

# Maximum Multiplicity of Matching Polynomial Roots and Minimum Path Cover in General Graphs

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## Abstract

Let  $G$  be a graph. It is well known that the maximum multiplicity of a root of the matching polynomial  $\mu(G, x)$  is at most the minimum number of vertex disjoint paths needed to cover the vertex set of  $G$ . Recently, a necessary and sufficient condition for which this bound is tight was found for trees. In this paper, a similar structural characterization is proved for any graph. To accomplish this, we extend the notion of a  $(\theta, G)$ -extremal path cover (where  $\theta$  is a root of  $\mu(G, x)$ ) which was first introduced for trees to general graphs. Our proof makes use of the analogue of the Gallai-Edmonds Structure Theorem for general root. By way of contrast, we also show that the difference between the minimum size of a path cover and the maximum multiplicity of matching polynomial roots can be arbitrarily large.

## 1 Introduction

All the graphs in this paper are simple. The vertex set and edge set of a graph  $G$  are denoted by  $V(G)$  and  $E(G)$  respectively. A *matching* of a graph  $G$  is a set of pairwise non-adjacent edges of  $G$ . Recall that for a graph  $G$  on  $n$  vertices, the *matching polynomial*  $\mu(G, x)$  of  $G$  is given by

$$\mu(G, x) = \sum_{k \geq 0} (-1)^k p(G, k) x^{n-2k},$$

where  $p(G, k)$  is the number of matchings with  $k$  edges in  $G$  and  $p(G, 0) = 1$  by convention. Let  $\text{mult}(\theta, G)$  denote the multiplicity of  $\theta$  as a root of  $\mu(G, x)$ .

The following result is well known. A proof of this assertion can be found in [2, Theorem 4.5 on p. 107].

**Theorem 1.1.** *The maximum multiplicity of a root of the matching polynomial  $\mu(G, x)$  is at most the minimum number of vertex disjoint paths needed to cover the vertex set of  $G$ .*

Consequently,

**Theorem 1.2.** *If  $G$  has a Hamiltonian path, then all roots of its matching polynomial are simple.*

The above is the source of motivation for our work. In this note, we give a necessary and sufficient condition for the maximum multiplicity of a root of the matching polynomial of a graph to be equal to the minimum number of vertex disjoint paths needed to cover it. The special case for trees (or forests) was previously proved by the authors in [6, Theorem 1.7]. Before stating the main result, we require some terminology and basic properties of matching polynomials.

If  $u \in V(G)$ , then  $G \setminus u$  is the graph obtained from  $G$  by deleting the vertex  $u$  and the edges of  $G$  incident to  $u$ . It is not difficult to prove that the roots of  $\mu(G \setminus u, x)$  *interlace* those of  $\mu(G, x)$ , that is, the multiplicity of a root changes by at most one upon deleting a vertex from  $G$  (see [2, Corollary 1.3 on p. 97]).

**Lemma 1.3.** *Suppose  $\theta$  is a root of  $\mu(G, x)$  and  $u$  is a vertex of  $G$ . Then*

$$\text{mult}(\theta, G) - 1 \leq \text{mult}(\theta, G \setminus u) \leq \text{mult}(\theta, G) + 1.$$

As a consequence of Lemma 1.3, we can classify the vertices in a graph by assigning a ‘sign’ to each vertex [3, Section 3].

**Definition 1.4.** Let  $\theta$  be a root of  $\mu(G, x)$ . For any vertex  $u \in V(G)$ ,

- $u$  is  $\theta$ -essential if  $\text{mult}(\theta, G \setminus u) = \text{mult}(\theta, G) - 1$ ,
- $u$  is  $\theta$ -neutral if  $\text{mult}(\theta, G \setminus u) = \text{mult}(\theta, G)$ ,
- $u$  is  $\theta$ -positive if  $\text{mult}(\theta, G \setminus u) = \text{mult}(\theta, G) + 1$ .

Note that even if  $\theta$  is not a root of  $\mu(G, x)$ , it is still valid to talk about  $\theta$ -neutral and  $\theta$ -positive vertices. A further classification of vertices plays an important role in establishing some structural properties of a graph:

**Definition 1.5.** Let  $\theta$  be a root of  $\mu(G, x)$ . For any vertex  $u \in V(G)$ ,  $u$  is  $\theta$ -special if it is not  $\theta$ -essential but has a neighbor that is  $\theta$ -essential.

It turns out that a  $\theta$ -special vertex must be  $\theta$ -positive (see [3, Corollary 4.3]).

We now introduce the following definition which is crucial in describing our main result.

**Definition 1.6.** Let  $G$  be a graph and  $\mathcal{P} = \{P_1, \dots, P_m\}$  be a set of vertex disjoint paths that cover  $G$ . For each  $i = 1, \dots, m$ , let  $G_i$  denote the subgraph induced by  $P_i$ . Then  $\mathcal{P}$  is said to be  $(\theta, G)$ -*extremal* if it satisfies the following:

- (a)  $\theta$  is a root of  $\mu(G_i, x)$  for all  $i = 1, \dots, m$ ;
- (b) for every edge  $e = \{u, v\} \in E(G)$  with  $u \in G_r$  and  $v \in G_s$ ,  $r \neq s$ , either  $u$  is  $\theta$ -special in  $G_r$  or  $v$  is  $\theta$ -special in  $G_s$ .

Note that if  $G$  is a tree, then  $G_i = P_i$  for all  $i = 1, \dots, m$ , so the definition of a  $(\theta, G)$ -extremal path cover coincides with that introduced in [6, Section 1] for forests.

Our main result is the following:

**Theorem 1.7.** *Let  $G$  be a graph and  $\mathcal{P} = \{P_1, \dots, P_m\}$  be a set of vertex disjoint paths covering  $G$ . Then  $m$  is the maximum multiplicity of a root of the matching polynomial  $\mu(G, x)$ , say  $\text{mult}(\theta, G) = m$  for some root  $\theta$ , if and only if  $\mathcal{P}$  is  $(\theta, G)$ -extremal.*

The outline of this paper is as follows: Section 2 contains some basic properties of matching polynomials and Section 3 gives an account of the Gallai-Edmonds Structure Theorem. Section 4 is devoted to graphs with a Hamiltonian path. The proof of the main result is presented in Section 5. We conclude by observing that there exist (connected) graphs such that the gap between the maximum multiplicity of matching polynomial roots and the minimum size of a path cover can be made arbitrarily large.

## 2 Basic Properties

In this section, we collect some useful results proved in [1], [2] and [3]. Recall that if  $u \in V(G)$ , then  $G \setminus u$  is the graph obtained from  $G$  by deleting the vertex  $u$  and the edges of  $G$  incident to  $u$ . We also denote the graph  $(G \setminus u) \setminus v$  by  $G \setminus uv$ . In general, we denote the graph obtained after deleting vertices  $u_1, \dots, u_r$  from  $G$  by  $G \setminus u_1 \cdots u_r$ . Note that the resulting graph does not depend on the order of which the vertices are deleted.

If  $e \in E(G)$ , the graph  $G - e$  is the graph obtained from  $G$  by deleting the edge  $e$ .

The matching polynomial satisfies the following basic identities.

**Proposition 2.1.** [2, Theorem 1.1] *Let  $G$  and  $H$  be graphs, with matching polynomials  $\mu(G, x)$  and  $\mu(H, x)$ , respectively. Then*

- (a)  $\mu(G \cup H, x) = \mu(G, x)\mu(H, x)$ ,
- (b)  $\mu(G, x) = \mu(G - e, x) - \mu(G \setminus uv, x)$  where  $e = \{u, v\}$  is an edge of  $G$ ,
- (c)  $\mu(G, x) = x\mu(G \setminus u, x) - \sum_{v \sim u} \mu(G \setminus uv, x)$  for any vertex  $u$  of  $G$ .

Suppose  $P$  is a path in  $G$ . Let  $G \setminus P$  denote the graph obtained from  $G$  by deleting the vertices of  $P$  and all the edges incident to these vertices. It is known that the multiplicity of a root decreases by at most one upon deleting a path.

**Lemma 2.2.** [3, Corollary 2.5] *For any root  $\theta$  of  $\mu(G, x)$  and a path  $P$  in  $G$ ,*

$$\text{mult}(\theta, G \setminus P) \geq \text{mult}(\theta, G) - 1.$$

If equality holds, we say that the path  $P$  is  $\theta$ -essential in  $G$ . Godsil [3] proved that if a vertex  $v$  is not  $\theta$ -essential in  $G$ , then no path with  $v$  as an end point is  $\theta$ -essential in  $G$ . In other words,

**Lemma 2.3.** [3, Lemma 3.3] *If  $P$  is a  $\theta$ -essential path in  $G$ , then its end points are  $\theta$ -essential in  $G$ .*

The following useful result appeared in [1]. We include its short proof here.

**Lemma 2.4.** [1, Lemma 3.4] *Let  $u$  be a  $\theta$ -positive vertex in  $G$ , adjacent to a  $\theta$ -essential vertex  $v$ . Let  $e = \{u, v\} \in E(G)$ . Then  $\text{mult}(\theta, G - e) = \text{mult}(\theta, G)$ , therefore  $u$  remains  $\theta$ -positive and  $v$  remains  $\theta$ -essential in  $G - e$ .*

*Proof.* Let  $k = \text{mult}(\theta, G)$  and  $G' = G - e$ . Notice that  $\text{mult}(\theta, G' \setminus u) = \text{mult}(\theta, G \setminus u) = k + 1$  and  $\text{mult}(\theta, G' \setminus v) = \text{mult}(\theta, G \setminus v) = k - 1$ . By interlacing (Lemma 1.3), it follows that  $\text{mult}(\theta, G') = k$ , so  $u$  is  $\theta$ -positive and  $v$  is  $\theta$ -essential in  $G'$ .  $\square$

### 3 Gallai-Edmonds Decomposition

The Gallai-Edmonds Structure Theorem describes a certain canonical decomposition of  $V(G)$  with respect to the zero root of  $\mu(G, x)$ . Its statement essentially consists of two lemmas, the Stability Lemma and Gallai's Lemma. For more information, see [7, Section 3.2]. Recently, Chen and Ku [1] extended these results to all nonzero roots of the matching polynomial. A recent application of this result can be found in [5]. The special case  $\theta = 0$  is the celebrated Gallai-Edmonds Decomposition.

Let

$$V(G) = B_\theta(G) \cup A_\theta(G) \cup P_\theta(G) \cup N_\theta(G)$$

be a partition of  $V(G)$  where

$B_\theta(G)$  is the set of all  $\theta$ -essential vertices in  $G$ ,

$A_\theta(G)$  is the set of all  $\theta$ -special vertices in  $G$ ,

$N_\theta(G)$  is the set of all  $\theta$ -neutral vertices in  $G$ ,

$P_\theta(G) = Q_\theta(G) \setminus A_\theta(G)$ , where  $Q_\theta(G)$  is the set of all  $\theta$ -positive vertices in  $G$ .

Note that there are no 0-neutral vertices. So  $N_0(G) = \emptyset$  and  $V(G) = B_0(G) \cup A_0(G) \cup P_0(G)$ .

**Theorem 3.1** ( $\theta$ -Stability Lemma, [1, Theorem 1.5]). *Let  $G$  be a graph with  $\theta$  a root of  $\mu(G, x)$ . If  $u \in A_\theta(G)$  then*

- (i)  $B_\theta(G \setminus u) = B_\theta(G)$ ,
- (ii)  $P_\theta(G \setminus u) = P_\theta(G)$ ,
- (iii)  $N_\theta(G \setminus u) = N_\theta(G)$ ,
- (iv)  $A_\theta(G \setminus u) = A_\theta(G) \setminus \{u\}$ .

**Theorem 3.2** ( $\theta$ -Gallai's Lemma, [1, Theorem 1.7]). *If every vertex of  $G$  is  $\theta$ -essential and  $G$  is connected, then  $\text{mult}(\theta, G) = 1$ .*

Suppose  $\theta$  is a root of  $\mu(G, x)$ . Call  $G$   $\theta$ -critical if every vertex of  $G$  is  $\theta$ -essential. In view of Theorem 3.2, if  $G$  is  $\theta$ -critical and connected then  $\text{mult}(\theta, G) = 1$ .

Suppose  $G$  has exactly  $s$   $\theta$ -special vertices and  $\text{mult}(\theta, G) = k$ . Then, by Theorem 3.1 and Theorem 3.2, after removing all the  $\theta$ -special vertices from  $G$ , we obtain  $k + s$  pairwise disjoint connected  $\theta$ -critical graphs. Call such a graph a  $\theta$ -critical component of  $G \setminus A_\theta(G)$ .

The Stability Lemma says that the 'sign' of a vertex does not change upon deleting a  $\theta$ -special vertex. Godsil proved a result very similar to the Stability Lemma by investigating how the sign changes when deleting a  $\theta$ -positive vertex.

**Proposition 3.3** (Theorem 4.2, [3]). *Let  $\theta$  be a root of  $\mu(G, x)$  and let  $u$  be a  $\theta$ -positive vertex in  $G$ . Then*

- (a) *if  $v$  is  $\theta$ -positive in  $G$  then it is  $\theta$ -essential or  $\theta$ -positive in  $G \setminus u$ ;*
- (b) *if  $v$  is  $\theta$ -essential in  $G$  then it is  $\theta$ -essential in  $G \setminus u$ ;*
- (c) *if  $v$  is  $\theta$ -neutral in  $G$  then it is  $\theta$ -essential or  $\theta$ -neutral in  $G \setminus u$ .*

Chen and Ku [1] investigated the effect on the sign of vertices when deleting a  $\theta$ -neutral vertex. Among other results, they gave the following statement which is analogous to Proposition 3.3. However, the proof of the following statement was omitted in [1]. For the sake of completeness, we supply below a proof which is similar to that of Godsil's [3].

**Proposition 3.4.** *Let  $\theta$  be a root of  $\mu(G, x)$  with non-zero multiplicity  $k$  and let  $u$  be a  $\theta$ -neutral vertex in  $G$ . Then*

- (a) *if  $v$  is  $\theta$ -positive in  $G$  then it is  $\theta$ -positive or  $\theta$ -neutral in  $G \setminus u$ ;*
- (b) *if  $v$  is  $\theta$ -essential in  $G$  then it is  $\theta$ -essential in  $G \setminus u$ ;*
- (c) *if  $v$  is  $\theta$ -neutral in  $G$  then it is  $\theta$ -neutral or  $\theta$ -positive in  $G \setminus u$ .*

*Proof.* (a) Suppose  $v$  is  $\theta$ -positive in  $G$ . By Proposition 3.3,  $u$  is either  $\theta$ -neutral or  $\theta$ -essential in  $G \setminus v$ . Therefore, either  $\text{mult}(\theta, G \setminus vu) = k + 1$  or  $\text{mult}(\theta, G \setminus vu) = k$ . This means that  $v$  is either  $\theta$ -positive or  $\theta$ -neutral in  $G \setminus u$ .

(b) Suppose  $v$  is  $\theta$ -essential in  $G$ . Since  $\text{mult}(\theta, G \setminus u) = k$ , we have  $\text{mult}(\theta, G \setminus vu) = \text{mult}(\theta, G \setminus uv) \geq k - 1$  by interlacing, so  $u$  is not  $\theta$ -essential in  $G \setminus v$ . Assume for the moment that  $u$  is  $\theta$ -positive in  $G \setminus v$ . Then  $\text{mult}(\theta, G \setminus uv) = k$ . As  $u$  is not  $\theta$ -essential in  $G$ , it follows from Lemma 2.2 and Lemma 2.3 that  $\text{mult}(\theta, G \setminus P) \geq k$  for every path  $P$  from  $u$  to  $v$  in  $G$ .

Recall the Heilmann-Lieb Identity (see [3, Lemma 2.4]):

$$\mu(G \setminus u, x)\mu(G \setminus v, x) - \mu(G, x)\mu(G \setminus uv, x) = \sum_{P \in \mathcal{P}(u, v)} \mu(G \setminus P, x)^2,$$

where  $\mathcal{P}(u, v)$  is the set of all paths in  $G$  from  $u$  to  $v$ .

Using the above identity, we deduce that  $\text{mult}(\theta, G \setminus u) + \text{mult}(\theta, G \setminus v) \geq 2k$ , contradicting the fact that  $u$  is  $\theta$ -neutral and  $v$  is  $\theta$ -essential in  $G$ . So  $u$  is  $\theta$ -neutral in  $G \setminus v$ , i.e.  $v$  is  $\theta$ -essential in  $G \setminus u$ .

(c) Suppose  $v$  is  $\theta$ -neutral in  $G$ . Since  $\text{mult}(\theta, G \setminus u) = k$ , by interlacing,  $\text{mult}(\theta, G \setminus uv) \geq k - 1$ . Since  $\text{mult}(\theta, G \setminus v) = k$ ,  $\theta$  has multiplicity at least  $2k - 1$  as a root of  $p(x)$  where

$$p(x) := \mu(G \setminus u, x)\mu(G \setminus v, x) - \mu(G, x)\mu(G \setminus uv, x).$$

On the other hand, by considering the right hand side of the Heilmann-Lieb Identity, the multiplicity of  $\theta$  as a root of  $p(x)$  must be even. So this multiplicity must be at least  $2k$ , whence  $\theta$  has multiplicity at least  $2k$  as a root of  $\mu(G, x)\mu(G \setminus uv, x)$ . Therefore,  $\text{mult}(\theta, G \setminus uv) \geq k$ , i.e.  $v$  is not  $\theta$ -essential in  $G \setminus u$ .  $\square$

**Remark 3.5.** The assertions of Proposition 3.3 and Proposition 3.4, excluding part (b), still hold even if  $\theta$  is not a root of  $\mu(G, x)$ .

**Lemma 3.6.** *A  $\theta$ -neutral vertex cannot be joined to any  $\theta$ -essential vertex.*

*Proof.* Suppose  $u$  is a  $\theta$ -neutral vertex and is joined to a  $\theta$ -essential vertex  $v$ . By Proposition 3.4, the path  $uv$  is  $\theta$ -essential in  $G$  whence  $u$  and  $v$  are  $\theta$ -essential in  $G$  (Lemma 2.3), which is a contradiction.  $\square$

The preceding implies that a  $\theta$ -special vertex must be  $\theta$ -positive ([3, Corollary 4.3]).

## 4 Graph with a Hamiltonian Path

In this section, we study the matching polynomial roots and their multiplicities in graphs with a Hamiltonian path. The results here will be needed in the proof of the main result in the next section.

**Proposition 4.1.** *Suppose  $G$  has a Hamiltonian path  $P$ . Let  $H$  be the graph obtained from  $G$  by deleting an end point of  $P$ . Then  $\mu(G, x)$  and  $\mu(H, x)$  have no common roots.*

*Proof.* We prove it by induction on the number  $n \geq 2$  of vertices of  $G$ . If  $n = 2$ , then  $G$  consists of a single edge and  $H$  is a point. Clearly, their matching polynomials have no roots in common. Let  $n > 2$ . Let  $u$  be an end point of  $P$  and  $H = G \setminus u$ . Also, let  $v$  be the vertex joined to  $u$  in  $P$ .

Assume, for a contradiction, that  $\theta$  is a root of  $\mu(G, x)$  and  $\mu(H, x)$ . By Theorem 1.2,  $\text{mult}(\theta, G) = 1 = \text{mult}(\theta, H)$ . This implies that  $u$  is  $\theta$ -neutral in  $G$ . By induction,  $\mu(H, x)$  and  $\mu(H \setminus v, x)$  have no common roots. Therefore,  $v$  is  $\theta$ -essential in  $H$ . By Proposition 3.4, we deduce that  $v$  is  $\theta$ -essential in  $G$ . But  $u$  is adjacent to  $v$  in  $G$ , contradicting Lemma 3.6.  $\square$

**Corollary 4.2.** *Suppose  $G$  has a Hamiltonian path  $P$ . Then the end points of  $P$  are  $\theta$ -essential in  $G$ .*

**Corollary 4.3.** *If  $G$  has a Hamiltonian cycle, then every vertex of  $G$  is  $\theta$ -essential.*

**Corollary 4.4.** *Suppose  $G$  has a Hamiltonian path  $P$  and  $\theta$  is a root of  $\mu(G, x)$ . Then every vertex of  $G$  which is not  $\theta$ -essential must be  $\theta$ -special.*

*Proof.* Let  $w$  be a vertex which is not  $\theta$ -essential. By Corollary 4.2,  $w$  is not an end point of  $P$ . Let  $u$  and  $v$  be the two neighbors of  $w$  in  $P$ . Let  $P_1$  and  $P_2$  denote the disjoint paths obtained after removing  $w$  from  $P$ . We may assume that  $u$  is an end point of  $P_1$ .

Consider the paths  $P_1$  and  $P_1uw$  in  $G$ . Suppose  $u$  is not  $\theta$ -essential in  $G$ . Then, by Lemma 2.3,  $P_1$  and  $P_1uw$  are not  $\theta$ -essential paths in  $G$ . By Lemma 2.2, both  $\text{mult}(\theta, G \setminus P_1)$  and  $\text{mult}(\theta, G \setminus P_1uw)$  is at least 1, i.e.  $\mu(G \setminus P_1, x)$  and  $\mu(G \setminus P_1uw, x)$  have at least one common root, contradicting Proposition 4.1. Therefore,  $u$  is  $\theta$ -essential in  $G$  and so  $w$  is  $\theta$ -special in  $G$ .  $\square$

**Lemma 4.5.** *Let  $u$  and  $u'$  be two distinct  $\theta$ -special vertices in  $G$ . Suppose  $u$  is adjacent to a  $\theta$ -essential vertex  $v$  such that  $G - e$  has a Hamiltonian path, where  $e = \{u, v\} \in E(G)$ . Then  $u$  and  $u'$  remain  $\theta$ -special in  $G - e$ . Moreover,  $\text{mult}(\theta, G - e) = \text{mult}(\theta, G)$ .*

*Proof.* Let  $k = \text{mult}(\theta, G) > 0$ . By Lemma 2.4,  $\text{mult}(\theta, G - e) = k$ ,  $u$  is  $\theta$ -positive and  $v$  is  $\theta$ -essential in  $G - e$ . By Corollary 4.4,  $u$  is  $\theta$ -special in  $G - e$ . By Theorem 3.1,  $\text{mult}(\theta, G \setminus uu') = k + 2$  and so  $u'$  is  $\theta$ -positive in  $G \setminus u$ . Note that  $G \setminus u = (G - e) \setminus u$ . Therefore,  $u'$  is  $\theta$ -positive in  $(G - e) \setminus u$ . Since  $u$  is  $\theta$ -positive in  $G - e$ , we deduce from Proposition 3.3 that  $u'$  is  $\theta$ -positive in  $G - e$ . By Corollary 4.4 again,  $u'$  is  $\theta$ -special in  $G - e$ .  $\square$

**Lemma 4.6.** *Suppose that  $G$  has a Hamiltonian path  $P = (u_1, \dots, u_n)$  and  $A_\theta(G) = \{u_{k_1}, \dots, u_{k_s}\}$ , where  $1 < k_1 < \dots < k_s < n$ . Then  $G \setminus A_\theta(G)$  is comprised of  $s + 1$*

$\theta$ -critical components  $C_1, \dots, C_{s+1}$  where each  $C_i$  is the subgraph of  $G$  induced by the path  $P_i = (u_{k_i+1}, \dots, u_{k_i-1})$ . Consequently, there are no edges of  $G$  between  $C_i$  and  $C_j$  for all  $i \neq j$ .

*Proof.* Clearly, each  $C_i$  is a connected subgraph of  $G \setminus A_\theta(G)$ , so  $G \setminus A_\theta(G)$  consists of at most  $s+1$  components. Since  $\text{mult}(\theta, G) = 1$ , by the Gallai-Edmonds Structure Theorem (Theorem 3.1 and Theorem 3.2) and Corollary 4.4,  $G \setminus A_\theta(G)$  consists of exactly  $s+1$   $\theta$ -critical components. Therefore, the subgraphs  $C_i$  must be pairwise disjoint and each of them is  $\theta$ -critical.  $\square$

**Proposition 4.7.** *Suppose  $G$  has a Hamiltonian path  $P = (u_1, \dots, u_n)$  and  $\theta$  is a root of  $\mu(G, x)$ . Let  $w$  be a  $\theta$ -special vertex of  $G$ . Let  $Q = wPu_n$  denote the subpath of  $P$  which starts from  $w$  and ends at  $u_n$ . Let  $u \in G \setminus Q$ . Then  $u$  is  $\theta$ -special in  $G \setminus Q$  if and only if  $u$  is  $\theta$ -special in  $G$ .*

*Proof.* Suppose there are  $s$   $\theta$ -special vertices in  $G$ . Let  $u_{k_1}, \dots, u_{k_s}$  denote these  $\theta$ -special vertices. By Corollary 4.2,  $1 < k_1 < k_2 < \dots < k_s < n$ . By Lemma 4.6,  $G \setminus u_{k_1} \dots u_{k_s}$  consists of  $s+1$   $\theta$ -critical components  $C_1, \dots, C_{s+1}$  such that each  $C_i$  has a Hamiltonian path  $P_i$  where

$$\begin{aligned} P_1 &= (u_1, \dots, u_{k_1-1}), \\ P_i &= (u_{k_{i-1}+1}, \dots, u_{k_i-1}) \quad \text{for all } i = 2, \dots, s, \\ P_{s+1} &= (u_{k_s+1}, \dots, u_n). \end{aligned}$$

Moreover, by Theorem 1.2,  $\text{mult}(\theta, C_i) = 1$  for all  $i = 1, \dots, s+1$ .

We may assume that  $w = u_{k_r}$  for some  $r \in \{1, \dots, s\}$ . Set  $H = G \setminus Q$ . Notice that  $Q$  is the path  $(w = u_{k_r}, u_{k_r+1}, \dots, u_n)$  and  $\text{mult}(\theta, H) = 1$ . We can view  $H$  as the subgraph of  $G$  induced by  $V(C_1) \cup \dots \cup V(C_r) \cup \{u_{k_1}, \dots, u_{k_{r-1}}\}$ .

( $\Leftarrow$ ) Suppose  $u$  is  $\theta$ -special in  $G$  and  $u \in V(H)$ . Then  $u \in \{u_{k_1}, \dots, u_{k_{r-1}}\}$ . Note that after removing  $u_{k_1}, \dots, u_{k_{r-1}}$  from  $H$ , we obtain a union of pairwise disjoint graphs  $C_1, \dots, C_r$ . Clearly,  $\text{mult}(\theta, H \setminus u_{k_1} \dots u_{k_{r-1}}) = r$ . This implies that each  $u_{k_i}$  with  $i \in \{1, \dots, r-1\}$  (one of which is  $u$ ) must be  $\theta$ -special in  $H$ ; otherwise  $u_{k_i}$  is  $\theta$ -essential in  $H$  for some  $i$  (by Corollary 4.4), and thus by first deleting  $u_{k_i}$  from  $H$  followed by removing  $u_{k_j}$  for all  $j \in \{1, \dots, r-1\}$ ,  $j \neq i$ , we would have  $\text{mult}(\theta, H \setminus u_{k_1} \dots u_{k_{r-1}}) < r$  by interlacing (Lemma 1.3), contradicting the fact that  $\text{mult}(\theta, H \setminus u_{k_1} \dots u_{k_{r-1}}) = r$ .

( $\Rightarrow$ ) Suppose  $u$  is  $\theta$ -special in  $H$ . First we see that if  $r = 1$  then  $w = u_{k_1}$ , whence  $H = C_1$  and it contains only  $\theta$ -essential vertices (by Theorem 3.1), contradicting the assumption that  $u$  is  $\theta$ -special in  $H$ . Therefore,  $r > 1$  and the set  $\{u_{k_1}, \dots, u_{k_{r-1}}\}$  is not empty. We need to prove that  $u \in \{u_{k_1}, \dots, u_{k_{r-1}}\}$ . Let  $\mathcal{F}$  denote the set of all edges  $\{x, y\} \in E(G) \setminus E(P)$  where  $x \in V(H)$ ,  $y \in V(C_{r+1}) \cup V(C_{r+2}) \cup \dots \cup V(C_{s+1})$ . By Lemma 4.6,  $x \in \{u_{k_1}, \dots, u_{k_{r-1}}\}$ , i.e.  $x$  must be  $\theta$ -special in  $G$ .

Now, consider removing the edges in  $\mathcal{F}$  from  $G$  one by one. At each step of removing such an edge, the resulting graph always has the Hamiltonian path  $P = (u_1, \dots, u_n)$ . Let  $G^*$  denote the graph obtained from  $G$  after removing all edges in  $\mathcal{F}$ . By repeated applications of Lemma 4.5,  $u_{k_1}, \dots, u_{k_s}$  remain  $\theta$ -special in  $G^*$  and  $\text{mult}(\theta, G^*) = \text{mult}(\theta, G)$ . Moreover, since  $G^* \setminus A_\theta(G) = G \setminus A_\theta(G)$ , by Theorem 3.1,  $\theta$ -essential vertices of  $G$  remain  $\theta$ -essential in  $G^*$ . Note that  $G^* \setminus u_{k_r} \cdots u_{k_s}$  is the union of  $H, C_{r+1}, \dots, C_{s+1}$ . Moreover, the set of  $\theta$ -special vertices of  $G^* \setminus u_{k_r} \cdots u_{k_s}$  is  $\{u_{k_1}, \dots, u_{k_{r-1}}\}$  which turns out to be  $A_\theta(H)$ . Hence  $u \in \{u_{k_1}, \dots, u_{k_{r-1}}\}$ . This completes the proof.  $\square$

## 5 Proof of Main Result

We proceed to establish the main result (Theorem 1.7) which will be given by Theorem 5.2 and Theorem 5.3 below. We begin by proving the following lemma:

**Lemma 5.1.** *Let  $G$  be a graph and  $\text{mult}(\theta, G) = m$ . Let  $\mathcal{P} = \{P_1, \dots, P_m\}$  be a set of vertex disjoint paths covering  $G$ . Then either  $G$  is  $\theta$ -critical or  $G$  has a  $\theta$ -special vertex.*

*Proof.* Suppose  $G$  is not  $\theta$ -critical. If  $G$  has a component  $C$  which has  $\theta$  as a root of its matching polynomial and is not  $\theta$ -critical, then  $C$  (and thus  $G$ ) contains a  $\theta$ -special vertex (see Lemma 3.6). For a contradiction, we may assume that  $G$  has a component  $C$  such that  $\text{mult}(\theta, C) = 0$ . Clearly,  $\text{mult}(\theta, G \setminus V(C)) = \text{mult}(\theta, G) = m$ . Observe that  $G \setminus V(C)$  can be covered by at most  $m - 1$  paths since at least one path of  $\mathcal{P}$  is required to cover  $C$ . But this contradicts Theorem 1.1.  $\square$

**Theorem 5.2.** *Let  $G$  be a graph and  $\text{mult}(\theta, G) = m$ . Let  $\mathcal{P} = \{P_1, \dots, P_m\}$  be a set of vertex disjoint paths covering  $G$ . Then  $\mathcal{P}$  is  $(\theta, G)$ -extremal.*

*Proof.* For each  $i = 1, \dots, m$ , let  $G_i$  denote the subgraph of  $G$  induced by  $P_i$ . Suppose all vertices of  $G$  are  $\theta$ -essential. Then,  $G$  is the disjoint union of all  $G_i$ ,  $i = 1, \dots, m$ ; otherwise,  $\text{mult}(\theta, G)$  would be strictly less than  $m$  by Theorem 3.2, a contradiction. Clearly,  $\mathcal{P}$  is  $(\theta, G)$ -extremal as  $G$  has no edges between  $G_i$  and  $G_j$  for all  $i \neq j$ . We may assume that not all vertices of  $G$  are  $\theta$ -essential, so  $G$  has a  $\theta$ -special vertex (Lemma 5.1). Also, the result holds if  $m = 1$ . So we may assume that  $m \geq 2$ .

We first claim that  $\theta$  is a root of  $\mu(G_i, x)$  for each  $i$ . We shall prove this by induction on  $m \geq 1$ . The case  $m = 1$  is obvious. Let  $m \geq 2$ . Since  $P_2, \dots, P_m$  cover  $G \setminus P_1$ , we deduce from Theorem 1.1 that  $\text{mult}(\theta, G \setminus P_1) \leq m - 1$ . On the other hand,  $\text{mult}(\theta, G \setminus P_1) \geq \text{mult}(\theta, G) - 1 = m - 1$  (Lemma 2.2). So  $\text{mult}(\theta, G \setminus P_1) = m - 1$ . By induction,  $\theta$  is a root of  $\mu(G_i, x)$  for all  $i = 2, \dots, m$ . Similarly,  $\theta$  is a root of  $\mu(G_i, x)$  for all  $i = 1, \dots, m - 1$  if we had deleted  $P_m$  instead of  $P_1$  in the preceding argument. This proves the claim. Moreover, by Theorem 1.2,  $\text{mult}(\theta, G_i) = 1$  for each  $i$ .

Now, let  $\{u, v\} \in E(G)$  with  $u \in V(G_r)$  and  $v \in V(G_s)$  for some  $r \neq s$ . We need to show that either  $u$  is  $\theta$ -special in  $G_r$  or  $v$  is  $\theta$ -special in  $G_s$ . Let  $w$  be a  $\theta$ -special vertex in  $G$ . Then  $\text{mult}(\theta, G \setminus w) = m + 1$ . Suppose  $w \in P_t$  for some  $t \in \{1, \dots, m\}$ .

Note that  $w$  is not an end point of  $P_t$ ; otherwise  $G \setminus w$  can be covered by at most  $m$  paths, whence  $\text{mult}(\theta, G \setminus w) \leq m$  by Theorem 1.1, a contradiction. Let  $H$  denote the graph obtained from  $G \setminus w$  after deleting all paths  $P_i$ ,  $i \neq t$ . By repeated applications of Lemma 2.2, we have  $\text{mult}(\theta, H) \geq \text{mult}(\theta, G \setminus w) - (m - 1) = 2$ . Note that  $H = G_t \setminus w$ . Since  $\text{mult}(\theta, G_t) = 1$ , we deduce that  $w$  is  $\theta$ -positive in  $G_t$ . By Corollary 4.4,  $w$  is  $\theta$ -special in  $G_t$ .

If  $w = u$  then  $r = t$  and  $u$  is  $\theta$ -special in  $G_r$ , so we are done. The case  $w = v$  can be proved similarly.

Therefore, we may assume that  $w \neq u$ ,  $w \neq v$ . We proceed by induction on the number of vertices. Since  $w$  is not an end point of  $P_t$ , let  $Q_1$  and  $Q_2$  denote the paths obtained from  $P_t$  after removing  $w$  from  $P_t$ . Note that  $\text{mult}(\theta, G \setminus w) = m + 1$  and  $\mathcal{Q} = \{Q_1, Q_2\} \cup \{P_i : i \neq t\}$  is a set of  $m + 1$  vertex disjoint paths that cover  $G \setminus w$ . By induction,  $\mathcal{Q}$  is  $(\theta, G \setminus w)$ -extremal. If  $t \neq r, s$ , then either  $u$  is  $\theta$ -special in  $G_r$  or  $v$  is  $\theta$ -special in  $G_s$ , so we are done. It remains to consider the following cases:

Case I.  $t = r$ .

Let  $H_1$  and  $H_2$  be the subgraphs of  $G_r$  induced by  $Q_1$  and  $Q_2$  respectively.

Without loss of generality, either  $u$  is  $\theta$ -special in  $H_1$  or  $v$  is  $\theta$ -special in  $G_s$ . If  $v$  is  $\theta$ -special in  $G_s$ , we are done. Otherwise, using the fact that  $w$  is  $\theta$ -special in  $G_r$  and Proposition 4.7, we deduce that  $u$  is  $\theta$ -special in  $G_r$ .

Case II.  $t = s$ .

An argument similar to Case I proves that either  $u$  is  $\theta$ -special in  $G_r$  or  $v$  is  $\theta$ -special in  $G_s$ .

We note that so long as  $w \neq u, v$ , the graph  $G \setminus w$  cannot be  $\theta$ -critical since  $G \setminus w$  consists of at most  $m$  components (because  $u$  is still joined to  $v$  in  $G \setminus w$ ); otherwise,  $\text{mult}(\theta, G \setminus w) \leq m$  which is not possible. So  $G \setminus w$  would always contain a  $\theta$ -special vertex (by Lemma 5.1). Therefore, the base cases of our induction occur when  $w = u$  or  $w = v$ .  $\square$

**Theorem 5.3.** *Let  $G$  be a graph and  $\mathcal{P} = \{P_1, \dots, P_m\}$  be a set of vertex disjoint paths covering  $G$ . Suppose  $\mathcal{P}$  is  $(\theta, G)$ -extremal. Then  $\text{mult}(\theta, G) = m$  and  $\theta$  is a root  $\mu(G, x)$  with the maximum multiplicity.*

*Proof.* By Theorem 1.1,  $\text{mult}(\theta, G) \leq m$ . It remains to show that  $\text{mult}(\theta, G) \geq m$ . As usual, for  $i = 1, \dots, m$ , let  $G_i$  denote the subgraph of  $G$  induced by  $P_i$ . We shall prove the theorem by induction on the number of vertices.

An edge  $\{u, v\}$  of  $G$  is said to be *crossing* if  $u$  and  $v$  belong to different paths in  $\mathcal{P}$ . Let  $C$  be the total number of crossing edges of  $G$ . If  $C = 0$ , then  $G$  consists of

disjoint components  $G_1, \dots, G_m$  such that each  $G_i$  contains  $P_i$  as a Hamiltonian path. By Theorem 1.2 and Proposition 2.1 (a), we must have  $\text{mult}(\theta, G) = m$ , as desired.

Therefore, we may assume that  $C > 0$ . Then, there exists a crossing edge  $\{u, v\}$ , say  $u \in V(P_1)$  and  $v \in V(P_2)$ . Since  $\mathcal{P}$  is  $(\theta, G)$ -extremal, without loss of generality, we may assume that  $u$  is  $\theta$ -special in  $G_1$ .

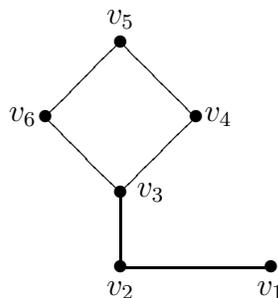
Since  $u$  is  $\theta$ -special in  $G_1$ ,  $u$  cannot be an end point of  $P_1$  (Corollary 4.2). So  $P_1 \setminus u$  consists of two disjoint paths  $Q_1$  and  $Q_2$ . Let  $H_1$  and  $H_2$  denote the subgraphs of  $G_1$  induced by  $Q_1$  and  $Q_2$  respectively. By Proposition 4.7,  $\theta$ -special vertices in  $H_1$  and  $H_2$  are precisely the  $\theta$ -special vertices of  $G$  in  $H_1$  and  $H_2$  respectively. Moreover, any edge between  $H_1$  and  $H_2$  must be incident to either a  $\theta$ -special vertex in  $H_1$  or a  $\theta$ -special vertex in  $H_2$  (Lemma 4.6). Therefore,  $\{Q_1, Q_2, P_2, P_3, \dots, P_m\}$  is  $(\theta, G \setminus u)$ -extremal. By induction,  $\text{mult}(\theta, G \setminus u) = m + 1$ . By interlacing (Lemma 1.3),  $\text{mult}(\theta, G) \geq m$ , as desired.

Notice that the base cases of our induction occur when there are no crossing edges.  $\square$

## 6 Conclusion

For a graph  $G$ , let  $\text{maxmult}(G)$  and  $\text{minpc}(G)$  denote the maximum multiplicity of a root of  $\mu(G, x)$  and the minimum size of a path cover of  $G$  respectively. Our main result (Theorem 1.7) gives a characterization of graphs  $G$  for which  $\text{maxmult}(G) = \text{minpc}(G)$ . The characterization is given in terms of the notion of a  $(\theta, G)$ -extremal path cover. Though the conditions of such a path cover do not seem easy to check in general, they do sometimes provide a quick way to identify graphs  $G$  for which  $\text{maxmult}(G) < \text{minpc}(G)$ . For example, take a graph  $H$  which has a Hamiltonian cycle and join one vertex, say  $v$ , of  $H$  to the second vertex  $u$  of the path  $P_4$  on four vertices to form the graph  $W$ . Clearly,  $\text{minpc}(W) = 2$ . By Corollary 4.3,  $v$  is not  $\theta$ -special in  $H$  for any root  $\theta$  of  $\mu(H, x)$ . It is also easy to check by hand that  $u$  is not  $\theta$ -special in  $P_4$  for any root  $\theta$  of  $\mu(P_4, x)$ . Therefore, in view of Theorem 1.7,  $\text{maxmult}(W) < 2$ .

It is worth mentioning that there exist connected graphs  $G$  for which the difference  $\text{minpc}(G) - \text{maxmult}(G)$  can be arbitrarily large. Indeed, consider the following graph  $S$ :



Let  $S_1, \dots, S_k$  be  $k$  disjoint copies of  $S$  and for each  $1 \leq i \leq k$ , let  $v_1^i, \dots, v_6^i$  denote the vertices of  $S_i$  corresponding to the vertices  $v_1, \dots, v_6$  of  $S$  respectively. Let  $P_i$  denote

the (Hamiltonian) path  $(v_1^i, v_2^i, v_3^i, v_4^i, v_5^i, v_6^i)$  in  $S_i$ .

For each  $k \geq 2$ , define the graph  $G_k$  as follows:

$$V(G_k) = \bigcup_{i=1}^k V(S_i), \quad E(G_k) = \left( \bigcup_{i=1}^k E(S_i) \right) \cup \left( \bigcup_{i=2}^k \{v_5^i, v_2^{i-1}\} \right).$$

It is not difficult to see that we may assume a minimum-sized path cover of  $G_k$  always contain  $P_1$ . Then a simple induction yields  $\min pc(G_k) = k$ . Next, we claim that  $\max mult(G_k) = 1$ . Let  $T_i = P_i \setminus v_1^i v_6^i$  for  $1 \leq i \leq k$ . Consider the path  $Z_k$  in  $G_k$  obtained by bridging the paths  $T_k, T_{k-1}, \dots, T_1$  with the edges  $\{v_5^k, v_2^{k-1}\}, \{v_5^{k-1}, v_2^{k-2}\}, \dots, \{v_5^2, v_2^1\}$ . Observe that  $G_k \setminus Z_k$  consists of isolated vertices and so  $\text{mult}(\theta, G_k \setminus Z_k) = 0$  provided  $\theta \neq 0$ . Therefore, if  $\theta$  is a root of  $G_k$  (note that  $\theta \neq 0$  since  $G_k$  has a perfect matching), then  $Z_k$  is a  $\theta$ -essential path in  $G_k$ . In view of Lemma 2.2, we deduce that  $\text{mult}(\theta, G_k) = 1$ , thus establishing the claim.

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