only need to consider the case k = 3. If k = 3, then $HM(G) \geq 2n^4 - 22n^3 + 126n^2 - 306n + 372$ and inequalities (4) and (5) both should be equalities. If (5) is an equality, then $d_1 = d_2 = 3$, $d_3 = \ldots = d_{n-3} = n-3$ and $d_{n-2} = d_{n-1} = d_n = n-1$, which implies $G = K_3 \vee (K_{n-5} + 2K_1)$. But this graph does not satisfy $2\sum_{uv \in E(G)} d_u d_v = \sum_{uv \in E(G)} (d_u^2 + d_v^2)$, which yields that (4) can not be an equality, a contradiction.

Case 2: $k \ge 4$. In this case, we get $6k^3 - (14n - 14)k^2 + (18n^2 - 36n + 42)k - 8n^3 + 42n^2 - 102n + 124 \ge 0$. Due to the proof of Case 1, we know that f(x) is strictly monotonically increasing and $f_{\max}(x) < 0$. Hence, when $4 \le k \le \frac{1}{2}n$, we still have $6k^3 - (14n - 14)k^2 + (18n^2 - 36n + 42)k - 8n^3 + 42n^2 - 102n + 124 < 0$, a contradiction.

This completes the proof.

4. Sufficient conditions on $HM(\overline{G})$

In [13], the author presented some sufficient conditions for graphs to be traceable and hamiltonian, respectively, by using the hyper-Zagreb index of the complement of graphs. In this section, we will use the hyper-Zagreb index of the complement of graphs to give sufficient condition for graphs to be Hamilton-connected.

Theorem 4.1. Let G be a connected graph of order $n \ge 6$ with minimum degree $\delta(G) \ge 3$. If

$$HM(\overline{G}) \leqslant (n-2)^2(2n-9),$$

then G is Hamilton-connected unless $G \in \{K_3 \lor 3K_1, K_6 \lor 6K_1, K_5 \lor 5K_1, K_4 \lor 4K_1\}$.

Proof. Suppose G is not Hamilton-connected. Let $H = cl_{n+1}(G)$. Then by Lemma 2.4, H is not Hamilton-connected, and then $H \neq K_n$. For any two nonadjacent vertices u and v in H, we have $d_H(u) + d_H(v) \leq n$. Hence, for any two adjacent vertices u and v in \overline{H} , we have

$$d_{\overline{H}}(u) + d_{\overline{H}}(v) = n - 1 - d_H(u) + n - 1 - d_H(v) \ge n - 2.$$

According to the definition of hyper-Zagreb index, we get

$$HM(\overline{H}) = \sum_{uv \in E(\overline{H})} (d_{\overline{H}}(u) + d_{\overline{H}}(v))^2 \ge (n-2)^2 m(\overline{H}).$$

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Since *H* is not Hamilton-connected, by Lemma 2.5, we have $m(H) \leq \binom{n-2}{2} + 5$ or $m(H) \geq \binom{n-2}{2} + 6$ and $H \in \mathcal{NP}$. If $m(H) \leq \binom{n-2}{2} + 5$, then

$$HM(\overline{G}) \ge HM(\overline{H}) \ge (n-2)^2 m(\overline{H}) \ge (n-2)^2 \left[\binom{n}{2} - \binom{n-2}{2} - 5 \right]$$
$$= 2(n-2)^2(n-4).$$

Combining with the condition of Theorem 4.1, it is easy to see that $(n-2)^2(2n-9) < 2(n-2)^2(n-4)$ for $n \ge 3$, a contradiction.

If $H \in \mathcal{NP}$ and $m(H) = \binom{n-2}{2} + 6$, then H belongs to the class $\mathcal{NP}_1 = \{K_3 \lor (K_{n-5} + 2K_1), K_6 \lor 6K_1, K_4 \lor (K_2 + 3K_1), K_4 \lor (K_{1,4} + K_1), K_4 \lor (K_{1,3} + K_2), K_3 \lor (K_{2,5}, K_3 \lor (K_1 + K_{1,3}), K_3 \lor (K_{1,2} + K_2), K_2 \lor K_{2,4}\}$. And we have

(6)
$$HM(\overline{G}) \ge HM(\overline{H}) \ge (n-2)^2 m(\overline{H}) \ge (n-2)^2 \left[\binom{n}{2} - \binom{n-2}{2} - 6 \right]$$
$$= (n-2)^2 (2n-9).$$

Due to the condition of Theorem 4.1, we know that all inequalities in (6) should be equalities. Then $d_{\overline{G}}(u) = d_{\overline{H}}(u)$ for every $u \in V(\overline{G}) = V(\overline{H})$; $d_{\overline{G}}(u)d_{\overline{G}}(v) = d_{\overline{H}}(u)d_{\overline{H}}(v)$ for $uv \in E(\overline{H})$, where $E(\overline{H}) \subseteq E(\overline{G})$; and $d_{\overline{H}}(u) + d_{\overline{H}}(v) = n - 2$ for $uv \in E(\overline{H})$. Hence, G = H and $G \in \{K_3 \lor 3K_1, K_6 \lor 6K_1\}$. If $H \in \mathcal{NP} \setminus \mathcal{NP}_1$, we know that $H = K_5 \lor 5K_1$ or $K_4 \lor 4K_1$. The hyper-Zagreb index of the complement of these two graphs is easy to calculate since they have a small number of vertices. After some simple calculations, we get that both $K_5 \lor 5K_1$ and $K_4 \lor 4K_1$ can enter the exceptional graphs list.

This completes the proof.

5. Concluding Remarks

Theorems 3.1–3.3 give sufficient conditions on HM(G) for graphs to be traceable, hamiltonian and Hamilton-connected, respectively. We do not know whether the results are sharp. For weakening the condition by (1), we have not found any exceptional graph. It is worthwhile to further study whether the bounds are sharp or they can be improved. Also, we might get more interesting results if the minimum degree of the graph is also involved. Further, can we use hyper-Zagreb index as conditions for other properties of graphs such as connectivity and toughness? We will leave these topics for our future work.

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