R E S E A R C H R E P O R T

SPECTRAL THEORY OF GRAPHS BASED ON THE SIGNLESS LAPLACIAN[1]

(*A QUICK OUTLINE: third draft*)

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Abstract. *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 with those based on the adjacency matrix A and the Laplacian L. The Q–theory can be composed using various connections to other theories: equivalence with A–theory and L–theory for regular graphs, or with L–theory for bipartite graphs, general analogies with A–theory and analogies with A–theory via line graphs and subdivision graphs. Within Q-theory we treat the following problems: graph operations, inequalities for eigenvalues, the largest eigenvalue, characterizations by eigenvalues, cospectral graphs, graph angles, integral graphs, enumeration of spanning trees, and miscellaneous problems.*

Keywords: graph theory, graph spectra, adjacency matrix, Laplacian, signless Laplacian

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Contents

Preface

This outline of the spectral theory of graphs based on the signless Laplacian has come out from the papers [26], [27], [28] with the common title "Towards a spectral theory of graphs based on the signless Laplacian". Texts from the previous papers of mine and of my coauthors on the same subject [14], [15], [23], [24] have been used as well. The intention when writing this report was to produce a summary of rapid developments in the area of the signless Laplacian eigenvalues as soon as possible.

The weakness of this report is that several important results of other authors are only briefly mentioned.

My initiative from [14] to build a spectral theory of graphs based on the signless Laplacian was motivated by the following three facts:

– computational results [31] have shown that spectral uncertainties are smaller in the signless Laplacian than in the adjacency matrix or the Laplacian;

– there is a simple connection between the signless Laplacian eigenvalues and spectra of line graphs implying that the existing well developed theory of graphs with least eigenvalue -2 [22] can help in building the new theory;

– apart for sporadic results almost nothing has been published on the signless Laplacian eigenvalues till that time.

I have presented the paper [14] at the 20-th British Combinatorial Conference in Durham in July 2005 and have been advocating the study of the subject in my talks on several occasions.

This text is put on Internet and thus is available to all interested researchers. The text might be revised and extended in the future.

The production of papers on the signless Laplacian eigenvalues in recent years was astonishingly high; the number of published papers is recently approaching one hundred.

January 2010 Author

Note on the second draft

The second draft of "Spectral theory of graphs based on the signless Laplacian" contains some improvements of the previous text and several additions.

The main additions are the following:

– Subsections 3.1, 3.4, 3.7 and 3.9 are extended,
– Subsection 3.2 is rewritten and extended,
– a proof of Theorem 3.6.2 is formulated,
– Appendix 2 is created,
– some references are updated and several new ones are added.

April 2010 Author

Note on the third draft

The third draft of "Spectral theory of graphs based on the signless Laplacian" contains only slight improvements of the previous text.

There are no plans to upgrade this version of the report.

December 2010 Author

1 Introduction

The idea of *spectral graph theory* (or *spectral theory of graphs*) is to exploit numerous relations between graphs and matrices in order to study problems with graphs by means of eigenvalues of some graph matrices, i.e. matrices associated with graphs in a prescribed way. Since there are several graph matrices which can be used for this purpose, one can speak about several such theories so that spectral theory of graphs is not unique. Of course, the spectral theory of graphs consists of all these special theories including their interactions.

By a spectral graph theory we understand, in an informal sense, a theory in which graphs are studied by means of the eigenvalues of some graph matrix M. This theory is called *M–theory.* Hence, there are several spectral graph theories (for example, the one based on the adjacency matrix, that based on the Laplacian, etc.). In that sense, the title "Towards a spectral theory of graphs based on the signless Laplacian" of papers [26], [27], [28], indicates the intention to build 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. The matrix $L = D - A$ is known as the *Laplacian* of G.

In order to give motivation for such a choice we introduce some notions and present some relevant computational results.

Graphs with the same spectrum of an associated matrix M are called *cospectral* graphs with respect to M, or *M–cospectral* graphs. A graph H cospectral with a graph G, but not isomorphic to G, is called a *cospectral mate* of G. Let $\mathcal{G}$ be a finite set of graphs, and let $\mathcal{G}'$ be the set of graphs in $\mathcal{G}$ which have a cospectral mate in $\mathcal{G}$ with respect to M. The ratio $|\mathcal{G}'|/|\mathcal{G}|$ is called the *spectral uncertainty* of (graphs from) $\mathcal{G}$ with respect to M (or, in general, *spectral uncertainty* of the M–theory).

The papers [31], [57] provide spectral uncertainties r_n with respect to the adjacency matrix A, s_n with respect to the Laplacian L and q_n with respect to the signless Laplacian Q of sets of all graphs on n vertices for $n \leq 11$ (see [7] for $n = 12$):

n	4	5	6	7	8	9	10	11	12
r_n	0	0.059	0.064	0.105	0.139	0.186	0.213	0.211	0.188
s_n	0	0	0.026	0.125	0.143	0.155	0.118	0.090	0.060
q_n	0.182	0.118	0.103	0.098	0.097	0.069	0.053	0.038	0.027

We see that numbers q_n are smaller than the numbers r_n and s_n for

$n \geq 7$. In addition, the sequence q_n is decreasing for $n \leq 12$ while the sequence r_n is increasing for $n \leq 10$. This is a strong basis for believing that studying graphs by Q–spectra is more efficient than studying them by their (adjacency) spectra.

Since the signless Laplacian spectrum performs better also in comparison to spectra of other commonly used graph matrices (Laplacian, the Seidel matrix), an idea was expressed in [31] that, among matrices associated with a graph (generalized adjacency matrices), the signless Laplacian seems to be the most convenient for use in studying graph properties.

This suggestion was accepted in [14] where it was also noted that almost no results in the literature on the spectra of signless Laplacian existed at that time. Moreover, connection with spectra of line graphs and the existence of a well developed theory of graphs with least eigenvalue -2 [22] were used as additional arguments for studying eigenvalues of the signless Laplacian.

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 a position to summarize the developments. In the first part [26](Part I) of our three part paper we have mentioned 15 papers (in particular, [10], [15], [24], [33], [41], [45], [46], [73], [84], [86], [89], [90], [92], [93], [107], where the signless Laplacian is used explicitly) in addition to our previous basic papers [14], [23]. In Part II [27] we have added the following 11 references: [1], [5], [47], [48], [49], [50], [68], [74], [98], [103], [105]. In Part III the following 16 papers [3],[29], [37], [38], [44], [52], [53], [56], [59], [60], [76], [87], [91], [94], [99], [104] have been recorded as published or in the process of publication at that moment. Together with [26], [27] and [28], there were in this moment about 50 papers on the signless Laplacian spectrum published since 2005. Several others have been published afterwards.

We are now in position to summarize the current development. We shall, in fact, outline a new spectral theory of graphs (based on the signless Laplacian), and call this theory the *Q–theory*.

The rest of the report is organized as follows. Section 2 presents the main spectral theories, including the Q–theory, and their interactions. In this way, the Q–theory is composed in part from several patches borrowed from other spectral theories. 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 Q-theory and relations to other spectral theories

In 2.1 we list existing spectral theories including A–theory and L–theory as the most developed theories. in Subsection 2.2 we survey basic properties of Q-eigenvalues. In the rest of the section we show how the Q–theory can be composed using various connections to other theories:

- equivalence with A–theory and L–theory for regular graphs (Subsection 2.3),
- equivalency with L-theory for bipartite graphs (Subsection 2.4),
- general analogies with A–theory (Subsection 2.5),
- analogies with A–theory via line graphs (Subsection 2.6),
- analogies with A–theory via subdivision graphs (Subsection 2.7).

This fragmentation appears in this presentation because the Q–theory has attracted the attention only after other theories had already been developed. It is quite possible to present the Q–theory smoothly if it is a primary goal.

We consider also the notions of *enriched* and *restricted* spectral theories (Subsection 2.8).

2.1 Particular theories

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

Let G be a simple graph with n vertices, and let M be a real symmetric matrix associated to G. The characteristic polynomial $\det(xI - M)$ of M 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.

In particular, if M is equal to one of the matrices A, L and Q (associated to a graph G on n vertices), then the corresponding eigenvalues (or spectrum) are called the A–eigenvalues (or A–spectrum), L–eigenvalues (or L–spectrum) and Q–eigenvalues (or Q–spectrum), respectively. Throughout the paper, these eigenvalues will be denoted by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ and $q_1 \geq q_2 \geq \cdots \geq q_n$, respectively. They are the roots of the corresponding characteristic polynomials $P_G(x) = \det(xI - A)$, $L_G(x) = \det(xI - L)$ and $Q_G(x) = \det(xI - Q)$ (note, $P_G(x)$ stands for $A_G(x)$). The largest eigenvalues, i.e. λ_1, μ_1 and q_1, are called the A–index, L–index and Q–index (of G), respectively.

Together with Q–theory we shall frequently consider the relevant facts from A–theory and L–theory as the most developed spectral theories and therefore useful in making comparisons between theories.

We shall mention in passing theories based on the matrix $\hat{L} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}}$, the *normalized* (or *transition*) *Laplacian matrix*[2]; (see [13]) and on the Seidel matrix $S = J - I - 2A$ (see, for example, [17]).

Since the eigenvalues of the matrix D are just vertex degrees, the D–theory is not, in practice, a spectral theory although it formally is. This example shows that the study of graphs by any sequence of structural graph invariants can be formally represented as a spectral theory.

As usual, K_n, C_n and P_n denote respectively the *complete graph*, the *cycle* and the *path* on n vertices. We write $K_{m,n}$ for the *complete bipartite* graph with parts of size m and n. The graph $K_{n-1,1}$ is called a *star* and is denoted by S_n.

A unicyclic graph containing an even (odd) cycle is called *even-unicyclic* (*odd-unicyclic*). The *union* of disjoint graphs G and H is denoted by $G \cup H$, while mG denotes the union of m disjoint copies of G. The *subdivision graph* $S(G)$ of a graph G is obtained from G when each edge of G is subdivided by a new vertex. $L(G)$ denotes the *line graph* of G. *Coalescence* of two rooted graphs is the graph obtained by identifying the roots.

2.2 Basic properties of Q-spectra

Let G be a graph on n vertices, having m edges and let R be its vertex–edge incidence matrix. The following relations are well–known:

$$RR^T = D + A, \quad R^T R = A(L(G)) + 2I, \tag{1}$$

where $A(L(G))$ is the adjacency matrix of $L(G)$, the line graph of G. Since the non–zero eigenvalues of RR^T and $R^T R$ are the same, we immediately get that

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

Basic facts on the signless Laplacian belong to mathematical folklore. Relations (1) and (2) can be found in many papers and books; we have included in the list of references only the items which contain a little more.

[2]Here we assume that G has no isolated vertices

In this section we present basic results arranged in accordance with our needs.

In virtue of (1), the signless Laplacian is a positive semi-definite matrix, i.e. all its eigenvalues are non-negative.

Let G be a graph with Q-eigenvalues $q_1, q_2, \ldots, q_n$ ($q_1 \geq q_2 \geq \cdots \geq q_n$). The largest eigenvalue q_1 is called the Q-index of G.

When applying the Perron-Frobenius theory of non-negative matrices (see, for example, Section 0.3 of [17]) to the signless Laplacian Q, we obtain the same or similar conclusions as in the case of the adjacency matrix. In particular, in a connected graph the largest eigenvalue is simple with a positive eigenvector. The Q-index of any proper subgraph of a connected graph is smaller than the Q-index of the original graph, an observation which follows from Theorems 0.6 and 0.7 of [17].

Concerning the least eigenvalue we have the following proposition.

Proposition 2.2.1 *The least eigenvalue of the signless Laplacian of a connected graph is equal to 0 if and only if the graph is bipartite. In this case 0 is a simple eigenvalue.*

Proof. Let $\mathbf{x}^T = (x_1, x_2, \ldots, x_n)$. For a non-zero vector $\mathbf{x}$ we have $Q\mathbf{x} = \mathbf{0}$ if and only if $R^T\mathbf{x} = \mathbf{0}$. The later holds if and only if $x_i = -x_j$ for every edge, i.e. if and only if G is bipartite. Since the graph is connected, $\mathbf{x}$ is determined up to a scalar multiple by the value of its coordinate corresponding to any fixed vertex i. ■

Remark. Assuming that the reader is familiar with the theory of graphs with least eigenvalue -2, the above proof can be rephrased as follows. By Theorem 2.2.4 of [22], the multiplicity of the eigenvalue -2 in $L(G)$ is equal to $m - n + 1$ if G is bipartite, and equal to $m - n$ if G is not bipartite. This together with formula (2) yields the assertion of the proposition. ■

Corollary 2.2.2. *In any graph the multiplicity of the eigenvalue* 0 *of the signless Laplacian is equal to the number of bipartite components.*

We shall also consider the eigenvectors (see [15]).

Proposition 2.2.3. *The eigenspace of the Q-eigenvalue 0 of a graph G determines sets of vertices and bipartitions in bipartite components of G.*

Proof. Let $\mathbf{x}^T = (x_1, x_2, \ldots, x_n)$. For a non-zero vector $\mathbf{x}$ we have $Q\mathbf{x} = \mathbf{0}$ if and only if $x_i = -x_j$ for every edge (as in the proof of Proposition 2.2.1). If the graph is connected (and then necessarily bipartite), $\mathbf{x}$ is determined up to a scalar multiple by the value of its coordinate corresponding to any fixed vertex i. If G is disconnected, at least one component is bipartite. If a vertex i belongs to a non-bipartite component, then $x_i = 0$. Using Corollary 2.2.2 we determine the number of bipartite components as the multiplicity of eigenvalue 0. For each bipartite component we have an eigenvector with non-zero coordinates exactly for vertices in this component. Now, vertex sets of bipartite components are determined by non-zero coordinates in vectors of a suitably chosen ortogonal basis of the eigencpace of 0. The sign of these coordinates determines colour classes within bipartite components. ■

The least eigenvalue of the signless Laplacan is studied in [40] as a measure of non-bipartiteness of a graph and Proposition 2.2.1 was obtained there as a corollary of a more general theorem (see Subsection 3.9).

Remark. In general, the Q-polynomial still does not contain information on the bipartiteness. It does if the graph is connected but we cannot recognize a connected graph from its Q-polynomial. ■

It is interesting to note that the Q-polynomial together with the information on one of the properties in question (connectedness and bipartiteness) enables us to recover the information on the other property: if we know the number of components we can decide whether the graph is bipartite and if we know whether the graph is bipartite we can find if it is connected.

Note also that for Laplacian eigenvalues it is known that the multiplicity of the eigenvalue 0 is equal to the number of components.

The proof of the following proposition can be found in many places (see, for example, [54]).

Proposition 2.2.4. *In bipartite graphs the Q-polynomial is equal to the characteristic polynomial of the Laplacian.*

One can formulate it more generally (see [15]):

Proposition 2.2.5. *The Q-polynomial of a graph is equal to the characteristic polynomial of the Laplacian if and only if the graph is bipartite.*

Proof. Suppose that the graph G is bipartite, with parts U and V. Consider the determinant defining $Q_G(x)$. Multiply by -1 all rows corresponding to vertices in U and then do the same with the corresponding columns. The transformed determinant now defines the characteristic polynomial of the Laplacian of G.

The multiplicity of the eigenvalue 0 in the Laplacian spectrum is equal to the number of components, while for the signless Laplacian, the multiplicity of 0 is equal to the number of bipartite components. Therefore in non-bipartite graphs the two polynomials cannot coincide. ■

However, this proposition is of limited use: since we cannot establish from the Q-polynomial of a graph G whether the graph is bipartite, we do not know whether $Q_G(\lambda)$ really equals the characteristic polynomial of the Laplacian of G.

Having in mind the above facts for a graph G it seems reasonable to prescribe, along with the Q-polynomial of G, the number of components of G. (In most situations we would normally consider connected graphs.) Then we can decide (using Proposition 2.2.1) whether G is bipartite and go on to calculate $P_{L(G)}(\lambda)$ using (2).

The following proposition can be useful.

Proposition 2.2.6. *The number of edges of a graph G on n vertices is equal to $-p_1/2$ where p_1 is the coefficient of λ^{n-1} in the Q-polynomial of G.*

Proof. The trace of the signless Laplacian is equal to the sum of vertex degrees of G. ■

Two graphs are said to be *Q-cospectral* if they have the same polynomial $Q_G(\lambda)$. By analogy with the notions of PING[3] and cospectral mate we introduce the notions of Q-PING and Q-cospectral mate with obvious meaning.

The graphs $K_{1,3}$ and $K_3 \cup K_1$ represent the smallest Q-PING and no other Q-PINGs on 4 vertices exist. There are two Q-PINGs on 5 vertices: one is provided by the graphs $K_{1,3} \cup K_1$ and $K_3 \cup 2K_1$ and the other by the graphs numbered 014 and 015 in Table 1 in the Appendix.

Note that the smallest PINGs (consisting of the graphs $K_{1,4}$ and $C_4 \cup K_1$ on 5 vertices and the well known PING of two connected graphs on 6 vertices [17, p. 157]) are not Q-PINGs. The paper [57] provides an example of two non-isomorphic (non-regular, non-bipartite) graphs on 10 vertices which are both cospectral and Q-cospectral (and, in addition, are cospectral with respect to the Laplacian, and have cospectral complements).

Two graphs are called *$\mathcal{L}$-cospectral* if their line graphs are cospectral.

Proposition 2.2.7. *If two graphs are Q-cospectral, then they are $\mathcal{L}$-cospectral.*

Proof. Since Q-cospectral graphs have the same number of vertices and the same number of edges, their $\mathcal{L}$-cospectrality follows from formula (2). ■

However, two $\mathcal{L}$-cospectral graphs need not be Q-cospectral. This is because two cospectral line graphs need not have the same number of vertices

[3]PING is an abbreviation for the “pair of isospectral non-isomorphic graphs”.

in their root graph. Such an example of cospectral line graphs is given in Fig. 1.

Fig. 1: Cospectral line graphs

Example. Cospectral line graphs of Fig. 1 have the characteristic polynomial $\lambda(\lambda^2 - \lambda - 4)(\lambda - 1)(\lambda + 1)^2$. The root graph of the first graph has 7 vertices with the Q-polynomial $\lambda(\lambda - 1)(\lambda - 2)(\lambda - 3)(\lambda^2 - 5\lambda + 2)$ while in the second case we have 8 vertices and the Q-polynomial $\lambda^2(\lambda - 1)(\lambda - 2)(\lambda - 3)(\lambda^2 - 5\lambda + 2)$.

The PING of Fig. 1 also shows that we cannot in general decide whether a graph is bipartite from the spectrum of its line graph while the Q-polynomial contains more information about that. ■

This example suggests that the polynomial $Q_G(\lambda)$ is more useful than $P_{L(G)}(\lambda)$. On the other hand, very few relations between $Q_G(\lambda)$ and the structure of G are known. Since we have just the opposite situation with eigenvalues of the adjacency matrix, we would still like to use $P_{L(G)}(\lambda)$ in spite of the fact that $L(G)$ usually has more vertices than G.

However, we have seen that $P_{L(G)}(\lambda)$ contains less information on the structure of G than $Q_G(\lambda)$. This disadvantage can be eliminated if, in addition to $P_{L(G)}(\lambda)$, we know the number of vertices of G. Then our information about G is the same as that provided by $Q_G(\lambda)$, since $Q_G(\lambda)$ can be calculated by formula (2), and either of the two polynomials can be considered.

In this way we can eliminate another uncertainty. Namely, by Theorem 4.3.1. of [22] a regular line graph could be cospectral with another line graph for which the root graph has a different number of vertices, and this fact would cause additional problems if the polynomial $P_{L(G)}(\lambda)$ alone were given.

Example. The graph $L(K_6)$ has the Q-polynomial $(\lambda - 16)(\lambda - 10)^5(\lambda - 6)^9$ while the graph $K_{10,6}$ has the Q-polynomial $(\lambda - 16)(\lambda - 10)^5(\lambda - 6)^9\lambda$. The line graph of either of these two graphs has the characteristic polynomial $(\lambda - 14)(\lambda - 8)^5(\lambda - 4)^9(\lambda + 2)^{45}$. ■

Now we see that for a graph G one should prescribe either (a) $Q_G(\lambda)$ and the number of components of G or, equivalently, (b) $P_{L(G)}(\lambda)$ together with the number n of vertices of G and the number of components of G.

See Subsection 2.8 for a formalization of this requirement.

2.3 Regular graphs

An important characteristic of a spectral theory is whether or not regular graphs can be recognized within that theory. Such a question is answered for a broad class of graph matrices in [31]. The answer is positive for matrices A, L and Q, but it is negative for the Seidel matrix S.

In particular, for the signless Laplacian we have the following proposition [23].

Proposition 2.3.1. *Let G be a graph with n vertices and m edges, and let q_1 be its largest Q-eigenvalue. Then G is regular if and only if $4m = nq_1$. If G is regular then its degree is equal to $q_1/2$, and the number of components equals the multiplicity of q_1.*

The proof is carried out in the same way as in the case of the adjacency matrix (cf. [17], Theorems 3.8, 3.22 and 3.23). In fact, one should compare the value of the relevant Rayleigh quotient for the all-one vector with the value of q_1.

In regular graphs it is not necessary to give explicitly the number of components since this can be calculated from $Q_G(\lambda)$ using Proposition 2.3.1.

The following characterization of regular graphs, known in the A–theory (cf. [17], p. 104), can be formulated also in the Q–theory.

Proposition 2.3.2. *A graph G is regular if and only if its signless Laplacian has an eigenvector all of whose coordinates are equal to 1.*

Of course, for regular graphs we can express the characteristic polynomial of the adjacency matrix and of the Laplacian in terms of the Q–polynomial and use them to study the graph. Thus for regular graphs the whole existing theory of spectra of the adjacency matrix and of the Laplacian matrix transfers directly to the signless Laplacian (by a translate of the spectrum). It suffices to observe that if G is a regular graph of degree r, then $D = rI$, $A = Q - rI$ and we have

$$P_G(x) = Q_G(x + r).$$

If $L_G(\lambda)$ is the characteristic polynomial of the Laplacian L of G, we have

$$L_G(x) = (-1)^n Q_G(2r - x)$$

since $L = 2D - Q = 2rI - Q$.

The mapping $\phi(q) = q - r$ maps the Q–eigenvalues to the A–eigenvalues and can be considered as an isomorphism of the Q–theory of regular graphs to the corresponding part of the A–theory.

Example. We shall give here A–eigenvalues, L–eigenvalues and Q–eigenvalues[4] for two representative classes of regular graphs: complete graphs and circuits. Provided one kind of eigenvalues is known, the other two kinds can be calculated by above formulas.

complete graph K_n $(n \geq 2)$:
A: $n-1, (-1)^{n-1}$
L: $0, n^{n-1}$,
Q: $2n-2, (n-2)^{n-1}$.

cycle C_n $(n \geq 3)$:
A: $2\cos\frac{\pi}{2n}j$ $(j = 0, 1, \ldots, n-1)$
L: $2 - 2\cos\frac{\pi}{2n}j$ $(j = 0, 1, \ldots, n-1)$
Q: $2 + 2\cos\frac{\pi}{2n}j$ $(j = 0, 1, \ldots, n-1)$.

For regular graphs many existing results from the A–theory can be reformulated in the Q–theory.

Proposition 2.3.3. *Let G be a regular bipartite graph of degree r. Then the Q–spectrum of G is symmetric with respect to the point r.*

This symmetry property is an immediate consequence of the well-known symmetry about 0 of the adjacency eigenvalues in bipartite graphs. Thus q is a Q–eigenvalue of multiplicity k if and only if $2r - q$ is also a Q–eigenvalue of multiplicity k; moreover, the eigenvalues 0 and $2r$ are always present.

We can go on and reformulate in the Q–theory, for example, all results from Section 3.3 of [17] and several related results for regular graphs.

2.4 Bipartite graphs

For bipartite graphs we have $L_G(x) = Q_G(x)$ (cf. Proposition 2.2.5). In this way, the Q–theory can be identified with the L–theory for bipartite graphs.

Hence, for non–regular and non–bipartite graphs the Q–polynomial really plays an independent role; for other graphs it can be reduced to either $P_G(x)$ or $L_G(x)$, or to both.

[4]Superscripts are used to denote the multiplicities of eigenvalues.

Unlike the situation with the regularity property, the problem here is that bipartite graphs cannot always be recognized by the Q–spectrum. This difficulty can be overcome by requiring that always, together with the Q–spectrum of a graph, the number of components is given, as explained in Subsection 2.2.

Among many results on bipartite graphs in the L–theory, let us mention a theorem from [65] (and [46]) saying that no starlike trees[5] are cospectral. (It was known before that the same statement holds also in the A–theory [66].) Now this statement holds also in the Q–theory.

Although the Q–theory looks to be identical with the L–theory for bipartite graphs, 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 that 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.

2.5 Analogies with A–theory

The results which we survey in this and in the next two subsections are obtained by applying to the signless Laplacian the same reasoning as for corresponding results concerning the adjacency matrix.

We consider graphs in general with special emphasis on the non-regular case. The results which we survey are of three types:

– results of *type a* are obtained by applying to the signless Laplacian

[5] A *starlike tree* is a tree with exactly one vertex of degree greater than two.

the same reasoning as for corresponding results concerning the adjacency matrix (Subsection 2.5),

– results of *type b* are obtained indirectly via line graphs (Subsection 2.6), and

– results of *type c* are obtained indirectly via subdivision graphs (Subsection 2.7).

First we shall give an interpretation of eigenvectors of Q.

From the relations (1) we see that if $\mathbf{x}$ is an eigenvector for the eigenvalue q of $A+D$, then the vector $\mathbf{u} = R^T\mathbf{x}$ is an eigenvector for the eigenvalue $q-2$ of A_L. It is convenient to consider coordinates of $\mathbf{u}$ as weights of edges of G. Let $\mathbf{x}^T = (x_1, x_2, \ldots, x_n)$ and $\mathbf{u}^T = (u_1, u_2, \ldots, u_m)$. If the edge k of G joins vertices i and j, then from the relation $\mathbf{u} = R^T\mathbf{x}$ we have $u_k = x_i + x_j$ and

$$(q-2)u_s = \sum_{t\sim s} u_t \quad (s = 1, 2, \ldots, m), \quad qu_s = 2u_s + \sum_{t\sim s} u_t \quad (s = 1, 2, \ldots, m),$$

where '$\sim$' denotes the adjacency relation for vertices of $L(G)$ and for edges of G. This is analogous to the well known relations for coordinates of eigenvectors of the adjacency matrix ('the eigenvalue equations').

Next we consider the enumeration of walks.

Definition. *A walk (of length k) in an (undirected) graph G is an alternating sequence $v_1, e_1, v_2, e_2, \ldots, v_k, e_k, v_{k+1}$ of vertices $v_1, v_2, \ldots, v_k, v_{k+1}$ and edges $e_1, e_2, \ldots, e_k$ such that for any $i = 1, 2, \ldots, k$ the vertices v_i and v_{i+1} are distinct end-vertices of the edge e_i.*

Such a walk can be imagined as an actual walk of a traveller along the edges in a diagrammatic representation of the graph under consideration. The traveller always walks along an edge from one end-vertex to the other. Suppose now that we allow the traveller to change his mind when coming to the midpoint of an edge: instead of continuing along the edge towards the other end-vertex, he could return to the initial end-vertex and continue as he wishes. Then the basic constituent of a walk is no longer an edge; rather we could speak of a walk as a sequence of *semi-edges*. Such walks could be called *semi-edge walks*. A semi-edge in a walk could be followed by the other semi-edge of the same edge (thus completing the edge) or by the same semi-edge in which case the traveller returns to the vertex at which he started. A formal definition of a semi-edge walk is obtained from the above definition of a walk by deleting the word "distinct" from the description of end-vertices. Hence we have the following definition.

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

In both definitions we shall say that the walk *starts* at the vertex v_1 and *terminates* at the vertex v_{k+1}.

The well known theorem concerning the powers of the adjacency matrix [17, p.44] has the following counterpart for the signless Laplacian (see [23]).

Theorem 2.5.1. *Let Q be the signless Laplacian of a graph G. The (i, j)-entry of the matrix Q^k is equal to the number of semi-edge walks of length k starting at vertex i and terminating at vertex j.*

Proof. For $k = 1$ the statement is obviously true. The result follows by induction on k just as in the proof of the corresponding theorem for the adjacency matrix. ■

Remark. The proof can also be carried out by applying the theorem concerning the powers of the adjacency matrix to the multidigraph $D(G)$ obtained by adding d_i loops to the vertex i for $i = 1, 2, \dots, n$, where d_i is the degree of the vertex i. Concerning the multidigraph $D(G)$ see the end of this subsection. ■

Let $T_k = \sum_{i=1}^{n} q_i^k$ $(k = 0, 1, 2, \dots)$ be the k-th spectral moment for the Q-spectrum. Since $T_k = \mathrm{tr} Q^k$, we have the following corollary.

Corollary 2.5.2. *The spectral moment T_k is equal to the number of closed semi-edge walks of length k.*

Corollary 2.5.3. *Let G be a graph with n vertices, m edges, t triangles and vertex degrees $d_1, d_2, \dots, d_n$. We have*

$$T_0 = n, \quad T_1 = \sum_{i=1}^{n} d_i = 2m, \quad T_2 = 2m + \sum_{i=1}^{n} d_i^2, \quad T_3 = 6t + 3\sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i^3.$$

Proof. The formulas for T_0 and T_1 are obvious. In T_2 the first term counts the semi-edge walks based on one edge while the second term counts those consisting of two semi-edges. In T_3 the terms are related to walks around a triangle, walks along one edge and one semi-edge, and walks consisting of three semi-edges. ■

Remark 1. Recall that $\mathrm{tr}MN = \mathrm{tr}NM$ for any two feasible matrices M, N. The formula for T_2 follows from $\mathrm{tr}Q^2 = \mathrm{tr}(A+D)^2 = \mathrm{tr}A^2 + \mathrm{tr}D^2$, since $\mathrm{tr}AD = 0$. We have $T_3 = \mathrm{tr}(A+D)^3 = \mathrm{tr}A^3 + 3\mathrm{tr}A^2D + 3\mathrm{tr}AD^2 + \mathrm{tr}D^3$. Since $\mathrm{tr}AD^2 = 0$, we obtain the above formula. Compare also the formula for T_1 with Proposition 2.2.6. ■

Remark 2. Expressions for the spectral moments from Corollary 2.5.3 can be used to determine vertex degrees if we know that vertex degrees can take only a limited number of values. In particular, suppose that a graph has n_i vertices of degree e_i for $i = 0, 1, 2, 3$ and no other vertices. If we specify e_0, e_1, e_2, e_3, the corresponding numbers of vertices n_0, n_1, n_2, n_3 can be determined from the system of equations (provided the spectral moments T_0, T_1, T_2, T_3 are known)

$$\sum_{i=0}^{3} n_i = T_0 = n, \quad \sum_{i=0}^{3} n_i e_i = T_1 = 2m,$$

$$\sum_{i=0}^{3} n_i e_i^2 = T_2 - 2m, \quad \sum_{i=0}^{3} n_i e_i^3 = T_3 - 6t - 3(T_2 - 2m).$$

Interesting conclusions could be made in the case $e_0 = 0, e_1 = 1, e_2 = 2, e_3 = 3$.

Such a situation occurs in graphs with vertex degrees at most 3. These graphs are of interest in chemical applications of graph theory. If such a graph is bipartite, we have $t = 0$ and vertex degrees are determined in terms of spectral moments by the above system. If the graph is connected, we have $n_0 = 0$ and we can treat non-bipartite case as well. (The first three equations suffice to determine vertex degrees and, in addition, the fourth equation yields the number of triangles t). ■

The following statement and its proof is analogous to an existing result related to the adjacency spectrum [17, Theorem 3.13]. The proof is taken from [15].

Theorem 2.5.4. *Let G be a connected graph of diameter D with e distinct Q–eigenvalues. Then $D \leq e - 1$.*

Proof. By Theorem 2.5.1 the (i, j)-entry $q_{i,j}^{(k)}$ of Q^k is the number of semi-edge walks of length k from i to j. By the definition of the diameter, for some vertices i and j there is no semi-edge walk of length k connecting i and j for $k < D$, whereas there is at least one for $k = D$. Hence we have $q_{i,j}^{(k)} = 0$

for $k < D$ and $q_{i,j}^{(k)} > 0$ for $k = D$. The minimal polynomial of the matrix Q is of degree $e(G) = e$ and yields a recursive relation connecting $e+1$ consecutive members of the sequence $q_{i,j}^{(k)}$, $k = 0, 1, 2, \ldots$. The assumption $D > e-1$ would cause that all members of the sequence $q_{i,j}^{(k)}$, $k = 0, 1, 2, \ldots$ are equal to 0 what is impossible. The obtained contradiction proves the theorem. ■

Let G be a connected graph with n vertices and m edges and let

$$Q_G(\lambda) = \sum_{j=0}^{n} p_j \lambda^{n-j} = p_0\lambda^n + p_1\lambda^{n-1} + \cdots + p_n$$

be the Q-polynomial of G.

A spanning subgraph of G whose components are trees or odd-unicyclic graphs is called a *TU-subgraph* of G. Suppose that a TU-subgraph H of G contain c unicyclic graphs and trees $T_1, T_2, \ldots, T_s$. Then the weight $W(H)$ of H is defined by $W(H) = 4^c \prod_{i=1}^{s}(1 + |E(T_i)|)$. Note that isolated vertices in H do not contribute to $W(H)$ and may be ignored.

We shall express coefficients of $Q_G(x)$ in terms of the weights of TU-subgraphs of G.

Theorem 2.5.5. *We have* $p_0 = 1$ *and*

$$p_j = \sum_{H_j} (-1)^j W(H_j), \quad j = 1, 2, \ldots, n,$$

where the summation runs over all TU*-subgraphs* H_j *of* G *with* j *edges.*

Proof. We shall need the formula

$$P_G^{(k)}(x) = k! \sum_{S_k} P_{G-S_k}(x) \tag{3}$$

where the summation runs over all k-vertex subsets S_k of the vertex set of G. (For $k = 1$ the formula is well-known [17, p.60], and then we obtain (3) by induction, as noted in [55].)

Starting from (2) and using the Maclaurin development we have

$$\begin{aligned} Q_G(x) &= x^{n-m} P_{L(G)}(x-2) \\ &= x^{n-m} \sum_{k=0}^{m} P_{L(G)}^{(k)}(-2) \frac{x^k}{k!} \\ &= x^{n-m} \sum_{k=m-n}^{m} x^k \frac{1}{k!} P_{L(G)}^{(k)}(-2) \end{aligned}$$

since the eigenvalue -2 of $L(G)$ has multiplicity[6] at least $m-n$. Applying (3) we obtain

$$Q_G(x) = x^{n-m} \sum_{k=m-n}^{m} x^k \sum_{S_k} P_{L(G)-S_k}(-2) \ . \tag{4}$$

All subgraphs $L(G) - S_k$ are, of course, line graphs and have -2 as an eigenvalue unless all components of $L(G) - S_k$ are line graphs of trees or of odd unicyclic graphs (see Corollary 2.2.5 of [22]).

The root graph of $L(G) - S_k$ is then a TU-subgraph H_{m-k} of G with $m-k$ edges. We have that $(-1)^{|E(Z)|}P_{L(Z)}(-2)$ is equal to 4 if Z is an odd-unicyclic graph and is equal to $1 + |E(Z)|$ if Z is a tree (see, for example, [22], p. 181). Hence, we have

$$P_{L(G)-S_k}(-2) = (-1)^{m-k} W(H_{m-k}) \ .$$

Now the formula (4) reduces to

$$Q_G(x) = x^{n-m} \sum_{k=m-n}^{m} x^k (-1)^{m-k} \sum_{H_{m-k}} W(H_{m-k}),$$

where in the second sum the summation runs over all TU-subgraphs H_{m-k} of G with $m-k$ edges. By substituting j for $m-k$ we obtain

$$Q_G(x) = \sum_{j=0}^{n} x^{n-j} (-1)^j \sum_{H_j} W(H_j).$$

This completes the proof. ■

This result appeared first in [39]; the proof given here stems from [23].

For $j = 1$ the only TU-subgraph H_1 is equal to K_2 with $W(H_1) = W(K_2) = 2$ and we readily obtain $p_1 = -2m$, thereby recovering Proposition 2.2.6. For $j = 2$, the possible TU-subgraphs H_2 are $2K_2$ and $K_{1,2,}$. Since $W(2K_2) = 4$ and $W(K_{1,2}) = 3$ we have $p_2 = 4a + 3b$ where a is the number of pairs of non-adjacent and b the number of pairs of adjacent edges in G. Since $a + b = \frac{m(m-1)}{2}$, we have the following result.

Corollary 2.5.6. *$p_1 = -2m$ and $p_2 = a + \frac{3}{2}m(m-1)$, where a is the number of pairs of non-adjacent edges in G.*

[6]Here we assume that G is not a tree. However, the proof remains valid also for trees since in that case the term for $k = -1$ in the last sum does not exist.

The following theorem is a direct reformulation of a well-known theorem from the Perron-Frobenius theory concerning relations between the largest eigenvalue and the row sums of non-negative matrices (cf., e.g., [51], vol. II, p. 63, or [17], p. 83).

Theorem 2.5.7. *Let G be a graph on n vertices with vertex degrees $d_1, d_2, \ldots, d_n$ and largest Q-eigenvalue q_1. Then*

$$2 \min d_i \leq q_1 \leq 2 \max d_i.$$

For a connected graph G, equality holds in either of these inequalities if and only if G is regular.

However, stronger inequalities can be derived using the very same result from the theory of non-negative matrices (see Subsection 2.6).

For other examples of analogies with A–theory, see also Theorems 3.3.5 and 3.3.5'.

Let G be a graph on n vertices with vertex degrees $d_1, d_2, \ldots, d_n$. Let $D(G)$ be the (multi-)digraph obtained from G by adding d_i loops to the vertex i for each $i = 1, 2, \ldots, n$. It was noted in [23] that the proof of Theorem 2.5.1 can be carried out by applying the theorem on powers of the adjacency matrix to the digraph $D(G)$.

This observation can be generalized. In fact, the Q–theory of graphs G is isomorphic to the A–theory of digraphs $D(G)$. In this way we have a useful tool in establishing analogies between the Q–theory and A–theory.

We shall provide some examples.

The interlacing theorem in its original form can be applied in a specific way in Q–theory. It is sufficient to use digraphs $D(G)$ instead of graphs G [26].

Theorem 2.5.8. *The Q–eigenvalues of a graph G and the A–eigenvalues of any vertex deleted subdigraph $D(G) - v$ of $D(G)$ interlace each other.*

The same applies to the divisor concept (see [17], Chapter 4). The theory of divisors anyway deals with multidigraphs. Hence we have the following theorem [26].

Theorem 2.5.9. *The A–polynomial of any divisor of $D(G)$ divides the Q–polynomial of G.*

This theorem was implicitly used in [93] (cf. Lemma 5.6. from that paper). For some related questions concerning graph homomorphisms see [33].

2.6 Line graphs

Let G be a graph on n vertices, having m edges. As we know, the following formula holds

$$P_{L(G)}(x) = (x+2)^{m-n} Q_G(x+2). \tag{5}$$

Therefore it follows that

$$q_1 - 2, q_2 - 2, \ldots, q_n - 2, \text{ and } -2^{m-n} \tag{6}$$

are the A–eigenvalues of $L(G)$; note, if $m - n < 0$ then $q_{m+1} = \cdots = q_n = 0$ and thus the multiplicity of -2 is non–negative.

The results which we survey in this subsection are obtained indirectly via line graphs using formula (5) and results from A–theory.

This method can be used to calculate Q–eigenvalues of some graphs.

Example. The A–eigenvalues of $L(P_n) = P_{n-1}$ are $2\cos\frac{\pi}{n}j$ $(j = 1, 2, \ldots, n-1)$ and by (6) the Q–eigenvalues of P_n are $2 + 2\cos\frac{\pi}{n}j = 4\cos^2\frac{\pi}{2n}j$ $(j = 1, 2, \ldots, n)$. Alternatively, one can say that Q–eigenvalues of P_n are $4\sin^2\frac{\pi}{2n}j$ $(j = 0, 1, \ldots, n-1)$.

Example. The A–eigenvalues of $L(K_{m,n})$ are $m+n-2, (n-2)^{m-1}, (m-2)^{n-1}, -2^{(m-1)(n-1)}$ and were obtained in [17], p. 175, via the sum of graphs. By formula (6) we see that Q–eigenvalues of $K_{m,n}$ are $m+n, n^{m-1}, m^{n-1}, 0$. ■

A specific form of the interlacing theorem for Q–eigenvalues was established in [23] and a proof using line graphs was given in [24]. In this version we delete edges instead of vertices. We have an interlacing of the Q-eigenvalues of a graph with the Q-eigenvalues of an edge-deleted subgraph. This can be seen by considering the corresponding line graph, for which the ordinary interlacing theorem holds, and shifting attention to the root graph. In fact, we have the following theorem.

Theorem 2.6.1. *Let G be a graph on n vertices and m edges and let e be an edge of G. Let $q_1, q_2, \ldots, q_n$ $(q_1 \geq q_2 \geq \cdots \geq q_n)$ and $s_1, s_2, \ldots, s_n$ $(s_1 \geq s_2 \geq \cdots \geq s_n)$ be Q-eigenvalues of G and $G - e$ respectively. Then*

$$0 \leq s_n \leq q_n \leq \cdots \leq s_2 \leq q_2 \leq s_1 \leq q_1.$$

Proof. We shall prove the assertion in the case that both G and $G - e$ are connected and $m \geq n + 1$. In other cases the argument remains valid with some technical modifications.

By formula (6) the eigenvalues of $L(G)$ and $L(G-e)$ are $q_1-2, q_2-2, \ldots, q_n-2, -2^{m-n}$ and $s_1-2, s_2-2, \ldots, s_n-2, -2^{m-1-n}$ respectively. Since $L(G-e)$ is an induced subgraph of $L(G)$ the (ordinary) interlacing theorem yields

$$q_1-2 \geq s_1-2 \geq q_2-2 \geq s_2-2 \geq \cdots \geq q_n-2 \geq s_n-2 \geq -2$$

and the result follows. ■

Suppose that G' is obtained from G by *splitting a vertex* v: namely if the edges incident with v are vw $(w \in W)$ then G' is obtained from $G-v$ by adding two new vertices v_1 and v_2 and edges v_1w_1 $(w_1 \in W_1)$, v_2w_2 $(w_2 \in W_2)$, where $W_1 \cup W_2$ is a non–trivial bipartition of W.

The following theorem from [26] is analogous to a theorem for A–index, proved in [80] (see also [21] p. 56).

Theorem 2.6.2. *If G' is obtained from the connected graph G by splitting any vertex then $q_1(G') < q_1(G)$.*

Proof. We first note that $L(G')$ is a proper (spanning) subgraph of $L(G)$. Thus $\lambda_1(L(G')) < \lambda_1(L(G))$. Then the proof follows from (2). ■

Theorem 2.6.3. *Let G be a graph on n vertices with vertex degrees $d_1, d_2, \ldots, d_n$ and largest Q-eigenvalue q_1. Then*

$$\min\ (d_i+d_j) \leq q_1 \leq \max\ (d_i+d_j),$$

where (i,j) runs over all pairs of adjacent vertices of G. For a connected graph G, equality holds in either of these inequalities if and only if G is regular or semi-regular bipartite.

Proof. The line graph $L(G)$ of G has largest eigenvalue q_1-2. Consider an edge u of G which joins vertices i and j. The vertex u of $L(G)$ has degree d_i+d_j-2. Hence we have

$$\min\ (d_i+d_j-2) \leq q_1-2 \leq \max\ (d_i+d_j-2),$$

which proves the theorem. ■

This theorem is taken from [23] and a version of it appears in [96]. Theorem 2.5.7 can be classified as a result of type a while Theorem 2.6.3 is of type b.

The paper [69] contains a new and shorter proof of the fact (previously known in the literature) that the multiplicity of the A-eigenvalue 0 in line graphs of trees is at most 1. Having in mind formula (1) one can say that the multiplicity of the Q-eigenvalue 2 in trees is at most 1.

Remark. Such a transformation of a result concerning the adjacency matrix to one concerning the signless Laplacian need not always to be successful. We give an example.

Example. Let $\chi(G)$ and $\chi'(G)$ be the chromatic number and the edge chromatic number of a graph G.

Let λ_1 and λ_n be the largest and the least eigenvalue of a graph H. Then (see Theorems 3.16 and 3.18 of [17])

$$1 + \frac{\lambda_1}{-\lambda_n} \le \chi(H) \le 1 + \lambda_1.$$

Let G be a connected graph containing an even cycle or two odd cycles, and let q_1 be the largest Q-eigenvalue of G.

By Theorem 6.11 of [17] the line graph $L(G)$ of G has least eigenvalue -2. By formula (2) $L(G)$ has largest eigenvalue $q_1 - 2$. Since $\chi(L(G)) = \chi'(G)$, we have

$$1 + \frac{q_1 - 2}{2} \le \chi'(G) \le 1 + (q_1 - 2),$$

from which the following assertion follows:

$$\frac{1}{2}q_1 \le \chi'(G) \le q_1 - 1$$

.

This assertion, a result of type b, is very weak although the initial inequalities are known to be good. In fact, we have $d_{max} \le \chi'(G) \le d_{max} + 1$ where d_{max} is the maximal vertex degree; these bounds are much better than those obtained from the assertion in conjunction with Theorem 2.5.7 (a result of type a).

See also Subsection 3.1 for further examples of using line graphs to derive results in the Q–theory.

2.7 Subdivision graphs

Let G be a graph on n vertices, having m edges. Let $S(G)$ be the subdivision graph of G. As noted in [24], the following formula appears implicitly in the literature (see e.g., [17, p. 63] and [106]):

$$P_{S(G)}(x) = x^{m-n} Q_G(x^2). \tag{7}$$

Therefore it follows that

$$\pm\sqrt{q_1}, \pm\sqrt{q_2}, \ldots, \pm\sqrt{q_n}, \text{ and } 0^{m-n} \tag{8}$$

are the A–eigenvalues of $S(G)$ (with the same comment as with (2) if $m-n<0$).

It is worth mentioning that formulas (5) and (7) provide a link between A–theory and Q–theory (and corresponding spectra, see (6) and (8)). While formula (5) has been used in this context in [23], first results in using (7) have been obtained in [15].

Here we first have the following observation [26].

Theorem 2.7.1. *Let G be a connected graph with A-index λ_1 and Q-index q_1. If G has no vertices of degree 1, then $q_1 < \lambda_1^2$. If G is a cycle, then $q_1 = \lambda_1^2 = 4$. If G is a starlike tree, then $q_1 > \lambda_1^2$.*

The proof of the theorem is based on the behaviour of the A-index when all edges are subdivided (see, [62], or [17] p. 79). Subdividing an edge which lies in the path appended to the rest of a connected graph increases the A–index, otherwise decreases except if the graph is a cycle. Since the A–index of $S(G)$ is equal to $\sqrt{q_1}$ we are done.

Let $\deg(v)$ be the degree of the vertex v. An *internal path* in some graph is a path $v_0, v_1, \ldots, v_{k+1}$ for which $\deg(v_0), \deg(v_{k+1}) \geq 3$ and $\deg(v_1) = \cdots = \deg(v_k) = 2$ (here $k \geq 0$, or $k \geq 2$ whenever $v_{k+1} = v_0$).

The following two theorems are also taken from [26].

Theorem 2.7.2. *Let G' be the graph obtained from a connected graph G by subdividing its edge uv. Then the following holds:*

(i) if uv belongs to an internal path then $q_1(G') < q_1(G)$;

(ii) if $G \neq C_n$ for some $n \geq 3$, and if uv is not on the internal path then $q_1(G') > q_1(G)$. Otherwise, if $G = C_n$ then $q_1(G') = q_1(G) = 4$.

Proof. Assume first that uv is on the internal path. Let w be a vertex inserted in uv (to obtain G'). Then $S(G')$ can be obtained from $S(G)$ by inserting two new vertices, one in the edge uw the other in the edge wv. Note that both of these vertices are inserted into edges belonging to the same internal path. But then $\lambda_1(S(G')) < \lambda_1(S(G))$ (by the result of Hoffman and Smith from A–theory). The rest of the proof of (i) immediately follows from (8).

To prove (ii), assume that uv is not on the internal path. Then, if $G \neq C_n$, G is a proper subgraph of G' and hence, $q_1(G') > q_1(G)$. Finally, if $G = C_n$, then $q_1(G') = q_1(G) = 4$, as required. ■

A direct proof of the above theorem has recently appeared in [45].

Theorem 2.7.3. *Let $G(k,l)$ $(k,l \geq 0)$ be the graph obtained from a non-trivial connected graph G by attaching pendant paths of lengths k and l at some vertex v. If $k \geq l \geq 1$ then*

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

Proof. Consider the graphs $S(G(k,l))$ and $S(G(k+1,l-1))$. By using the corresponding result of [67] for the A-index, we immediately get that $\lambda_1(S(G(k,l))) > \lambda_1(S(G(k+1,l-1)))$. The rest of the proof immediately follows from (8). ■

We continue to exploit this link between the A–theory and Q–theory.

The A–indices of all graphs topologically equivalent (or homeomorphic) to some fixed graph, say G are examined in [62]. 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 [62] (which is reproduced in [17], p. 79), we arrived in [27] at:

Theorem 2.7.4. *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 $(a^{\frac{1}{2}} + a^{-\frac{1}{2}})^2$, where $a = \frac{1}{2}(d_i - 2 + \sqrt{d_i^2 - 4f_i})$, 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 2.7.5. *Let G be a connected graph without vertices of degree 1, with maximum degree Δ and the Q–index q_1. Then*

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

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 Subsection 3.2): $q_1 \geq \Delta + 1$ with equality if and only if G is a star.

Some other results of the same type will be considered in Subsection 3.3.

2.8 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 [21].

The Q–theory is usually enriched by the number of components c, as recommended at the end of Subsection 2.2 (see also [23]). This minor enrichment strengthens considerably the theory. The Q–PING, 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 [14], [23]: this is important because in the case of bipartite graphs the Q–theory is reduced to L–theory (see Subsection 2.4).

This enrichment was exploited to prove in [15] the following theorem concerning graphs with the Q–index not exceeding 4. By Proposition 6.1 of [23] 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 $K_{1,3}$.

Let n_i be the number of vertices of degree i and k_q the multiplicity of the Q-eigenvalue q.

The following relations connecting these parameters with the spectrum:

$$k_0 = b, \qquad k_4 = e + t + u + s.$$

Next, we have some relations connecting these parameters with quantities n_0, n_1, n_2, n_3:

$$v = n_0, \quad p = \frac{n_1 - 3n_3}{2}, \quad s = n_3,$$

Note also that $b = v + p + e + s$ and $c = b + t + u$.

¿From all these relations it is easy to derive the following equation:

$$2n_0 + n_1 - 3n_3 = 2c - 2k_4.$$

Previous equations for n_0, n_1, n_2, n_3 (see Remark 2 to Corollary 2.5.3) read now

$$n_0 + n_1 + n_2 + n_3 = T_0 = n, \quad n_1 + 2n_2 + 3n_3 = T_1 = 2m,$$

$$n_1 + 4n_2 + 9n_3 = T_2 - 2m, \quad n_1 + 8n_2 + 27n_3 = T_3 - 6t - 3(T_2 - 2m).$$

Using the above equations we can determine vertex degrees and, in particular, numbers of components of each type, provided the Q-spectrum and the number of components c are known. In fact, the first four out of these five equations are independent and yield unique values for n_0, n_1, n_2, n_3 and the fifth equation yields t. Then gradually all other parameters can be calculated.

Hence, we have proved the following theorem [15].

Theorem 2.8.1. *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 $k, l \geq 2,\ k \neq l$, what can be verified since the Q–spectra of cycles and paths are known [23]. ■

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 Section 1) of the Q–theory restricted to starlike trees is equal to 0.*

3 Treating problems within Q–theory

Our survey in [26], [27] and [28] shows that several important developments concerning the Q-theory have recently taken place.

Remarkable results have been obtained in finding extremal graphs for the Q-index in various classes of graphs (graphs with given numbers of vertices and edges, in particular, trees, unicyclic and bicyclic graphs, with various additional conditions, such as prescribing the values of diameter, the number of pendant edges, independence number, etc.) The basic tool is a lemma (Lemma 3.3.3) describing the behaviour of the Q-index under edge rotation. Another important tool is Theorem 3.3.5 saying that extremal graphs are nested split graphs.

Spectral characterizations of graphs and classes of graphs, together with the phenomenon of cospectrality, have been studied extensively.

The subject of Q-integral graphs has also attracted attention of researchers.

The technique of reducing problems from Q-theory to A-theory using subdivisions of graphs appears to be very fruitful as demonstrated in all three parts [26], [27] and [28] .

The divisor technique (see Theorem 2.5.9) has been used in various occasions for computing Q-eigenvalues (see, for example, [50], [74], [94]).

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 Subsection 3.3). 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 [5] 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 3.3.10 and 3.3.11: a result from A–theory has been transformed into Q–theory using subdivisions (Theorem 3.3.10) and then back into A–theory (Theorem 3.3.11).

The long derivation of the lower bound for the least eigenvalue of the signless Laplacian of a non-bipartite graph in [10] 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 [15].

Proposition 3.1. *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 [17], 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. ∎

Of course, Proposition 3.1 can be proved easily without the use of eigenvalues (by induction on the number m of edges, using a pendant edge).

It would be interesting to find other problems where Q-spectral techniques could help.

Although the Q–theory has a smaller spectral uncertainty than other frequently used spectral theories (as can be expected by the computational results from [31] – see Section 1), it seems that we do not have enough tools at the moment to exploit this advantage. Results presented in this section support such feelings.

The subsections of this section treat the following problems:
– graph operations,
– inequalities for eigenvalues,
– the largest eigenvalue,
– characterizations by eigenvalues,
– cospectral graphs,
– graph angles,
– integral graphs
– enumeration of spanning trees, and
– miscellaneous problems.

3.1 Graph operations

There are very few formulas for Q–spectra of graphs obtained by some operations on other graphs. This is quite different from the situation with A–spectrum (see, for example, [17], where the whole Chapter 2 is devoted to such formulas). Even with the L–spectrum the situation is better than in the Q-spectrum.

First, in common with many other spectral theories, the Q-polynomial of the union of two or more graphs is the product of Q–polynomials of the starting graphs (i.e. the spectrum of the union is the union of spectra of original graphs). In other words, the Q–polynomial of a graph is the product of Q–polynomials of its components.

Formula (5) connects the Q–eigenvalues of a graph with the A–eigenvalues of its line graph, while formula (7) does the same thing with respect to its subdivision graph.

If G is a regular graph of degree r, then its line graph $L(G)$ is regular of degree $2r-2$ and we have $Q_{L(G)}(x) = P_{L(G)}(x-2r+2)$. Formula (5) yields

$$Q_{L(G)}(x) = (x-2r+4)^{m-n} Q_G(x-2r+4).$$

Thus if $q_1, q_2, \ldots, q_n$ are the Q–eigenvalues of G, then the Q–eigenvalues of $L(G)$ are $q_1+2r-4, q_2+2r-4, \ldots, q_n+2r-4$ and $2r-4$ repeated $m-n$ times. We see that in line graphs of regular graphs the least Q–eigenvalue could be very large.

We do have a useful result in the case of the *sum* of graphs (for the definition and the corresponding result for the adjacency spectra see, for example, [17], pp. 65-72).

Let G_1, G_2 be graphs with adjacency matrices A_1, A_2, degree matrices D_1, D_2 and signless Laplacans Q_1, Q_2, respectively. We have $Q_1 = A_1 + D_1, Q_2 = A_2 + D_2$.

It is known that $A_1 \otimes I_2 + I_1 \otimes A_2$ is the adjacency matrix of the sum $G_1 + G_2$ of graphs G_1 and G_2. Here I_1, I_2 are identity matrices with the same order as G_1, G_2 respectively. If $\lambda_i^{(1)}, \lambda_j^{(2)}$ are eigenvalues of G_1, G_2, then the eigenvalues of $G_1 + G_2$ are all possible sums $\lambda_i^{(1)} + \lambda_j^{(2)}$.

In a quite analogous manner, $(A_1 + D_1) \otimes I_2 + I_1 \otimes (A_2 + D_2) = Q_1 \otimes I_2 + I_1 \otimes Q_2$ is the signless Laplacian of the sum $G_1 + G_2$ and if $q_i^{(1)}, q_j^{(2)}$ are Q-eigenvalues of G_1, G_2, then the Q-eigenvalues of $G_1 + G_2$ are all possible sums $q_i^{(1)} + q_j^{(2)}$, as noted in [15].

Example. The Q-eigenvalues of a path have been determined in Subsection 2.6. The sum of paths $P_m + P_n$ has eigenvalues $4(\sin^2 \frac{\pi}{2m} i + \sin^2 \frac{\pi}{2n} j)$ $(i =$

$0, 1, \ldots, m-1,\ j = 0, 1, \ldots, n-1)$. ■

For the product we have the following interesting formula [26]

$$Q_{G\times K_2}(x) = Q_G(x)L_G(x) = L_{G\times K_2}(x). \tag{9}$$

The formula is easily obtained by elementary determinantal transformations. Therefore it follows that

$$q_1, q_2, \ldots, q_n \text{ and } \mu_1, \mu_2, \ldots, \mu_n$$

are the Q–eigenvalues (and as well the L–eigenvalues) of the graph $G \times K_2$. In particular, we have that the Q–indices of G and $G \times K_2$ are equal (as is the case for A–indices of these graphs; see [17], p. 69).

While for the L–polynomial there is a formula involving the complement of the graph (see, for example, [17], p. 58), no similar formula for the Q–polynomial seems possible.

Let G be a graph rooted at vertex u and let H be a graph rooted at vertex v. $GuvH$ denotes the graph obtained from disjoint union of graphs G and H by adding the edge uv. Let $G+v$ be obtained from G by adding a pendant edge uv and let $H+u$ be obtained from H by adding a pendant edge vu. Then the following formula holds [26]

$$Q_{GuvH}(x) = \frac{1}{x}(Q_{G+v}(x)Q_H(x) + Q_G(x)Q_{H+v}(x) - (x-2)Q_G(x)Q_H(x)) \tag{10}$$

This formula is derived by applying to the line graph $L(GuvH)$ the well–known formula for the A–polynomial of the coalescence of two graphs (see, for example, [17], p. 159).

Another expression for $Q_{GuvH}(x)$ has been found in [98].

If we put $H = K_1$, we get a useless identity for $Q_{G+v}(x)$, indicating that no simple formula for $Q_{G+v}(x)$ could exist (in contrast to the formula $P_{G+v}(x) = xP_G(x) - P_{G-u}(x)$, see, for example, [17], p. 59). However, if we take $H = K_2$, we obtain $Q_{GuvH}(x) = (x-2)Q_{G+v}(x) - Q_G(x)$, which is analogous to the mentioned formula in the A–theory.

We shall need the formula

$$P_G^{(k)}(x) = k!\sum_{S_k} P_{G-S_k}(x), \tag{11}$$

where the summation runs over all k-vertex subsets S_k of the vertex set of G. For $k = 1$ the formula is well-known [17, p. 60] and says that the first derivative of the A–polynomial of a graph is equal to the sum of A–polynomials of its vertex deleted subgraphs. We can obtain (10) by induction, as noted in [23]. If we apply (11) to the line graph $L(G)$ of a graph G and use (5), we immediately obtain

$$Q_G^{(k)}(x) = k! \sum_{S_k} Q_{G-U_k}(x), \tag{12}$$

where the summation runs over all k-edge subsets U_k of the edge set of G. In particular, the first derivative of the Q–polynomial of a graph is equal to the sum of Q–polynomials of its edge deleted subgraphs. The last statement is of interest in reconstruction problems presented in Subsection 3.9.

The next theorem (see, for example, [17], p. 62) shows that a relation between $P_G(x)$ and $P_{L(G)}(x)$ can be established for certain non-regular graphs.

Theorem 3.1.1. *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*

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

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, [22], p. 15, for the source).

Theorem 3.1.2. *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*

$$P_{L(G)}(x) = (x - r_1 - r_2 + 2)(x - r_1 + 2)^{n_1-n_2}(x+2)^{n_1r_1-n_1-n_2+1}$$

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

Proof. It is easy to see that $\lambda_1 = \sqrt{r_1r_2}$ 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 3.1.2 from Theorem 3.1.1 by a straightforward calculation. ■

In addition, we obtain a formula for the Q–polynomial of a semi-regular bipartite graph [27].

Theorem 3.1.3. *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 (5) to Theorem 3.1.2. ■

A formula for the Q–polynomial of the join of two regular graphs has been obtained in [50].

The *complete product* or *join* of graphs G_1 and G_2 is the graph $G_1 \triangledown G_2$ obtained from $G_1 \cup G_2$ by joining each vertex of G_1 with every vertex of G_2.

Henceforth, $\mathbf{1}_j$ and $\mathbf{0}_j$ are the vectors of order j with all elements equal to 1 and 0, respectively, and $\mathbf{0}_{j,k}$ denotes the $j \times k$ all zeros matrix. Moreover, we denote the $j \times j$ all ones matrix by $\mathbb{J}_j$, and the $j \times k$ all ones matrix by $\mathbb{J}_{j,k}$.

Theorem 3.1.4. For $i = 1, 2$, let G_i be a r_i-regular graph on n_i vertices. Then, the characteristic polynomial of the matrix $Q(G_1 \triangledown G_2)$ is

$$Q_{G_1 \triangledown G_2}(x) = \frac{Q_{G_1}(x - n_2) Q_{G_2}(x - n_1)}{(x - 2r_1 - n_2)(x - 2r_2 - n_1)} f(x),$$

where $f(x) = x^2 - (2(r_1 + r_2) + (n_1 + n_2))x + 2(2r_1 r_2 + r_1 n_1 + r_2 n_2)$.

Proof. For $i = 1, 2$, let G_i be a r_i-regular graph with n_i vertices. Then, the signless Laplacian matrix of $G_1 \triangledown G_2$ can be represented as follows

$$Q = Q(G_1 \triangledown G_2) = \begin{bmatrix} Q(G_1) + n_2 \mathbb{I}_{n_1} & \mathbb{J}_{n_1, n_2} \\ \mathbb{J}_{n_2, n_1} & Q(G_2) + n_1 \mathbb{I}_{n_2} \end{bmatrix}.$$

Note that $\mathbf{1}_{n_i}$ is a Q-eigenvector of G_i associated to $2r_i$, $i = 1, 2$. If $\mathbf{v}$ is orthogonal to $\mathbf{1}_{n_1}$ and satisfies $Q(G_1)\mathbf{v} = q\mathbf{v}$, then $\mathbf{w} = \begin{bmatrix} \mathbf{v} \\ \mathbf{0}_{n_2} \end{bmatrix}$ is such that $Q\mathbf{w} = (q + n_2)\mathbf{w}$. Analogously, if $\mathbf{u}$ is an eigenvector of $Q(G_2)$ orthogonal to $\mathbf{1}_{n_2}$, associated to an eigenvalue q, then $\mathbf{z} = \begin{bmatrix} \mathbf{0}_{n_1} \\ \mathbf{u} \end{bmatrix}$ satisfies $Q\mathbf{z} = (q + n_1)\mathbf{z}$.

Now, for $a, b \in \mathbb{R}$, $\mathbf{w} = \begin{bmatrix} a\mathbf{1}_{n_1} \\ b\mathbf{1}_{n_2} \end{bmatrix}$ is an eigenvector of Q corresponding to an eigenvalue λ if and only if $\mathbf{w}' = \begin{bmatrix} a \\ b \end{bmatrix}$ is an eigenvector of the matrix

$M = \begin{bmatrix} 2r_1 + n_2 & n_2 \\ n_1 & 2r_2 + n_1 \end{bmatrix}$ associated to λ. Since the characteristic polynomial of M is $f(x) = x^2 - (2(r_1+r_2)+(n_1+n_2))x + 2(2r_1r_2+r_1n_1+r_2n_2)$, the result is proved. ■

Note that M is the adjacency matrix of a divisor of $D(G_1 \bigtriangledown G_2)$ (cf. Theorem 2.5.9).

3.2 Inequalities for eigenvalues

There are several ways to establish inequalities for Q–eigenvalues. This area of investigation is very promising as is the case of the other spectral theories.

Recall from Theorems 2.5.7 and 2.6.3 that the following statements hold.

Let G be a graph on n vertices with vertex degrees $d_1, d_2, \ldots, d_n$ and largest Q-eigenvalue q_1. Then

$$2 \min d_i \leq q_1 \leq 2 \max d_i.$$

For a connected graph G, equality holds in either of these inequalities if and only if G is regular.

With the same notation we have

$$\min\,(d_i + d_j) \leq q_1 \leq \max\,(d_i + d_j),$$

where (i, j) runs over all pairs of adjacent vertices of G. For a connected graph G, equality holds in either of these inequalities if and only if G is regular or semi-regular bipartite.

Some basic inequalities can be obtained from the following well-known inequality for the Rayleigh quotient

$$q_n \leq \frac{\mathbf{x}^T Q \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \leq q_1$$

which holds for any non-zero vector $\mathbf{x}$ of the corresponding dimension. Equality holds for relevant eigenvectors.

Note that if $\mathbf{x}^T = (x_1, x_2, \ldots, x_n)$, then

$$\mathbf{x}^T Q \mathbf{x} = \sum_{i \sim j,\ i<j} (x_i + x_j)^2.$$

We also have

$$q = \sum_{i \sim j,\ i<j} (x_i + x_j)^2$$

if $\mathbf{x}$ is a normalized eigenvector belonging to eigenvalue q of Q.

Let us label vertices of a graph G on n vertices so that vertex 1 has maximal degree Δ, and vertices $2, \ldots, \Delta + 1$ are the neighbours of vertex 1. Now consider the Rayleigh quotient $\mathbf{x}^T((D + A)\mathbf{x})/\mathbf{x}^T\mathbf{x}$, where $\mathbf{x} = (\Delta, 1, \ldots, 1, 1, 0, \ldots, 0)^T$, with Δ entries equal to 1. Since each vertex has degree at least 1, this quotient is at least $(\Delta(\Delta^2{+}\Delta){+}\Delta(\Delta{+}1))/(\Delta^2 + \Delta) =$

$\Delta+1$. When equality holds, vertices $2,\ldots,\Delta+1$ have degree 1 and so G is a star. Hence we have proved

$$q_1 \geq \Delta+1$$

with equality if and only if G is the star S_n.

This inequality has been derived in [24] and confirms Conjecture 4 from that paper. For an improvement see Corollary 2.7.5.

Let us now label vertices of the graph G so that vertex 1 has minimal degree δ. The value of the Rayleigh quotient for the vector $\mathbf{x}=(1,0,\ldots,0)$ is equal to δ and we arrive at the following inequality, noted in [37],

$$q_n \leq \delta.$$

The well known Courant-Weyl inequalities (cf. [17], pp. 51-52) are useful in our context.

Let $\lambda_1(X) \geq \lambda_2(X) \geq \cdots \geq \lambda_n(X)$ be the eigenvalues of a real symmetric matrix X. If A and B are real symmetric matrices of order n and if $C = A+B$, then

$$\lambda_{i+j+1}(C) \leq \lambda_{i+1}(A) + \lambda_{j+1}(A),$$

$$\lambda_{n-i-j}(C) \geq \lambda_{n-i}(A) + \lambda_{n-j}(B),$$

where $0 \leq i, j, i+j+1 \leq n$. In particular we have

$$\lambda_i(A) + \lambda_n(B) \leq \lambda_i(C) \leq \lambda_i(A) + \lambda_1(B),$$

$$\lambda_1(C) \leq \lambda_1(A) + \lambda_1(B).$$

Paper [24] is devoted to inequalities involving Q–eigenvalues. It presents 30 computer generated conjectures in the form of inequalities for Q–eigenvalues. Conjectures that are confirmed by simple results already recorded in the literature, explicitly or implicitly, are identified. Some of the remaining conjectures have been resolved by elementary observations; for some quite a lot of work had to be invested. The conjectures left unresolved appear to include some difficult research problems.

One of such difficult conjectures (Conjecture 24) has been confirmed in [10] by a long sequence of lemmas. The corresponding result reads:

Theorem 3.2.1. *The minimal value of the least Q–eigenvalue among connected non–bipartite graphs of prescribed order is attained for the odd–unicyclic graph obtained from a triangle by appending a hanging path.*

By the Interlacing Theorem (see Theorem 2.6.1) it is clear that such an extremal graph is an odd-unicyclic graph, and so one should discuss the least eigenvalue in odd-unicyclic graphs. The extremal graph is a lollipop graph. Lollipop graphs are characterized by their Q-spectra (see Subsection 3.4).

Many of the inequalities contain eigenvalues of more than one graph matrix. In particular, largest eigenvalues λ_1, μ_1 and q_1 of matrices A, L and Q, respectively, satisfy the following inequalities:

$$\mu_1 \leq q_1, \qquad 2\lambda_1 \leq q_1,$$

with equality in the first place if and only if the graph is bipartite. The first inequality was derived in [77], [79] while the second one stems from [12].

To derive the first inequality recall that

$$q_1 = \sum_{i \sim j,\ i<j} (x_i + x_j)^2$$

if $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ is a normalized eigenvector belonging to eigenvalue q_1 of Q. In a similar way we have

$$\mu_1 = \sum_{i \sim j,\ i<j} (w_i - w_j)^2$$

if $\mathbf{w} = (w_1, w_2, \ldots, w_n)^T$ is a normalized eigenvector belonging to eigenvalue μ_1 of L. The inequality follows from the obvious relation

$$\sum_{i \sim j,\ i<j} (w_i - w_j)^2 \leq \sum_{i \sim j,\ i<j} (|w_i| + |w_j|)^2 \leq \sum_{i \sim j,\ i<j} (x_i + x_j)^2.$$

Moreover, equality could hold only if $(w_i - w_j)^2 = (|w_i| + |w_j|)^2$ for each edge ij. Equivalently, we have $w_i w_j < 0$ for each edge ij and the graph is bipartite. In other direction, we have by Proposition 2.2.5 that in bipartite graphs $\mu_1 = q_1$.

The inequality $2\lambda_1 \leq q_1$, is obtained by applying the Courant-Weyl inequalities to the matrix Q represented as the sum $Q = 2A + (D - A) = 2A + L$.

The above inequalities imply that any lower bound on μ_1 is also a lower bound on q_1 and that doubling any lower bound on λ_1 also yields a valid lower bound on q_1. Similarly, upper bounds on q_1 yield upper bounds on μ_1 and λ_1. Paper [73] checks whether known upper bound on μ_1 hold also for q_1 and establishes that many of them do hold.

For example, we have the following result from [71] concerning the largest eigenvalue μ_1 of the Laplacian matrix: $\mu_1 \geq \Delta + 1$, with equality if and only if $\Delta = n - 1$. As we have seen, the same upper bound holds for q_1 but note that the case of equality for the signless Laplacian is more restrictive than that for the Laplacian.

In the next theorem we use Theorem 3.3.5' to provide an analogue of Hong's inequality from A–theory (see [63]) in Q–theory. This theorem appeared in [26].

Theorem 3.2.2. *Let G be a connected graph on n vertices and m edges. Then*

$$q_1(G) \leq \sqrt{4m + 2(n-1)(n-2)}.$$

The equality holds if and only if G is a complete graph.

Proof. Recall first that

$$\lambda_1(M) \leq \max_{1 \leq i \leq n} \{\sum_{j=1}^{n} m_{ij}\},$$

holds for any non–negative and symmetric $n \times n$ matrix $M = (m_{ij})$. In addition, the equality holds if and only if all–one vector is an eigenvector for the M–index of M.

By Theorem 3.3.5' we may assume that G is a nested split graph. Consider the matrix $Q^2 (= (D + A)^2 = D^2 + DA + AD + A^2)$. Let d_i the degree of a vertex i of G. Consider next a multigraph G^2 corresponding to matrix Q^2. Then, for the vertex i in the G^2 we have

$$\sum_{j=1}^{n} (Q^2)_{ij} = (d_i^2) + (\sum_{j \sim i} d_j) + (d_i^2) + (\sum_{j \sim i} (d_j - 1) + d_i),$$

or

$$\sum_{j=1}^{n} (Q^2)_{ij} = 2[d_i^2 + \sum_{j \sim i} d_j].$$

Assume now that $d_i < d_k$. By the definition of nested split graphs we now have:

$$d_i^2 + \sum_{j\sim i} d_j < d_k^2 + \sum_{l\sim k} d_l,$$

since this is equivalent to

$$d_i^2 - d_i + \sum_{j\in\bar{\Gamma}(i)} d_j < d_k^2 - d_k + \sum_{l\in\bar{\Gamma}(k)} d_l,$$

where $\bar{\Gamma}(v)$ stands for the closed neighbourhood of v (observe also that $\bar{\Gamma}(i) \subset \bar{\Gamma}(k)$ in our situation.

Let s be a vertex of G of maximum degree ($= n-1$). such a vertex exists since G is a nested split graph. Then we have (for any vertex i)

$$\sum_{j=1}^{n} (Q^2)_{ij} \leq 2[d_s^2 + \sum_{t\sim s} d_t] = 4m + 2(n-1)(n-2),$$

and thus

$$q_1(G)^2 \leq 4m + 2(n-1)(n-2),$$

as required.

The equality can hold only if G is a nested split graph (indeed, any other graph has the Q–index strictly less than some nested split graph). In addition, this nested split graph should be regular (otherwise, all–one vector is not its eigenvector of Q^2 for q_1^2; note $q_1^2 = 2(d_i^2 + \sum_{j\sim i} d_j)$ should hold for each i). The only graph G with these properties is a complete graph.

This completes the proof. ∎

Next we prove an inequality relating the algebraic connectivity (the second smallest L–eigenvalue) and the second largest Q-eigenvalue of a graph.

Theorem 3.2.3. *Let a be the second smallest L–eigenvalue and q_2 the second largest Q–eigenvalue of a graph G with n ($n \geq 2$) vertices. We have $a \leq q_2 + 2$ with equality if and only if G is a complete graph.*

Proof. Since $2A = Q - L$, the Courant–Weyl inequality for the third eigenvalue of $2A$ yields $2\lambda_3 \leq q_2 - a$, i.e. $a \leq q_2 - 2\lambda_3$. It was proved in [9] that for graphs with at least four vertices the inequality $\lambda_3 \geq -1$ holds with equality if and only if $G = \overline{K_{p,q} \cup rK_1}$. Now we obtain $a \leq q_2 + 2$ but equality holds only for K_n. Namely, if $p, q \geq 1$ we have by direct calculation that $a \leq n-2$ and $q_2 = n-2$. (In this case Q–eigenvalue 0 of $\overline{G}$ has the multiplicity at least 2 with an eigenvector x orthogonal to all–one vector. The vector x is an eigenvector of $q_2 = n-2$ in G). For $n = 2,\ 3$ the theorem trivially holds. ■

Theorem 3.2.3 appears in [26] and confirms Conjecture 19 of [24].

Also Conjecture 20 of [24] was treated in a similar way in [26].

Theorem 3.2.4. *Let a be the second smallest L–eigenvalue and q_2 the second largest Q–eigenvalue of a non–complete graph G with n $(n \geq 2)$ vertices. We have $a \leq q_2$.*

Proof. The inequality $a \leq q_2 - 2\lambda_3$ immediately confirms the statement of the theorem for graphs with $\lambda_3 \geq 0$. It was proved in [9] that for graphs with at least four vertices the inequality $\lambda_3 < 0$ holds if and only if the complement of G has exactly one non-trivial component which is bipartite. The case $G = \overline{K_{p,q} \cup rK_1}$ from the previous theorem is excluded here. Hence $\overline{G}$ contains a subgraph isomorphic to P_3 whose Q–eigenvalues are 3, 1, 0. By the interlacing theorem the Q–index of $\overline{G}$ is at least 3. As in the proof of previous theorem we have $q_2 = n - 2$ while $a \leq n - 3$. ■

The question of equality $(a = q_2)$ in Theorem 3.2.4 remains unsolved. Graphs for which equality holds are among the graphs with $\lambda_3 = 0$. To this group belong the graphs mentioned with Conjecture 20 in [24] (stars , cocktail–party graphs, complete bipartite graphs with equal parts). We can add here regular complete multipartite graphs in general (cocktail–party graphs and complete bipartite graphs with equal parts are special cases).

Paper [37] settled completely the question of equality in Theorem 3.2.4.

The same paper confirmed the lower bound of Conjecture 14 together with Conjectures 15, 22 and 23. This was achieved using the following lower bound for the second largest Q-eigenvalue in terms of vertex degrees:

$$q_2 \geq \frac{\Delta_1 + \Delta_2 - \sqrt{(\Delta_1 - \Delta_2)^2 + 4}}{2},$$

where Δ_1 is the largest vertex degree and Δ_2 is the second largest vertex degree. This inequality was proved by applying the interlacing theorem to matrix Q and its 2×2 principal submatrix corresponding to vertices of degrees Δ_1 and Δ_2.

A consequence of the last inequality is the inequality $q_2 \geq \Delta_2 - 1$, which is weaker but useful.

Conjectures 6,7 and 10 from [24] have been confirmed in [49].

Crucial to the resolution of these conjectures was the following result related to the largest Q-eigenvalue q_1 of a graph G.

Theorem 3.2.5. *Let G be a connected graph with n vertices and m edges. Then*

$$q_1(G) \leq \frac{2m}{n-1} + n - 2$$

with equality if and only if G is $K_{1,n-1}$ or K_n.

The inequality of Theorem 3.2.5 is better than the bound in Theorem 3.2.2. The two bounds are equal only for complete graphs. The best upper bound for q_1 in terms of n and m is implicitly given by Theorems 3.3.5 and 3.3.5'.

In order to prove Theorem 3.2.5, the authors of [49] derive first the bound

$$q_1(G) \leq max\{d_v + m_v | v \in V(G)\} \tag{13}$$

where d_v is the degree of the vertex v and m_v the average degree of neighbors of v.

The key observation in proving inequality (13) is that in the matrix $D^{-1}QD$ the row sums are equal to $d_i + m_i$ for $i = 1, 2, \ldots, n$. By the Perron-Frobenius theory of non-negative matrices the largest eigenvalue is bounded above by the maximal row sum and we obtain (13) since the largest eigenvalue of $D^{-1}QD$ is equal to $q_1(G)$.

As noted, paper [73] checks whether known upper bounds on largest Laplacian eigenvalue μ_1 hold also for q_1 and establishes that many of them do hold, in particular inequality (13). However, the authors of [73] claim that (13) was implicitly proved in [34]. Actually, the bound (13) was derived explicitly in [37].

To complete the proof of Theorem 3.2.5 the authors of [49] use another inequality by K.Ch. Das [35]:

$$max\{d_v + m_v | v \in V(G)\} \leq \frac{2m}{n-1} + n - 2.$$

Some results related to Conjecture 7 can be found in [1].

At the moment the following conjectures of [24] remain unconfirmed: parts related to upper bounds in Conjectures 8, 9, 11, 14 together with Conjectures 17, 18, 21, 25, 26. See Appendix 2 for a detailed survey on the current status of the conjectures.

The paper [3] discusses the same set of conjectures and presents some new ones.

A new set of conjectures involving the largest Q–eigenvalue appears in [59]. The Q-index is considered in connection with various structural invariants, such as diameter, radius, girth, independence and chromatic number, etc. Out of 152 conjectures, generated by computer (i.e. the system AGX), many of them are simple or proved in [59], so that only 18 remained unsolved. An additional conjecture of this type has been resolved in [60]; it is proved that $q_1(G) \leq 2n(1 - 1/k)$, where k is the chromatic number, thus improving an analogous inequality for the A-index (cf. [17], p. 92).

Recall that the *total* graph of G, denoted by $T(G)$, is the graph with vertex set corresponding to union of vertex and edge sets of G, with two vertices of $T(G)$ adjacent if the corresponding elements in G are adjacent or incident. It is also well known that $T(G) = S(G)^2$ (see [61]), where $S(G)$ is a subdivision of G, while square stands for the 2-power graph (so H^2 has the same vertex set as H, with two vertices being adjacent if their distance in H is ≤ 2). The above relation implies that

$$Q(T(G)) = A^2(S(G)) + Q(S(G))$$

where $A(H)$ and $Q(H)$ denote the adjacency matrix and the signless Laplacian of the graph H respectively. Therefore by using the Courant-Weyl inequalities we get that

$$q_1(T(G)) \leq \lambda_1(A^2(S(G))) + q_1(S(G)) = \lambda_1^2(S(G)) + q_1(S(G)).$$

Since $\lambda_1(S(G)) = \sqrt{q_1(G)}$ (see (8)), we arrive at the following result [28].

Theorem 3.2.6. *Let $S(G)$ and $T(G)$ be the subdivision and total graph of G. Then*

$$q_1(T(G)) \leq q_1(G) + q_1(S(G)).$$

This inequality is best possible since equality holds for cycles C_n $(n \geq 3)$.

Some further inequalities for other eigenvalues can be obtained in the same way.

Inequalities involving the clique number, independence number and the signless Laplacian eigenvalues are obtained in [68].

3.3 The largest eigenvalue

When applying the Perron-Frobenius theory of non-negative matrices (see, for example, Section 0.3 of [17]) to the signless Laplacian Q, we obtain the same or similar conclusions as in the case of the adjacency matrix. In particular, in a connected graph the largest eigenvalue is simple with a positive eigenvector. The largest eigenvalue of any proper subgraph of a connected graph is smaller than the largest eigenvalue of the original graph, an observation which follows from Theorems 0.6 and 0.7 of [17].

The following proposition was proved in [23].

Proposition 3.3.1 *Let q_1 be the largest Q-eigenvalue of a graph G. The following statements hold:*
(i) $q_1 = 0$ if and only if G has no edges,
(ii) $0 < q_1 < 4$ if and only if all components of G are paths,
(iii) for a connected graph G we have $q_1 = 4$ if and only if G is a cycle or $K_{1,3}$.

Proof. (i) is trivial. In this case, of course, all Q-eigenvalues of G are equal to 0.

The eigenvalues of $L(P_n) = P_{n-1}$ are $2\cos\frac{\pi}{n}j$ $(j = 1, 2, \ldots, n-1)$ and by (2) the Q-eigenvalues of P_n are $2+2\cos\frac{\pi}{n}j$ $(j = 1, 2, \ldots, n)$. Hence for paths we have $q_1 < 4$. For cycles and for $K_{1,3}$ we have $q_1 = 4$. By the interlacing theorem these graphs are forbidden subgraphs in graphs for which $q_1 < 4$, and this completes the proof of (ii).

To prove the sufficiency in (iii) we use the strict monotonicity of the largest Q-eigenvalue when adding edges to a connected graph. First, G cannot contain a cycle without being itself a cycle. If G does not contain a cycle, it must contain $K_{1,3}$ since otherwise G would be a path and we would have $q_1 < 4$. Finally G must be $K_{1,3}$ since otherwise we would have $q_1 > 4$.

This completes the proof. ■

Several elementary inequalities for Q-eigenvalues are given in [12]. Among other things, it is proved that the Q-index q_1 of a connected graph on n vertices satisfies the inequalities

$$2 + 2\cos\frac{\pi}{n} \le q_1 \le 2n - 2.$$

The lower bound is attained for P_n, and the upper for K_n. The first fact is a consequence of Proposition 3.3.1 while the other follows from the mentioned behaveour of the largest eigenvalue. Q-spectra of P_n and K_n have been determined in Subsections 2.3 and 2.6.

By Proposition 3.3.1, 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 [98] managed to obtain results in the range up to 4.5. We first give some definitions.

Following [101], 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 [98].

Theorem 3.3.2. *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 [98] which says that a connected graph whose A–index lies in the interval $(2, \frac{3}{2}\sqrt{2})$ is an open or a closed quipu, or a dagger. Daggers are eliminated by the Corollary to Theorem 2.7.5 and the rest immediately follows by the use of formula (8). Note that $(\frac{3}{2}\sqrt{2})^2 = 4.5$.

The paper [98] contains several refinements of Theorem 3.3.2. The interval $(4, 4.5)$ is subdivided by points $\tau = 2 + \sqrt{5} \approx 4.24$ and $\epsilon = 2 + \frac{1}{3}((54 - 6\sqrt{33})^{\frac{1}{3}} + (54 + 6\sqrt{33})^{\frac{1}{3}}) \approx 4.38$ into intervals $(4, \tau]$, $(\tau, \epsilon]$ and $(\epsilon, 4.5)$. In the interval $(4, \tau]$ we have only open quipus with exactly one vertex od degree 3 and this vertex has two neighbours of degree 1. In the interval $(\tau, \epsilon]$ appear only some of the open quipus with at most 3 vertices od degree 3 while in the interval $(\epsilon, 4.5)$ we encounter only open or closed quipus. The results are obtained by considering limit points of the Q-index of graphs in question.

We shall consider now the behavior of the largest eigenvalue q_1 of Q under some graph perturbations. We have

$$q_1 = \sup_{\mathbf{x} \in I\!R^n \setminus \{\mathbf{0}\}} \frac{\mathbf{x}^{\mathbf{T}} Q \mathbf{x}}{\mathbf{x}^{\mathbf{T}} \mathbf{x}} = \max_{||\mathbf{x}||=1} \mathbf{x}^{\mathbf{T}} Q \mathbf{x}. \tag{14}$$

(see, for example, [21]). The equality holds here if and only if $\mathbf{x}$ is an eigenvector of G for q_1. Generally, it is natural to expect that q_1 changes when G is perturbed, and we can ask whether q_1 increases or decreases if

G is modified. Here we consider how q_1 changes when some edges of G are relocated.

Let G' be a modification of G, and let Q' be the corresponding signless Laplacian $A' + D'$, with largest eigenvalue q_1'. In what follows, we assume (without loss of generality) that G is connected, and we take $\mathbf{x}$ to be the principal eigenvector of G (that is, the unit positive eigenvector corresponding to q_1). From (14) we obtain:

$$q_1' - q_1 = \max_{||\mathbf{y}||=1} \mathbf{y}^T Q' \mathbf{y} - \mathbf{x}^T Q \mathbf{x} \geq \mathbf{x}^T (A' - A)\mathbf{x} + \mathbf{x}^T (D' - D)\mathbf{x}, \qquad (15)$$

with equality if and only if $\mathbf{x}$ is also the principal eigenvector for Q'.

On basis of this observation, we obtain [23]:

Lemma 3.3.3. *Let G' be a graph obtained from a connected graph G (on n vertices) by rotating the edge rs (around r) to the position of a non-edge rt. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ be the principal eigenvector of G. If $x_t \geq x_s$ then $q_1' > q_1$.*

Proof: From (15) we immediately obtain

$$q_1' - q_1 \geq 2(2x_r + x_s + x_t)(x_t - x_s).$$

Since x_r, x_s and x_t are positive and $x_t \geq x_s$ we obtain $q_1' \geq q_1$. Equality holds only if $\mathbf{x}$ is an eigenvector of G' for $q_1' = q_1$. But then, from the eigenvalue equations applied to the vertex t (or s) in G' and G we find $(q_1' - q_1)x_t = x_r + x_t$ (or $(q_1' - q_1)x_s = -x_r - x_s$), and this is a contradiction. This completes the proof. ∎

Lemma 3.3.3 appeared in a bit different form also in [64].

In addition, we can prove [23]:

Proposition 3.3.4. *Let G' be a graph obtained from a graph G by a local switching of edges ab and cd to the positions of non-edges ad and bc. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ be a principal eigenvector of G. If $(x_a - x_c)(x_b - x_d) \geq 0$ then $q_1' \geq q_1$, with equality if and only if $x_a = x_c$ and $x_b = x_d$.*

Proof: From (15) we have

$$q_1' - q_1 \geq 2(x_a - x_c)(x_b - x_d),$$

and the first assertion follows. The second assertion follows from the eigenvalue equations for G and G'. ∎

The following two theorems have been proved in [23], [24] in the same way as the corresponding results in A-theory (Theorems 2.4 and 2.4' from [83]).

Theorem 3.3.5. *Let G be a graph with fixed numbers of vertices and edges, with maximal largest Q-eigenvalue. Then G does not contain, as an induced subgraph, any of the graphs: $2K_2$, P_4 and C_4.*

Moreover, we also have

Theorem 3.3.5$'$. *Let G be a connected graph with fixed numbers of vertices and edges, with maximal largest Q-eigenvalue. Then G does not contain, as an induced subgraph, any of the graphs: $2K_2$, P_4 and C_4.*

The proof of these theorems is given in the following two lemmas.

Assume now that G is a graph whose Q–index is maximal among all graphs with n vertices and m edges ($m > 0$).

Lemma 3.3.6. *Under the above assumptions, either G is a connected graph or G has exactly one non-trivial component.*

Proof: Let C be a component of G with index $\mu_1 = \mu_1(G)$. Suppose, by the way of contradiction, that G has another non-trivial component C'. Then G has an eigenvector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ corresponding to μ_1 such that $x_i > 0$ for all $i \in V(C)$ and $x_i = 0$ for all $i \notin V(C)$.

Now let t be a vertex of C and let rs be an edge in C'. Consider the graph G' obtained from G by replacing rs with the edge rt. Since $x_t > 0$ and $x_r = x_s = 0$, Equation (14) shows that $q_1(G') > q_1$, what represents a contradiction. ■

In view of this lemma, it suffices to consider the unique non-trivial component of G, and so we now assume further that G is connected.

Lemma 3.3.7. *The graph G does not contain P_4, $2K_2$ or C_4 as an induced subgraph.*

Proof. Let u be a vertex of G corresponding to a maximal coordinate of the principal eigenvector. The vertex u has degree $n-1$ for if there were a vertex v, non-adjacent to u, by rotating an edge vw to the position vu and applying Lemma 3.3.3 we would force a contradiction.[7]

[7]This observation, communicated to us by B.-S.Tam, has shortened the original proof of this lemma from [24].

Now suppose, by the way of contradiction, that G contains a graph $F \in \{P_4, 2K_2, C_4\}$ as an induced subgraph. Let $\mathbf{x}$ be the principal eigenvector of G, and let r, s, t, w be the vertices of F. Without loss of generality, $x_s = \min_{v \in V(F)} x_v$. Additionally, the structure of F allows us to assume that r is a neighbour of s but not of t. Now let G' be the graph obtained from G by rotating the edge rs (around r) to the non–edge position rt. By Lemma 3.3.3, we have $q_1(G') > q_1(G)$. Since G' is connected, this is a contradiction and we are done. ■

In order to explain these results we need the following definition.

Definition. A *nested split graph* with parameters n, q, k; $p_1, p_2, \ldots, p_k$; $q_1, q_2, \ldots, q_k$, denoted by $NS(n, q, k; p_1, p_2, \ldots, p_k; q_1, q_2, \ldots, q_k)$, is a graph on n vertices consisting of a clique on q vertices and k cocliques $S_1, S_2, \ldots, S_k$ of cardinalities $p_1, p_2, \ldots, p_k$ respectively; vertices in these cocliques have $q_1, q_2, \ldots, q_k$ neighbors in the clique respectively, the set of neighbors of S_{i+1} being a proper subset of the set of neighbors of S_i for $i = 1, 2, \ldots, k-1$.

We have also an equivalent definition.

Definition. A graph G with the edge set E_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 $p \leq q$.

This definition is used in [21], where the graphs in question were called graphs with a *stepwise* adjacency matrix. Some other definitions and terms are used in the literature, e.g. degree maximal graphs, threshold graphs. Note that graphs with a stepwise adjacency matrix are exactly the nested split graphs. Moreover, S.Simić et al. [83] have recently proved the following proposition. Alternatively, it follows immediately from the stepwise nature of an adjacency matrix.

Proposition A. *A graph is a nested split graph if and only if it does not contain as an induced subgraph any of the graphs $P_4, 2K_2, C_4$.*

Since the set of forbidden subgraphs in this proposition, namely $\{P_4, 2K_2, C_4\}$, is closed under the operation of complementation the following proposition is straightforward.

Proposition B. *The complement of a nested split graph is also a nested split graph.*

From Theorems 3.3.5 and 3.3.5′ we see that a graph G with maximal largest Q-eigenvalue is a nested split graph in the first case and a nested split graph with possibly some isolated vertices added, in the second.

Theorems 3.3.5 and 3.3.5′ have been announced in [23] and complete proofs appear in [24]. The result has been repeated independently in [93]. In particular, by Theorem 3.3.5′ we easily identify the graphs with maximal Q–index within trees, unicyclic graphs and bicyclic graphs (on a fixed number of vertices). Namely, each of these sets of graphs has a unique nested split graph (see [24]).

Theorem 3.3.8. *Let G be a graph with maximal Q–index among connected graphs with n vertices and m edges.*

(i) If $m = n - 1$ then G is the star $S_n = K_{1,n-1}$.

(ii) if $m = n$ then G is the graph S_n^+ obtained from S_n by adding an edge;

(iii) if $m = n + 1$ then G is the graph obtained from S_n by adding two adjacent edges.

The result for bicyclic graphs has again been independently rediscovered in [41].

Thus Theorem 3.3.8 identifies the trees, the unicyclic graphs and the bicyclic graphs of order n with maximal Q-index. In particular, we can confirm the upper bounds in Conjectures 2 and 3 from [24]: the only tree which is a nested split graph is a star and the only unicyclic graph which is a nested split graph is a star together with an additional edge. The lower bounds in Conjectures 1 and 2 are confirmed by Proposition 3.3.1: the graphs with minimal Q-index among trees and among unicyclic graphs are the path and the cycle respectively.

Next we shall compare the considered problem with the corresponding one in A-theory. For that purpose we define some special nested split graphs.

A *pineapple* with parameters n, q ($q \leq n$), denoted by $PA(n, q)$, is a graph on n vertices consisting of a clique on q vertices and a stable set on the remaining $n-q$ vertices in which each vertex of the stable set is adjacent to a unique vertex of the clique.

A *fanned pineapple of type* i ($i = 1, 2$) with parameters n, q, t ($n \geq q \geq t$) , denoted by $FPA_i(n, q, t)$, is a graph (on n vertices) obtained from a pineapple $PA(n, q)$ by connecting a vertex from the stable set by edges to t vertices of the

1) clique, with $0 \leq t \leq q - 2$, for $i = 1$,

2) stable set, with $0 \leq t < n - q$, for $i = 2$.

We have $FPA_i(n, q, 0) = PA(n, q)$ for $i = 1, 2$.

Let $\mathcal{H}(n, n+k)$ be the set of all connected graphs with n vertices and $n+k$ edges, and let $G_{n,k}$ and $H_{n,k}$ be the graphs defined in [20]. These graphs are fanned pineapple graphs of types 1 and 2 respectively: using above notation we have $G_{n,k} = FPA_1(n, d, t)$ and $H_{n,k} = FPA_2(n, 1, k + 1)$.

It was proved in [20] that for given k and sufficiently large n the graph $H_{n,k}$ has maximal A-index among graphs in $\mathcal{H}(n, n + k)$. Otherwise, the graph $G_{n,k}$ can play this role. It was conjectured in [2] that for all n, k the extremal graph is either $G_{n,k}$ or $H_{n,k}$ or both.

Generally, we know that extremal graphs for the problem of maximizing the A-index among graphs with fixed numbers of vertices and edges have a *stepwise* adjacency matrix (cf. [21], pp. 60–74).

We see that both the A–index and Q–index attain their maximal values for nested split graphs. The question arises whether these extremal nested split graphs are the same in both cases. For small number of vertices this is true as existing graph data show. However, among graphs with $n = 5$ vertices and $m = 7$ edges there are two graphs (No. 14 and No. 15 in Table 1 in Appendix) with maximal Q–index while only one of them (No. 14) yields maximal A–index. In fact, for any $n \geq 5$ and $m = n + 2$ there are two graphs with a maximal Q–index [93].

Papers [11] and [94] further elaborate these problems.

Explicit expression for the characteristic polynomial of the signless Laplacian of a nested split graph (or threshold graphs) in terms of vertex degrees is derived in [94]. In addition, it was proved that $q_1(G_{n,k}) < q_1(H_{n,k})$ for $3 \leq k \leq n - 3$ what is quite different from the situation in A-theory. It is announced in [11] that with the same limitation the graph $H_{n,k}$ has maximal Q-index among graphs in $\mathcal{H}(n, n+k)$. Graphs which maximize the Q-index among graphs in $\mathcal{H}(n, n + k)$ are completely determined for $k = 0, 1, 2, 3$.

The announced result indicates that the problem of maximizing the index in $\mathcal{H}(n, n + k)$, although very difficult in both cases, is easier in Q-theory than in A-theory.

Next we present a result in Q-theory which is analogous to a result in A-theory from [67]. According to [27] we have

Theorem 3.3.9. *Let u, v be the adjacent vertices of a connected graph G, both of degree at least two. Let $G(k, l)$ $(k, l \geq 0)$ be the graph obtained from G by attaching pendant paths of lengths k and l at u and v, respectively. If $k \geq l \geq 1$ 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 [67], 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. ■

Similarly, we can use a result for θ–graphs from [82] 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 $m_1 \geq m_2 \geq \cdots \geq m_{k-1} \geq 2$; in contrast $m_k \geq 1$). Now we have [27]:

Theorem 3.3.10. *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 $G' = \Theta(m'_1, m'_2, \ldots, m'_k)$. Consider the graphs $S(G)$ and $S(G')$. Using Theorem 1 from [82] (see also [21] 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. ■

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 [82] 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 $\Theta(m_1 + 1, m_2 + 1, \ldots, m_k + 1)$.

Then, since $\lambda_1(L(G)) = q_1(G) - 2$, we immediately get [27]:

Theorem 3.3.11. *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 $\hat{B}$).

First we have that the minimum vertex degree of $\hat{B}$ is greater than 1, for otherwise we can delete any such vertex from $\hat{B}$ (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 2.7.2). Thus we get a graph from $\mathcal{B}_n$ with a smaller Q–index, a contradiction. Therefore, $\hat{B}$ 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 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 $q_1(G) = \lambda_1^2(S(G))$ (for any G) we can, in order to identify $\hat{B}$, 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 [82] the minimal A–index of graphs of type (i) is less than the minimal A–index of graphs of type (ii). So $\hat{B}$ cannot be of type (ii). From [81] (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 [82], 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 $\hat{B}$ 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 [27]:

Theorem 3.3.12. *Let $\mathcal{B}_n$ be the set of bicyclic graphs on n vertices. If $\hat{B} \in \mathcal{B}_n$ is a graph with minimal Q–index, then $\hat{B}$ 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 $\frac{n}{3} \leq p \leq \frac{n+2}{3}$.

The study of the largest Q-eigenvalue remains an attractive topic for researchers. In particular, the extremal values of the Q-index in various classes of graphs, and corresponding extremal graphs, have been investigated.

The maximal signless Laplacian spectral radius of graphs with given diameter has been determined in [48].

The maximal signless Laplacian spectral radius of graphs with given matching number has been determined in [103].

In [47] the class of unicyclic graphs with a given number of pendant vertices or given independence number was considered. Graphs with maximal Q-index are determined.

Independently, the same results have been obtained in [104], in a more general setting. Graphs with maximal Q-index in the class of graphs with given vertex degrees are determined and these results are applied to unicyclic graphs.

In [44] the class of bicyclic graphs with a given number of pendant vertices was considered. Graphs with maximal Q-index are determined.

A graph G is a *quasi-k-cyclic* graph if it contains a vertex (say r, the root of G) such that $G - r$ is a k-cyclic graph, i.e. a connected graph with cyclomatic number k ($= m - n + 1$, where n is the number of vertices and m the number of its edges). For example, if $k = 0$, the corresponding graph is a *quasi-tree*. In [52] quasi-k-cyclic graphs having the largest Q-index are identified for $k \leq 2$.

The task of finding maximal Q-index in various classes of graphs has been considered also in the references [8], [42], [102] (see the titles of these papers to identify the classes considered).

3.4 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 [31] 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 ($m = \binom{n}{2}$) are Q–DS. In addition, the same holds for $m = 1$ and for $m = \binom{n}{2} - 1$.

Let $e(G)$ be the number of distinct Q-eigenvalues of a graph G.

If $e(Q) = 1$ then obviously G is a graph without edges.

If $e(Q) = 2$ then the minimal polynomial of Q has the form $x^2 + ax + b$, and so $A^2 + AD + DA + D^2 + aA + aD + bI = O$. For distinct i, j this gives $a_{ij}^{(2)} + (d_j + d_i + a)a_{ij} = 0$, and so there are no vertices i, j at distance 2. Hence $G = K_n$.

Alternatively, by Theorem 2.5.4 , the diameter D of G is bounded above by $e(Q) - 1$, and if $e(Q) = 2$ it follows that $D = 1$ what means that G is a complete graph.

This statement has been obtained in [24] (cf. Conjecture 27) and also earlier in [30].

The path P_n, and, more generally, the union of paths is Q–DS. The proof, given in [31], is longer than necessary. It is sufficient to refer to Proposition 3.3.1 which says that in graphs with Q–index smaller than 4 all components are paths.

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 [18]. Due to this fact, it is not true[8] that the union of paths is A–DS, as

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

wrongly stated in [31]. 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 [16]). 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" [27].

Theorem 3.4.1. *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.

Starlike trees are DS in the L–theory [75], while this is not proved for the A–theory [100]. Recently the paper [76] has appeared where it is proved that T–shape trees (starlike trees with maximal degree equal to 3) are Q-DS except for $K_{1,3}$ and an infinite series of T-shape trees. One can verify this assertion by reducing the problem via subdivision graphs to A–theory and then using results of [100]. Indeed, the subdivision graph of a T–shape tree is again a T–shape tree and A–cospectral mates, described in [100], yield the corresponding Q–cospectral mates from [76]. Hence, our method of using subdivision graphs and results from [100] proves these results in a much simpler way. [9]

[9] As a curiosity we quote related paragraphs from [27] and [28].

Part II: Concerning the Q–theory, a private communication of G.R. Omidi is cited in [32] 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 [100]. Indeed, the subdivision graph of a T–shape tree is again a T–shape tree and an A–cospectral mate, described in [100], is not a subdivision graph except for $K_{1,3}$.

Part III: Recently the paper [76] has appeared. Contrary to his previous private communication, mentioned above, G.R. Omidi proves now that not only $K_{1,3}$ but an infinite series of T-shape trees which are not DS does exist. When confirming the original private communication we made a mistake. The mistake was that the A–cospectral mate, The content of this example can be formulated more generally (cf. also [99]):

Proposition 3.4.2. *(i) If the subdivision graph $S(G)$ is A–*DS*, then the graph G is Q–*DS*.*

*(ii) If any graph A-cospectral to $S(G)$ is not a subdivision of some graph, then the graph G is Q–*DS*.*

*(iii) If the graph G is Q–*DS *and if any graph A-cospectral to $S(G)$ is a subdivision of some graph, then $S(G)$ is A-*DS*.*

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 Subsection 2.4, 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 [105]. It was proved that the lollipop graph is determined by its Q–spectrum. Note that the lollipop graph is determined by its A–spectrum, as proved in [6] and [58] before, so that characterization with Q-spectrum follows immediately by Proposition 4.3.2,(i), since the subdivision of a lollipop graph is again a lollipop graph. However, this technique was not known at the time when [105] was written so that the problem is solved within the Q-theory. Nevertheless, it seems that this proof is much shorter than the corresponding one in A-theory and [105] is still important. Unfortunately, the proof cannot be carried out to A-theory via subdivision graphs since a subdivision graph could be A-cospectral to a graph which is not a subdivision graph. (This remark provides a negative solution to the Problem 3.1 from [99]).

Remark. With our own modification a sketch of the proof that the lollipop graph is determined by its Q–spectrum could look as follows.

By Theorem 2.6.3 we have $q_1 < 5$ for a lollipop graph H. If we delete an edge from the cycle incident to the vertex of degree 3 of H and apply the Interlacing Theorem (see Theorem 2.6.1), we get $q_2 < 4$.

---

mentioned above, is still a subdivision graph yielding the Q-cospectral mate found in [76]. Hence, our method of using subdivision graphs and results from [100] do confirm the results from [76]. In fact our method proves these results in a much simpler way.

Given the spectrum of a lollipop graph H, the inequality $q_1 \geq \Delta+1$ from Subsection 3.2 yields $\Delta \leq 3$ for any graph G with such a spectrum. Now we can apply equations from Remark 2 in Subsection 2.5 to determine vertex degrees of G. The case $n_0 > 0$ leads to a contradiction and with $n_0 = 0$ we get vertex degrees of H.

If G is disconnected, a cycle would appear as a component and we would get $q_2 \geq 4$, a contradiction. Hence G is connected. If $q_n = 0$, G is a lollipop graph with an even cycle and the girth is determined by Proposition 3.9.2. In the remaining case we apply the formula from the proof of Proposition 3.9.5. to determine the girth.

Hence G is a lollipop graph. ∎

Graphs consisting of two cycles with just a vertex in common are called ∞-*graphs* in [99]. It is proved that ∞-graphs without triangles are characterized by their Laplacian spectra and that all ∞-graphs, with one exception, are characterized by their signless Laplacian spectra.

3.5 Cospectral graphs

Statistics on cospectral graphs, given in the introduction, 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 [23]. Five Q–PINGs, all consisting of connected graphs on 6 vertices, were identified in [15]. All these PINGs can be found in the Appendix.

Formulas (5) and (7) 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 [15]) yield two A–PINGs whose graphs belong to restricted classes of graphs (line and subdivision graphs).

Note that formula (7) immediately verifies

Proposition 3.5.1. *Graphs G and H are Q-cospectral if and only if $S(G)$ and $S(H)$ are A-cospectral.*

This statement is a bit different from the corresponding statement for line graphs based on formula (5) (cf. Proposition 2.2.7).

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 Subsection 3.1, 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 [107] 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 $8 \leq n \leq 21$:

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 [107] cannot be justified since it is known [70] 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 [18]. 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 [86] 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.

The paper [76] provides an infinite series of pairs of Q-cospectral graphs, one graph in each pair being bipartite and the other non-bipartite. The only such pair of Q-cospectral graphs, previously noted in the literature, consists of the graphs $K_{1,3}$ and $C_3 \cup K_1$.

Assume that G is not DS. We shall say that G is *minimal* graph which is not determined by its spectrum if removing of any subset of its components implies that the remaining graph is DS. In what follows, only the minimal graphs which are not DS will be considered, since any other such graph can be easily recognized by the presence of some of minimal graphs.

We consider the class of graphs whose each component is either a path or a cycle. We shall classify the graphs from the considered class into those which are determined, or not determined, by their spectrum.

For signless Laplacian spectra the problem is implicitly solved in [27] (see here Theorem 2.8.1 and the example after it) and explicitly in [29]. It follows that $C_{2k} \cup 2P_l$ and $C_3 \cup K_1$ are minimal non-DS graphs. Using subdivisions of graphs (which reduces the problem to usual spectrum), and having in mind relations between the spectra, one can see that no other minimal non–DS graphs exist. Moreover, these considerations solve also the problem for the set of graphs whose largest signless Laplacian eigenvalue does not exceed 4 (cf. Theorem 3.3.1). The only additional connected non-DS graph is $K_{1,3}$ which is cospectral to $C_3 \cup K_1$.

As shown in [29], where A-, L- and Q-eigenvalues are considered, in the class of graphs whose each component is a path or a cycle, the cospectrality as a phenomenon the most rarely appears in the case of signless Laplacian spectrum.

3.6 Q-theory enriched by angles

This subsection is completely written following the corresponding parts from [27], [28].

Graph angles can be introduced for the signless Laplacian matrix in the same way as for the adjacency matrix (see, for example, [21] 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 $P_i P_j = O$ if $i \neq j$, and $P_i^2 = P_i = P_i^T$ $(1 \leq i, j \leq m)$. If $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$ are the vectors of the standard basis in $\mathbb{R}^n$, 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 3.6.1. *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*

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

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

$$Q^k = \kappa_1^k P_1 + \kappa_2^k P_2 + \cdots + \kappa_m^k P_m \quad (k = 0, 1, 2, \ldots). \tag{16}$$

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 (16) (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 (16), 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. ■

This theorem from [27] is quite analogous to a similar theorem proved in the A–theory [88]. 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 vertex eccentricities 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 Groetzsch-Graph (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

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 Theorem 2.5.4 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, [21], 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

$$Q_{G+v}(x) = Q_G(x)(x - 1 - x\sum_i \frac{\gamma_{ij}^2}{x - \kappa_i}). \tag{17}$$

This formula can be used to rewrite formula (10) and also independently, for calculating $Q_{G+v}(x)$. (Recall also from Subsection 3.1 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, [21], 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.

T

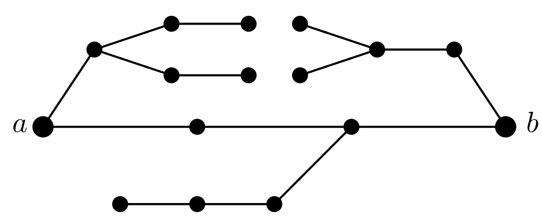

Fig. 1: The smallest Q-endospectral tree

By formula (10) 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 [70] to prove that also almost all trees have a Q–cospectral mate. The difference 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 (17) 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.

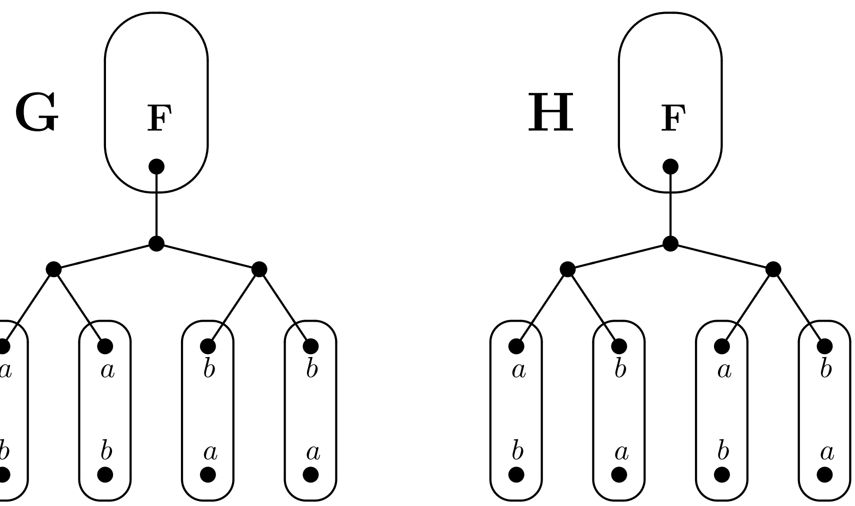

Fig. 2: Q–cospectral graphs with same angles

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 [21], pp. 112-113, can be adapted to work also in the

Q–theory.

We have considered in Subsection 2.8 the enriched theory Q_c, the Q-theory enriched by the number of components c. Now we consider the enriched theory Q_Γ, the Q-theory enriched by the Q–angle matrix Γ.

The next theorem shows that the theory Q_Γ is at least as strong as the theory Q_c, i.e. everything that can be proved for a graph in Q_c can also be proved in Q_Γ [28].

Theorem 3.6.2. *The number of components c of a graph can be determined by Q-eigenvalues and Q-angles.*

Proof. We need some definitions and a lemma.

A partition of the vertex set of G is called *admissible* if no edge of G connects vertices from different parts; and subgraphs induced by parts of an admissible partition are called *partial graphs*. (Thus a partial graph is a union of components, and the components are induced by the parts of the finest admissible partition.) The spectra and angles of these partial graphs are called the *partial spectra* and *partial angles* corresponding to the original partition.

Given a graph G, there is a uniquely determined admissible partition of G such that (i) in each partial graph all components have the same index, and (ii) any two partial graphs have different indices. This partition is called *index separating partition.*

Lemma 3.6.3. Given the eigenvalues, angles and an admissible partition of the graph G, the corresponding partial spectra and partial angles of G are determined uniquely.

Proof. We know from formula (16) that the (j,j)-entry $q_{jj}^{(k)}$ of Q^k is $\sum_{i=1}^{m} \gamma_{ij}^2 \kappa_i^k$ $(j = 1, 2, ..., n)$. Let $j \in \tilde{V}$, where $\tilde{V}$ is the set of vertices of a partial graph $\tilde{G}$: then by Theorem 2.5.1 $q_{jj}^{(k)}$ is the number of j-j semi-edge walks of length k in G and hence also in $\tilde{G}$. The spectral moments of $\tilde{G}$ are therefore $\sum_{j\in\tilde{V}} q_{jj}^{(k)}$ $(k \in I\!N)$, and these determine the spectrum of $\tilde{G}$. Moreover $q_{jj}^{(k)} = \sum_{i=1}^{t} \tilde{\gamma}_{ij}\tilde{\kappa}_i^k$ $(j \in \tilde{V})$ where $\tilde{\kappa}_1, ..., \tilde{\kappa}_t$ are the distinct eigenvalues of $\tilde{G}$ and $\tilde{\gamma}_{ij}$ is the angle of $\tilde{G}$ corresponding to $\tilde{\kappa}_i$ and j. These equations now determine $\tilde{\gamma}_{1j}, \ldots, \tilde{\gamma}_{tj}$ $(j \in \tilde{V})$.

This completes the proof of the lemma. ■

Vertices belonging to components whose index coincides with the index κ_1 of G can be identified from the angle sequence for κ_1: they are the vertices j for which the angle γ_{1j} is non-zero. The bipartition of G in which one part consists of these vertices is an admissible partition, and so we can apply Lemma 3.6.3 to determine the corresponding partial spectra and partial angles. In particular, we obtain the eigenvalues and angles of the subgraph induced by the other part of the bipartition. We can now apply the above arguments to this subgraph and repeat the procedure until we obtain the index separating partition.

In each partial graph determined by the index separating partition the number of components is equal to the multiplicity of its index. Hence we obtain the number of components of the whole graph.

This completes the proof of Theorem 3.6.2. ■

The proof is carried out analogously to the proof of the corresponding result for A-theory (see [21], Lemma 4.4.1, Theorem 4.4.3 and Remark 4.4.4). In the proofs the walks are replaced by semi-edge walks.

In fact, the theory Q_Γ is much stronger than the theory Q_c. As noted before, the numbers of triangles, quadrangles and pentagons can be determined from eigenvalues and angles in the Q–theory. In addition, the vertex degrees can also be determined in Q_Γ.

Next theorem, taken from [28], strengthens Theorem 2.8.1.

Theorem 3.6.4. *Let G be a graph whose Q-index does not exceed 4. Then G is characterized by its Q-eigenvalues and Q-angles.*

Proof. If $q_1 < 4$, all components are paths and the graph is uniquely determined by eigenvalues only. Otherwise, we can have among the components some cycles and stars $K_{1,3}$. The vertices belonging to these components are identified by non-zero angles of the eigenvalue 4. We determine vertex degrees and then the number of stars is equal the the number of vertices of degree 3. The angle of the eigenvalue 4 in a cycle of length s is equal to $1/\sqrt{s}$.

This completes the proof. ■

It would be interesting to investigate the case when the Q-index does not exceed 4.5. If Q–index lies in the interval $(4, 4.5)$ then the graph is an open or a closed quipu (cf. Theorem 3.3.2 or [98]).

3.7 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 [4].

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 [4], while 37 are L–integral [71]; according to a table of Q–eigenvalues of the 112 connected graphs on 6 vertices from [15], 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 (5) 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 [89], [90] that there are exactly 172 connected Q–integral graphs up to 10 vertices[10]. 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 [92], Problem AWGS.2-C. For a more tractable problem we can require, in addition, that the graphs are non-bipartite.

The next proposition stems from [27].

Proposition 3.7.1. *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 (9) and the corresponding formula for A–eigenvalues.

It was proved in [84] 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.

[10] There are exactly 150 connected A–integral graphs up to 10 vertices [4].

Some infinite series of ALQ-integral graphs have been constructed in [91]. In addition, semi-regular bipartite Q-integral graphs are considered and this investigation is continued in [87].

All Q–integral complete split graphs have been identified in [50]. Several infinite families of Q–integral graphs have been found in some related classes of graphs using the join of regular graphs.

Next theorem gives a necessary and sufficient condition for the join of two Q-integral regular graphs to be Q-integral.

Theorem 3.7.2. For $i = 1, 2$, let G_i is a r_i-regular graph with n_i vertices. The graph $G_1 \bigtriangledown G_2$ is Q-integral if and only if G_1 and G_2 are Q-integral and $((2r_1 - n_1) - (2r_2 - n_2))^2 + 4n_1n_2$ is a perfect square.

Proof. From Theorem 3.1.4, $G_1 \bigtriangledown G_2$ is Q-integral if and only if G_1 and G_2 are Q-integral and the roots of $f(x) = x^2 - (2(r_1 + r_2) + (n_1 + n_2))x + 2(2r_1r_2 + r_1n_1 + r_2n_2)$ are integers. So, $G_1 \bigtriangledown G_2$ is Q-integral if and only if both graphs G_1 and G_2 are Q-integral and the roots

$$\frac{(2r_1 + 2r_2 + n_1 + n_2) \pm \sqrt{(2r_1 + 2r_2 + n_1 + n_2)^2 - 8(2r_1r_2 + r_1n_1 + r_2n_2)}}{2}$$

are integers.

Since $2r_1+2r_2+n_1+n_2$ and $(2r_1+2r_2+n_1+n_2)^2-8(2r_1r_2+r_1n_1+r_2n_2)$ have the same parity, in order for $f(x)$ to have integer roots it is only necessary and sufficient that $(2r_1 + 2r_2 + n_1 + n_2)^2 - 8(2r_1r_2 + r_1n_1 + r_2n_2) = ((2r_1 - n_1) - (2r_2 - n_2))^2 + 4n_1n_2$ is a perfect square. ■

If G_1 and G_2 are both r-regular Q-integral graphs, we have $((2r - n_1) - (2r - n_2))^2 + 4n_1n_2 = (n_1 + n_2)^2$. So, $G_1 \bigtriangledown G_2$ is also a Q-integral graph.

Example. As a consequence of Theorem 3.7.2, for every $n \neq 4$ and 7, the *wheel* graphs $W_n = K_1 \bigtriangledown C_{n-1}$ are not Q-integral, i.e. the wheel graph W_n is Q-integral if and only if $n = 4, 7$.

Indeed, it is well known that the cycle C_{n-1} is Q-integral if and only if n = 4, 5 or 7. Therefore, from Theorem 3.7.2. $W_n \cong K_1 \bigtriangledown C_{n-1}$ is Q-integral if and only if $((2r_1 - n_1) - (2r_2 - n_2))^2 + 4n_1n_2 = (n - 4)^2 + 16$ is a perfect square. Consequently, the only Q-integral wheels are W_4 and W_7.

The corresponding Q-spectra are $6, 2^3$ and $8, 4^2, 3, 2^2, 1$, where exponents denote multiplicities. ■

3.8 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.

Proposition 1.3 of [17] gives $t(G)$ in terms of L–eigenvalues while Proposition 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 2.3.3, these formulas coincide for regular bipartite graphs.

Example. The Q–spectrum of $K_{m,n}$ was determined in Subsection 2.6 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 2.3 and the second of these formulas yields $t(K_n) = n^{n-2}$ (the Cayley formula). ■

Example. Similarly we have

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

■

The aforementioned Proposition 1.3 of [17] shows that $t(G) = \frac{(-1)^{n-1}}{n}L'_G(0)$. For a non-bipartite graph G formula (9) 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

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

Since $Q_G(0) = (-1)^n \det Q$, we get an expression [27] 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 2.5.5) 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 2.5.5.

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

3.9 Miscellaneous

Ad. 1. Studying graph reconstruction from collections of subgraphs of various kind is a traditional challenge in the graph theory.

It was proved in [39] that the Q–polynomial of a graph G is reconstructible from the collection of vertex deleted subgraphs $G - v$ of G. The same result for the A–theory is well known [95].

Next result involves edge deleted subgraphs.

Theorem 3.9.1. *The Q–polynomial of a graph G is reconstructible from the collection of the Q–polynomials of edge deleted subgraphs of G.*

Proof. Given the Q–polynomials of edge deleted subgraphs of G, we can calculate by formula (2) the A–polynomials of vertex deleted subgraphs of the line graph $L(G)$ of G. As is well–known, the A-eigenvalues of line graphs are bounded from below by -2. By results of [85] the A–polynomial of $L(G)$ can now be reconstructed. Again by formula (2), we obtain the Q–polynomial of G. ∎

The reconstruction of the Q–polynomial of a graph G from the collection of the Q–polynomials of edge deleted subgraphs of G corresponds to the reconstruction of the A–polynomial of a graph G from the collection of the A–polynomials of vertex deleted subgraphs of G. While the first problem is positively solved by Theorem 3.9.1, the corresponding problem in the A–theory remains unsolved in the general case. Therefore Theorem 3.9.1 says much about the usefulness of the Q–theory.

Ad. 2. The *Q–spectral spread* $s_Q(G) = q_1 - q_n$ has been studied in [74]. 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 [24]:

Over the set of all connected graphs of order $n \geq 6$, $q_1 - q_n$ 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 [74] have derived a weaker upper bound for $s_Q(G)$ but they believe that the best upper bound is as expressed in Conjecture 25.

Note that the calculation of the Q-spectrum of the extremal graph $K_{n-1} + v$ has been carried out independently by different methods in [74] (the graph divisor technique) and in Subsection 3.6 (using Q-angles) with the same result.

Another relaxation appears in [53], where the conjecture was confirmed for unicyclic graphs.

Ad. 3. For a subset S of $V = V(G)$, let $e_{min}(S)$ be the minimum number of edges whose removal from the subgraph of G induced by S results in a bipartite graph. Let $\mathrm{cut}(S)$ be the set of edges with one vertex in S and the other in its complement $V - S$. Thus $|\mathrm{cut}(S)| + e_{min}(S)$ is the minimum number of edges whose removal from $E(G)$ disconnects S from $V - S$ and results in a bipartite subgraph induced by S. Let ψ be the minimum over all non-empty proper subsets S of $V(G)$ of the quotient

$$\frac{|\mathrm{cut}(S)| + e_{min}(S)}{|S|}.$$

The parameter ψ was introduced in [40] as a measure of non-bipartiteness. It is shown that the least eigenvalue q_n of the signless Laplacian Q is bounded above and below by functions of ψ. In particular, it is proved that, for a connected graph,

$$\frac{\psi^2}{4d_{max}} \leq q_n \leq 4\psi,$$

where d_{max} is the maximal vertex degree.

Ad. 4. Next, for a graph G let p be the number of vertices of degree 1 and q the number of their neighbors. It is proved in [43] that the difference $p-q$ is equal to the multiplicity of the root 1 of the permanental polynomial $\mathrm{per}(xI - Q)$ of the signless Laplacian of G. It is shown by examples that such a result is impossible if we use the characteristic polynomial or other graph matrices (the adjacency matrix or Laplacian).

Ad. 5. An upper bound on maximal entry of the eigenvector of the largest Q-eigenvalue q_1 of a graph has been obtained in [38].

Ad. 6. The quantity $IE(G) = \sum_1^n \sqrt{q_i}$ is called the *incidence energy* of a graph G in [56] (see also references cited therein). The incidence energy is related to the well known quantity $E(G)$ called the *energy* defined as the sum of absolute values of A-eigenvalues of a graph. Having in view relations (8) we have $IE(G) = \frac{1}{2}E(S(G))$, where $S(G)$ is the subdivision of G. Several lower and upper bounds and Nordhaus-Gaddum type results are obtained for the incidence energy in [56].

Ad. 7. We write $\Gamma(v)$ for the neighbourhood of v, and we call $\{v\}\cup\Gamma(v)$ the *closed* neighbourhood of v. Vertices with the same neighbourhood are called *duplicate* vertices; they necessarily induce a co-clique. Vertices with the same closed neighbourhood are called *co-duplicate* vertices; they necessarily induce a clique. The following two assertions have been proved in [24] (Conjectures 28 and 29).

(i) If G has k duplicate vertices ($k > 1$), with neighbourhood of size d, then d is an eigenvalue of Q with multiplicity $e(d) \geq k - 1$.

(ii) If G has k co-duplicate vertices ($k > 1$), with closed neighbourhood of size d, then $d-1$ is an eigenvalue of Q with multiplicity $e(d-1) \geq k-1$.

Assertion (i) is true, because $Q - dI$ has k repeated rows, and assertion (ii) is true, because $Q - (d-1)I$ has k repeated rows. The validity of these assertions follows also from a remark in [96].

Ad. 8. The theory of star complements of graphs is presented in the book [22], Chapter 5. The paper [23] offers a few observations indicating possibilities to extend the theory to signless Laplacians.

For a graph G we describe the relation between the eigenspaces $\mathcal{E}_L(\lambda)$ ($\lambda \neq -2$) of an eigenvalue λ of the line graph $L(G)$ and the eigenspaces $\mathcal{E}_{D+A}(\lambda)$ ($\lambda \neq 0$) of the signless Laplacian $D + A$. (In each case, the remaining eigenspace is found as an orthogonal complement.) The first part of the following Proposition is well known.

Proposition 3.9.1. *(i) The map* $\mathbf{x} \mapsto R\mathbf{x}$ *is an isomorphism* $\mathcal{E}_L(\lambda) \to \mathcal{E}_{D+A}(\lambda+2)$ $(\lambda \neq -2)$.
(ii) If P represents the orthogonal projection $\mathbb{R}^m \to \mathcal{E}_L(\lambda)$ and P' denotes the orthogonal projection $\mathbb{R}^n \to \mathcal{E}_{D+A}(\lambda+2)$ $(\lambda \neq -2)$ then $RP = P'R$.

Proof. (i) See [21, Theorem 2.6.1].
(ii) Let $\mathbf{y}$ be an arbitrary element of $\mathbb{R}^m$, say $\mathbf{y} = \mathbf{w} + \mathbf{z}$, where $\mathbf{w} \in \mathcal{E}_L(\lambda)$ and $\mathbf{z} \in \mathcal{E}_L(\lambda)^\perp$. Then $P\mathbf{y} = \mathbf{w}$ and $RP\mathbf{y} = R\mathbf{w} = P'R\mathbf{w}$, while $P'R\mathbf{y} = P'R\mathbf{w} + P'R\mathbf{z}$. It remains to show that $P'R\mathbf{z} = \mathbf{0}$, equivalently $R\mathbf{z} \in \mathcal{E}_{D+A}(\lambda+2)^\perp$. But if $\mathbf{v} \in \mathcal{E}_{D+A}(\lambda+2)$ then $\mathbf{v} = R\mathbf{x}$ for some $\mathbf{x} \in \mathcal{E}_L(\lambda)$, and we have $\mathbf{v}^T(R\mathbf{z}) = \mathbf{x}^T R^T R\mathbf{z} = (\lambda+2)\mathbf{x}^T\mathbf{z} = 0$. ■

Ad. 9. We write $\mathcal{U}_{e,f}$ for the set of unicyclic graphs on $e + f$ vertices with a cycle of length e. $E_{e,f}$ is a unicyclic graph with $e + f$ vertices obtained by a coalescence of a vertex in C_e with an end-vertex of P_{f+1}.

By the Interlacing Theorem (Theorem 2.6.1) we have

$$0 = q_n(P_n) \leq q_n(E_{e,n-e}) \leq q_{n-1}(P_n), \quad e = 3, 5, \ldots, e_{\max} \leq n.$$

Hence
$$0 \leq q_n(E_{e,n-e}) \leq 2\left(1-\cos\frac{\pi}{n}\right) = 4\sin^2\frac{\pi}{2n}.$$

Having in mind Ad. 3, for an odd-unicyclic graph we have $\psi = 1/n$ and so we obtain the following double inequality :
$$\frac{1}{12n^2} \leq q_n(E_{e,n-e}) \leq \frac{4}{n}.$$

We conclude that
$$\frac{1}{12n^2} \leq q_n(E_{e,n-e}) \leq 4\sin^2\frac{\pi}{2n} \approx \frac{\pi^2}{n^2},$$
i.e. $n^2 q_n(E_{e,n-e}) = O(1)$.

The following proposition is easily obtained from Theorem 2.5.5.

Proposition 3.9.2. *For a graph G on n vertices, with girth g, we have:*
$$p_n(G) = 0, \quad (-1)^{n-1}p_{n-1}(G) = ng$$
if G is an even-unicyclic graph, and
$$(-1)^n p_n(G) = 4, \quad (-1)^{n-1}p_{n-1}(G) = ng + 4\sum t_i$$
if G is an odd-unicyclic graph, t_i being the number of vertices of the tree obtained by deleting an edge i outside the cycle.

We mention in passing that the girth can be determined from the Q-eigenvalues in the case of even-unicyclic graphs but not in the case of odd-unicyclic graphs. For (adjacency) eigenvalues we have exactly the opposite situation. However, Laplacian eigenvalues perform best: the girth of a unicyclic graph can be determined in all cases. (Then the coefficient of the linear term in the characteristic polynomial is equal to $-n$ times the number N of spanning trees, and for unicyclic graphs, N is equal to the girth. Note that results concerning such coefficients for some other classes of graphs, in particular for trees, have been obtained in [72].)

The following lemma is a straightforward consequence of Proposition 3.9.2.

Lemma 3.9.3. *Let G be an odd-unicyclic graph on n vertices. Let u be a vertex of degree at least 3 and v a vertex of degree 1 in G. Let T be the tree attached at u. Let G' be the graph obtained by relocating the tree T from u to v. Then*
$$(-1)^{n-1}p_{n-1}(G') > (-1)^{n-1}p_{n-1}(G).$$

Using Lemma 3.9.3 repeatedly, we obtain:

Proposition 3.9.4. *For $G \in \mathcal{U}_{e,f}$, e odd, and $G \neq E_{e,f}$ we have*

$$(-1)^{n-1} p_{n-1}(E_{e,f}) > (-1)^{n-1} p_{n-1}(G),$$

where $n = e + f$.

In addition, we have the following observation.

Proposition 3.9.5. *For n odd and $e = 5, 7, \ldots, n$ we have*

$$(-1)^{n-1} p_{n-1}(E_{3,n-3}) > (-1)^{n-1} p_{n-1}(E_{e,n-e}).$$

Proof: From Proposition 3.9.2 we have $(-1)^{n-1} p_{n-1}(E_{e,n-e}) =$

$$ne + 4((n-e) + (n-e-1) + \cdots + 1) = 2e^2 - (3n+2)e + 2n^2 + 2n,$$

and the maximum value of this function is attained when $e = 3$. ■

Now, for sufficiently small x, the equation $Q_G(x) = 0$ can be reduced to $p_{n-1}(G)x + p_n(G) = 0$, whose solution $-p_n(G)/p_{n-1}(G)$ could be considered as an approximation for $q_n(G)$. By Propositions 3.9.2, 3.9.4 and 3.9.5, this approximation value is minimal for the graph $E_{3,n-3}$. These arguments were quoted in [24] to support Conjecture 24 before it was proved in [10].

We note in passing that extremal results concerning the coefficients $p_i(T)$ for a tree T have been obtained in [107]. In particular, it is proved that for $i = 3, 4, \ldots, n-1$ the coefficient $(-1)^i p_i$ is minimal in paths and maximal in stars.

Appendix 1

We present Q-spectra of graphs on up to 5 vertices (Table 1) and of graphs on 6 vertices (Table 2).

TABLE 1: SPECTRUM AND Q-SPECTRUM OF CONNECTED GRAPHS WITH $n = 2, 3, 4, 5$ VERTICES

The graphs are ordered in the same way as in the book [17] and are given here in Fig. 1. For each graph G_i the first line contains the subscript i and A-eigenvalues while Q-eigenvalues are contained in the second line.

This table stems from [23]

```
**********************************************************************
                        n = 2
**********************************************************************

001   1.0000  -1.0000
      2.0000   0.0000

**********************************************************************
                        n = 3
**********************************************************************

002   2.0000  -1.0000  -1.0000
      4.0000   1.0000   1.0000

003   1.4142   0.0000  -1.4142
      3.0000   1.0000   0.0000

**********************************************************************
                        n = 4
**********************************************************************

004   3.0000  -1.0000  -1.0000  -1.0000
      6.0000   2.0000   2.0000   2.0000

005   2.5616   0.0000  -1.0000  -1.5616
      5.2361   2.0000   2.0000   0.7639
```

```
006   2.1701   0.3111  -1.0000  -1.4812
      4.5616   2.0000   1.0000   0.4384

007   2.0000   0.0000   0.0000  -2.0000
      4.0000   2.0000   2.0000   0.0000

008   1.7321   0.0000   0.0000  -1.7321
      4.0000   1.0000   1.0000   0.0000

009   1.6180   0.6180  -0.6180  -1.6180
      3.4142   2.0000   0.5858   0.0000

*********************************************************************
                        n = 5
*********************************************************************

010   4.0000  -1.0000  -1.0000  -1.0000  -1.0000
      8.0000   3.0000   3.0000   3.0000   3.0000

011   3.6458   0.0000  -1.0000  -1.0000  -1.6458
      7.3723   3.0000   3.0000   3.0000   1.6277

012   3.3234   0.3579  -1.0000  -1.0000  -1.6813
      6.8284   3.0000   3.0000   2.0000   1.1716

013   3.2361   0.0000   0.0000  -1.2361  -2.0000
      6.5616   3.0000   3.0000   2.4384   1.0000

014   3.0861   0.4280  -1.0000  -1.0000  -1.5141
      6.3723   3.0000   2.0000   2.0000   0.6277

015   3.0000   0.0000   0.0000  -1.0000  -2.0000
      6.3723   3.0000   2.0000   2.0000   0.6277

016   2.9354   0.6180  -0.4626  -1.4728  -1.6180
      6.1249   3.0000   2.6367   1.2384   1.0000

017   2.8558   0.3216   0.0000  -1.0000  -2.1774
      5.7785   3.0000   2.7108   2.0000   0.5107
```

018	2.6855	0.3349	0.0000	-1.2713	-1.7491
	5.7785	2.7108	2.0000	1.0000	0.5107
019	2.6412	0.7237	-0.5892	-1.0000	-1.7757
	5.4679	2.9128	2.0000	1.2011	0.4182
020	2.5616	1.0000	-1.0000	-1.0000	-1.5616
	5.5616	3.0000	1.4384	1.0000	1.0000
021	2.4812	0.6889	0.0000	-1.1701	-2.0000
	5.1149	2.7459	2.6180	1.1392	0.3820
022	2.4495	0.0000	0.0000	0.0000	-2.4495
	5.0000	3.0000	2.0000	2.0000	0.0000
023	2.3429	0.4707	0.0000	-1.0000	-1.8136
	5.3234	2.3579	1.0000	1.0000	0.3187
024	2.3028	0.6180	0.0000	-1.3028	-1.6180
	4.9354	2.6180	1.5374	0.5272	0.3820
025	2.2143	1.0000	-0.5392	-1.0000	-1.6751
	4.6412	2.7237	1.4108	1.0000	0.2243
026	2.1358	0.6622	0.0000	-0.6622	-2.1358
	4.4812	2.6889	2.0000	0.8299	0.0000
027	2.0000	0.6180	0.6180	-1.6180	-1.6180
	4.0000	2.6180	2.6180	0.3820	0.3820
028	2.0000	0.0000	0.0000	0.0000	-2.0000
	5.0000	1.0000	1.0000	1.0000	0.0000
029	1.8478	0.7654	0.0000	-0.7654	-1.8478
	4.1701	2.3111	1.0000	0.5188	0.0000
030	1.7321	1.0000	0.0000	-1.0000	-1.7321
	3.6180	2.6180	1.3820	0.3820	0.0000

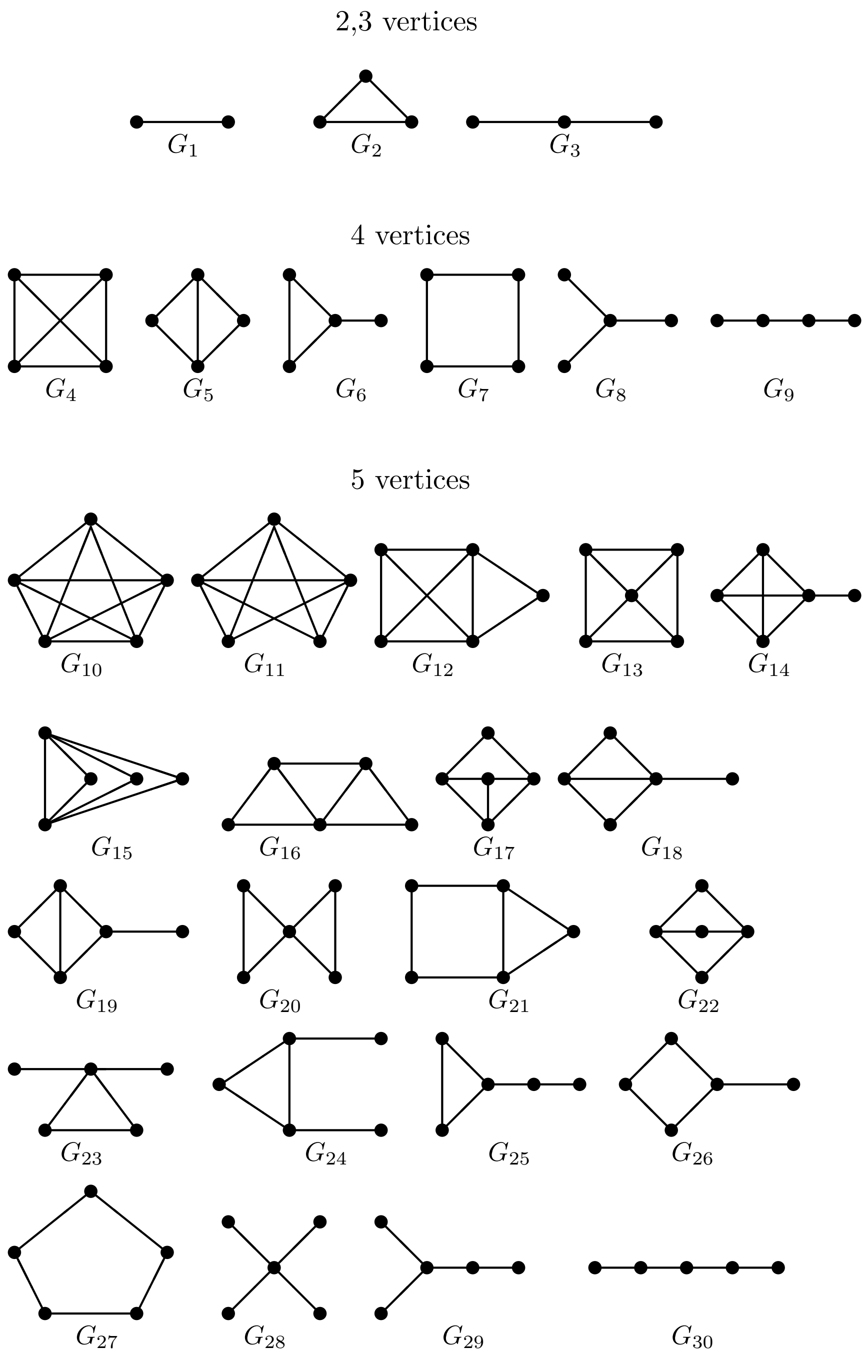

Fig. 1: Graphs with up to 5 vertices

TABLE 2: Q-SPECTRA OF CONNECTED GRAPHS WITH 6 VERTICES

The graphs are ordered and labelled in the same way as in the paper [19] and the reader is referred to this paper for drawings of the graphs. (In fact, the graphs are ordered lexicographically by spectral moments of the adjacency matrix.) Diagrams of these graphs can be found also in the appendix of the book [25]. The number of edges m is also given.

The following 5 pairs of graphs form Q-PINGs: 5 6, 14 16, 53 56, 65 71, 82 88.

This table stems from [15].

m=15	001.	10.0000	4.0000	4.0000	4.0000	4.0000	4.0000
m=14	002.	9.4641	4.0000	4.0000	4.0000	4.0000	2.5359
m=13	003.	9.0000	4.0000	4.0000	4.0000	3.0000	2.0000
	004.	8.8284	4.0000	4.0000	4.0000	3.1716	2.0000
m=12	005.	8.6056	4.0000	4.0000	3.0000	3.0000	1.3944
	006.	8.6056	4.0000	4.0000	3.0000	3.0000	1.3944
	007.	8.4495	4.0000	4.0000	3.5505	2.0000	2.0000
	008.	8.2588	4.0000	4.0000	3.2518	3.0000	1.4894
	009.	8.0000	4.0000	4.0000	4.0000	2.0000	2.0000
m=11	010.	8.2749	4.0000	3.0000	3.0000	3.0000	0.7251
	011.	8.1355	4.0000	3.6532	3.0000	2.0000	1.2113
	012.	7.9651	4.0000	3.7180	3.0000	2.0000	1.3169
	013.	8.0000	4.0000	4.0000	2.0000	2.0000	2.0000
	014.	7.7588	4.0000	3.3054	3.0000	3.0000	0.9358
	015.	7.7913	4.0000	3.6180	3.2087	2.0000	1.3820
	016.	7.7588	4.0000	3.3054	3.0000	3.0000	0.9358
	017.	7.5616	4.0000	3.4384	3.0000	3.0000	1.0000
	018.	7.5047	4.0000	4.0000	3.1354	2.0000	1.3600
m=10	019.	7.7264	3.8577	3.0000	3.0000	1.7093	0.7066
	020.	7.5446	3.8329	3.0000	3.0000	2.0000	0.6224
	021.	7.7588	4.0000	3.3054	2.0000	2.0000	0.9358
	022.	7.5742	3.7337	3.6180	2.5076	1.3820	1.1845
	023.	7.3723	4.0000	3.0000	3.0000	1.6277	1.0000
	024.	7.4279	4.0000	3.3757	2.0000	2.0000	1.1965
	025.	7.3919	3.7904	3.2106	3.0000	1.6815	0.9256
	026.	7.1859	3.7200	3.3007	3.0000	2.0000	0.7933
	027.	7.1190	4.0000	3.6180	2.5684	1.3820	1.3126
	028.	7.2361	3.6180	3.6180	2.7639	1.3820	1.3820
	029.	7.0839	4.0000	3.2132	3.0000	2.0000	0.7029
	030.	6.8951	4.0000	3.3973	3.0000	1.7076	1.0000
	031.	6.8284	4.0000	4.0000	2.0000	2.0000	1.1716

	032.	6.9095	3.6093	3.0000	3.0000	3.0000	0.4812
m=9	033.	7.2724	3.7245	3.0000	2.0000	1.3437	0.6594
	034.	7.0604	3.6395	3.0000	2.4522	1.2270	0.6208
	035.	6.9095	3.6093	3.0000	2.0000	2.0000	0.4812
	036.	7.0000	4.0000	2.0000	2.0000	2.0000	1.0000
	037.	7.4641	4.0000	2.0000	2.0000	2.0000	0.5359
	038.	7.0839	3.2132	3.0000	3.0000	1.0000	0.7029
	039.	6.7982	3.7904	3.0000	2.5025	1.3626	0.5463
	040.	7.1156	3.6701	3.0971	2.0000	1.2393	0.8780
	041.	6.7321	3.4142	3.2679	2.0000	2.0000	0.5858
	042.	6.8284	3.6180	3.6180	1.3820	1.3820	1.1716
	043.	6.9576	3.6180	3.1215	2.0000	1.3820	0.9209
	044.	6.6458	4.0000	3.0000	2.0000	1.3542	1.0000
	045.	6.6648	3.3011	3.0000	3.0000	1.5713	0.4628
	046.	6.6058	3.7197	3.1897	2.4767	1.3225	0.6856
	047.	6.4081	3.6180	3.2934	2.5573	1.3820	0.7411
	048.	6.3234	4.0000	3.3579	2.0000	1.3187	1.0000
	049.	6.4940	4.0000	3.1099	2.0000	2.0000	0.3961
	050.	6.3419	3.5959	3.0000	3.0000	1.6324	0.4298
	051.	6.0000	4.0000	3.0000	3.0000	1.0000	1.0000
	052.	6.0000	3.0000	3.0000	3.0000	3.0000	0.0000
m=8	053.	6.9095	3.6093	2.0000	2.0000	1.0000	0.4812
	054.	6.6728	3.4142	2.6481	2.0000	0.6791	0.5858
	055.	6.3923	3.3254	2.0000	2.0000	2.0000	0.2823
	056.	6.9095	3.6093	2.0000	2.0000	1.0000	0.4812
	057.	6.4940	3.1099	3.0000	2.0000	1.0000	0.3961
	058.	6.7494	3.1469	3.0000	1.4577	1.0000	0.6460
	059.	6.4317	3.6180	2.7995	1.3820	1.2245	0.5443
	060.	6.2422	3.5496	2.6524	2.0000	1.0855	0.4703
	061.	6.6262	3.5151	2.0000	2.0000	1.0000	0.8587
	062.	6.0000	4.0000	2.0000	2.0000	1.0000	1.0000
	063.	6.1779	3.1905	3.0000	2.4204	0.7828	0.4284
	064.	6.1159	3.7195	2.7379	2.0000	1.0648	0.3619
	065.	5.8781	3.5834	3.0000	2.0000	1.2296	0.3089
	066.	6.2491	3.4142	2.8536	2.0000	0.8972	0.5858
	067.	6.0280	3.2953	3.0000	2.0000	1.2849	0.3918
	068.	5.9452	3.6180	3.0856	1.3820	1.2963	0.6728
	069.	5.7093	3.4142	3.1939	2.0000	1.0968	0.5858
	070.	5.5616	4.0000	3.0000	1.4384	1.0000	1.0000
	071.	5.8781	3.5834	3.0000	2.0000	1.2296	0.3089
	072.	5.5887	3.5463	3.0000	2.4537	1.0000	0.4113
	073.	6.0000	4.0000	2.0000	2.0000	2.0000	0.0000
	074.	5.5616	3.0000	3.0000	3.0000	1.4384	0.0000
m=7	075.	6.4940	3.1099	2.0000	1.0000	1.0000	0.3961
	076.	6.1563	3.4142	2.0000	1.3691	0.5858	0.4746
	077.	5.9452	3.0856	2.6180	1.2963	0.6728	0.3820

	078.	5.8781	3.5834	2.0000	1.2296	1.0000	0.3089
	079.	6.3723	3.0000	2.0000	1.0000	1.0000	0.6277
	080.	5.6458	3.4142	2.0000	2.0000	0.5858	0.3542
	081.	5.8154	3.0607	2.0000	2.0000	0.8638	0.2602
	082.	5.4893	3.2892	2.0000	2.0000	1.0000	0.2215
	083.	5.7217	3.5127	2.0000	1.3098	1.0000	0.4558
	084.	5.0000	4.0000	2.0000	1.0000	1.0000	1.0000
	085.	5.6597	3.1461	2.7357	1.3736	0.7772	0.3077
	086.	5.3615	3.1674	2.6180	2.0000	0.4711	0.3820
	087.	5.2647	3.5378	2.6491	1.2987	1.0000	0.2497
	088.	5.4893	3.2892	2.0000	2.0000	1.0000	0.2215
	089.	5.0664	3.2222	3.0000	1.3478	1.0000	0.3636
	090.	5.5141	3.5720	2.0000	2.0000	0.9139	0.0000
	091.	5.2361	3.0000	3.0000	2.0000	0.7639	0.0000
	092.	5.0000	3.0000	3.0000	2.0000	1.0000	0.0000
	093.	4.9032	3.4142	2.8061	2.0000	0.5858	0.2907
m=6	094.	6.2015	2.5451	1.0000	1.0000	1.0000	0.2534
	095.	5.5344	3.0827	1.5929	1.0000	0.4889	0.3010
	096.	5.2361	2.6180	2.6180	0.7639	0.3820	0.3820
	097.	5.3839	2.7424	2.0000	1.0000	0.6721	0.2015
	098.	4.9809	3.0420	2.0000	1.2938	0.4629	0.2204
	099.	4.8422	3.5069	1.4931	1.0000	1.0000	0.1578
	100.	4.6554	3.2108	2.0000	1.0000	1.0000	0.1338
	101.	5.2361	3.0000	2.0000	1.0000	0.7639	0.0000
	102.	4.8136	3.0000	2.5293	1.0000	0.6571	0.0000
	103.	4.7321	3.4142	2.0000	1.2679	0.5858	0.0000
	104.	4.5616	3.0000	2.0000	2.0000	0.4384	0.0000
	105.	4.4383	3.1386	2.6180	1.1798	0.3820	0.2434
	106.	4.0000	3.0000	3.0000	1.0000	1.0000	0.0000
m=5	107.	6.0000	1.0000	1.0000	1.0000	1.0000	0.0000
	108.	5.0861	2.4280	1.0000	1.0000	0.4859	0.0000
	109.	4.5616	3.0000	1.0000	1.0000	0.4384	0.0000
	110.	4.3028	2.6180	2.0000	0.6972	0.3820	0.0000
	111.	4.2143	3.0000	1.4608	1.0000	0.3249	0.0000
	112.	3.7321	3.0000	2.0000	1.0000	0.2679	0.0000

Appendix 2

The thirty AGX Conjectures from the paper [24]

The following 30 conjectures related to the Q-eigenvalues of a graph have been formulated after some experiments with the system AGX. Almost all the conjectures are in the form of inequalities which provide upper or lower bounds for spectrally based graph invariants. The notation is as follows.

As above, Q denotes the signless Laplacian of a graph G and $(q_1, q_2, \ldots q_n)$ the spectrum of Q, where the eigenvalues are such that $q_1 \geq q_2 \geq \ldots \geq q_n$.

Let L denote the Laplacian of a graph G and $(\mu_1, \mu_2, \ldots \mu_n)$ the spectrum of L, where the eigenvalues are such that $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n$.

Let A denote the adjacency matrix of a graph G and $(\lambda_1, \lambda_2, \ldots \lambda_n)$ the spectrum of A, where the eigenvalues are such that $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$.

Sometimes we shall use the notation $q_i = q_i(G), i = 1, 2, \ldots, n$. Also, we write a for μ_{n-1}, called the *algebraic connectivity* of G (see [17, p. 265]).

The *double star* $DS(m, n)$ is obtained from two disjoint stars $K_{m-1,1}$, $K_{n-1,1}$ by adding an edge between their central vertices. The *double comet* $DC(n, r, s)$ is the graph of order n obtained from two disjoint stars $K_{r-1,1}$, $K_{s-1,1}$ by adding a path (of length $n - r - s + 1$) between their central vertices.

A *complete split graph* with parameters n, q ($q \leq n$), denoted by $CS(n, q)$, is a graph on n vertices consisting of a clique on q vertices, a co-clique on the remaining $n - q$ vertices, and all $q(n - q)$ possible edges between the clique and the co-clique.

The conjectures apply to graphs with at least 4 vertices, and they are classified according to the graph invariants involved.

Conjectures on the largest eigenvalue

Conjecture 1:
If G is a connected graph of order $n \geq 4$, then

$$2 + 2\cos\frac{\pi}{n} = q_1(P_n) \leq q_1(G) \leq q_1(K_n) = 2n - 2$$

with equality if and only if G is the path P_n for the lower bound, and if and only if G is the complete graph K_n for the upper bound.

Conjecture 2:
If T is a tree of order $n \geq 4$, then

$$2 + 2\cos\frac{\pi}{n} = q_1(P_n) \leq q_1(T) \leq q_1(S_n) = n$$

with equality if and only if T is the path P_n for the lower bound, and if and only if T is the star S_n for the upper bound.

Conjecture 3 :
Let S_n^+ denote the graph consisting of a star and an additional edge. If G is a unicyclic graph of order $n \geq 4$, then

$$4 = q_1(C_n) \leq q_1(G) \leq q_1(S_n^+)$$

with equality if and only if G is the cycle C_n for the lower bound, and if and only if G is S_n^+ for the upper bound.

Conjecture 4 :
If G is a connected graph of order $n \geq 4$ and maximum degree Δ, then

$$q_1 \geq \Delta + 1$$

with equality if and only if G is the star S_n.

Conjecture 5 :
If G is a connected graph of order $n \geq 4$, with minimum, average and maximum degree $\delta, \overline{d}$ and Δ respectively,

$$2\delta \leq 2\overline{d} \leq q_1 \leq 2\Delta$$

with equality in any instance if and only if G is regular.

Conjecture 6 :
If G is a connected graph of order $n \geq 4$ and average degree $\overline{d}$, then

$$q_1 - 2\overline{d} \leq n - 4 + 4/n$$

with equality if and only if G is the star S_n.

Conjecture 7 :
If G is a connected graph of order $n \geq 5$ and average degree $\overline{d}$, then

$$2 \leq q_1 - \overline{d} \leq n - 1$$

with equality if and only if G is the cycle C_n for the lower bound, and if and only if G is the complete graph K_n for the upper bound.

Conjecture 8 :
If G is a connected graph of order $n \geq 4$, index λ_1 and average degree $\overline{\mathrm{d}}$, then

$$0 \leq q_1 - \overline{\mathrm{d}} - \lambda_1 \leq n - 2 + 2/n - \sqrt{n-1}$$

with equality if and only if G is regular for the lower bound, and if and only if G is the star S_n for the upper bound.

Conjecture 9 :
If G is a connected graph of order $n \geq 4$, index λ_1 with maximum Laplacian eigenvalue μ_1, then

$$1 \leq \mu_1 + \lambda_1 - q_1 \leq \sqrt{\lceil n/2 \rceil \lfloor n/2 \rfloor}$$

with equality if and only if G is the complete graph K_n for the lower bound, and if and only if G is the complete bipartite graph $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$ for the upper bound.

Conjecture 10 :
If G is a connected graph of order $n \geq 4$ with maximum Laplacian eigenvalue μ_1, then

$$0 \leq q_1 - \mu_1 \leq n - 2$$

with equality if and only if G is bipartite for the lower bound, and if and only if G is the complete graph K_n for the upper bound.

Conjecture 11 :
If G is a connected graph of order $n \geq 4$ and index λ_1, then

$$0 \leq q_1 - 2\lambda_1 \leq n - 2\sqrt{n-1}$$

with equality if and only if G is regular for the lower bound, and if and only if G is the star S_n for the upper bound.

Conjectures on the second largest eigenvalue

Conjecture 12 :
If G is a connected graph of order $n \geq 4$, then $q_2 \geq 1$, with equality if and only if G is the star S_n.

Conjecture 13 :
Over all trees on n vertices ($n \geq 4$), q_2 is maximum for the graphs $DS(\frac{1}{2}n, \frac{1}{2}n)$ and $DC(n, \frac{1}{2}n - 1, \frac{1}{2}n - 1)$ if n is even (in which case $q_2 = \frac{1}{2}n$), and for the graph $DC(n, \frac{1}{2}(n-1), \frac{1}{2}(n-1))$ if n is odd.

Conjecture 14:
If G is a connected graph of order $n \geq 7$, then

$$-1 \leq q_2 - \overline{d} \leq n - 6 + \frac{8}{n}$$

with equality if and only if G is the complete graph K_n for the lower bound, and if and only if G is the complete bipartite graph $K_{n-2,2}$ for the upper bound.

Conjecture 15:
If G is a connected graph of order $n \geq 7$, then

$$-1 \leq q_2 - \delta \leq n - 3$$

with equality if and only if G is the complete graph K_n for the lower bound, and if and only if G is $K_{n-1} + e$ for the upper bound.

Conjecture 16:
If G is a connected graph of order $n \geq 4$, then $\Delta - q_2 \leq n - 2$, with equality if and only if G is the star S_n.

Conjecture 17:
Over all connected graphs on n vertices ($n \geq 4$), the graph H, described below, minimizes $\Delta - q_2$.
If n is even, H is constructed as follows from two copies of $K_{\frac{n}{2}}$. Delete an edge uv from one copy and an edge $u'v'$ from the other; then add the two edges uu' and vv'.
If n is odd, H is constructed as follows from two copies of $K_{\frac{n-1}{2}}$ and an isolated vertex w. Delete an edge uv from one copy of $K_{\frac{n-1}{2}}$ and an edge $u'v'$ from the other; then add the four edges uw,vw, $u'w$ and $v'w$.

Conjecture 18:
If G is a connected graph of order $n \geq 9$, then

$$1 - \sqrt{n-1} \leq q_2 - \lambda_1 \leq n - 2 - \sqrt{2n-4}$$

with equality if and only if G is the star S_n for the lower bound, and if and only if G is the complete bipartite graph $K_{n-2,2}$ for the upper bound.

Conjecture 19:
If G is a connected graph of order $n \geq 9$ and algebraic connectivity a, then

$$q_2 - a \geq -2$$

with equality if and only if G is the complete graph K_n.

Conjecture 20 :
If G is a connected graph and not complete of order $n \geq 9$ and algebraic connectivity a, then

$$q_2 - a \geq 0.$$

The bound is attained by the star S_n, by the complement of a matching of $\lfloor n/2 \rfloor$ edges and, if n is even, by the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$.

Conjecture 21 :
Over all connected graphs on n vertices ($n \geq 4$), the graph K, described below, maximizes $q_2 - a$.
If n is even, K is obtained from two copies of $K_{\frac{n}{2}}$ by adding a single edge connecting the two cliques.
If n is odd, K is obtained from two copies of $K_{\frac{n-1}{2}}$ and an isolated vertex w by adding two edges between w and each clique $K_{\frac{n-1}{2}}$.

Conjecture 22 :
If G is a connected graph of order $n \geq 4$, then

$$q_1 - q_2 \leq n$$

with equality if and only if G is the complete graph K_n.

Conjecture 23 :
If T is a tree order $n \geq 4$, then

$$q_1 - q_2 \leq n - 1$$

with equality if and only if T is the star S_n.

Conjectures on the least eigenvalue

Conjecture 24 :
If G is of order $n \geq 4$, connected and not bipartite then

$$q_n \geq q_n(E_{3,n-3})$$

where $E_{e,f}$ is a unicyclic graph with $e + f$ vertices obtained by a coalescence of a vertex in C_e with an endvertex of P_{f+1}.

Conjecture 25 :
Over the set of all connected graphs of order $n \geq 6$, $q_1 - q_n$ is minimum for a path P_n and for an odd cycle C_n, and is maximum for the graph $K_{n-1}+e$.

Conjecture 26 :
For any connected graph G of order $n \geq 4$ with independence number α,

$$q_1 + q_n + 2\alpha \leq 3n - 2$$

with equality if and only if G is a complete split graph $CS(n, n-\alpha)$.
If G has m edges then $q_1 + q_2 + \cdots + q_n = 2m$, and so the conjecture is equivalent to:

$$\sum_{i=2}^{n-1} q_i \geq 2(m + \alpha + 1) - 3n$$

with equality if and only if G is a complete split graph $CS(n, n-\alpha)$.

Conjectures related to the multiplicities of eigenvalues

Conjecture 27 :
Let $e(Q)$ denote the number of distinct eigenvalues of the matrix Q and $m(q_i)$ the multiplicity of the eigenvalue q_i. Then

$$e(Q) = 2 \quad \Longleftrightarrow \quad m(q_2) = n-1 \quad \Longleftrightarrow \quad G \equiv K_n \ .$$

In this case, $q_2 = n - 2$.

Conjecture 28 :
If G has k duplicate vertices ($k > 1$), with neighbourhood of size d, then d is an eigenvalue of Q with $m(d) \geq k - 1$.

Conjecture 29 :
If G has k co-duplicate vertices ($k > 1$), with closed neighbourhood of size d, then $d - 1$ is an eigenvalue of Q with $m(d-1) \geq k - 1$.

Conjecture 30 :
If G is a connected graph of order $n \geq 4$ with at least two dominating vertices, then $q_2 = \Delta - 1 = n - 2$ with multiplicity at most $\lceil n/2 \rceil - 2$.

Comments on the conjectures

Here we identify conjectures that are resolved, explicitly or implicitly. The conjectures left unresolved appear to include some difficult research problems.

Conjecture 1. Several elementary inequalities for Q-eigenvalues are given in [12]. Among other things, it is proved that the Q-index q_1 of a connected graph on n vertices satisfies the inequalities

$$2 + 2\cos\tfrac{\pi}{n} \leq q_1 \leq 2n - 2.$$

The lower bound is attained in P_n, and the upper bound in K_n.

This double inequality is the content of **Conjecture 1**, which is therefore confirmed as noticed in [24].

Conjectures 2 and 3 are resolved in [24]. Theorem 3.3.8 identifies the trees, the unicyclic graphs and the bicyclic graphs of order n with maximal Q-index. In particular, we can confirm the upper bounds in **Conjectures 2 and 3**: the only tree which is a nested split graph is a star and the only unicyclic graph which is a nested split graph is a star together with an additional edge. The lower bounds in Conjectures 1 and 2 are confirmed by Proposition 3.3.1: the graphs with minimal Q-index among trees and among unicyclic graphs are the path and the cycle respectively.

Conjecture 4 has been confirmed in [24] (see Subsection 3.2). Alternatively, we can confirm Conjecture 4 by using the inequality $\mu_1 \leq q_1$ (see Subsection 3.2) and the following result from [71] concerning the largest eigenvalue μ_1 of the Laplacian matrix: $\mu_1 \geq \Delta + 1$, with equality if and only if $\Delta = n - 1$. We note that the case of equality for the signless Laplacian is more restrictive than that for the Laplacian.

Conjecture 5. By theorem 2.5.7 we have the following statement.

Let G be a graph on n vertices with vertex degrees $d_1, d_2, \ldots, d_n$ and largest Q-eigenvalue q_1. Then

$$2\delta = 2 \min d_i \leq q_1 \leq 2 \max d_i = 2\Delta.$$

If G is connected, then equality holds in either of these inequalities if and only if G is regular.

Now let $\overline{d}$ be the mean degree of G, and recall that

$$q_1 = \sup_{\mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{0}\}} \frac{\mathbf{x}^{\mathbf{T}} Q \mathbf{x}}{\mathbf{x}^{\mathbf{T}} \mathbf{x}} = \sup_{||\mathbf{x}||=1} \mathbf{x}^{\mathbf{T}} Q \mathbf{x},$$

with equality if and only if $\mathbf{x}$ is an eigenvector of G corresponding to q_1. Taking $\mathbf{x}$ to be the all-1 vector, we see that $q_1 \geq \overline{d}$, with equality if and only if G is regular (cf. Proposition 2.3.1). The quoted facts confirm **Conjecture 5** as noticed in [24].

Conjecture 6 and the upper bound in **Conjecture 7** have been confirmed in [49] using Theorem 3.2.5.

Concerning **Conjecture 7**, the lower bound holds for graphs which are not trees because we can take the all-1 vector in a Rayleigh quotient for Q to obtain $q_1 \geq \overline{d} + 2$. In fact, for $\overline{d} \geq 2$ by (the confirmed statement of) Conjecture 5 we have $q_1 \geq 2\overline{d} \geq \overline{d} + 2$ and equality holds if and only if G is regular of degree 2. For trees of order $n \geq 5$ we use (the confirmed statement of) Conjecture 1 to obtain $q_1 \geq 2 + 2\cos\frac{\pi}{n} > 4 - \frac{2}{n} = \overline{d} + 2$.

The upper bounds in Conjectures 6 and 7 may be regarded as upper bounds for q_1 as a function of m and n, where m is the number of edges; in view of Theorem 3.3.5, it suffices to verify the bounds for nested split graphs.

The lower bound in **Conjecture 8** is also verified using (the confirmed statement of) Conjecture 1: we have $q_1 \geq 2\lambda_1 \geq \lambda_1 + \overline{d}$, with equality if and only if G is regular. The upper bound is not yet confirmed.

The lower bound in **Conjecture 9** follows from (the confirmed statement concerning) the lower bound in Conjecture 10, since $1 \leq \lambda_1$ for graphs with at least one edge. We note that the upper bound holds for bipartite graphs, because then $\mu_1 = q_1$ by Proposition 2.2.5. The upper bound is not yet confirmed.

Conjecture 10. The following statement was proved implicitly in [79] (see Subsection 3.2): *We have $\mu_1 \leq q_1$ with equality if and only if G is bipartite.*

This inequality confirms the lower bound in **Conjecture 10**.

The upper bound has been confirmed in [49] using Theorem 3.2.5.

Conjecture 11. The lower bound is confirmed by Theorem 3.4 of [12] (see Subsection 3.2). The upper bound is not yet confirmed.

Conjecture 12 is verified by Theorem 3.2 of [12]. Note that equality holds also for the graph K_3. (Theorem 3.2 of [12] contains also the inequality $q_2 \leq n-2$ with equality if the graph is complete. Theorem 3.7 of [12] provides an upper bound for q_2 in the case of bipartite graphs, namely again $n-2$, which is attained solely for $K_{2,n-2}$).

Conjecture 13 is resolved by results of [78](see also references cited therein). The result is obtained in the context of the Laplacian spectrum but in view of Proposition 2.2.5 it can be immediately reformulated for the signless Laplacian. It turned out that there are three extremal graphs for n even.

Conjecture 14. The lower bound has been confirmed in [37]. The upper bound is not yet confirmed.

Conjecture 15. has been confirmed in [37].

Conjecture 16 has been confirmed in [24]. Suppose first that $\Delta \leq n-2$. Since $q_2 \geq 0$, we have $\Delta - q_2 \leq n-2$, with equality if and only if $q_2 = 0$ and $\Delta = n-2$. However, if $q_2 = 0$ then Proposition 2.2.1 provides a contradiction. It remains to deal with the case $\Delta = n-1$, when the Conjecture reduces to: $q_2 \geq 1$ with equality if and only if G is a star. This is just Conjecture 12, confirmed above.

Conjecture 17. remains unresolved.

Conjecture 18. remains unresolved.

Conjecture 19. has been confirmed by Theorem 3.2.3.

Conjecture 20. has been confirmed by Theorem 3.2.4 and the case of equality in [37].

Conjecture 21. remains unresolved.

Conjecture 22. has been confirmed in [37].

Conjecture 23. has been confirmed in [37].

A few of the conjectures are related to the least Q-eigenvalue, and among them is **Conjecture 24**. This conjecture has been confirmed in [10] (cf. Theorem 3.2.1).

Conjecture 25 seems to be interesting and difficult to resolve. It is related to the difference between the largest and the least eigenvalue which is known as *spectral spread* (for any matrix). The corresponding conjecture for eigenvalues of the adjacency matrix is identified in [2] as a hard conjecture (also produced by AGX). It seems that we have enough evidence that system AGX can produce difficult conjectures. Some related work is done in [74] and [53] (cf. Subsection 3.9). the part related to the minimal value of the spectral spread is confirmed while in general the conjecture remains unresolved.

Conjecture 26. remains unresolved.

In contrast, we can deal easily with the conjectures concerning eigenvalue multiplicities as noticed in [24]. First, one can confirm **Conjecture 27** as follows. If $e(Q) = 2$ then the minimal polynomial of Q has the form $x^2 + ax + b$, and so $A^2 + AD + DA + D^2 + aA + aD + bI = O$. For distinct i, j this gives $a_{ij}^{(2)} + (d_j + d_i + a)a_{ij} = 0$, and so there are no vertices i, j at distance 2. Conjecture 27 has also been confirmed in [30].

More generally, the diameter of G is bounded above by $e(Q) - 1$ (see Theorem 2.5.4).

Conjecture 28 is true, because $Q - dI$ has k repeated rows, and **Conjecture 29** is true, because $Q - (d-1)I$ has k repeated rows. The validity of these conjectures follows also from a remark in [96].

Conjecture 30 is false, with K_n $(n > 5)$ a counterexample since then $d-1 = n-2$ with multiplicity $n-1$. (Note that the hypotheses are a special case of those of Conjecture 29.)

As already said in Subsection 3.2, at the moment the following conjectures of [24] remain unconfirmed: parts related to upper bounds in Conjectures 8, 9, 11, 14 together with Conjectures 17, 18, 21, 25, 26.

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