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Towards a spectral theory of graphs based on the signless Laplacian, II ☆

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A B S T R A C T

A spectral graph theory is a theory in which graphs are studied by means of eigenvalues of a matrix M which is in a prescribed way defined for any graph. This theory is called *M-theory*. We outline a spectral theory of graphs based on the signless Laplacians Q and compare it with other spectral theories, in particular to those based on the adjacency matrix A and the Laplacian L. As demonstrated in the first part, the Q-theory can be constructed in part using various connections to other theories: equivalency with A-theory and L-theory for regular graphs, common features with L-theory for bipartite graphs, general analogies with A-theory and analogies with A-theory via line graphs and subdivision graphs. In this part, we introduce notions of enriched and restricted spectral theories and present results on integral graphs, enumeration of spanning trees, characterizations by eigenvalues, cospectral graphs and graph angles.

1. Introduction

This is the second part of our work with a common title. The first part [14] will be also referred in the sequel as Part I.

By a spectral graph theory we understand, in an informal sense, a theory in which graphs are studied by means of eigenvalues of a matrix M which is in a prescribed way defined for any graph. This theory is called *M-theory*. Hence, there are several spectral graph theories (for example, those based on the adjacency matrix, the Laplacian, etc.). In that sense, the title "Towards a spectral theory of graphs based

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on the signless Laplacian" indicates the intention to built such a spectral graph theory (the one which uses the signless Laplacian without explicit involvement of other graph matrices).

Recall that, given a graph, the matrix $Q = D + A$ is called the *signless Laplacian*, where A is the adjacency matrix and D is the diagonal matrix of vertex degrees.

We shall, in fact, outline a new spectral theory of graphs (based on the signless Laplacian Q). We shall call this theory the *Q-theory*.

Only recently has the signless Laplacian attracted the attention of researchers. As our bibliography shows, several papers on the signless Laplacian spectrum have been published since 2005 and we are now in position to summarize the development. In the first part of this paper we have mentioned 15 papers (in particular, [4,6,13,17–20,30,35,36,38–41,48], where the signless Laplacian is explicitly used) in addition to our basic papers [5,12,14]. In the meantime the following 11 papers [1,3,21–24,27,31,42,45,46] have been published or are in the process of publishing.

This paper is organized in a similar way as Part I. In Section 2, we give some more accounts to the considerations from the same section of Part I. Section 3 contains several comparisons of the effectiveness of solving various classes of problems within particular spectral theories with an emphasis on the performance of the Q-theory.

2. More on the fundamentals of the *Q*-theory

In Section 2 of Part I (see [14]) we have shown how the Q-theory can be composed using various connections to other theories: equivalency with A-theory and L-theory for regular graphs, common features with L-theory for bipartite graphs, general analogies with A-theory, analogies with A-theory via line graphs, and analogies with A-theory via subdivision graphs.

Here, after recalling some definitions (Section 2.1) and after extending the previous survey concerning bipartite graphs, the subdivision graphs, operations on graphs and inequalities for eigenvalues (Sections 2.2–2.5), we complete our description of the Q-theory by considering enriched and restricted spectral theories in 2.6. Some comments on the present stage of the theory are given in 2.7.

2.1. Recalling some definitions

We shall start with some definitions related to a general M-theory.

Let G be a simple graph with n vertices. The characteristic polynomial $\det(xI - M)$ of a real symmetric matrix M associated to G is called the *M-characteristic polynomial* (or *M-polynomial*) of G and is denoted by $M_G(x)$. The eigenvalues of M (i.e. the zeros of $\det(xI - M)$) and the spectrum of M (which consists of the n eigenvalues) are also called the *M-eigenvalues of G* and the *M-spectrum of G*, respectively. The M-eigenvalues of G are real because M is symmetric, and the largest eigenvalue is called the *M-index* of G.

Let A denote the adjacency matrix of a graph G. In view of the above notation the eigenvalues and the spectrum of A will be called the A-eigenvalues and the A-spectrum of G. The A-polynomial $A_G(x) = \det(xI - A)$ will be mostly denoted by $P_G(x)$.

Let $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ be the A-spectrum of G, where the eigenvalues are such that $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. The largest eigenvalue λ_1 is called the A-index of G.

The matrix $L = D - A$, known as the *Laplacian* of G, while the matrix $Q = D + A$ is called the *signless Laplacian* of G.

Following the adopted general notation, the polynomial $Q_G(x)$ will be called the *Q-polynomial* of G. The eigenvalues and the spectrum of Q will be called the *Q-eigenvalues* and the *Q-spectrum*, respectively.

Let $(q_1, q_2, \ldots, q_n)$ be the Q-spectrum of G, where the eigenvalues are such that $q_1 \geqslant q_2 \geqslant \cdots \geqslant q_n$. The largest eigenvalue q_1 is called the Q-index of G.

Together with some facts from the Q-theory we shall frequently consider in parallel the relevant facts from the A-theory and the L-theory as mostly developed spectral theories, just for making comparisons between these theories.

2.2. Bipartite graphs

For bipartite graphs we have $L_G(x) = Q_G(x)$ (cf. Proposition 2.3 of [12]). In this way, the Q-theory looks to be identical with the L-theory for bipartite graphs. However, the following remarks seem to be interesting.

Given the L-spectrum (or the Q-spectrum what is the same) of a tree, in the L-theory we can recognize from the spectrum that the graph in question is a tree (by establishing that the graph is connected and has the number of edges smaller by 1 than the number of vertices), while in the Q-theory we cannot be sure whether the graph is connected (which opens the possibility that in the case of non-connectedness it is not bipartite). Hence, for trees the L-theory is superior although in both theories trees have the same spectra.

Recall the second smallest L-eigenvalue is called the *algebraic connectivity* of a graph. This important graph parameter has been treated extensively in the literature. An interesting question arises when trying to establish an analogous quantity for the Q-spectrum. Since in bipartite graphs the two spectra coincide, one could think that the second smallest Q-eigenvalue plays the role of algebraic connectivity. However, in regular graphs the second largest A-eigenvalue λ_2 is mapped into the second smallest L-eigenvalue $r - \lambda_2$ and to the second largest Q-eigenvalue $q_2 = r + \lambda_2$. Hence, one should think that the second largest Q-eigenvalue plays the role of algebraic connectivity! The question remains whether q_2 really has in general the properties analogous to those of the algebraic connectivity.

2.3. Subdivision graphs

As noted in [13], the following formula appears implicitly in the literature (see e.g., [8, p. 63] and [47]):

$$P_{S(G)}(x) = x^{m-n} Q_G(x^2), \tag{1}$$

where G is a graph with n vertices and m edges, and $S(G)$ is the subdivision graph of G. We continue to exploit this link between the A-theory and Q-theory. In what follows we exploit the connection between indices of graphs based on the A and Q spectra; namely, we have that $\lambda_1(S(G)) = \sqrt{q_1(G)}$ (see (1)).

The A-indices of all graphs topologically equivalent (or homeomorphic) to some fixed graph, say G are examined in [25]. Since the A-index of $S(G)$ is greater than or equal to the infimum of the A-indices of the graphs as considered above, by using the relevant result from [25] (which is reproduced in [8, p. 79]), we arrive at:

Theorem 2.1. *Let d_i be the degree of the vertex i in a connected graph G having at least one vertex of degree greater than 2. Let f_i be the number of vertices of degree 1 adjacent to i. Then for any vertex i of degree greater than 2, the quantity $\left(a^{\frac{1}{2}} + a^{-\frac{1}{2}}\right)^2$, where $a = \frac{1}{2}\left(d_i - 2 + \sqrt{d_i^2 - 4f_i}\right)$, is a lower bound for the Q-index of G.*

For graphs with no vertices of degree 1 we have $f_i = 0$ for any i and so we arrive at the following corollary.

Corollary 1. *Let G be a connected graph without vertices of degree 1, with maximum degree Δ and the Q-index q_1. Then*

$$q_1 \geqslant \Delta + 1 + \frac{1}{\Delta - 1}.$$

Equality holds if and only if G is a cycle.

Equality cannot hold if $\Delta > 2$ since Q-eigenvalues should be either irrational numbers or integers. However, in this case q_1 could be arbitrarily close to the bound which follows from the considerations on limit points of the A-index of graphs which are the iterated subdivisions of some fixed graph.

The bound in the last corollary is an improvement for graphs without vertices of degree 1 of a known lower bound (see [13, Conjecture 4]): $q_1 \geqslant \Delta + 1$ with equality if and only if G is a star.

We next show that Theorem 6 from [26] also holds for Q-index. Our proof is based on Theorem 7 from [26].

Theorem 2.2. *Let u, v be the adjacent vertices of a connected graph G, both of degree at least two. Let $G(k, l)$ $(k, l \geqslant 0)$ be the graph obtained from G by attaching pendant paths of lengths k and l at u and v, respectively. If $k \geqslant l \geqslant 1$ then*

$$q_1(G(k, l)) > q_1(G(k + 1, l - 1)).$$

Proof. Let $S_1 = S(G(k, l))$ and $S_2 = S(G(k + 1, l - 1))$. Then u and v are in the latter two graphs the vertices of degree at least three and at distance 2, having pendant paths at u and v of lengths $2k$ and $2l$, respectively (in S_1), and of lengths $2k + 2$ and $2l - 2$, respectively (in S_2). Observe also that S_2 can be obtained from S_1 by relocating the last two edges from the path of length $2l$ to the path of length $2k$. But then, see Theorem 7 [26], we have that

$$\lambda_1(S_1) > \lambda_1(S_2)$$

and consequently

$$q_1(G(k, l)) > q_1(G(k + 1, l - 1)),$$

as required. $\square$

Similarly, we can use a result for θ-graphs from [34] to get an analogous result for the Q-index. Let $\Theta(m_1, m_2, \ldots, m_k)$ be graph obtained from k paths of lengths $m_1, m_2, \ldots, m_k$, by identifying the end vertices of each path with two fixed vertices. (Note, without loss of generality we can assume that $m_1 \geqslant m_2 \geqslant \cdots \geqslant m_{k-1} \geqslant 2$; in contrast $m_k \geqslant 1$.) Now we have:

Theorem 2.3. *Let $\Theta(m_1, m_2, \ldots, m_k)$ be a θ-graph defined as above, and let $\Theta(m'_1, m'_2, \ldots, m'_k)$ be a θ-graph obtained from the former one by taking $m'_i = m_i + 1$, $m'_j = m_j - 1$ and $m'_p = m_p$ for $p \neq i, j$. Then, whenever $m_j - m_i > 1$, we have*

$$q_1(\Theta(m'_1, m'_2, \ldots, m'_k)) > q_1(\Theta(m_1, m_2, \ldots, m_k)).$$

Proof. Let $G = \Theta(m_1, m_2, \ldots, m_k)$ and $G\prime = \Theta(m'_1, m'_2, \ldots, m'_k)$. Consider the graphs $S(G)$ and $S(G')$. Using Theorem 1 from [34] (see also [10, p. 64]) we get that $\lambda_1(S(G')) > \lambda_1(S(G))$. Note, we have now to move in two steps one vertex from the longer path to the shorter one, in order to apply the corresponding result for the A-index. The rest of the proof follows immediately. $\square$

Remark. Similar reasoning can be used for some other classes of homeomorphic graphs. For example, we can consider graphs homeomorphic to the graph consisting of several loops at a single vertex (see [34] for the corresponding result for the A-index).

There is also a possibility of exploiting further the above ideas, now going back to the A-theory via line graphs. Let $L(m_1, m_2, \ldots, m_k)$ be the line graph of the θ-graph $\Theta(m_1 + 1, m_2 + 1, \ldots, m_k + 1)$. Recall from Part I that

$$P_{L(G)}(x) = (x + 2)^{m-n} Q_G(x + 2). \quad (2)$$

Then, since $\lambda_1(L(G)) = q_1(G) - 2$, we immediately get:

Theorem 2.4. *Let $L(m_1, m_2, \ldots, m_k)$ be a graph defined as above, and let $L(m'_1, m'_2, \ldots, m'_k)$ be a graph obtained from the former one by taking $m'_i = m_i + 1$, $m'_j = m_j - 1$ and $m'_p = m_p$ for $p \neq i, j$. Then, whenever $m_j - m_i > 1$, we have*

$$q_1(L(m_1', m_2', \ldots, m_k')) > q_1(L(m_1, m_2, \ldots, m_k)).$$

A *bicyclic* graph is a connected graph on n vertices and $n+1$ edges. Let $\mathcal{B}_n$ be the set of all bicyclic graphs on n vertices.

Our next aim is to identify in $\mathcal{B}_n$ the graph(s) whose Q-index is minimal (further on denoted by $\widehat{B}$).

First we have that the minimum vertex degree of $\widehat{B}$ is greater than 1, for otherwise we can delete any such vertex from $\widehat{B}$ (this reduces the Q-index), and then insert that vertex into the reduced subgraph by subdividing some edge belonging to a cycle (this again reduces the Q-index by Theorem 2.9 from [14]). Thus we get a graph from $\mathcal{B}_n$ with a smaller Q-index, a contradiction. Therefore, $\widehat{B}$ has one of the following forms:

(i) $\Theta(a, b, c)$, where $a + b + c = n + 1$ (θ-graph);
(ii) $C_d \cdot C_e$, where $d + e = n + 1$ (coalescence[1] of two cycles);
(iii) $D(f, g, h)$, where $f + g + h = n + 1$ (cycles C_f and C_h joined by a path of length g).

Since $q_1(G) = \lambda_1(S(G))^2$ (for any G) we can, in order to identify $\widehat{B}$, consider the A-spectrum of the subdivisions of the graphs from (i)-(iii), i.e. the graphs $\Theta(2a, 2b, 2c)$, $C_{2d} \cdot C_{2e}$ and $D(2f, 2g, 2h)$.

As observed in [34] the minimal A-index of graphs of type (i) is less than the minimal A-index of graphs of type (ii). So $\widehat{B}$ cannot be of type (ii). From [33] (see Corollary 1) we have that $\lambda_1(D(a+b, a+b, 2c)) < \lambda_1(D(2a, 2b, 2c))$ whenever $a \neq b$. In addition we have that $\lambda_1(\Theta(a+b, a+b, 2c) = \lambda_1(D(a+b, a+b, 2c))$, as can be seen by comparing the eigenvalue equations (for indices) of the latter two graphs. Using Theorem 1 from [34], we easily get that $\lambda_1(\Theta(2a, 2b, 2c)$ is minimal if either $2a = 2b = 2c (=2k)$ or $2a = 2b (= 2k)$, $2c = 2k \pm 2$. Hence $\widehat{B}$ is one of the graphs $\Theta(k, k, k)$ and $D(k, k, k)$, or $\Theta(k, k, k \pm 1)$ and $D(k, k, k \pm 1)$, depending on n. So we have arrived at the following result:

Theorem 2.5. *Let $\mathcal{B}_n$ be the set of bicyclic graphs on n vertices. If $\widehat{B} \in \mathcal{B}_n$ is a graph with minimal Q-index, then $\widehat{B}$ is either of the graphs*

$$\Theta(p, p, n + 1 - 2p), D(p, p, n + 1 - 2p),$$

where p is an integer chosen so that $\frac{n}{3} \leqslant p \leqslant \frac{n+2}{3}$.

2.4. Graph operations

The next theorem (see, for example, [8, p. 62]) shows that a relation between $P_G(x)$ and $P_{L(G)}(x)$ can be established for certain non-regular graphs.

Theorem 2.6. *Let G be a semi-regular bipartite graph with n_1 mutually non-adjacent vertices of degree r_1 and n_2 mutually non-adjacent vertices of degree r_2, where $n_1 > n_2$. Then*

$$P_{L(G)}(x) = (x+2)^{\beta} \sqrt{\left(-\frac{\alpha_1}{\alpha_2}\right)^{n_1 - n_2} P_G\left(\sqrt{\alpha_1 \alpha_2}\right) P_G\left(-\sqrt{\alpha_1 \alpha_2}\right)},$$

where $\alpha_i = x - r_i + 2$ $(i = 1, 2)$ and $\beta_1 r_1 - n_1 - n_2$.

We apply now this theorem to semi-regular bipartite graphs (see, for example, [11, p. 15], for the source).

Theorem 2.7. *If G is a semi-regular bipartite graph with parameters n_1, n_2, r_1, r_2 $(n_1 > n_2)$ and if $\lambda_1, \lambda_2, \ldots, \lambda_{n_2}$ are the first n_2 largest eigenvalues of G, then*

[1] *Coalescence* of two rooted graphs is the graph obtained by identifying the roots.

$$P_{L(G)}(x) = (x - r_1 - r_2 + 2)(x - r_1 + 2)^{n_1 - n_2}(x + 2)^{n_1 r_1 - n_1 - n_2 + 1} \times \prod_{i=2}^{n_2 - 1}((x - r_1 + 2)(x - r_2 + 2) - \lambda_i^2).$$

Proof. It is easy to see that $\lambda_1 = \sqrt{r_1 r_2}$ and that the spectrum of G contains at least $n_1 - n_2$ eigenvalues equal to 0. Having in mind that the spectrum of a bipartite graph is symmetric with respect to 0, we get Theorem 2.7 from Theorem 2.6 by a straightforward calculation. □

In addition, we obtain a formula for the Q-polynomial of a semi-regular bipartite graph.

Theorem 2.8. *If G is a semi-regular bipartite graph with parameters n_1, n_2, r_1, r_2 $(n_1 > n_2)$ and if $\lambda_1, \lambda_2, \ldots, \lambda_{n_2}$ are the first n_2 largest eigenvalues of G, then*

$$Q_G(x) = x(x - r_1 - r_2)(x - r_1)^{n_1 - n_2} \prod_{i=2}^{n_2 - 1}((x - r_1)(x - r_2) - \lambda_i^2).$$

Proof. Apply formula (2) to Theorem 2.7.

A formula for the Q-polynomial of the join of two regular graphs has been obtained in [24].

2.5. Inequalities for eigenvalues

We continue the survey on inequalities for eigenvalues from the corresponding subsection of [14].

Conjectures 6,7 and 10 from [13] have been proved in [23].

The maximal signless Laplacian spectral radius of graphs with given diameter has been determined in [22].

The maximal signless Laplacian spectral radius of graphs with given matching number has been determined in [45].

Inequalities involving the clique number, independence number and the signless Laplacian eigenvalues are obtained in [27].

2.6. Enriched and restricted spectral theories

Let M be a graph matrix and consider the corresponding spectral M-theory of graphs. The theory can be *enriched* by assuming that for any graph G, together with eigenvalues of M, some other graph invariants are given.

An M-theory of graphs can be *restricted* by considering within that theory not all graphs but a restricted class of graphs.

Finally, a theory can be both enriched and restricted by combining these two definitions.

To be more precise, we introduce the following notation.

The M-theory, enriched by a family $\mathcal{E}$ of graph invariants and restricted to the set $\mathcal{G}$, will be denoted by $M_{\mathcal{E}}(\mathcal{G})$. If $\mathcal{E} = \emptyset$, we shall omit the subscript and write $M(\mathcal{G})$. If $\mathcal{G}$ is the set of all graphs, we shall write $M_{\mathcal{E}}$. The M-theory, without any enrichment or restriction, would be the union over all positive integers n of theories $M(\mathcal{G}_n)$, where $\mathcal{G}_n$ is the set of graphs on n vertices. If the family $\mathcal{E}$ consists of a single element a, we shall write $M_a(\mathcal{G})$.

For example, the A-theory can be enriched by graph angles [10].

The Q-theory is usually enriched by the number of components c, as recommended in [12]. This minor enrichment strengthens considerably the theory. The Q-PING[2], consisting of the graphs $K_{1,3}$ and $C_3 \cup K_1$ on 4 vertices, is no longer a PING in the enriched theory Q_c. In particular, bipartite graphs can be recognized in theory Q_c [5,12]: this is important because in the case of bipartite graphs the Q-theory is reduced to L-theory (see Section 2.3).

[2] PING is an abbreviation for the "pair of isospectral non-isomorphic graphs".

This enrichment was exploited to prove in [6] the following theorem concerning graphs with the Q-index not exceeding 4. By Proposition 6.1 of [12] components of such graphs are paths (including isolated vertices), cycles and stars $K_{1,3}$.

Let us introduce the following notation:

v – the number of isolated vertices.
p – the number of (non-trivial) paths,
e – the number of even cycles,
t – the number of triangles,
u – the number of of odd cycles of length greater or equal to 5,
s – the number of components isomorphic to the star $K_{1,3}$.

Theorem 2.9. *Let the Q-spectrum and the number c of components of a graph with the Q-index not exceeding 4 be given. Then the numbers v, p, e, t, u, s, defined above, are uniquely determined.*

However, all this is not sufficient to determine the graph up to isomorphism.

Example. Graphs $C_4 \cup 2P_3$ and $C_6 \cup 2K_2$ are Q-cospectral. This is the smallest of the following family of Q-PINGs: $C_{2k} \cup 2P_l$ and $C_{2l} \cup 2P_k$ for $k, l \geqslant 2, k \neq l$, what can be verified since the Q-spectra of cycles and paths are known [12].

This example shows that although the numbers of components of each type are determined, the distribution of vertices between components (in these cases between paths and even cycles) is not unique. The Q-PING, consisting of the graphs $K_{1,3}$ and $C_3 \cup K_1$ shows that the conclusion of Theorem 2.7 does not hold unless the Q-theory is enriched.

The result that no starlike trees are Q-cospectral can be stated in the following way: *The spectral uncertainty (as defined in Part I) of the Q-theory restricted to starlike trees is equal to 0.*

2.7. First signs of maturity

Some of the results obtained in the Q-theory have been already used to derive new results.

In particular, this applies to the characterization of graphs with maximal Q-index among graphs with a fixed number of vertices and edges (see Part I). As shown, such graphs are nested split graphs. An upper bound for the Q-index has been derived for a class of graphs in [1] in such a way that a known bound for the A-index has been applied to line graphs of nested split graphs.

The next example is even more suggestive. In [3] the problem of finding necklaces with maximal A-index has been reduced to the search for a caterpillar with maximal Q-index since necklaces are line graphs of caterpillars. In this way the Q-theory starts to be helpful to the A-theory: so far the help has been going only in the other direction! See also the way of reasoning in Theorems 2.3 and 2.4: a result from A-theory has been transformed into Q-theory using subdivisions (Theorem 2.3) and then back into A-theory (Theorem 2.4).

The long derivation of the lower bound for the least eigenvalue of the signless Laplacian of a non-bipartite graph in [4] (see also Part I) appears to be without a parallel in the A-theory and other spectral theories. It was necessary to prove a lot of lemmas on eigenvectors of the least eigenvalue without any paradigm before the proof of the main result was achieved.

One should also note the first case of a statement not involving eigenvalues which has been proved using Q-eigenvalues (*Q-spectral techniques*). The following proposition has been proved in [6].

Proposition 2.1. *The subdivision of a tree with m edges has a matching of size m.*

Proof. If T is a tree on n vertices formula (1) yields $P_{S(T)}(x) = x^{-1}Q_T(x^2)$. Let $\eta(G)$ be the multiplicity of the eigenvalue 0 in the spectrum of a graph G. Since T is a bipartite graph $Q_T(x)$ has a simple root 0 and we have $\eta(S(T)) = 1$. The quantity $\eta(T)$ is an important parameter of a tree T since it determines the size of the maximal matching. By Theorem 8.1 of [8], the size of the maximal matching of a tree T on n vertices is equal to $\frac{1}{2}(n - \eta(T))$ and we are done. $\square$

Of course, Proposition 2.1 can be proved easily without the use of eigenvalues (by induction on the number m of edges, using a pendant edge).

3. Solving problems within Q-theory

Although the Q-theory has a smaller spectral uncertainty than other frequently used spectral theories (see the Introduction in Part I), it seems that we do not have enough tools at the moment to exploit this advantage. In this section we present examples supporting such a feeling. In particular, we present results on integral graphs, enumeration of spanning trees, characterizations by eigenvalues, cospectral graphs, graph angles and miscellaneous topics. Together with results presented in Section 3 of Part I (graph operations, inequalities for eigenvalues and reconstruction problems) this survey completes the picture of the Q-theory as it exists at the moment.

3.1. Integral graphs

A graph is called *M-integral* if all its M-eigenvalues are integers.

Originally, only A-integral graphs have been studied. For a survey of results see the paper [2].

A-integral graphs are very rare. Other kinds of integral graphs could be more frequent. For example, out of 112 connected graphs on 6 vertices there are only 6 A-integral graphs [2], while 37 are L-integral [29]; according to a table of Q-eigenvalues of the 112 connected graphs on 6 vertices from [6], just 13 are Q-integral.

The reason for the high number of L-integral graphs is, among other things, the fact that the complement of an L-integral graph is also L-integral. As we already noted, there are no corresponding formulas for the A-polynomial and for the Q-polynomial which would preserve the property of being integral and this is reflected in statistics for integral graphs.

By formula (2) a graph is Q-integral if and only if its line graph is A-integral. If a graph is regular then it is at the same time A-integral, L-integral and Q-integral.

A graph which is at the same time A-integral, L-integral and Q-integral is called *ALQ-integral*.

It is established by a computer search [38], [39] that there are exactly 172 connected Q-integral graphs up to 10 vertices[3]. Among them there exists exactly one graph which is ALQ-integral but not regular and not bipartite. It has 10 vertices. There is another ALQ-integral graph (on 10 vertices) which is bipartite (and not regular).

The problem of determining all connected, non-regular ALQ-integral graphs was posed in [40], Problem AWGS.2-C. For a more tractable problem we can require, in addition, that the graphs are non-bipartite.

Proposition 3.1. *If G is an ALQ-integral graph, then the product $G \times K_2$ is a bipartite ALQ-integral graph.*

The proof is based on formula (5) from Part I and the corresponding formula for A-eigenvalues.

It was proved in [35] that there are exactly 26 connected Q-integral graphs with maximum edge-degree at most four. Some partial results on graphs with maximum edge-degree five are also obtained.

All Q-integral complete split graphs have been identified in [24]. Other Q-integral graphs have been found in some related classes of graphs.

3.2. Enumeration of spanning trees

Let $t(G)$ be the number of spanning trees in a graph G. Spectral techniques are known to be efficient in enumerating spanning trees.

[3] There are exactly 150 connected A-integral graphs up to 10 vertices [2].

Theorem 1.3 of [8] gives $t(G)$ in terms of L-eigenvalues while Theorem 1.4 does this for regular graphs in terms of A-eigenvalues. The first theorem yields the following formula

$$t(G) = \frac{1}{n}\prod_{i=1}^{n-1} q_i$$

for bipartite graphs G on n vertices, while on the basis of the second theorem we have

$$t(G) = \frac{1}{n}\prod_{i=2}^{n}(2r - q_i)$$

for regular graphs G of degree r (also with n vertices). In view of Theorem 2.2 of Part I, these formulas coincide for regular bipartite graphs.

Example. The Q-spectrum of $K_{m,n}$ was determined in Subsection 2.5 of Part I and the first of these formulas yields $t(K_{m,n}) = m^{n-1}n^{m-1}$. The Q-spectrum of K_n was determined in Subsection 2.2 of Part I and the second of these formulas yields $t(K_n) = n^{n-2}$ (the Cayley formula). $\square$

Example. Similarly we have

$$t(P_m + P_n) = 4^{(m-1)(n-1)}\prod_{i=1}^{m-1}\prod_{j=1}^{n-1}\left(\sin^2\frac{\pi}{2m}i + \sin^2\frac{\pi}{2n}j\right). \quad \square$$

The aforementioned Proposition 1.3 of [8] shows that $t(G) = \frac{(-1)^{n-1}}{n}L'_G(0)$. For a non-bipartite G formula (5) from Part I yields for the product $G \times K_2$ the expression $L_{G\times K_2}(x) = L_G(x)Q_G(x)$. Now we have

$$t(G \times K_2) = \frac{(-1)^{2n-1}}{2n}(L_G(x)Q_G(x))'\Big|_{x=0} = \frac{(-1)^n}{2}Q_G(0)t(G).$$

Since $Q_G(0) = (-1)^n \det Q$, we get an expression for the determinant of matrix Q

$$\det Q = 2\frac{t(G \times K_2)}{t(G)}.$$

Note that the coefficient theorem for $Q_G(x)$ (see Theorem 4.4 of [12]) gives for $\det Q$ a much more complicated expression. Of course, we have $\det Q = 0$ if G is bipartite.

Example. For $G = C_{2k+1}$ we have that $G \times K_2 = C_{4k+2}$. Since $t(C_{2k+1}) = 2k + 1$ and $t(C_{4k+2}) = 4k + 2$, we have $\det Q = 4$. The same result we get also by Theorem 4.4 from [12].

Hence, a number of results can be derived nicely using Q-eigenvalues.

3.3. Characterizations by eigenvalues

A graph G is said to be *characterized by its spectrum* in M-theory (or with respect to the matrix M) if any graph H, which is M-cospectral to G, is also isomorphic to G. This definition is extended in an obvious way to enriched and restricted spectral theories. Instead of the traditional phrase "characterized by the spectrum", the authors of [15] launched recently the term "determined by the spectrum" (abbreviated DS). We shall extend it to an M-DS notation.

There are many spectral characterization results in A-theory and slightly fewer in L-theory. Since Q-theory has a low spectral uncertainty, one can expect many such results in this theory. We shall survey results which can be formulated using connections with A-theory and L-theory. There are also some new results specific to Q-theory.

Given the Q-spectrum of a graph G, one can immediately determine the number n of vertices and the number m of edges. Then we immediately get that graphs determined by n and m are also characterized by Q-spectrum. In particular, graphs without edges ($m = 0$) and complete graphs $\left(m = \binom{n}{2}\right)$ are Q-DS. In addition, the same holds for $m = 1$ and for $m = \binom{n}{2} - 1$.

The path P_n, and, more generally, the union of paths is Q-DS. The proof, given in [15], is longer than necessary. It is sufficient to refer to Proposition 6.1 of [12] which says that in graphs with Q-index smaller than 4 all components are paths (see also Theorem 2.9).

Note that in A-theory the interval of reals containing all eigenvalues of paths (i.e. the interval $(-2, 2)$) contains the spectra of some other graphs [9]. Due to this fact, it is not true[4] that the union of paths is A-DS, as wrongly stated in [15]. For example, $P_5 \cup P_1$ and $K_{1,3} \cup K_2$ form an A-PING. Hence, the Q-theory is more efficient if we restrict ourselves to the union of paths.

Characterizations of regular graphs in A-theory are transferred immediately to Q-theory. This is because regular graphs can be recognized in Q-theory and we may use the isomorphism with A-theory.

In particular, this applies to regular graphs of degree $r = 0, 1, 2$ and $n-1, n-2, n-3$ (n is the number of vertices). All graphs mentioned are DS in all three theories considered.

There is a theorem that summarizes many of the results in the theory of graphs with least A-eigenvalue -2 (see [7]). It remains literally in the same form when translated from A-theory to Q-theory: only the word "A-spectrum" is replaced by the word "Q-spectrum".

Theorem 3.1. *The Q-spectrum of a graph G determines whether or not it is a regular, connected line graph except for 17 cases. In these cases G has the spectrum of $L(H)$ where H is one of the 3-connected regular graphs on 8 vertices or H is a connected, semi-regular bipartite graph on* $6 + 3$ *vertices*.

The situation becomes more complicated if we consider non-regular graphs. While regular graphs of degree 2 are DS, we lose this property if we consider graphs with the Q-index equal to 4 (see Theorem 2.9).

Starlike trees are DS in the L-theory [32], while this is not proved for the A-theory [43]. Concerning the Q-theory, a private communication of Omidi is cited in [16] by which T-shape trees (starlike trees with maximal degree equal to 3) are DS except for $K_{1,3}$. We can verify this assertion by reducing the problem via subdivision graphs to A-theory and then using results of [43]. Indeed, the subdivision graph of a T-shape tree is again a T-shape tree and an A-cospectral mate, described in [43], is not a subdivision graph except for $K_{1,3}$.

Here we need some caution. Namely, if a bipartite graph is proved to be L-DS, this does not mean that it is Q-DS since it could be cospectral to a non-bipartite graph. The situation is especially curious in trees. As pointed out in Section 2.2, given the L-spectrum (or the Q-spectrum, which is the same) of a tree, in L-theory we can recognize that it is a tree, while in the Q-theory we cannot be sure whether the graph is connected (which opens the possibility that in the case of non-connectedness it is not bipartite).

The lollipop graph (a cycle with a path attached by an end-vertex) was considered in [46]. It was proved that the lollipop graph is determined by its Q-spectrum.

3.4. Cospectral graphs

Statistics on cospectral graphs, given in the introduction of Part I, indicates that cospectral graphs are less frequent in the Q-theory than in the A-theory or L-theory. In this subsection we shall document and partially explain this phenomenon.

The basic Q-PING, consisting of the graphs $K_{1,3}$ and $C_3 \cup K_1$ on 4 vertices, is already mentioned. A Q-PING, consisting of connected graphs on 5 vertices, was identified in [12]. Five Q-PINGs, all consisting of connected graphs on 6 vertices, were identified in [6].

Formulas (1) and (2) explain partially the fact that A-PINGs are more frequent than Q-PINGs. Namely, for any Q-PING these formulas (as stated in Proposition 3.5 of [6]) yield two A-PINGs whose graphs belong to restricted classes of graphs (subdivision and line graphs).

[4] Nevertheless, the assertion becomes true if one excludes trivial paths P_1 from consideration.

Various constructions of A-PINGs using formulas for the spectra of graphs obtained by graph operations are known in the literature. As we saw in Section 3.1 of Part I, such formulas are not so frequent for the Q-polynomial. Hence, many of the constructions of A-PINGs cannot be repeated for the Q-polynomial, again supporting the idea that PINGs are less frequent in the Q-theory.

The paper [48] provides spectral uncertainties r_n with respect to the adjacency matrix and $s_n = q_n$ with respect to the Laplacian and the signless Laplacian of sets of all trees on n vertices for $8 \leqslant n \leqslant 21$:

n	8	9	10	11	12	13	14
r_n	0.087	0.213	0.075	0.255	0.216	0.319	0.261
q_n	0	0	0	0.0255	0.0109	0.0138	0.0095

n	15	16	17	18	19	20	21
r_n	0.319	0.272	0.307	0.261	0.265	0.219	0.213
q_n	0.0062	0.0035	0.0045	0.0019	0.0014	0.0008	0.0005

Again, spectral uncertainties q_n are much smaller than r_n but the optimism expressed in [48] cannot be justified since it is known [28] that both r_n and q_n tend toward 1 when n tends to the infinity. It is interesting that there are no (non-isomorphic) Q-cospectral trees on fewer than 11 vertices while smallest A-cospectral trees have 8 vertices.

The next example also illustrates the frequency of PINGs. The spectral structure of graphs whose A-index does not exceed 2 (known as *Smith* graphs) has been studied in [9]. Cospectral Smith graphs are very frequent and they have been described by some algebraic means in the same paper. Let S be the set of Smith graphs excluding cycles and the subdivision of $K_{1,3}$. It was proved in [36] that the set S essentially contains only three graphs which are not DS in Q-theory. For PINGs containing cycles see Theorem 2.9. and Example after it. The Q-index of the subdivision of $K_{1,3}$ is approximately equal to 4.4142 and the characterization of graphs whose Q-index lies around this value seems to be a hard problem.

3.5. Graph angles

Graph angles can be introduced for the signless Laplacian matrix in the same way as for the adjacency matrix (see, for example, [10, p. 75]).

The spectral decomposition of the matrix Q reads:

$$Q = \kappa_1 P_1 + \kappa_2 P_2 + \cdots + \kappa_m P_m,$$

where $\kappa_1, \kappa_2, \ldots, \kappa_m$ are the distinct Q-eigenvalues of a graph G, and $P_1, P_2, \ldots, P_m$ the projection matrices (of the whole space to the corresponding eigenspaces); so $P_iP_j = O$ if $i \neq j$, and $P_i^2 = P_i = P_i^T$ ($1 \leqslant i, j \leqslant m$). If $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$ are the vectors of the standard basis in $\boldsymbol{R}^n$, then the quantities $\gamma_{ij} = \|P_i\mathbf{e}_j\|$, are called the Q-*angles* ; in fact γ_{ij} is the cosine of the angle between the unit vector $\mathbf{e}_j$ (corresponding to vertex j of G) and the eigenspace for κ_i. We also define the Q-angle matrix of G, i.e. an $m \times n$ matrix (m is the number of its distinct eigenvalues, while n is the order of G) as a matrix (γ_{ij}). This matrix is a graph invariant if its columns are ordered lexicographically.

If G is a regular graph of degree r, any eigenvector of the A-eigenvalue λ is also an eigenvector of the Q-eigenvalue $\lambda + r$. Hence, eigenspaces of a regular graph are the same in the A-theory and in the Q-theory and also Q-angles coincide with A-angles.

We shall now consider the vertex eccentricities of a connected graph in the context of the Q-angles. Let $ecc(u)$ be the eccentricity of the vertex u.

Theorem 3.2. *Let G be a connected graph and u an arbitrary vertex. If $m(u)$ is the number of non-zero entries in the u-th column (corresponding to the vertex u) of the angle matrix, then*

$$ecc(u) \leqslant m(u) - 1.$$

Proof. Suppose by the way of contradiction that $e \geqslant m(u)$, where $e = ecc(u)$. From the spectral decomposition of the signless Laplacian of G we have

$$Q^k = \kappa_1^k P_1 + \kappa_2^k P_2 + \cdots + \kappa_m^k P_m \quad (k = 0, 1, 2, \ldots). \tag{3}$$

Suppose that v is a vertex of G at distance e from u. Then the (u, v)-entries of Q^k for all $k \in \{0, 1, \ldots, e-1\}$ are equal to zero (there are no semi-edge walks between u and v). Let x_j $(j = 1, 2, \ldots, m)$ be the (u, v)-entry of P_j. Comparing the (u, v)-entries of matrices from both sides of (3) (for $k = 0, 1, \ldots, e-1$) we obtain a system of e equations in m unknowns $x_1, x_2, \ldots, x_m$, which reads

$$\sum_{j=1}^{m} \kappa_j^k x_j = 0 \quad (k = 0, 1, \ldots, e-1).$$

Note next that $x_j = (P_j\mathbf{e}_u)^T(P_j\mathbf{e}_v)$, which is zero if $\gamma_{ju} = 0$. Accordingly, the above system reduces to a system of e equations in $m(u)$ unknowns. The system consisting of the first $m(u)$ equations has a Vandermonde determinant, and so all the remaining x_js are also zero. From (3), we see that the (u, v)-entry of Q^k is zero for all k. Hence G is not connected, a contradiction.

This completes the proof. $\square$

This theorem is quite analogous to a similar theorem proved in the A-theory [37]. On the other hand, in literally the same way, we can prove the analogous theorem for the L-theory. In the following example we will show that neither theory offers the bound which is in the general case the best possible (in other words they are incomparable). For this purpose we will take three graphs which are contained in the computer package Mathematica.

Example. The graphs considered will be named as in Mathematica. In the tables below the first three (inner) rows correspond to upper bounds for $m(u)$ obtained by using matrices A, L and Q, respectively; the fourth row gives the exact values of eccentricities (e stands for *ecc*). The (inner) columns correspond to the vertices of the graph under consideration.

(i) We first give an example where A-theory is superior. Consider the GroetzschGraph (or the MycielskiGraph[4] of chromatic number 4) - the smallest triangle-free graph of chromatic number 4.

	1	2	3	4	5	6	7	8	9	10	11
A	4	4	4	4	4	2	4	4	4	4	4
L	6	6	6	6	6	2	6	6	6	6	6
Q	6	6	6	6	6	2	6	6	6	6	6
e	2	2	2	2	2	2	2	2	2	2	2

(ii) We next give an example where L-theory is superior. Consider the graph called the NoPerfectMachingGraph – the connected graph on 16 vertices without perfect matching.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
A	7	7	7	7	6	3	6	6	7	7	7	7	7	7	7	7
L	6	6	7	7	6	3	6	6	7	7	6	6	7	7	6	6
Q	7	7	7	7	6	3	6	6	7	7	7	7	7	7	7	7
e	6	6	5	5	4	3	4	4	5	5	6	6	5	5	6	6

(iii) Finally, we give an example where Q-theory is superior. Consider the graph called the Uniquely3ColorableGraph – the triangle-free graph on 12 vertices, with chromatic number 3 that is uniquely 3-colourable.

	1	2	3	4	5	6	7	8	9	10	11	12
A	10	10	10	10	10	10	10	10	10	10	10	10
L	8	8	7	7	8	8	7	7	8	8	8	8
Q	5	5	5	5	5	5	5	5	5	5	5	5
e	2	2	2	2	2	2	2	2	3	3	3	3

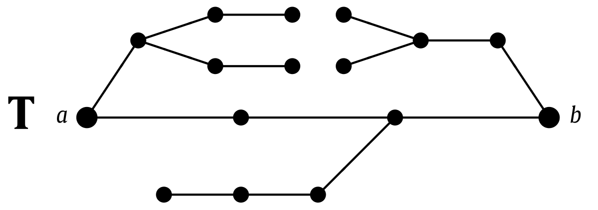

Fig. 1. The smallest endospectral tree.

It is worth noting that the diameters of the above graphs are: 2, 6, and 3, respectively, while the bounds based on the number of distinct eigenvalues (equal to $m - 1$, see [14], Theorem 2.4 for the Q-theory) are depending of spectra: 4, 6 and 6, respectively in (i); 7, 7 and 8, respectively in (ii); 10, 8 and 5, respectively in (iii). On the other hand, the best bounds for the diameter (for the same graphs) based on angles are: 4, 7 and 5, respectively (so the same as former above – a surprising fact). □

Several other results on angles from A-theory can be imitated also in the Q-theory. For example, the numbers of triangles, quadrangles and pentagons can be determined from eigenvalues and angles in the Q-theory.

Let G be a graph rooted at vertex u and let $G + v$ be obtained from G by adding a pendant edge uv.

Consider the characteristic polynomials $Q_G(x) = \det(xI - Q)$ and $Q_{G+v}(x)$ as determinants. Let $Q_u^-(x)$ be the (principal) minor of $Q_G(x)$ obtained by deleting the row and column corresponding to the vertex u. Although we have that $Q_G'(x) = \sum_u Q_u^-(x)$, this formula is not very interesting since $Q_u^-(x)$ is not the Q-polynomial of vertex deleted subgraph $G - u$. Using the same procedure as in A-theory (see, for example, [10, p. 83]), we can derive the formula

$$Q_j^-(x) = Q_G(x) \sum_i \frac{\gamma_{ij}^2}{x - \kappa_i}.$$

However, we have $Q_{G+v}(x) = (x-1)Q_G(x) - xQ_u^-(x)$ which together with the previous formula yields

$$Q_{G+v}(x) = Q_G(x) \left(x - 1 - x \sum_i \frac{\gamma_{ij}^2}{x - \kappa_i} \right). \tag{4}$$

This formula can be used to rewrite formula (6) in Part I and also independently, for calculating $Q_{G+v}(x)$. (Recall also from Part I that no simple formula for $Q_{G+v}(x)$ could exist.)

Example. Consider $K_n + v$, the graph obtained from K_n by adding a pendant edge. The distinct Q-eigenvalues of K_n are $2n - 2$ and $n - 2$. For any vertex the corresponding angles are $\sqrt{\frac{1}{n}}$ and $\sqrt{\frac{n-1}{n}}$ (see, for example, [10, p. 76]). Applying (4) we get that the Q-eigenvalues of $K_n + v$ are the roots of the equation $x^2 - (2n-1)x + 2(n-2) = 0$, $n - 1$ and $n - 2$ of multiplicity $n - 2$. □

Let G be a graph containing a vertex a, and let now $G(a)$ be the graph obtained from G by adding a pendant edge at vertex a. Vertices a and b of a connected graph G are called *M-cospectral* if the graphs $G(a)$ and $G(b)$ are non-isomorphic and M-cospectral. A graph having M-cospectral vertices is called M-endospectral.

We found by computer search that the smallest Q-endospectral tree has 16 vertices and it is given on Fig. 1 as the tree T with cospectral vertices a and b. There are no other Q-endospectral graphs on 16 or 17 vertices.

By formula (6) in Part I the graphs $TavH$ and $TbvH$ are Q-cospectral for any graph H rooted at the vertex v. This is an imitation of the well known procedure for constructing cospectral graphs in A-theory by which it was proved a long time ago that almost all trees have an A-cospectral mate. In fact, the tree T was used in [28] to prove that also almost all trees have a Q-cospectral mate. The difference

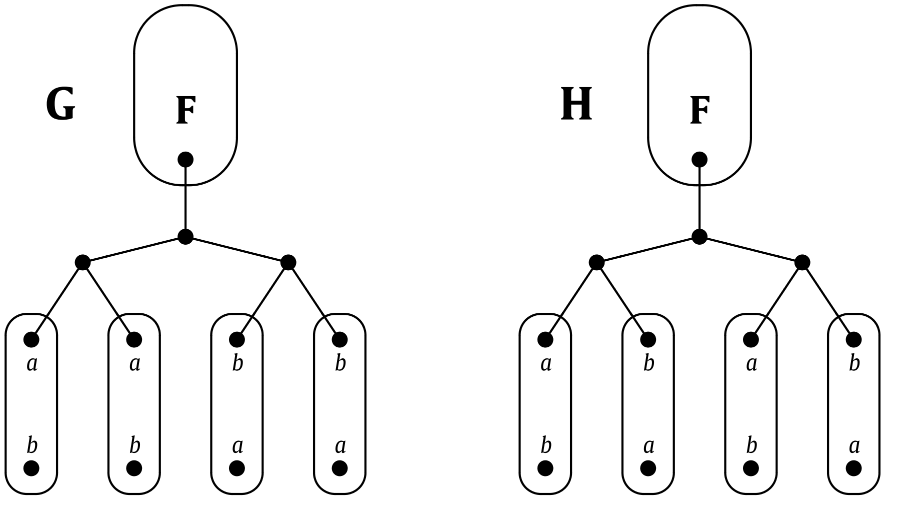

Fig. 2. Q-cospectral graphs with same angles.

between the two theories is that the smallest A-endospectral tree has 9 vertices, many fewer than in the Q-theory. This explains the data given in the previous subsection on spectral uncertainties of trees. One should go well beyond 16 in order to get a high probability that the tree T appears as a limb in a random tree which would then ensure that the spectral uncertainty starts to approach to 1.

One can also repeat the construction from A-theory of cospectral trees with the same angles. By formula (4) we see that knowledge of $Q_G(x)$ allows us to obtain the angles corresponding to a vertex u from the eigenvalues of $G(u)$, and vice versa. Hence Q-cospectral graphs G and H on n vertices have the same angles if the collection of supergraphs $G(i), i = 1, 2, \ldots, n$ can be mapped by a bijection f into the collection of supergraphs $H(i), i = 1, 2, \ldots, n$ in such a way that $G(i)$ and $f(G(i))$ are Q-cospectral. Such a pair of graphs is presented in Fig. 2.

Both graphs G and H in Fig. 2 are composed of four copies of the tree T and an arbitrary but fixed graph F. Each copy is represented by an oval and is attached at the rest of the graph by the vertex a or b. In all cases related to this example, attaching a copy of T at vertex a instead of vertex b, or vice versa, results in a Q-cospectral graph. Therefore, clearly, G and H are Q-cospectral. To see that they have the same angles we provide the function f mentioned above: vertices of a copy of T in G are mapped by f to corresponding vertices of a copy of T in H which has the same type of attachment to the rest of the graph.

A consequence of the existence of the above construction is that almost all trees have a Q-cospectral mate with the same angles.

The algorithm for constructing trees with given A-eigenvalues and angles, described in [10, pp. 112–113], can be adapted to work also in the Q-theory.

3.6. Miscellaneous

As mentioned in Section 2.6, the graphs with Q-index not exceeding 4 have, as components, paths (including isolated vertices), cycles and stars $K_{1,3}$. The authors of the paper [42] managed to obtain results in the range up to 4.5. We first give some definitions.

Following [44], an *open quipu* is a tree with maximal vertex degree 3 such that all vertices of degree 3 lie on a path. A *closed quipu* is a connected graph with maximal vertex degree 3 such that all vertices of degree 3 lie on a cycle, and no other cycle exists. A *dagger* is obtained from the star $K_{1,3}$ by attaching a hanging path at its central vertex.

The following theorem stems from [42].

Theorem 3.3. *Let G be a connected graph whose Q-index lies in the interval* $(4,4.5)$. *Then G is an open or a closed quipu*.

This theorem follows from the corresponding result in *A*-theory from [42] which says that a connected graph whose *A*-index lies in the interval $\left(2, \frac{3}{2}\sqrt{2}\right)$ is an open or a closed quipu, or a dagger. Daggers are eliminated by the Corollary to Theorem 2.1 and the rest immediately follows by the use of formula (1). Note that $\left(\frac{3}{2}\sqrt{2}\right)^2 = 4.5$.

The *Q-spectral spread* $s_Q(G) = q_1 - q_n$ has been studied in [31]. It was proved that, for a connected graph G other than K_4 or C_4, the inequality $s_Q(G) < 2n - 4$ holds.

The same problem appears in Conjecture 25 of [13]:

Over the set of all connected graphs of order $n \geqslant 6$, $q_1 - q_n$ *is minimum for a path* P_n *and for an odd cycle* C_n, *and is maximum for the graph* $K_{n-1} + v$.

In fact the authors of [31] have derived a weaker upper bound for $s_Q(G)$ but they believe that the best upper bound is as expressed in Conjecture 25.

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