



## Graphs for which the least eigenvalue is minimal, II<sup>☆</sup>

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Received 14 November 2007; accepted 9 June 2008

Available online 8 August 2008

Submitted by R.A. Brualdi

Dedicated to Michael Doob on his 65th birthday.

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### Abstract

We continue our investigation of graphs  $G$  for which the least eigenvalue  $\lambda(G)$  is minimal among the connected graphs of prescribed order and size. We provide structural details of the bipartite graphs that arise, and study the behaviour of  $\lambda(G)$  as the size increases while the order remains constant. The non-bipartite graphs that arise were investigated in a previous paper [F.K. Bell, D. Cvetković, P. Rowlinson, S.K. Simić, Graphs for which the least eigenvalue is minimal, I, *Linear Algebra Appl.* (2008), doi:10.1016/j.laa.2008.02.032]; here we distinguish the cases of bipartite and non-bipartite graphs in terms of size.

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*AMS classification:* 05C50

*Keywords:* Bipartite graph; Graph spectrum; Largest eigenvalue; Least eigenvalue

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<sup>☆</sup> Research supported by EPSRC Grant EP/D010748/1 and by the Serbian Ministry for Science Grant 144015G.

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### 1. Introduction

Let  $G = (V_G, E_G)$  be a simple graph, with vertex set  $V_G$  and edge set  $E_G$ . Its *order* is  $|V_G|$ , denoted by  $n$ , and its *size* is  $|E_G|$ , denoted by  $m$ . We write  $u \sim v$  to indicate that vertices  $u$  and  $v$  are adjacent, and we write  $A_G$  for the  $(0, 1)$ -adjacency matrix of  $G$ . The characteristic polynomial  $\det(xI - A_G)$  is denoted by  $\phi_G(x)$ . The zeros of  $\phi_G(x)$  are called the *eigenvalues* of  $G$ ; recall that they are real since  $A_G$  is symmetric. We write  $\lambda(G)$  for the least eigenvalue of  $G$ ,  $\rho(G)$  for the largest eigenvalue (the *index*) of  $G$ , and  $\lambda_i(G)$  for the  $i$ th largest eigenvalue of  $G$  ( $i = 1, 2, \dots, n$ ). The degree of a vertex  $v$  is denoted by  $\deg(v)$ .

In a previous paper [1] we investigated the graphs  $G$  for which  $\lambda(G)$  is minimal among the connected graphs of prescribed order and size. We showed that if  $G$  is not complete then  $\lambda(G)$  is a simple eigenvalue and  $G$  is either bipartite or a join of two graphs of a simple form. In this paper, we provide structural details of the bipartite graphs that arise, and study the behaviour of  $\lambda(G)$  as the size increases while the order remains constant.

The main structural result in [1] is Theorem 3.7 which reads:

**Theorem 1.1.** *Let  $G$  be a connected graph whose least eigenvalue is minimal among the connected graphs of order  $n$  and size  $m$  ( $0 < m < \binom{n}{2}$ ). Then  $G$  is either*

- (i) *a bipartite graph, or*
- (ii) *a join of two nested split graphs (not both totally disconnected).*

A graph  $G$  is called a *nested split graph* if its vertices can be ordered so that  $jq \in E_G$  implies  $ip \in E_G$  whenever  $i \leq j$  and  $p \leq q$ . The nested split graphs are the graphs without  $2K_2, P_4$  or  $C_4$  as an induced subgraph (cf. [5]); they are precisely the graphs with a stepwise adjacency matrix (see [4, Section 3.3]). For subsequent reference we provide further details from [1] of the graphs that arise in case (ii) of Theorem 1.1. Here, let  $\mathbf{x} = (x_1, \dots, x_n)^T$  be an eigenvector corresponding to  $\lambda(G)$ , and let  $V^- = \{u \in V_G : x_u < 0\}$ ,  $V^0 = \{u \in V_G : x_u = 0\}$ ,  $V^+ = \{u \in V_G : x_u > 0\}$ . Let  $H^-, H^+$  be the subgraphs of  $G$  induced by  $V^-, V^+$ , respectively. By [1, Proposition 3.5], if  $H^-, H^+$  are not both totally disconnected then every vertex in  $V^-$  is adjacent to every vertex in  $V^+$ . Otherwise,  $V_0 \neq \emptyset$  (since  $G$  is non-bipartite), and each vertex  $v$  in  $V^- \cup V^+$  has a neighbour outside  $V_0$  (by consideration of the corresponding eigenvalue equation  $\lambda(G)x_v = \sum_{u \sim v} x_u$ ). Recall also that each vertex in  $V^0$  is adjacent to all other vertices [1, Lemma 3.1]. Accordingly we can deduce the following:

**Proposition 1.2.** *In case (ii) of Theorem 1.1,  $G$  has an edge  $e = vw$  such that  $x_v x_w \geq 0$ ,  $x_v \neq 0$  and  $G - e$  is connected.*

For a bipartite graph  $G$ , we have  $\lambda(G) = -\rho(G)$ , and so in Section 2 we determine the structure of connected bipartite graphs with maximal index for prescribed  $n$  and  $m$ . Here,  $m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ , with equality if and only if  $G = K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ . In Section 3, we investigate how the minimal least eigenvalue of bipartite graphs varies with  $m$  when  $n$  is fixed, while in Section 4 we use these results to study the same question for all connected graphs; in particular, we are in a position to distinguish cases (i) and (ii) of Theorem 1.1 when  $m$  varies.

## 2. The structure of extremal bipartite graphs

Before we state our main result in this section we need a definition.

Let  $G$  be a bipartite graph with colour classes  $U$  and  $V$ . We say that  $G$  is a *double nested graph* if there exist partitions  $U = U_1 \dot{\cup} U_2 \dot{\cup} \dots \dot{\cup} U_h$  and  $V = V_1 \dot{\cup} V_2 \dot{\cup} \dots \dot{\cup} V_h$ , such that the neighbourhood of each vertex in  $U_1$  is  $V_1 \dot{\cup} V_2 \dot{\cup} \dots \dot{\cup} V_h$ , the neighbourhood of each vertex in  $U_2$  is  $V_1 \dot{\cup} \dots \dot{\cup} V_{h-1}$ , and so on. If  $|U_i| = m_i$  ( $i = 1, 2, \dots, h$ ) and  $|V_i| = n_i$  ( $i = 1, 2, \dots, h$ ) then  $G$  is denoted by  $D(m_1, m_2, \dots, m_h; n_1, n_2, \dots, n_h)$ .

**Theorem 2.1.** *If  $G$  is a graph for which  $\lambda(G)$  is minimal (equivalently,  $\rho(G)$  is maximal) among all connected bipartite graphs of order  $n$  and size  $m$ , then  $G$  is a double nested graph.*

Thus double nested graphs play the same role among bipartite graphs (with respect to the index) as nested split graphs among non-bipartite graphs. The proof of Theorem 2.1 is based on the following lemmas, the first of which is taken from [6]. Recall that the index  $\rho$  of a connected graph  $G$  is a simple eigenvalue, and that there exists a unique unit eigenvector corresponding to  $\rho$  having only positive entries; this eigenvector is called the *Perron eigenvector* of  $G$ .

**Lemma 2.2.** *Let  $G'$  be the graph obtained from a connected graph  $G$  by rotating the edge  $r_i$ s around  $r_i$  to the non-edge position  $r_i t$  for each  $i \in \{1, \dots, k\}$ . Let  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$  be the Perron eigenvector of  $G$ . If  $x_t \geq x_s$  then  $\rho(G') > \rho(G)$ .*

The next lemma will be very helpful when we encounter a bridge in a graph whose index is assumed to be maximal. Given two rooted graphs  $P(=P_u)$  and  $Q(=Q_v)$  with  $u$  and  $v$  as roots, let  $G$  be the graph obtained from the disjoint union  $P \dot{\cup} Q$  by adding the edge  $uv$ . Let  $G'$  be the graph obtained from the coalescence of  $P_u$  and  $Q_v$  by attaching a pendant edge at the vertex identified with  $u$  and  $v$ .

**Lemma 2.3.** *With the above notation, if  $P$  and  $Q$  are two non-trivial connected graphs then  $\rho(G) < \rho(G')$ .*

**Proof.** Let  $(x_1, x_2, \dots, x_n)^T$  be the Perron eigenvector of  $G$ . Without loss of generality, we may suppose that  $x_u \leq x_v$ . Let  $\Delta$  be the neighbourhood of  $u$  in  $P$ ; since  $P$  is non-trivial,  $\Delta \neq \emptyset$ . Now  $G'$  is obtained from  $G$  by replacing the edges  $uw$  ( $w \in \Delta$ ) by the edges  $vw$  ( $w \in \Delta$ ), and so  $\rho(G) < \rho(G')$  by Lemma 2.2, as required.  $\square$

In what follows we assume that  $G$  has maximal index among the connected bipartite graphs of fixed order and size.

**Lemma 2.4.** *Let  $G$  be a graph satisfying the above assumptions, and let  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$  be the Perron eigenvector of  $G$ . If  $v, w$  are vertices in the same colour class such that  $x_v \geq x_w$  then  $\deg(v) \geq \deg(w)$ .*

**Proof.** Let  $U, V$  be the colour classes of  $G$  and suppose, by way of contradiction, that  $v, w$  are vertices in  $V$  such that  $x_v \geq x_w$  and  $\deg(v) < \deg(w)$ . Then  $\deg(w) > 1$  and there exists

$u \in U$  such that  $v \not\sim u \sim w$ . By Lemma 2.1, we may rotate  $uw$  to  $uv$  to obtain a graph  $G'$  such that  $\rho(G') > \rho(G)$ . If  $uw$  is a bridge then  $\deg(u) = 1$  by Lemma 2.3, and so  $G'$  is necessarily connected; but now the maximality of  $\rho(G)$  is contradicted, and the proof follows.  $\square$

From now on we take the colour classes to be  $U = \{u_1, u_2, \dots, u_p\}$  and  $V = \{v_1, v_2, \dots, v_q\}$ , with  $x_{u_1} \geq x_{u_2} \geq \dots \geq x_{u_p}$  and  $x_{v_1} \geq x_{v_2} \geq \dots \geq x_{v_q}$ . By Lemma 2.4, this ordering coincides with the ordering by degrees in each colour class, and in the next lemma we note some consequences.

**Lemma 2.5.** *Let  $G$  be a graph satisfying the above assumptions including those on vertex ordering. Then*

- (i) *the vertices  $u_1$  and  $v_1$  are adjacent;*
- (ii)  *$u_1$  is adjacent to every vertex in  $V$ , and  $v_1$  is adjacent to every vertex in  $U$ ;*
- (iii) *if the vertex  $u$  is adjacent to  $v_k$  then  $u$  is adjacent to  $v_j$  for all  $j < k$ , and if the vertex  $v$  is adjacent to  $u_k$  then  $v$  is adjacent to  $u_j$  for all  $j < k$ .*

**Proof.** First we consider bridges in  $G$ : by Lemma 2.3, all bridges are pendant edges. By Lemma 2.2, all pendant edges are attached at the same vertex, and this vertex  $w$  is such that  $x_w$  is maximal. Without loss of generality,  $x_{u_1} \geq x_{v_1}$  and  $w = u_1$ . It follows that the result holds if  $G$  is a tree, for then  $G$  is a star. Accordingly, we suppose that  $G$  is not a tree.

To prove (i), suppose by way of contradiction that  $u_1 \not\sim v_1$ . Then  $v_1$  is adjacent to some vertex  $u \in U$ , and  $uv_1$  is not a bridge. By Lemma 2.2, we may rotate  $v_1u$  to  $v_1u_1$  to obtain a connected bipartite graph  $G'$  such that  $\rho(G') > \rho(G)$ , contradicting the maximality of  $\rho(G)$ .

To prove (ii), suppose that  $u$  is a vertex of  $U$  not adjacent to  $v_1$ . Then  $u \neq u_1$  by (i),  $uv$  is not a bridge, and  $u$  is adjacent to some vertex  $v$  in  $V$  other than  $v_1$ . Now we can rotate  $uv$  to  $uv_1$  to obtain a contradiction as before. Secondly, suppose that  $v$  is a vertex of  $V$  not adjacent to  $u_1$ . Then  $v \neq v_1$  by (i), again  $vu_1$  is not a bridge, and a rotation about  $v$  yields a contradiction.

To prove (iii), suppose that  $u \in U, u \sim v_k$  and  $u \not\sim v_j$  for some  $j < k$ . Now  $u \neq u_1$  by (ii), and so  $uv_k$  is not a bridge. Then we can rotate  $uv_k$  to  $uv_j$  to obtain a contradiction. Finally, suppose that  $v \in V, v \sim v_k$  and  $v \not\sim u_j$  for some  $j < k$ . In this case,  $vu_k$  is not a bridge because  $k > 1$ , and the rotation of  $vu_k$  to  $vu_j$  yields a contradiction.

This completes the proof.  $\square$

The proof of Theorem 2.1. follows now directly from Lemma 2.5 and the definition of a double nested split graph.

We conclude this section with two remarks.

First, with the notation of Lemma 2.5, let  $d_i = \deg(u_i)$  ( $i = 1, \dots, p$ ) and  $e_j = \deg(v_j)$  ( $j = 1, \dots, q$ ). Let  $\Pi_U$  be the integer partition  $m = d_1 + d_2 + \dots + d_p$ , and let  $\Pi_V$  be the integer partition  $m = e_1 + e_2 + \dots + e_q$ . We have  $d_1 \geq d_2 \geq \dots \geq d_p$  and  $e_1 \geq e_2 \geq \dots \geq e_q$ ; moreover, the structure of a double nested graph ensures that  $\Pi_U$  and  $\Pi_V$  are conjugate, i.e. the Ferrers diagram for  $\Pi_U$  is the transpose of the Ferrers diagram for  $\Pi_V$ .

Secondly, we can give an algorithm for constructing the double nested graphs of order  $n$  and size  $m$ . For each integer partition  $\Pi : m = d_1 + d_2 + \dots + d_p$  with  $d_1 \geq d_2 \geq \dots \geq d_p$  and  $d_1 + p = n$ , we can construct the double nested graph with  $U = \{u_1, u_2, \dots, u_p\}$ ,  $V = \{v_1, v_2, \dots, v_q\}$ ,  $q = d_1$  and  $\Pi_U = \Pi$  as follows. Considering the vertices  $u_1, u_2, \dots, u_p$  in succession, we join  $u_k$  to the first  $d_k$  of the vertices  $v_1, v_2, \dots, v_q$ .

### 3. The behaviour of the least eigenvalue of extremal connected bipartite graphs

We may summarize the results of this section as follows.

**Theorem 3.1.** *For fixed  $n \geq 7$ , let  $G_m$  be a graph whose least eigenvalue is minimal (equivalently, whose index is maximal) among the connected bipartite graphs of order  $n$  and size  $m < \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ . Then*

- (i) if  $m \neq t(n - t)$  for all  $t \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1\}$  then  $\rho(G_m) < \rho(G_{m+1})$ ;
- (ii) if  $m = t(n - t)$  for some  $t \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1\}$  then  $\rho(G_m) > \rho(G_{m+1})$  unless  $G_{m+1}$  has the form  $D(p, q; r, s)$ , where

$$\{t, n - t\} = \{p + q, r + s\}, t(n - t) = pr + ps + qr - 1 \leq pqrs.$$

The proof follows from sequence of lemmas in which we discuss how  $\rho(G_m)$  varies with (for fixed  $n$ ).

**Lemma 3.2.** *Under the above assumptions we have:*

- (i)  $\rho(G_m) \leq \sqrt{m}$ , with equality if and only if  $G_m$  is a complete bipartite graph  $K_{t, n-t}$ , for some  $t \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor\}$ ;
- (ii)  $\rho(G_m) < \rho(G_{m+1})$  whenever  $t(n - t) + 1 \leq m < (t + 1)(n - t - 1)$ , where  $t \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1\}$ .

**Proof.** Let  $\lambda_1 > \lambda_2 \geq \dots \geq \lambda_{n-1} > \lambda_n$  be the eigenvalues of a connected bipartite graph  $G$ . Since  $G$  is bipartite we have

$$m = \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} \lambda_i^2. \tag{1}$$

It follows that  $\rho(G_m) \leq \sqrt{m}$ , with equality if and only if  $\lambda_1^2 = m$  and  $\lambda_2^2 = \dots = \lambda_{\lfloor \frac{n}{2} \rfloor} = 0$ . In this case,  $G_m = K_{t, n-t}$  for some  $t$  (see, e.g. [2, Theorem 6.5]), and this completes the proof of (i).

In (ii),  $m \neq t(n - t)$  for all  $t$ , and so  $G_m$  is not a complete bipartite graph. Thus  $G_m$  is a proper spanning subgraph of some complete bipartite graph  $K$  (of order  $n$ ). Accordingly we may add to  $G$  some edge of  $K$  to obtain a connected bipartite graph  $G'$  of order  $n$  for which  $\rho(G_m) < \rho(G')$ . Since  $\rho(G') \leq \rho(G_{m+1})$ , the proof of (ii) is complete.  $\square$

**Remark.** Computational data obtained by F. Marić shows that if  $m = t(n - t)$  for some  $t \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1\}$  then both possibilities (namely  $\rho(G_m) < \rho(G_{m+1})$  and  $\rho(G_m) > \rho(G_{m+1})$ ) can arise. For  $n = 9$  we have the situation presented in Fig. 1, where points at which  $m = t(n - t) + 1$  for some  $t$  are indicated by vertical lines.

In considering the situation left unresolved by Lemma 3.2, we let  $m = t(n - t)$  for some  $t \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1\}$ . Then  $G_m = K_{t, n-t}$ , while  $G_{m+1}$  is a double nested graph  $D(m_1, m_2, \dots, m_h; n_1, n_2, \dots, n_h)$ .

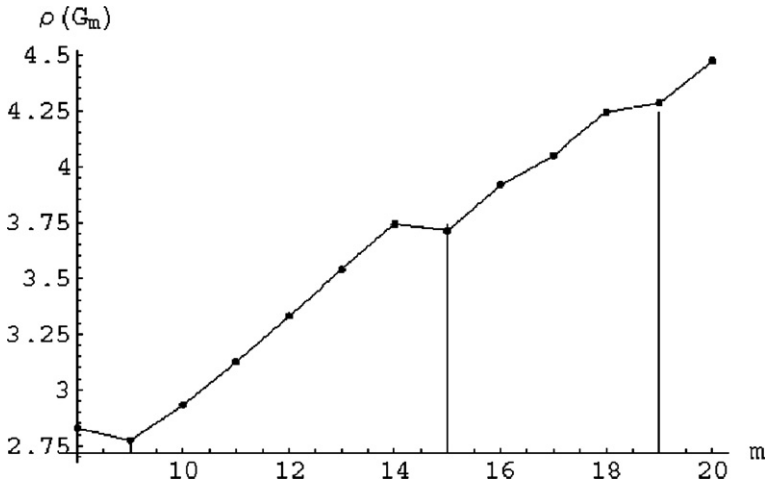


Fig. 1. The behavior of  $\rho(G_m)$  when  $n = 9$ .

In the next two lemmas and Theorem 3.1, we assume that  $n \geq 7$ ; when  $n < 7$ , we may refer to the tables of eigenvalues in [2,3].

**Lemma 3.3.** *Suppose that  $m = t(n - t)$  and  $n \geq 7$ . If  $h \geq 3$  then  $\rho(G_m) > \rho(G_{m+1})$ .*

**Proof.** We write  $G = G_m$  and  $G' = G_{m+1}$ . Let  $\lambda_1 > \lambda_2 \geq \dots \geq \lambda_{n-1} > \lambda_n$  and  $\lambda'_1 > \lambda'_2 \geq \dots \geq \lambda'_{n-1} > \lambda'_n$  be the eigenvalues of  $G$  and  $G'$ , respectively.

From (1) we have immediately:

$$\sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} (\lambda'_i)^2 - \lambda_1^2 = 1.$$

From this it follows that

$$\rho(G)^2 - \rho(G')^2 = \sum_{i=2}^{\lfloor \frac{n}{2} \rfloor} (\lambda'_i)^2 - 1. \tag{2}$$

In considering the relation (2), we distinguish two cases.

*Case 1:  $h \geq 4$ .* In this case,  $G'$  has an induced subgraph  $D_1$ , where  $D_1 = D(1, 1, 1, 1; 1, 1, 1, 1)$ , and we have  $\lambda'_2 \geq \lambda_2(D_1)$ . But  $\lambda_2(D_1) > 1$ , and so  $\rho(G)^2 > \rho(G')^2$  by (2).

*Case 2:  $h = 3$ .* In this case,  $G'$  contains, as an induced subgraph, one of the graphs  $D_2 = D(1, 1, 1; 1, 1, 2)$ ,  $D_3 = D(1, 1, 1; 1, 2, 1)$  and  $D_4 = D(1, 1, 1; 2, 1, 1)$ . Since  $\lambda_2(D_i) > 1$  ( $i = 2, 3, 4$ ), we have  $\rho(G)^2 > \rho(G')^2$  as before.

This completes the proof.  $\square$

**Remark.** Note that the graphs  $D_i$  ( $i = 1, 2, 3, 4$ ) appearing in the above lemma are not the smallest induced subgraphs which can be used to obtain the required inequality.

When  $h = 1$ ,  $G_{m+1}$  is itself a complete bipartite graph,  $n = 2t + 2$  and  $\rho(G_m) < \rho(G_{m+1})$ . The next lemma deals with the remaining case,  $h = 2$ .

**Lemma 3.4.** *Suppose that  $m = t(n - t)$  and  $G_{m+1} = D(p, q; r, s)$  (so that  $m + 1 = pr + ps + qr$ ). Then we have:*

- (i)  $\rho(G_m) < \rho(G_{m+1})$  if  $m > pqrs$ ;
- (ii)  $\rho(G_m) = \rho(G_{m+1})$  if  $m = pqrs$ ;
- (iii)  $\rho(G_m) > \rho(G_{m+1})$  if  $m < pqrs$ .

**Proof.** We write  $G = G_m$ ,  $G' = G_{m+1}$  as before, and we use the divisor technique (see [2, Chapter 4]) to compute the eigenvalues of  $G'$ . Note that  $V_{G'}$  has  $U_1 \dot{\cup} U_2 \dot{\cup} V_1 \dot{\cup} V_2$  as an equitable partition, and the corresponding divisor has adjacency matrix

$$A_D = \begin{pmatrix} 0 & 0 & r & s \\ 0 & 0 & r & 0 \\ p & q & 0 & 0 \\ p & 0 & 0 & 0 \end{pmatrix}.$$

We find easily that  $\phi_{A_D^2}(x) = (x^2 - m'x + pqrs)^2$ , where  $m' = m + 1$ .

The vertices in each of the four cells of the equitable partition are duplicate vertices of  $G'$ , and together they give rise to  $n - 4$  eigenvalues equal to 0. We deduce that there are just four non-zero eigenvalues in  $G'$ , namely  $\pm\lambda'_1, \pm\lambda'_2$  where

$$\lambda'_{1,2} = \frac{1}{2} \left( m' \pm \sqrt{m'^2 - 4pqrs} \right).$$

Now the result follows from (2).  $\square$

On the basis of Lemmas 3.3 and 3.4 the proof of Theorem 3.1 readily follows.

In case (ii) of Theorem 3.1, we can use a program written in *Mathematica* to check, for each 4-tuple  $(p, q, r, s)$ , whether the corresponding graph exists. If at least one such graph exists then  $\rho(G_m) \leq \rho(G_{m+1})$  by Lemma 3.4. We show that, in this situation, at least two of the parameters  $p, q, r, s$  are subject to an absolute bound.

By Lemma 3.4, we have the following basic requirement:

$$pr + ps + rq \geq 1 + pqrs. \tag{3}$$

In addition to this, we can assume

$$p + r \geq 3, \quad r \geq p. \tag{4}$$

The first condition in (4) follows from the fact that  $D(p, q, r, s)$  is not a tree, while the second follows from the fact that we may interchange  $U$  and  $V$  if necessary. We consider the following three cases:

- (a)  $ps = 1$  (equivalently,  $p = s = 1$ );
- (b)  $qs = 1$  (equivalently,  $q = s = 1$ );
- (c)  $ps \neq 1$  and  $qs \neq 1$ .

Note that  $rq \neq 1$ , by (4).

In cases (a) and (b), respectively, we obtain immediately:

- (a')  $p = 1, q \geq 1, r \geq \max\{2, p\}$  and  $s = 1$ ;
- (b')  $p \geq 1, q = 1, r \geq \max\{2, p\}$  and  $s = 1$ .

In case (c) we can prove the following:

**Proposition 3.5.** *If (c) holds, then  $p, q$  and  $s$  are bounded above; indeed, we have*

$$(c') \quad p \leq 2, q \leq 2, r \geq p \text{ and } s \leq 3.$$

Additionally, if  $s = 1$  then  $q \leq 2$ ; and if  $2 \leq s \leq 3$  then  $q = 1$ .

**Proof.** We can rewrite (3) in the form

$$\frac{1}{qs} + \frac{1}{ps} + \frac{1}{rq} \geq 1 + \frac{1}{pqrs}. \tag{5}$$

If  $q$  is not bounded, then by letting  $q \rightarrow +\infty$  we see that  $ps \leq 1$ , a contradiction to (c). Similarly,  $s$  is bounded, for otherwise  $rq = 1$ . Next, if  $p$  (and hence also  $r$ ) is unbounded, then by letting  $p, r \rightarrow +\infty$  we find that  $qs \leq 1$ , contradicting (c) again.

We now determine the upper bounds for  $p, q$  and  $s$ . First, if  $s = 1$  then from (5) we obtain

$$q \leq \frac{1}{r} + \frac{p}{p-1} \leq \frac{5}{2}.$$

Here the second inequality holds because  $p \geq 2$  (by (c)), while  $r \geq 2$  (by (4)). Thus  $q = 2$  (by (c)). Now from (4) and (3) (with  $q = 2$  and  $s = 1$ ) we find that  $p < 3$ , and hence that  $p = 2$ .

Secondly, if  $s \geq 2$ , we first use the relation

$$\frac{1}{qs} + \frac{1}{ps} + \frac{1}{rq} > 1 \tag{6}$$

to obtain

$$s < \frac{1 + \frac{1}{p}}{1 - \frac{1}{rq}} \leq 4.$$

Thus  $s \in \{2, 3\}$ , as required. From (6) we find that

$$q < \frac{1 + \frac{s}{r}}{s - \frac{1}{p}} < 2.$$

Thus  $q = 1$ . If  $s = 2$ , then from (4) and (3) (with  $q = 1, s = 2$ ), we find that  $p \leq 2$ . Similarly, if  $s = 3$  then we find that  $p = 1$ .

This completes the proof.  $\square$

#### 4. The behaviour of the least eigenvalue of extremal connected graphs

In this section, we establish several propositions which serve to prove the following theorem.

**Theorem 4.1.** *Let  $G$  be a graph whose least eigenvalue is minimal among the connected graphs of order  $n$  and size  $m$ . Then*



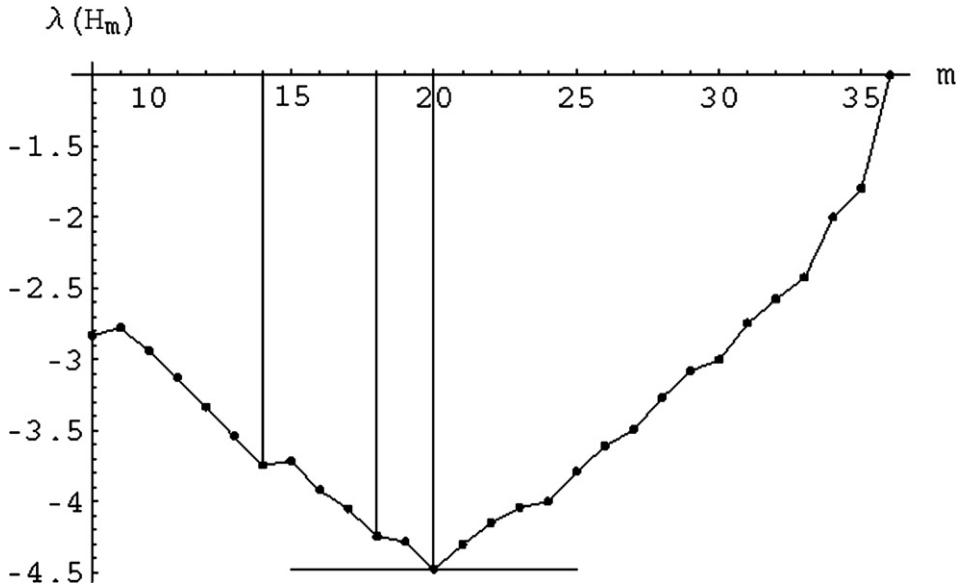


Fig. 2. The behavior of  $\rho(H_m)$  when  $n = 9$ .

- (i) if  $n - 1 \leq m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$  and  $m \neq t(n - t) + 1$  for all  $t \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1\}$ , then  $G$  is bipartite and hence a double nested graph;
- (ii) if  $m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$  and  $m = t(n - t) + 1$  for some  $t \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1\}$ , then  $G$  is either bipartite or the non-bipartite graph  $K_{t,n-t} + e$ , where  $e$  is an edge joining two vertices of degree  $\min\{t, n - t\}$  in  $K_{t,n-t}$ ;
- (iii) if  $\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil < m < \binom{n}{2}$  then  $G$  is non-bipartite and hence the join of two nested split graphs.

The bipartite graphs which appear in the case (ii) of Theorem 4.1 are more precisely described in Theorem 3.1(ii); see also Lemma 3.4 and Proposition 3.5.

We fix  $n$  and take  $H_m$  to be a graph whose least eigenvalue is minimal among the connected graphs of order  $n$  and size  $m$ . Fig. 2 shows the behaviour of  $\lambda = \lambda(H_m)$  for  $n = 9$  (obtained by direct calculation).

It was observed that, for  $m \leq 20$ ,  $H_m$  is always a bipartite graph; of course, for  $m > 20$  this is impossible. In the following proposition, we give a partial result which explains this phenomenon in a more general setting.

**Proposition 4.2.** *If  $m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$  and  $m \neq t(n - t) + 1$ , where  $t \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1\}$ , then  $H_m$  is a bipartite graph.*

**Proof.** Assume the contrary, and let  $H = H_m$  where  $m$  is the least integer for which the assertion is false. Let  $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$  be a unit eigenvector of  $H$  corresponding to  $\lambda(H)$ . From Proposition 1.2, we know that  $H$  contains an edge  $e = vw$  such that  $x_v x_w \geq 0$  and  $H - e$  is connected. Writing  $H^* = H - e$ , we have

$$\lambda(H^*) \leq \mathbf{x}^T A_{H^*} \mathbf{x} = \mathbf{x}^T A_H \mathbf{x} - 2x_v x_w \leq \mathbf{x}^T A_H \mathbf{x} = \lambda(H). \tag{7}$$

Now  $H_{m-1}$  is bipartite (by the choice of  $m$ ), and so we have

$$\lambda(G_{m-1}) = \lambda(H_{m-1}) \leq \lambda(H^*) \leq \lambda(H) \leq \lambda(G_m).$$

On the other hand, since  $m - 1 \geq s(n - s) + 1$ , we have  $\lambda(G_m) < \lambda(G_{m-1})$  by Lemma 3.2. This contradiction completes the proof.  $\square$

**Remark.** Note that the arguments in the above proof cannot always be used when  $m = t(n - t) + 1$  for some  $t$ , since then we may have  $\lambda(G_{m-1}) < \lambda(G_m)$  (see Lemma 3.4).

When  $n = 9$ , we can see that, for  $m > 20$ ,  $\lambda(H_m)$  increases strictly with  $m$  (up to  $-1$ ). This property is easily established in the general case:

**Proposition 4.3.** *For fixed  $n$ , and for  $m > \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ ,  $\lambda(H_m)$  increases strictly with  $m$  (to a maximum of  $-1$ ).*

**Proof.** We use the notation of Proposition 4.2, with  $H = H_m$ ,  $H^* = H - e$ ,  $e = vw$  and  $\mathbf{x}$  a unit eigenvector of  $H$  corresponding to  $\lambda$ . By Proposition 1.2 we may choose  $v, w$  such that  $x_v x_w \geq 0$  and  $x_v \neq 0$ . Now Eq. (7) holds, and we deduce that  $\lambda(H^*) \leq \lambda(H)$ . If  $\lambda(H^*) = \lambda(H)$  then  $\mathbf{x}$  is an eigenvector of  $H^*$  corresponding to  $\lambda$ ; but then the eigenvalue equations for  $w$  in  $H$  and  $H^*$  are inconsistent since  $x_v \neq 0$ . Thus  $\lambda(H^*) < \lambda(H)$ , and since  $\lambda(H_{m-1}) \leq \lambda(H^*)$ , the proof is complete.  $\square$

**Remark.** Let  $\hat{H}_m$  be a graph whose least eigenvalue is minimal among the connected non-bipartite graphs of order  $n$  and size  $m$ . If  $n$  is fixed and  $m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$  then  $\lambda(\hat{H}_m)$  does not necessarily increase with  $m$ .

Finally, we resolve the situation not covered by Proposition 4.2.

**Proposition 4.4.** *If  $m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$  and  $H_m$  is a non-bipartite graph, then  $m = t(n - t) + 1$  for some  $t \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1\}$  and  $H_m = K_{t, n-t} + e$ , where  $e$  is an edge joining two vertices of degree  $\min\{t, n - t\}$  in  $K_{t, n-t}$ .*

**Proof.** First, by Proposition 4.2 we have  $m = t(n - t) + 1$  for some  $t \in \{1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1\}$ . On the other hand, from Theorem 1.1 we know that  $H_m$  has a complete bipartite graph  $B = K_{u, n-u}$  ( $u \leq \lfloor \frac{n}{2} \rfloor$ ) as a proper spanning subgraph. Thus  $u \leq t$ , and it suffices to show that  $u = t$ . We suppose by way of contradiction that  $u < t$ .

Let  $H = H_m$ , and let  $\mathbf{x}$  be a unit eigenvector for  $\lambda(H)$ . Then we have

$$\lambda(H) = \mathbf{x}^T A_H \mathbf{x} = 2 \sum_{vw \in E_H} x_v x_w \geq 2 \sum_{vw \in E_B} x_v x_w \geq \lambda(B).$$

Now consider a graph  $K = K_{t, n-t} + e$ , where  $e$  is an edge joining two vertices in a colour class. We obtain the contradiction  $\lambda(K) < \lambda(H)$  by showing that  $\lambda(K) < \lambda(B)$ . Note that  $\lambda(B) \geq -\sqrt{c}$  where  $c = (t - 1)(n - t + 1)$ .

First we compute the spectrum of a graph  $G = K_{a,b} + e$ , where  $e$  is added to the colour class of size  $b$ . Counting the number of duplicate and co-duplicate vertices of  $G$ , we see that at least

$a + b - 3$  eigenvalues are equal to 0 or  $-1$ . On the other hand, if  $b > 2$ , three eigenvalues can be determined from the divisor with adjacency matrix

$$A_D = \begin{pmatrix} 0 & b - 2 & 2 \\ a & 0 & 0 \\ a & 0 & 1 \end{pmatrix}.$$

Thus the three remaining eigenvalues are the solutions of  $f(x) = 0$ , where

$$f(x) = x^3 - x^2 - abx + a(b - 2).$$

If  $b = 2$  then  $A_D = \begin{pmatrix} 0 & 2 \\ a & 1 \end{pmatrix}$ , and again the least eigenvalue is a solution of  $f(x) = 0$ .

Taking  $a = t, b = n - t$ , we have

$$f(-\sqrt{c}) = \sqrt{c}(n - 2t + 1) + (n - 4t + 1) > (t - 1)(n - 2t + 1) + (n - 4t + 1) \geq 0.$$

Hence  $\lambda(K) < -\sqrt{c} \leq \lambda(B)$ , and so  $\lambda(K) < \lambda(H)$  as required.

Finally, suppose that  $a > b$ . If we interchange  $a$  and  $b$  above,  $f(x)$  is replaced by  $g(x)$ , where  $g(x) = f(x) + 2(a - b)$ . Since  $g(x) > f(x)$ , the smallest root of  $g(x)$  is less than the smallest root of  $f(x)$ . Accordingly,  $\lambda(K)$  is minimal when  $e$  joins two vertices of smaller degrees.

This completes the proof.  $\square$

**Remark.** We give an example due to F. Marić which illustrates Proposition 4.4. If  $n = 12$  and  $m = 21$  then  $H_m = K_{2,10} + e$ , where  $e$  is an edge joining two vertices of degree 2 in  $K_{2,10}$ . Actually, now  $\lambda(H_m) = -4.38835\dots$ , while any connected bipartite graph of order 12 and size 21 has all eigenvalues greater than  $-4.37228\dots$ , as required. Among all graphs  $G$  of order 12 and size 21 (not necessarily connected), the minimal value of  $\lambda(G)$  is not attained by  $H_{21}$  because  $\lambda(K_{3,7} \dot{\cup} 2K_1) = -\sqrt{21} = -4.58275\dots$

In view of Theorem 1.1 and Propositions 4.2, 4.4, the proof of Theorem 4.1 clearly follows.

**Remark.** Let  $\mathcal{G}(n, m)$  be the set of graphs of order  $n$  and size  $m$ , and define

$$f(n, m) = \min\{\lambda(G) : G \in \mathcal{G}(n, m)\},$$

$$g(n, m) = \min\{\lambda(G) : G \in \mathcal{G}(n, m) \text{ and } G \text{ is connected}\}.$$

We noted in [1] that  $f(n, m) = \min\{g(k, m) : k \leq n \text{ and } \mathcal{G}(k, m) \text{ contains at least one connected graph}\}$ . Since  $k - 1 \leq m \leq k(k - 1)/2$ , we have

$$\frac{1}{2}(1 + \sqrt{1 + 8m}) \leq k \leq \min\{n, m + 1\}.$$

To find the value of  $k$  for which the minimum of  $g(k, m)$  is attained, we need to know the behaviour of  $\min\{\lambda(G) : G \in \mathcal{G}(k, m)\}$  as a function of  $k$  when  $m$  is constant. In principle, this can be deduced from Theorem 4.1 but we do not attempt an explicit formulation.

**Acknowledgement**

The authors are grateful to Filip Marić for undertaking some calculations used in the preparation of this paper.

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