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TOWARDS A SPECTRAL THEORY OF GRAPHS BASED ON THE SIGNLESS LAPLACIAN, I

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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: equivalency 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. We present results on graph operations, inequalities for eigenvalues and reconstruction problems.

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" indicates the intention to build such a spectral graph theory

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(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 [**11**], [**17**] 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 $n \leqslant 11$:

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

We see that numbers q_n are smaller than the numbers r_n and s_n for $n \geqslant 7$. In addition, the sequence q_n is decreasing for $n \leqslant 11$ while the sequence r_n is increasing for $n \leqslant 10$. 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 [**11**] 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 [**4**] 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 [**8**] were used as additional arguments for studying eigenvalues of the signless Laplacian.

In order to avoid repetitions and to reduce the list of references we shall refer to our previous papers, in particular to the survey paper [**9**]. (Concerning the papers on the signless Laplacian published before 2003, here we mention only [**13**]). The present paper extends the surveys [**9**] and [**10**] by providing further results and comments.

Only recently has the signless Laplacian attracted the attention of researchers. As our bibliography shows, several papers on the signless Laplacian spectrum (in particular, [**2**], [**5**], [**10**], [**12**], [**14**], [**15**], [**16**], [**24**], [**26**], [**28**], [**29**], [**30**], [**31**], [**32**], [**35**], where the signless Laplacian is explicitly used) have been published since 2005. We are also aware that several other papers are being prepared, or are already in the process of publication. Therefore, 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 this paper 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 mostly composed 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. This survey will be continued in the second part of this paper.

2. Main spectral theories and their interactions

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

- equivalency with A-theory and L-theory for regular graphs (Subsection 2.2),
- equivalency with L-theory for bipartite graphs (Subsection 2.3),
- general analogies with A-theory (Subsection 2.4),
- analogies with A-theory via line graphs (Subsection 2.5),
- analogies with A-theory via subdivision graphs (Subsection 2.6).

This fragmentation appears in this presentation because the Q-theory has attracted 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.

The notions of *enriched* and *restricted* spectral theories will be considered in the second part of this paper.

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 $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$, $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_n$ and $q_1 \geqslant q_2 \geqslant \cdots \geqslant q_n$, 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 $\hat{L} = D^{-1/2}LD^{-1/2}$, the *normalized* (or *transition*) *Laplacian matrix*[1]; (see [**3**]) and on the Seidel matrix $S = J - I - 2A$ (see, for example, [**6**]).

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.

2.2. 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 [**11**]. The answer is positive for matrices A, L and Q, but it is negative for the matrix S. For the signless Laplacian see Proposition 3.1 of [**9**], where it is also stated that the number of components in regular graphs is equal to the multiplicity of the Q-index.

The following characterization of regular graphs, known in the A-theory (cf. [**6**, p. 104]), can be formulated also in the Q-theory.

PROPOSITION 2.1. *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

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

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 give A-eigenvalues, L-eigenvalues and Q-eigenvalues[2] 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.

[1] Here we assume that G has no isolated vertices.

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

complete graph K_n $(n \geqslant 2)$:		cycle C_n $(n \geqslant 3)$:	
$A:$	$n-1, (-1)^{n-1}$	$A:$	$2\cos\frac{\pi}{2n}j \;\; (j=0,1,\ldots,n-1)$
$L:$	$0,\ n^{n-1}$	$L:$	$2-2\cos\frac{\pi}{2n}j \;\; (j=0,1,\ldots,n-1)$
$Q:$	$2n-2, (n-2)^{n-1}$	$Q:$	$2+2\cos\frac{\pi}{2n}j \;\; (j=0,1,\ldots,n-1)$

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

PROPOSITION 2.2. *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 [**6**] and several related results for regular graphs.

2.3. Bipartite graphs. For bipartite graphs we have $L_G(x) = Q_G(x)$ (cf. Proposition 2.3 of [**9**]). In this way, the Q-theory can be identified with the L-theory for bipartite graphs.

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.

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 [**4**] (and [**9**]).

Among many results on bipartite graphs in the L-theory, let us mention a theorem from [**20**] (and [**16**]) saying that no starlike trees[3] are cospectral. (It was known before that the same statement holds also in the A-theory [**21**].) Now this statement holds also in the Q-theory.

2.4. Analogies with A-theory. The results which we survey in this subsection are obtained by applying to the signless Laplacian the same reasoning as for corresponding results concerning the adjacency matrix.

For example, the well known theorem concerning the powers of the adjacency matrix [**6**, p. 44] has the following counterpart for the signless Laplacian.

THEOREM 2.3. *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.*

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

For the proof and definition of *semi-edge walks* see [**9**].

The following statement and its proof is analogous to an existing result related to the adjacency spectrum [**6**, Theorem 3.13].

THEOREM 2.4. *Let G be a connected graph of diameter D with k distinct Q-eigenvalues. Then $D \leqslant k-1$.*

The proof uses Theorem 2.3 (see [**5**]).

For other examples of analogies with A-theory, see also Theorems 3.2 and 3.3.

Let G be a graph on n vertices with vertex degrees $d_1, d_2, \dots, d_n$. Let $D(G)$ be the (multi-)digraph obtained from G by adding d_i loops to the vertex i for each $i = 1, 2, \dots, n$. It was noted in [**9**] that the proof of Theorem 2.3 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.

THEOREM 2.5. *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 [**6**, Chapter 4]). The theory of divisors anyway deals with multidigraphs. Hence we have the following theorem.

THEOREM 2.6. *The A-polynomial of any divisor of $D(G)$ divides the Q-polynomial of G.*

This theorem was implicitly used in [**32**] (cf. Lemma 5.6 from that paper). For some related questions concerning graph homomorphisms see [**12**].

2.5. Line graphs. 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:

$$RR^T = D + A, \ R^T R = A(L(G)) + 2I,$$

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

$$P_{L(G)}(x) = (x+2)^{m-n} Q_G(x+2). \tag{1}$$

Therefore it follows that

$$q_1 - 2, q_2 - 2, \dots, q_n - 2, \text{ and } (-2)^{m-n} \tag{2}$$

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 (1) 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 (2) 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 $4\sin^2\frac{\pi}{2n}j$ ($j = 0, 1, ..., n-1$).

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 [**6**, p. 175] via the sum of graphs. By formula (1) we see that the 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 [**9**] and a proof using line graphs was given in [**10**]. In this version we delete edges instead of vertices.

Another example of deriving results on Q-eigenvalues via line graphs is Theorem 4.7 of [**9**] giving a lower and an upper bound on the Q-index in terms of vertex degrees.

The paper [**23**] 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.

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 is analogous to a theorem for A-index, proved in [**25**] (see also [**7**, p. 56]).

Theorem 2.7. *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). $\square$

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

2.6. 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 [**10**], the following formula appears implicitly in the literature (see e.g., [**6**, p. 63] and [**34**]):

$$P_{S(G)}(x) = x^{m-n}Q_G(x^2), \tag{3}$$

Therefore it follows that

$$\pm\sqrt{q_1}, \pm\sqrt{q_2}, \ldots, \pm\sqrt{q_n}, \quad \text{and} \quad 0^{m-n} \tag{4}$$

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

It is worth mentioning that formulas (1) and (3) provide a link between A-theory and Q-theory (and corresponding spectra, see (2) and (4)). While formula (1) has been already used in this context [**9**], the connection with subdivision graphs remains to be exploited. Some results in this direction have been obtained in [**5**].

Here we first have the following observation.

THEOREM 2.8. *Let G be a connected graph with A-index λ_1 and Q-index q_1. If G has no vertices of degree 1 and is not a cycle, 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, [**18**], or [**6**, 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 $\deg(v_0), \deg(v_{k+1}) \geqslant 3$ and $\deg(v_1) = \cdots = \deg(v_k) = 2$ (here $k \geqslant 0$, or $k \geqslant 2$ whenever $v_{k+1} = v_0$).

THEOREM 2.9. *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 $n \geqslant 3$, 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 (4).

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 [**15**].

THEOREM 2.10. *Let $G(k,l)$ $(k,l \geqslant 0)$ 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 $k \geqslant l \geqslant 1$ then $q_1\big(G(k,l)\big) > q_1\big(G(k+1,l-1)\big)$.*

PROOF. Consider the graphs $S(G(k,l))$ and $S(G(k+1,l-1))$. By using the corresponding result of [**22**] for the A-index, we immediately get that $\lambda_1\big(S(G(k,l))\big) > \lambda_1\big(S(G(k+1,l-1))\big)$. The rest of the proof immediately follows from (4). □

Some other results of the same type will be considered in the second part of this paper.

3. Solving problems within *Q*-theory

Although the Q-theory has a smaller spectral uncertainty than other frequently used spectral theories (as can be expected by the computational results from [**11**]-see Section 1), it seems that we do not have enough tools at the moment to exploit this advantage. In this section we present some results supporting such feelings. Our results refer to graph operations, inequalities for eigenvalues and reconstruction 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, [**6**], 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 (1) connects the Q-eigenvalues of a graph with the A-eigenvalues of its line graph, while formula (3) 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 (1) yields

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

Thus if $q_1, q_2, \dots, q_n$ are the Q-eigenvalues of G, then the Q-eigenvalues of $L(G)$ are $q_1+2r-4, q_2+2r-4, \dots, q_n+2r-4$ 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, [**6**, pp. 65–72]).

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 [**5**].

Example. The Q-eigenvalues of a path have been determined in Subsection 2.5. The sum of paths $P_m + P_n$ has eigenvalues $4\big(\sin^2 \frac{\pi}{2m} i + \sin^2 \frac{\pi}{2n} j\big)$ $(i = 0, 1, \dots, m-1,\ j = 0, 1, \dots, n-1)$.

For the product we have the following interesting formula

$$Q_{G\times K_2}(x) = Q_G(x) L_G(x) = L_{G\times K_2}(x). \tag{5}$$

The formula is easily obtained by elementary determinantal transformations. Therefore it follows that $q_1, q_2, \dots, q_n$ and $\mu_1, \mu_2, \dots, \mu_n$ 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 [**6**, p. 69]).

While for the L-polynomial there is a formula involving the complement of the graph (see, for example, [**6**, 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

$$Q_{GuvH}(x) = \frac{1}{x}\big(Q_{G+v}(x)Q_H(x) + Q_G(x)Q_{H+u}(x) - (x-2)Q_G(x)Q_H(x)\big) \tag{6}$$

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, [**6**, p. 159]).

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, [**6**, 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

$$P_G^{(k)}(x) = k! \sum_{S_k} P_{G-S_k}(x), \tag{7}$$

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 [**6**, 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 (7) by induction, as noted in [**9**]. If we apply (7) to the line graph $L(G)$ of a graph G and use (2), we immediately obtain

$$Q_G^{(k)}(x) = k! \sum_{S_k} Q_{G-U_k}(x), \tag{8}$$

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 3.3.

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.

Paper [**10**] 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 [**2**] by a long sequence of lemmas. The corresponding result reads:

THEOREM 3.1. *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.*

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 inequalities $\mu_1 \leqslant q_1$ and $2\lambda_1 \leqslant q_1$, with equality in the first place if and only if the graph is bipartite. See [**10**] for references (Conjectures 10 and 11).

These 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 [**24**] checks whether known upper bound on μ_1 hold also for q_1 and establishes that many of them do hold.

Best upper bounds for q_1 under some conditions are given in an implicit way by the following two theorems. First we need a definition.

A graph G with the edge set E_G is called a *nested split graph*[4] if its vertices can be ordered so that $jq \in E_G$ implies $ip \in E_G$ whenever $i \leqslant j$ and $p \leqslant q$.

The following theorem can be proved in the same way as the corresponding result in A-theory [**9**].

THEOREM 3.2. *Let G be a graph with fixed numbers of vertices and edges, with maximal Q-index. Then G does not contain, as an induced subgraph, any of the graphs: $2K_2$, P_4 and C_4. Equivalently, G is a nested split graph.*

Moreover, we also have [**9**]:

THEOREM 3.3. *Let G be a connected graph with fixed numbers of vertices and edges, with maximal Q-index. Then G does not contain, as an induced subgraph, any of the graphs: $2K_2$, P_4 and C_4. Equivalently, G is a nested split graph.*

Theorems 3.2 and 3.3 have been announced in [**9**] and complete proofs appear in [**10**]. The result has been repeated independently in [**32**]. In particular, by Theorem 3.3 we easily identify the graphs with maximal Q-index within trees, unicyclic graphs and bicyclic graphs (of a fixed number of vertices). Namely, each of these sets of graphs has a unique nested split graph (see [**10**]). The result for bicyclic graphs has again been independently rediscovered in [**14**].

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. 5 and No. 6 for $n = 5$ in Appendix of [**9**]) with maximal Q-index while only one of them (No. 5) yields maximal A-index. In fact, for any $n \geqslant 5$ and $m = n + 2$ there are two graphs with a maximal Q-index [**32**].

In the next theorem we demonstrate another use of Theorem 3.3 by providing an analogue of Hong's inequality from A-theory (see [**19**]) in Q-theory.

THEOREM 3.4. *Let G be a connected graph on n vertices and m edges. Then*

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

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

[4]This term was used in [**10**] with an equivalent definition. The present definition is used in [**7**], where the graphs in question were called graphs with a *stepwise* adjacency matrix.

PROOF. Recall first that

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

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 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

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

or

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

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)

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

and thus $q_1(G)^2 \leqslant 4m + 2(n-1)(n-2)$, 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 $q_1^2 = 2\big(d_i^2 + \sum_{j\sim i} d_j\big)$ should hold for each i). The only graph G with these properties is a complete graph. □

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

THEOREM 3.5. *Let a be the second smallest L-eigenvalue and q_2 the second largest Q-eigenvalue of a graph G with n $(n \geqslant 2)$ vertices. We have $a \leqslant q_2 + 2$ 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 $2\lambda_3 \leqslant q_2 - a$, i.e., $a \leqslant q_2 - 2\lambda_3$. It was proved in [**1**] that for graphs with at least four vertices the inequality $\lambda_3 \geqslant -1$ holds with equality if and only if $G = \overline{K_{p,q} \cup rK_1}$. Now we obtain $a \leqslant q_2 + 2$ but equality holds only for K_n. Namely, if $p, q \geqslant 1$ we have by direct calculation that $a \leqslant n - 2$ 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 3.5 confirms Conjecture 19 of [**10**].

We can treat in a similar way Conjecture 20 of [**10**] as well.

Theorem 3.6. *Let a be the second smallest L-eigenvalue and q_2 the second largest Q-eigenvalue of a non-complete graph G with n $(n \geqslant 2)$ vertices. We have $a \leqslant q_2$.*

Proof. The inequality $a \leqslant q_2 - 2\lambda_3$ immediately confirms the statement of the theorem for graphs with $\lambda_3 \geqslant 0$. It was proved in [**1**] 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 $a \leqslant n - 3$. □

The question of equality in Theorem 3.6 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 [**10**] (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).

3.3. Reconstruction problems. Studying graph reconstruction from collections of subgraphs of various kind is a traditional challenge in the graph theory.

It was proved in [**13**] 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 [**33**].

Next result involves edge deleted subgraphs.

Theorem 3.7. *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 [**27**] 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 3.7, the corresponding problem in the A-theory remains unsolved in the general case. Therefore Theorem 3.7 says much about the usefulness of the Q-theory.

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