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

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This part of our work further extends our project of building a new spectral theory of graphs (based on the signless Laplacian) by some results on graph angles, by several comments and by a short survey of recent results.

## 1. INTRODUCTION

This is the third part of our work with a common title. The first [**11**] and the second part [**12**] will be also referred in the sequel as Part I and Part II, respectively.

This third part was not planned at the beginning, but a lot of recently published papers on the signless Laplacian eigenvalues of graphs and some observations of ours justify its preparation.

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

In fact, we outlined in [**11**], [**12**] a new spectral theory of graphs (based on the signless Laplacian $Q$). We shall call this theory the *$Q$–theory*.

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We have also compared the $Q$-theory with other spectral theories, in particular to those based on the adjacency matrix $A$ and the Laplacian $L$. As demonstrated in the first part, the $Q$–theory can be constructed in part using various connections to other theories: equivalence with $A$–theory and $L$–theory for regular graphs, common features with $L$–theory for bipartite graphs, general analogies with $A$–theory and analogies with $A$–theory via line graphs and subdivision graphs. In Part I we also presented results on graph operations, inequalities for eigenvalues and reconstruction problems. In Part II we introduced notions of enriched and restricted spectral theories and presented results on integral graphs, enumeration of spanning trees, characterizations by eigenvalues, cospectral graphs and graph angles. This part further extends our project by some results on graph angles, by several comments and by a short survey of recent results.

We use here the terminology and notation from Parts I and II although a part of that we repeat here.

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 of this paper we have mentioned 15 papers (in particular, [**4**], [**6**], [**10**], [**15**], [**20**], [**22**], [**23**], [**35**], [**39**], [**41**], [**43**], [**44**], [**46**], [**47**], [**55**], where the signless Laplacian is used explicitly) in addition to our previous basic papers [**5**], [**9**]. In Part II we have added the following 11 references: [**1**], [**3**], [**24**], [**25**], [**26**], [**27**], [**34**], [**36**], [**48**], [**52**], [**54**]. In the meantime the following 16 papers [**2**], [**13**], [**18**], [**19**], [**21**], [**28**], [**29**], [**30**], [**31**], [**32**], [**38**], [**42**], [**45**], [**49**], [**51**], [**53**] have been published or are in the process of publication at this moment. Together with [**11**], [**12**] and this paper, there are in this moment about 50 papers on the signless Laplacian spectrum published since 2005. Several others are forthcoming.

The rest of the paper is organized as follows. Section 2 surveys the progress in resolving some conjectures on the signless Laplacian eigenvalues which are generated by computer. Recent results on spectral characterizations are presented in Section 3. The largest eigenvalue is the subject of Section 4. We present in Section 5 new results related to graph angles. Other results are noted in Section 6. Section 7 contains some concluding remarks.

## 2. RESOLVING CONJECTURES

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 others quite a lot of work had to be invested. The conjectures left unresolved appear to include some difficult research problems. One difficult conjecture (Conjecture 24) has been confirmed in [**4**] by a long sequence of lemmas.

Conjecture 25 appears also to be a difficult one. It remains unsolved but some related work is described in Section 6.

Conjectures 6, 7 and 10 from [**10**] have been proved in [**26**].

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

**Theorem 1.** *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 1 is better than our bound in Theorem 3.4 of Part I. 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 3.2 and 3.3 of Part I.

In order to prove Theorem 1, the authors of [**26**] derive first the bound

$$q_1(G) \leq \max\{d_v + m_v | v \in V(G)\}, \tag{1}$$

where $d_v$ is the degree of the vertex $v$ and $m_v$ the average degree of neighbors of $v$. As noted in Part I, paper [**35**] checks whether known upper bounds on largest Laplacian eigenvalue $\mu_1$ hold also for $q_1$ and establishes that many of them do hold, in particular inequality (1). However, the authors of [**35**] claim that (1) was implicitly proved in [**16**].

To complete the proof of Theorem 1 the authors of [**26**] use another inequality by K. Ch. Das [**17**]:

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

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

Theorems 3.5 and 3.6 of Part I confirm Conjecture 19 and 20 of [**10**], respectively.

The question of equality in Theorem 3.6. ($a = q_2$) remained unresolved in Part I. Graphs for which equality holds are among the graphs with $\lambda_3 = 0$. To this group belong the graphs mentioned in Conjecture 20 of [**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).

Paper [**18**] settled completely the question of equality in Theorem 3.6 of Part I (Conjecture 20).

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

At the moment the following conjectures of [**10**] remain unconfirmed: those parts related to upper bounds in Conjectures 8, 9, 11, 14 together with Conjectures 16, 17, 18, 21, 25, 26.

The paper [**2**] discusses the same set of conjectures and presents some new ones.

A new set of conjectures involving the largest $Q$–eigenvalue appears in [**31**]. 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. by the system AGX), many of them are simple or proved in [**31**], so that only 18 remained unsolved. An additional conjecture of this type has been resolved in [**32**]; 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. [**7**], p. 92).

## 3. SPECTRAL CHARACTERIZATIONS

In Part II we had the following paragraph.

Starlike trees are DS in the $L$–theory [**37**], while this is not proved for the $A$–theory [**50**]. Concerning the $Q$–theory, a private communication of Omidi is cited in [**14**] 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 [**50**]. Indeed, the subdivision graph of a $T$–shape tree is again a $T$–shape tree and an $A$–cospectral mate, described in [**50**], is not a subdivision graph except for $K_{1,3}$.

Recently the paper [**38**] 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, mentioned above, is still a subdivision graph yielding the $Q$-cospectral mate found in [**38**]. Hence, our method of using subdivision graphs and results from [**50**] do confirm the results of [**38**]. In fact our method proves these results in a much simpler way.

The paper [**38**] 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 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 [**12**] (see Subsection 3.3, Theorem 2.9 and the example after it) and explicitly in [**13**]. It follows that $C_{2k} \cup 2P_\ell$ 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. The only additional non-DS graph is $K_{1,3}$ which is cospectral to $C_3 \cup K_1$.

As shown in [**13**], 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.

Graphs consisting of two cycles with just a vertex in common are called $\infty$-*graphs* in [**49**]. It is proved that $\infty$-graphs without triangles are characterized by their Laplacian spectra and that all $\infty$-graphs, with one exception, are characterized by their signless Laplacian spectra.

## 4. THE LARGEST EIGENVALUE

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.

In [**24**] the class of unicyclic graphs with a given number of pendant vertices or given independence number was considered. Graphs with maximal $Q$-index and corresponding extremal graphs are determined.

Independently, the same results have been obtained in [**53**], 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 [**21**] the class of bicyclic graphs with a given number of pendant vertices was considered. Graphs with maximal $Q$-index and corresponding extremal graphs 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 $m$ is the number of edges). For example, if $k = 0$, the corresponding graph is a *quasi-tree*. In [**28**] quasi-$k$-cyclic graphs having the largest $Q$-index are identified for $k \leq 2$.

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 [**51**].

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 [**33**]), 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 $\leq 2$). 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 signless Laplacian of the graph $H$, respectively. Therefore (by using the Courant-Weyl inequalities - see [**7**], pp. 51-52) we get that

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

Since $\lambda_1(S(G)) = \sqrt{q_1(G)}$ (see Part I, Section 2.6), we arrive at the following result.

**Proposition 1.** *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.

## 5. $Q$-THEORY ENRICHED BY ANGLES

As explained in Part II the $Q$-angles of a graph are defined in the following way.

The spectral decomposition of the matrix $Q$ reads:

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

where $\kappa_1, \kappa_2, \ldots, \kappa_m$ are the distinct $Q$–eigenvalues of a graph $G$, and $P_1, P_2, \ldots, P_m$ the projection matrices (of the whole space to the corresponding eigenspaces); so $P_iP_j = O$ if $i \neq j$, and $P_i^{\,2} = P_i = P_i^{\,T}$ $(1 \leq i, j \leq m)$. 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 $\gamma_{ij}$ is the cosine of the angle between the unit vector $\mathbf{e}_j$ (corresponding to vertex $j$ of $G$) and the eigenspace for $\kappa_i$. 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 the matrix $\Gamma = (\gamma_{ij})$. This matrix is a graph invariant if its columns are ordered lexicographically.

We have considered in Part II the enriched theory $Q_c$, the $Q$-theory enriched by the number of components $c$. Now we consider the enriched theory $Q_\Gamma$, the $Q$-theory enriched by the $Q$–angle matrix $\Gamma$.

The next theorem shows that the theory $Q_\Gamma$ 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 $Q_\Gamma$.

**Theorem 2.** *The number of components $c$ of a graph can be determined by $Q$-eigenvalues and $Q$-angles.*

The proof can be carried out analogously to the proof of the corresponding result for $A$-theory (see [**8**], 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 $Q_\Gamma$ is much stronger than the theory $Q_c$. As noted in Part II, 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 $Q_\Gamma$.

Next, we are in position to strengthen Theorem 2.9 from Part II.

**Theorem 3.** *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 $1/\sqrt{s}$. $\square$

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 in Part II or [**48**]).

## 6. OTHER RECENT RESULTS

Several infinite families of $Q$-integral graphs have been constructed in [**27**] using the join of regular graphs. The formula for the join of regular graphs was derived by the graph divisor technique.

Some infinite series of $ALQ$-integral graphs[2] have been constructed in [**45**]. In addition, semi-regular bipartite $Q$-integral graphs are considered and this investigation is continued in [**42**].

As pointed out in Part II, the *$Q$–spectral spread* $s_Q(G) = q_1 - q_n$ has been studied in [**36**]. Now, when we have the whole text of this paper at our disposal, we can see that the calculation of the $Q$-spectrum of the extremal graph $K_{n-1} + v$ has been carried out independently by different methods in [**36**] (the graph divisor technique) and in Part II (using $Q$-angles) with the same result.

Conjecture 25 of [**10**] concerning the spectral spread $s_Q(G)$ [3] was relaxed in [**36**] by proving a weaker inequality. Another relaxation appears in [**29**], where the conjecture was confirmed for unicyclic graphs.

An upper bound on maximal entry of the eigenvector of the largest $Q$-eigenvalue $q_1$ of a graph has been obtained in [**19**].

The quantity $IE(G) = \sum_{1}^{n} \sqrt{q_i}$ is called the *incidence energy* of a graph $G$ in [**30**] (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

[2] Integral graphs with respect to all three graph matrices $A, L, Q$, as defined in Part II.

[3] Conjecture 25 reads: *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 $K_{n-1} + v$.*

of $A$-eigenvalues of a graph. Having in view relation (3) from Part I 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 [**30**].

## 7. CONCLUSION

Our survey in [**11**], [**12**] and this paper 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 5.1 from [**10**]) describing the behaviour of the $Q$-index under edge rotation. Another important tool is Theorem 3.3 from Part I 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 of this survey.

The divisor technique (see Theorem 2.6 of Part I) has been used in various occasions for computing $Q$-eigenvalues (see, for example, [**27**], [**36**], [**51**]).

*Bibliographical note.* Reference [**27**] of Part I was incorrectly given and the correct form reads as here in [**40**].

[**27**] is updated reference [**24**] of Part II.

[**35**] is updated reference [**30**] of Part II, i.e. [**24**] of Part I.

[**36**] is updated reference [**31**] of Part II.

[**41**] is updated reference [**36**] of Part II, i.e. [**28**] of Part I.

[**43**] is corrected reference [**38**] of Part II, i.e. [**29**] of Part I.

*Note added in proof.* Between submission of this paper (October 2009) and its revision (December 2009) the authors became aware of the existence of the papers [**56**] - [**67**] in which signless Laplacian eigenvalues appear. In this way the number of papers on the signless Laplacian spectrum published since 2005 raises to over 60. As noticed by the referee, the $Q$-theory, and in particular "the 30 conjectures in . . . [**10**], have attracted a new generation of researchers to spectral graph theory".

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