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On Graphs with Exactly Three Q-main Eigenvalues

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Abstract. For a simple graph G, the Q-eigenvalues are the eigenvalues of the signless Laplacian matrix Q of G. A Q-eigenvalue is said to be a Q-main eigenvalue if it admits a corresponding eigenvector non orthogonal to the all-one vector, or alternatively if the sum of its component entries is non-zero. In the literature the trees, unicyclic, bicyclic and tricyclic graphs with exactly two Q-main eigenvalues have been recently identified. In this paper we continue these investigations by identifying the trees with exactly three Q-main eigenvalues, where one of them is zero.

1. Introduction

All graphs considered here are simple, undirected and finite. Let $G = G(V(G), E(G))$ be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. For a graph G the order is $|V(G)| = n$ and the size is $|E(G)| = m$; by $\deg(v_i) = d_i$ we denote the degree of the vertex v_i. The cyclomatic number ω of G is defined as $m - n + t$ where t is the number of connected components of G. If G is a connected graph, then for $\omega(G)$ equal to 0, 1, 2 and 3, G is said to be a tree, unicyclic, bicyclic and tricyclic graph, respectively. In Spectral graph Theory, the graphs are studied by means of the eigenvalues of some prescribed graph matrix $M = M(G)$. The M-polynomial of G is defined as $\det(\lambda I - M)$, where I is the identity matrix. The roots of the M-polynomial are the M-eigenvalues and the M-spectrum, denoted also by $\mathrm{Spec}_M(G)$, of G is a multiset consisting of the M-eigenvalues. A M-eigenvalue λ is said to be M-main if it admits an eigenvector $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ non orthogonal to the all-one vector $\mathbf{j}$, that is, $\sum_{i=1}^{n} x_i \neq 0$.

The most common graph matrix is the adjacency matrix defined as the $n \times n$ matrix $A(G) = [a_{ij}]$ where $a_{ij} = 1$ if v_i is adjacent to v_j, and $a_{ij} = 0$ otherwise. Another graph matrix of great interest is $Q(G) = A(G) + D(G)$, where $D(G) = \mathrm{diag}(d_1, d_2, \ldots, d_n)$, known as the signless Laplacian (or, quasi-Laplacian) of G. For general results on graphs spectra and definitions not given here, we refer the reader to [1]; for basic result on the signless Laplacian matrix, we refer the reader to [3].

In this paper we focus our attention to the main eigenvalues associated to the signless Laplacian of graphs. Note that the main eigenvalues have been largely studied in the literature, since relevant structural properties are related to such eigenvalues, for example the A-main eigenvalues are related to the number of walks. Hence studying the so-called main spectrum, namely the multiset of the main eigenvalues, has attracted the attention of many researchers, and in the years this problem has become one of the most

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attractive studies in the field of the algebraic graph theory. For some historical important papers on the A-main eigenvalues, we refer the reader to see [2, 5], while we refer to see [13] for a survey collecting many relevant results on the A-main eigenvalues. More recently, Hou and Zhou characterized all the trees with exactly two A-main eigenvalues [9]. One year later, Nikiforov showed that G is harmonic and irregular if and only if G has two A-main eigenvalues, one being zero and the other one non-zero. Recall that a graph G is harmonic if the degree vector $\mathbf{d} = (d_1, d_2, \ldots, d_n) = A\mathbf{j}$ is an A-eigenvector (see [12], for example). Later, the unicyclic, bicyclic and tricyclic graphs with exactly two A-main eigenvalues were characterized and classified in [10, 11].

The main eigenvalues have been considered in the context of signless Laplacian matrix, and similar studies to the adjacency case have been conducted for the matrix Q. For example, graphs with two Q-main eigenvalues are considered in [6–8]. Here, we consider the connected graphs with exactly three Q-main eigenvalues, and we give a necessary and sufficient condition for graphs to have exactly three Q-main eigenvalues. Recall that Q is a positive semi-definite matrix, and 0 appears as an eigenvalue of multiplicity k if and only if the graph has k bipartite components. Therefore, we identify all the trees with q_1, q_2 and $q_3 = 0$ as Q-main eigenvalues and we show that there are only two kinds of such trees.

2. Preliminaries

In this section we give some further definitions and results useful for the remainder of the paper.

In the signless Laplacian theory, the notion of semi-edge walk replaces that of ordinary walks. The difference is that while traversing an edge one can decide to go back (so the end vertices are repeated), which is equivalent to have a loop (cf. Figure 1).

Definition 2.1 ([3]). *A semi-edge walk of length k in an undirected graph G is an alternating sequence $v_1, e_1, v_2, \ldots, e_k, v_{k+1}$ of vertices $v_1, v_2, \ldots, v_{k+1}$ and edges $e_1, e_2, \ldots, e_k$ that for any $i = 1, 2, \ldots, k$ the vertices v_i and v_{i+1} are end-vertices (not necessarily distinct) of the edge e_i.*

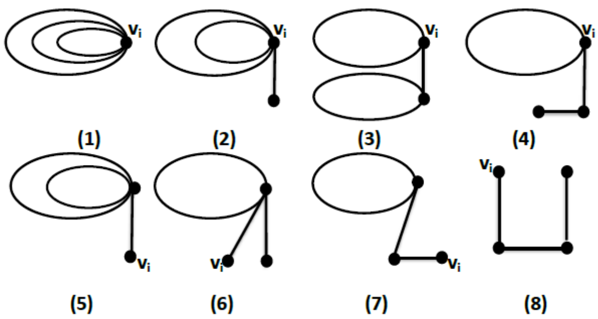

Figure 1: Semi-edge walks of length 3 that start from v_i.

In the following theorem we synthesize some information about Q, its entries and the Q-main eigenvalues. Also, it characterizes all the graphs with exactly one Q-main eigenvalue.

Theorem 2.2. *Let G be a graph with Q as its signless Laplacian matrix, then:*

(a) (Perron-Ferobenius Theorem) For a non-negative irreducible square matrix the spectral radius is a simple eigenvalue and a corresponding eigenvector can be taken with positive entries.

(b) [3] The (i,j)-entry of the matrix Q^k is equal to the number of semi-edge walks of length k starting at vertex v_i and terminating at vertex v_j.

(c) [3] G has exactly one Q-main eigenvalues if and only if G is regular.

(d) [6] If G has exactly s Q-main eigenvalues q_k for $k = 1, 2, \ldots, s$ then $[\prod_{k=1,k\neq i}^{s}(Q - q_k I)]\ \mathbf{j}$ is an eigenvector corresponding to q_i for $i = 1, 2, \ldots, s$. In particular, $[\prod_{k=1}^{s}(Q - q_k I)]\ \mathbf{j} = 0$.

(e) [6] *G has exactly s Q-eigenvalues* q_k *for* $k = 1, 2, \ldots, s$ *if and only if the vectors* $\mathbf{j}, Q\mathbf{j}, \ldots, Q^{s-1}\mathbf{j}$ *are linearly independant and* $[\prod_{k=1}^{s}(Q - q_k I)]\ \mathbf{j} = 0$.

In [6, 8] all the graphs with exactly two Q-main eigenvalues are characterized.

Theorem 2.3 ([6]). *A graph G has exactly two Q-main eigenvalues if and only if there exists a unique pair of integers a and b such that for any* $v \in V(G)$ *we have* $s(v) = ad(v) + b - d^2(v)$ *where* $s(v) = \sum_{u \in N(v)} d(u)$.

Theorem 2.4. *Let G be a connected bipartite graph with bi-partion* V_1 *and* V_2 *such that* V_1 *and* V_2 *has* n_1 *and* n_2 *members, respectively. Then* 0 *is a Q-main eigenvalue of G if and only if* $n_1 \neq n_2$.

Proof. It is well known that $Q(G) = RR^{\top}$, where R is the vertex-edge incident matrix of G. Recall that the multiplicity of 0 counts the number of bipartite components of G, so from G being bipartite (and connected) we have that 0 is a (simple) Q-eigenvalue of G. Now, let X be an eigenvector corresponding to 0. Thus $QX = 0$ if and only if $R^t X = 0$ if and only if $x_i = -x_j$ for every edges due to G being bipartite. Without loss of generality, we can ordered the entries of X as follows:

$$X = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

such that x_1 corresponds to vertices of V_1 and x_2 corresponds to vertices of V_2. By linearity we can assign $x_1 = 1$ and $x_2 = -1$. Hence $\sum_{i=1}^{n} x_i = 0$ if and only if $n_1 = n_2$. Evidently, 0 is a Q-main eigenvalue of G if and only if $n_1 \neq n_2$. This ends the proof. □

3. Graphs with Three Q-main Eigenvalues

If v_i is an arbitrary vertex of G, then there are 8 cases for semi-edge walks of length 3 that start at v_i as shown in Figure 1. Consider first Case (1), the number of different choices of the outer circle is equal to the number of neighbors of v_i, that is $d(v_i)$. Similarly, there are $d(v_i)$ choices for the second and $d(v_i)$ choices for the third circle. So there are in total $d^3(v_i)$ different semi-edge walks from v_i from Case (1), by the Counting Principle. The other cases can be similarly counted.

We synthesize the number of length 3 semi-edge walks starting from a vertex in the table below:

Cases	number of semi-edge walks
(1)	$d^3(v_i)$
(2)	$d^3(v_i)$
(3)	$d(v_i) \sum_{u \in N(v_i)} d(u)$
(4)	$d(v_i) \sum_{u \in N(v_i)} d(u)$
(5)	$\sum_{u \in N(v_i)} d^2(u)$
(6)	$\sum_{u \in N(v_i)} d^2(u)$
(7)	$d^2(v_i) + \sum_{u \in N(v_i)} \sum_{w \in N(u)/v_i} d(w)$
(8)	$d^2(v_i) + \sum_{u \in N(v_i)} \sum_{w \in N(u)/v_i} d(w)$

TABLE 1: The number of semi-edge walks of length 3 that start at v_i.

We are ready to state the main theorem about all graphs with exactly three Q-main eigenvalues.

Theorem 3.1. *A graph G has exactly three Q-main eigenvalues if and only if there exist unique nonnegative integers a, b and c such that for every $v \in V(G)$,*

$$d^3(v) + d^2(v) + s(v)d(v) + s'(v) + s''(v) = a(s(v) + d^2(v)) - bd(v) + c, \tag{1}$$

where $s(v) = \sum_{u\in N(v)} d(u)$, $s'(v) = \sum_{u\in N(v)} d^2(v)$ and $s''(v) = \sum_{u\in N(v)} \sum_{w\in N(u)/v} d(w)$.

Proof. If G has exactly three Q-main eigenvalues q_1, q_2 and q_3, then $(Q-q_1I)(Q-q_2I)(Q-q_3I)\mathbf{j} = 0$ by Theorem 2.2. So,

$$Q^3\mathbf{j} = (q_1 + q_2 + q_3)Q^2\mathbf{j} - (q_1q_2 + q_1q_3 + q_2q_3)Q\mathbf{j} + (q_1q_2q_3)\mathbf{j}. \tag{2}$$

By Theorem 2.2, we have that $Q^3\mathbf{j}$ is the vector whose i-th entry is the number of semi-edge walks in G of length 3 that start at v_i. By combining the computation of these semi-edge walks from Table 1 and (2), for every vertex v_i, we have:

$$\begin{aligned} d^3(v_i) + d^2(v_i) + s(v_i)d(v_i) + s'(v_i) + s''(v_i) &= (q_1 + q_2 + q_3)(s(v_i) + d^2(v_i)) + \\ &\quad -(q_1q_2 + q_1q_3 + q_2q_3)(d(v)) + \frac{q_1q_2q_3}{2}. \end{aligned} \tag{3}$$

Set $a = q_1 + q_2 + q_3$, $b = q_1q_2 + q_1q_3 + q_2q_3$ and $2c = q_1q_2q_3$. We have the following result by (3),

$$d^3(v_i) + d^2(v_i) + s(v_i)d(v_i) + s'(v_i) + s''(v_i) = a(s(v_i) + d^2(v_i)) - bd(v_i) + c, \tag{4}$$

a, b and c may be viewed as the unique solution of the linear equation (2) of integer coefficients because as previously mentioned, the (i,j)-entry of Q^k is the number of semi-edge walks of lenght k starting at v_i and ending at v_j. So $Q^k\mathbf{j}$ is a vector whoes i-th entry is the number of semi-edge walks of lenght k starting at v_i. Therefore the equation (2) essentially is a system of linear equations of integer cofficients of the form:

$$m_ix + n_iy + z = p_i,$$

where p_i, m_i, n_i are respectively the number of semi-edge walks of lenght 3,2,1 starting at v_i for $i = 1, ..., n$. The coefficient matrix of this system has $Q^2\mathbf{j}$, $Q\mathbf{j}$ and $\mathbf{j}$ as it's columns. These columns are linearly independant by Theorem 2.2. Thus the determinant of the coefficient matrix is non-zero which means the system has a unique solution (a, b, c). So a, b and c must be rational numbers. Since the eigenvalues q_1, q_2 and q_3 are algebraic integers and the set of all algebraic integers is a ring, therefore a, b and c are algebraic integers. But every rational algebraic integer is an integer, so a, b and c are integers and of course nonnegative .
If there exist unique nonnegative numbers a, b and c such that (4) holds, then $Q^3\mathbf{j} = aQ^2\mathbf{j} - bQ\mathbf{j} + c\mathbf{j}$. We know that $\mathbf{j}$, $Q\mathbf{j}$ are linearly independant otherwise, G is a regular graph and has one Q-main eigenvalue which is a contradiction.

Now let $Q^2\mathbf{j} = pQ\mathbf{j} + q\mathbf{j}$ for some real numbers p and q. Then,

$$Q^3\mathbf{j} = Q(pQ\mathbf{j} + q\mathbf{j}) = pQ^2\mathbf{j} + qQ\mathbf{j} = p(pQ\mathbf{j} + q\mathbf{j}) + q\mathbf{j} = p^2Q\mathbf{j} + pq\mathbf{j}$$

and by (3),

$$Q^3\mathbf{j} = aQ^2\mathbf{j} - bQ\mathbf{j} + c\mathbf{j} = a(pQ\mathbf{j} + q\mathbf{j}) - bQ\mathbf{j} + c\mathbf{j} = (ap - b)Q\mathbf{j} + (aq + c)\mathbf{j}.$$

So $\mathbf{j}$, $Q\mathbf{j}$ and $Q^2\mathbf{j}$ are linearly independant, which implies that G has exactly three Q-main eigenvalues by Theorem 2.2 (e). This completes the proof. □

4. Trees with Exactly Three Q-main Eigenvalues

Let T be a tree with exactly three Q-main eigenvalues $q_1 = 0$, q_2 and q_3. If $P_T = v_0 v_1 \dots v_k$ is the longest pendant path of T as defined in [6], then by applying (1) for v_0, we have:

$$d(v_2) = a(1 + d(v_1)) - d^2(v_1) - 2d(v_1) - b. \tag{5}$$

Note that every neighbor of v_1 other than v_2 are pendant vertices, because otherwise T has the longest pendant path longer than P_T. We want to characterize all the trees with this property. Thus we need to prove two following Lemmas first.

Lemma 4.1. *Let T be a tree with the above assumptions and $P_T = v_0 v_1 \dots v_k$ is the longest pendant path of T. Then $d(v_2) = 2$.*

Proof. On the contrary, let $d(v_2) > 2$. So $a(1 + d(v_1)) - d^2(v_1) - 2d(v_1) - b > 2$ by (5). Solving this inequality in terms of $d(v_1)$ leads to:

$$\frac{2 - a + \sqrt{\Delta}}{-2} < d(v_1) < \frac{2 - a - \sqrt{\Delta}}{-2}, \tag{6}$$

where $\Delta = a^2 - 4b - 4$. We claim that if v_2 has an arbitrary neighbor v_1' other than v_1 and v_3, then either $d(v_1') = 1$ or $d(v_1') = d(v_1)$. Let $d(v_1') \neq 1$, so v_1' has at least one neighbor v_0' other than v_2. Now $P_T' = v_0' v_1' v_2 ... v_n$ is the longest pendant path for T. By using (1) for v_0', we get:

$$d(v_2) = a(1 + d(v_1')) - d^2(v_1') - 2d(v_1') - b. \tag{7}$$

Comparing equations (5) and (7) gives us:

$$(d(v_1) - d(v_1'))(a - 2 - d(v_1) - d(v_1')) = 0.$$

So $d(v_1) = d(v_1')$ or $d(v_1) + d(v_1') = a - 2$ or both of them are established at the same time. If $d(v_1) = d(v_1')$, there is nothing left to prove. So let $d(v_1) \neq d(v_1')$. Then by using (1) for v_1 and v_1', subtracting them from each other and again using of (5) and (7), we have:

$$d(v_2) = a - b - 1 + d(v_1)d(v_1'),$$

and then,

$$-d^2(v_1) + (a - 2 - d(v_1'))d(v_1) + 1 = 0,$$

by (5). This equation may be viewed as a quadratic equation of $d(v_1)$. The discriminant of this is $(a - 2 - d(v_1'))^2 + 4$, which has a perfect square value only if $d(v_1') = a - 2$, and so $d(v_1) = 1$ which is impossible. Thus $d(v_1) = d(v_1')$. Therefore there are three modes for every neighbor of v_2 other than v_1 and v_3 as in the following:

(1) all of them are pendant vertices;

(2) all of them have degree equal to $d(v_1)$;

(3) there is at least one neighbor of degree 1 and one neighbor with equal degree to $d(v_1)$.

Assume that (1) occurs, and u be a pendant neighbor of v_2. We have:

$$d(v_3) = a(1 + d(v_2)) - b + 1 - 2d(v_2) - d^2(v_2) - d(v_1), \tag{8}$$

by using (1) for u. Similarly by using (1) for v_1 and applying (8), the quadratic equation in terms of $d(v_1)$ is obtained as follows:

$$d^2(v_1) + (1 - b - a)d(v_1) + a - 2 = 0,$$

and by solving this equation, we get:

$$d(v_1) = \frac{a + b - 1 + \sqrt{\Delta'}}{2} \text{ or } d(v_1) = \frac{a + b - 1 - \sqrt{\Delta'}}{2},$$

where $\Delta' = 9 + a^2 + b^2 + 2ab - 6a - 2b$.

Now let $d(v_1) = \frac{a + b - 1 + \sqrt{\Delta'}}{2}$. If $d(v_1) \in (\frac{2 - a + \sqrt{\Delta}}{-2}, \frac{2 - a - \sqrt{\Delta}}{-2})$ as in (6), then,

$$\frac{2 - a + \sqrt{\Delta}}{-2} < \frac{a + b - 1 + \sqrt{\Delta'}}{2} < \frac{2 - a - \sqrt{\Delta}}{-2}.$$

So, $1 - \sqrt{\Delta} < -b - \sqrt{\Delta'} < 1 + \sqrt{\Delta}$. Consider the two left-hand sides of these inequalities, we have,

$$b^2 + 9 + a^2 + b^2 + 2ab - 6a - 2b + 2b\sqrt{\Delta'} < 1 + a^2 - 4b - 4 - 2\sqrt{\Delta}.$$

Thus, $2b^2 + 12 + 2ab - 6a - 2b + 2b\sqrt{\Delta'} < -2\sqrt{\Delta} < 0$, which leads to $b^2 + 6 + ab - 3a - b < -b\sqrt{\Delta'} < 0$. So $b^2 + 6 + ab - 3a - b$ always has a negative value or we can say that $(b - 3)a < b - b^2 - 6$. But if $b > 3$, then $a < -b - 2 - \frac{12}{b - 3} < 0$ which is in contradiction with a being positive. So $b \le 3$. If $b = 1$, Then $\Delta' = a^2 - 4a + 8$, which has a perfect square value only if $a = 2$. Then $d(v_1) = 2$ and subsequently $d(v_2) < 0$ by (5), a contradiction. Similarly if $b = 2$, then $a = 2$, $d(v_1) = 3$ and then $d(v_2) < 0$, which is a impossible too. Also $b = 3$ leads to a same contradiction too. So $d(v_1) = \frac{a + b - 1 - \sqrt{\Delta'}}{2}$. On the other hand we know that,

$$\Delta' = (a + b)^2 + 9 - 6a - 2b > (a + b)^2 - 6a - 2b > (a + b)^2 - 6a - 6b = (a + b)^2 - 6(a + b) = (a + b)(a + b - 6).$$

If $a + b \ge 6$, then $\Delta' > (a + b - 6)^2$ and so $d(v_1) < \frac{5}{2}$. Thus $d(v_1) = 2$ and so $a + 2b = 4$, a contradiction. Therefore $a + b < 6$ and all the possible cases for a and b are: $\{a = 1, b = 1, 2, 3, 4\}$, $\{a = 2, b = 1, 2, 3\}$, $\{a = 3, b = 1, 2\}$ and $\{a = 4, b = 1\}$. But if $a = 1, 3, 4$ then Δ' never has a perfect square value. So the only possible case is $\{a = 2, b = 1, 2, 3\}$. In this case Δ' must be $4, 9, 16$, respectively and then $d(v_1)$ is 0 or $\frac{1}{2}$ which is impossible too. In this way (1) is rejected. Similarly (2) is rejected.

Now let (3) occurs and v_2 has $u_1, u_2, ..., u_x$ pendant neighbors and $v_1, v_2, ..., v_y$ neighbors other than v_1 and v_3 with $d(v_i) = d(v_1)$ for $i = 1, ..., y$. So by using (1) for u_1, we have:

$$d(v_3) = a(x + y + 3) - b - 3 - 2x - y - (x + y + 2)^2 - (y + 1)d(v_1), \tag{9}$$

and again by using (1) for v_1, and replace (9) in it, we get,

$$d(v_1) = -4 - x + 2a - b - y. \tag{10}$$

On the other hand $d(v_1) \geq 2$ means,

$$d(v_2) \leq 2a - b, \tag{11}$$

or $-d^2(v_1) + (a-2)d(v_1) - a \leq 0$ by (5). Let $a \geq 8$. By solving above inequality in term of $d(v_1)$, one of two following conditions occurs:

$$d(v_1) < \frac{2-a+\sqrt{\delta'}}{-2} \text{ or } d(v_1) > \frac{2-a-\sqrt{\delta'}}{-2},$$

where $\delta' = a^2 - 8a + 4$. We always have $\frac{2-a+\sqrt{\Delta}}{-2} < \frac{2-a+\sqrt{\delta'}}{-2}$. So if $d(v_1) < \frac{2-a+\sqrt{\delta'}}{-2}$, then $d(v_1)$ must be in the interval $(\frac{2-a+\sqrt{\Delta}}{-2}, \frac{2-a+\sqrt{\delta'}}{-2})$, by (6). But $\delta' > a^2 - 8a = a(a-8) > (a-8)^2$ and subsequently,

$$d(v_1) < \frac{2-a+\sqrt{\delta'}}{-2} < \frac{2-a+a-8}{-2} = 3,$$

which means $d(v_1) = 2$. So $2a - b = x + y + 6 = d(v_2) + 4$, by (10) and then $d(v_2) = 2a - b - 4$. On the other side $d(v_2) = 3a - 8 - b$ by (5). By comparing these two equations, we obtain $a = 4$ which is a contradiction.

Now let $d(v_1) > \frac{2-a-\sqrt{\delta'}}{-2}$. By the same argument, we see that $d(v_1)$ belongs to the interval $(\frac{2-a-\sqrt{\delta'}}{-2}, \frac{2-a-\sqrt{\Delta}}{-2})$, and so,

$$a-5 < \frac{2-a-a-8}{-2} < \frac{2-a-\sqrt{\delta'}}{-2} < d(v_1) < \frac{2-a-\sqrt{\Delta}}{-2} < \frac{2-a-a}{-2} = a-1$$

Therefore $a - 5 < d(v_1) < a - 1$. If $d(v_1) = a - 4$, then $d(v_2) = 3a - b - 8$ by (5). But $a \geq 8$, so $d(v_2) > 2a - b$. This is a contradiction with (11).

Now let $d(v_1) = a - 2$. So $d(v_2) = x + y + 2 = a - b$ by (5). If we use (1) for v_1, we have,

$$-a + ab - b^2 + 1 = d(u_1) + d(u_2) + \cdots + d(u_x) + d(v_1) + \ldots + d(v_y) + d(v_3).$$

But,

$$d(u_1) + d(u_2) + \cdots + d(u_x) + d(v_1) + \ldots + d(v_y) + d(v_3) > 1 + \cdots + 1 + d(v_1) + d(v_3) > a - b - 3 + d(v_1) + 1.$$

This means $-a + ab - b^2 + 1 > a - b - 4$ or equally $(3-b)(a-b-2) + 1 < 0$. If $b > 3$, then $d(v_2) = a - b < a - 3 = d(v_1) - 1$. So $8(1 + d(v_1)) - d^2(v_1) - 2d(v_1) - b \leq d(v_2) < d(v_1) - 1$ and then $-d^2(v_1) + 5d(v_1) - b + 9 < 0$. Now if $b \geq 16$, then,

$$2 < d(v_2) < a(1 + d(v_1)) - d^2(v_1) - 2d(v_1) - 16,$$

or equally $-d^2(v_1) - 2d(v_1) + a - 18 > 0$. By solving this inequality in terms of $d(v_1)$ we have,

$$-1-\frac{\sqrt{4a-28}}{2}<d(v_1)<-1+\frac{\sqrt{4a-28}}{2}.$$

But $4a-28<a(4a-28)<(2a-4)^2$, so,

$$-1-\frac{\sqrt{4a-28}}{2}<d(v_1)<-1+\frac{\sqrt{4a-28}}{2}<a-3,$$

which is a contradiction with $d(v_1)=a-2$. So $3<b<16$. By using (1) for v_1, we obtain:

$$(1+y)(a-1)-(b-1)(x+y+2)=0.$$

If $b=4$, then

$$-2a+ay-y-3a+12=0. \tag{12}$$

On the other hand $x+y+2=d(v_2)=a-b=a-4$ or $a=x+y+6$. So by replacing a in (12), $y^2+(x+3)y-2x-1=0$, a quadratic equation of y is obtained. Its discriminant has a perfect square value only if $x=2$. This leads to $y=\frac{3}{2}$ which is impossible. The case $4<b<16$ is rejected by the same way. Therefore $b\leq 3$ and $(3-b)(a-b-2)+1>0$, a contradiction too.
For $d(v_1)=a-3$ we can act similarly to the case $d(v_1)=a-2$, and we show that this must be rejected too.
Now Let $a\leq 7$. If $a=1,2$ then $d(v_2)<0$ by (5), which is impossible. If $a=3$ then $\Delta=5-4b\geq 9$, so $0<d(v_1)<2$ by (6). This means $d(v_1)=1$ which is impossible too. If $a=4$ then $\Delta\geq 16$ and so $d(v_1)=2$. This satisfied in (5) according to assumption if $b=1$ and subsequently $d(v_2)=3$. Now by using (1) for v_1 we get $s(v_2)=2$ which is never happen. In this way we can see that $a\leq 7$ leads to a contradiction. Therefore the proof is complete and $d(v_2)=2$. □

Lemma 4.2. *If T is a tree with exactly three Q-main eigenvalues 0, q_2 and q_3 and $P_T=v_0v_1...v_k$ is the longest pendant path of T, then $a-b=\pm 2$.*

Proof. On the contrary let $a-b\neq\pm 2$. By using of (5) and Lemma 4.1, we have $-d^2(v_1)+(a-2)d(v_1)+a-b=2$. By solving this equation in terms of $d(v_1)$ we get $d(v_1)=\frac{2-a\pm\sqrt{\Delta}}{-2}$, where $\Delta=a^2-4b-4$. Now if $a<5$, then $\Delta<21-4b$ and so $b\leq 5$. If $b=1$ then Δ has a perfect square value only if $a=3$, but this leads to $d(v_1)=0,1$ which is impossible. Similarly if $b=2$, then Δ has a perfect square value only if $a=4$ and this results $d(v_1)=0,1$ which is impossible too. The cases $b=3$ and $b=4$ give contradiction to a being less than 5. Finally if $b=5$, the only possible value for a is 5 and then $d(v_1)=2$. By using (1) for v_2, we have $d(v_4)=1$. So T is a path of length 4 which never has three Q-main eigenvalues. Thus $a>5$. We consider these possible cases for a and b and show that no one of these cases is happen:

(a) $a=b$;

(b) $a-b=1$ or -1;

(c) $a-b>2$;

(d) $a-b<-2$.

Assume (a) is true. Then $\Delta=(a-2)^2-8$ and it has a perfect square value only if $a=5$. But it leads to $d(v_1)=\frac{-3}{2}$ which is impossible. If $a-b=1$, then Δ has a perfect value only if $a=4$, which is a contradiction and if $a-b=-1$, then Δ has a perfect square value only if $a=6$. Then $b=7$ and subsequently $d(v_1)=6$.

Finally $d(v_2) < 0$ by (5), a contradiction too. So (b) is rejected.

Let (c) holds and $d(v_1) = \frac{2-a-\sqrt{\Delta}}{-2}$. We always have, $ad(v_1) - d^2(v_1) - 2d(v_1) < 0$ by (5) and previous Lemma. Then $d(v_1)(-d(v_1) + a - 2) < 0$ which leads to $d(v_1) > a - 2$. On the other side,

$$d(v_1) = \frac{2-a-\sqrt{\Delta}}{-2} < \frac{2-a-a}{-2} = a - 1.$$

So $a - 2 < d(v_1) < a - 1$, a contradiction. Also $d(v_1) = \frac{2-a+\sqrt{\Delta}}{-2}$ in (d) leads to a contradiction, as well. Now let $d(v_1) = \frac{2-a+\sqrt{\Delta}}{-2}$. we know that,

$$\Delta > a^2 - 4b^2 - 4 = a^2 - 4(b^2 + 1) > a^2 - 4(b^2 + 1 + 2b) = a^2 - 4(b + 1)^2 = (a - 2b - 2)(a + 2b + 2).$$

If $a - 2b - 2 > 0$, then $\Delta > (a - 2b - 2)^2$ and so $d(v_1) < \frac{2-a+a-2b-2}{-2} < a - 2$, and of course,

$$d(v_1) = \frac{2-a+\sqrt{\Delta}}{-2} > \frac{2-a-a}{-2} = a - 1,$$

this is a contradiction too. But if $a - 2b - 2 < 0$, then,

$$-d^2(v_1) + (a - 2)d(v_1) + b < 0,$$

by (5) and previous Lemma. By solving this equation in terms of $d(v_1)$, we have:

$$\frac{2-a+\sqrt{\Delta'}}{-2} < d(v_1) < \frac{2-a-\sqrt{\Delta'}}{-2},$$

where $\Delta' = (a - 2)^2 + 4b$. But $a - b > 2$, so $\Delta' < a^2 - 4 < a^2$. So,

$$d(v_1) < \frac{2-a\sqrt{\Delta'}}{-2} < \frac{2-a-a}{-2} = a - 1,$$

a contradiction. Also $d(v_1) = \frac{2-a-\sqrt{\Delta}}{-2}$ in (d) leads to a contradiction, as well. Therefore (c) and (d) do not happen. Hence, $a - b = \pm 2$.
□

Theorem 4.3. *If T is a tree with exactly three Q-main eigenvalues $q_1 = 0$, q_2 and q_3, then T is a tree with diameter 4 with $a = q_2 + q_3$ and $b = q_2 + q_3 - 2$ or T is a tree with diameter 6 with $a = 5$ and $b = 3$ as Fig. 2.*

Proof. Let T be a tree with three Q-main eigenvalues 0, q_2 and q_3 and let $P_T = v_0v_1...v_k$ be the longest pendant path of T. Then by using (1) for v_k we get:

$$d(v_{k-2}) = a(1 + d(v_{k-1})) - d^2(v_{k-1}) - 2d(v_{k-1}) - b. \quad (13)$$

Similar to the proof of Lemma 4.1 we can show that $d(v_{k-2}) = 2$. So we have $d(v_1) = d(v_{k-1})$ or $d(v_1)+d(v_{k-1}) = a - 2$ by subtracting (5) and (13). We can easily show that $d(v_1) = d(v_{k-1})$ as before. So $d(v_1) = d(v_{k-1})$. Assume first that $k = 4$, then $d(v_0) = d(v_4) = 1$, $d(v_1) = d(v_3)$ and $d(v_2) = 2$. Now if $a - b = -2$ then Δ has a perfect square value only if $a = 7$. Then $b = 9$ and $d(v_1) = 4$. So by using of (1) for v_1 we get $111 = 121$ which is a contradiction but if $a - b = 2$ then $d(v_1) = d(v_3) = a - 2$ by using of (1) for v_0. Thus we have a bunch of trees with exactly three Q-main eigenvalues $q_1 = 0$, q_2 and q_3 such that $a = q_2 + q_3$ and $b = q_2 + q_3 - 2$, cf. Fig. 2 (1).

Now let $k > 4$. First of all we want to show that $d(v_3) = a - 3 = 2$ for $k > 4$. Let $d(v_3) > 2$. Therefore v_3 has at least one neighbor like u other than v_2 and v_4. If $d(u) = 1$, then by using of (1) for u we get $s(v_3) = 3a - b - 7$. On the other hand by using of (1) for v_2 we get $s(v_3) = 4a - b - 10 - d(v_1)$. Therefore $d(v_1) = a - 3 = d(v_3)$. But $a - b = 2$ leads to $\Delta = (a - 2)^2$ and $d(v_1) = a - 2$ which is a contradiction. Therefore u has at least a neighbor like w other than v_3. We want to show that all of the neighbors of w have equal degree to $d(v_1)$. Let $d(w) \neq 1$. Every neighbors of w are pendant, because if they are not pendant, then there is a longest pendant path longer than P_T, a contradiction. So by use of (1) for an arbitrary neighbor of w, we have $d(u) = a(1 + d(w)) - d^2(w) - 2d(w) - b$. Similar to the proof of Lemma 4.1 we can show that $d(u) = 2$. So $a(1 + d(w)) - d^2(w) - 2d(w) - b = a(1 + d(v_1)) - d^2(v_1) - 2d(v_1) - b$ and quickly $d(w) = d(v_1)$. Now by using of (1) for v_3, we have $s(v_4) = -380a^2 + 733a - 361$ which always has negative value, a contradiction too. It is easy to see that $d(w) = 1$ leads to a contradiction. So $d(v_3) = 2, a = 5, b = 3$ and $d(v_1) = 3$ by Lemmas 4.1 and 4.2. So $d(v_2) = d(v_3) = 2$, $d(v_4) = 2$, $d(v_5) = 3$ and $d(v_6) = 1$ by using (1) for v_2, v_3 and v_4 respectively. Therefore $k = 6$, $q_2 + q_3 = 5$ and $q_2q_3 = 3$ and then $q_2 = 0.6972$ and $q_3 = 4.3028$. This tree is depicted in Fig. 2 (2). Therefore, all the trees with our desired property are classified. □

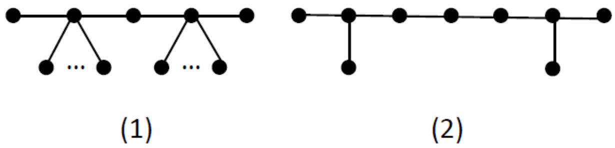

Figure 2: The trees with exactly three Q-main eigenvalues $q_1 = 0$, q_2 and q_3

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