TOWARDS A SPECTRAL THEORY OF GRAPHS BASED ON THE SIGNLESS LAPLACIAN, III[1]

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Abstract. *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.*

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

AMS Classification: 05C50

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.*

[1]Research supported by the Serbian Ministry of Science and Technological Development, grant 144015G

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: equivalency with A–theory and L–theory for regular graphs, common features with L–theory for bipartite graphs, general analogies with A–theory and analogies with A–theory via line graphs and subdivision graphs. In 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 position to summarize the development. 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 explicitly used) 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 publishing. Together with [11], [12] and this paper, there are in this moment about 50 papers on the signless Laplacian spectrum published since 2005. Several other are coming.

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. The progress in studying Q-integral graphs is described in Section 5. We present in Section 6 new results related to graph angles. Other results are commented in Section 7. Section 8 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 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 [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].

The crucial role in resolving these conjectures had 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 bound on largest Laplacian eigenvalue μ_1 hold also for q_1 and establishes that many of them do hold, in particular inequality (1). However, 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 related results 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 the equality in Theorem 3.6. ($a = q_2$) remained unsolved in Part I. 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).

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

The same paper confirmed lower bound of Conjecture 14 and 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 unsolved: parts related to upper bounds in Conjectures 8, 9, 11, 14 and Conjectures 16, 17, 18, 21, 25, 26.

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 to various structural invariants, such as diameter, radius, girth, independence and chromatic number, etc. Out of 152 conjectures, generated by computer (i.e. 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 G.R. 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 original private communication we made a mistake. The mistake was that the A–cospectral mate, mentioned above, is still a subdivision graph yielding Q-cospectral mate found in [38]. Hence, our method of using subdivision graphs and results of [50] do confirm the results of [38]. In fact our method proves these results in 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, being noted in the literature so far, consists of 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 further, only the minimal graphs which are not DS will be considered, since any other such a graph can be easily recognized if it contains 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 [12] (see Subsection 3.3, Theorem 2.9 and the example after it) and explicitly in [13]. 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. 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 ∞-*graphs* in [49]. It is proved that ∞-graphs without triangles are characterized by their Laplacian spectra and that all ∞-graphs, with one unique exception, are characterized by their signless Laplacian spectra. Again, we see the advantage of 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 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 set of graphs with given vertex degrees are determined and these results 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 *quasi-k-cyclic graph* if it contains a vertex (say r, the 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 a number of its vertices, while m a number of its edges). For example, if $k = 0$, the corresponding graph is a *quasi-tree*. In [28] quasi-k-cyclic graph 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, a *total* graph of G, denoted by $T(G)$, is a 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 ≤ 2). The above relation implies that

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

Therefore (by using Courant-Weyl inequalities - see [7], pp. 51-52) we get that

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

Since $\lambda_1(S(G)) = (\sqrt{q_1(G)})^2$, 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 Integral graphs

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].

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

6 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 $P_i P_j = O$ 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 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_Γ, the Q-theory enriched by the Q–angle matrix Γ.

Next theorem shows that the theory Q_Γ is strong at least as the theory Q_c, i.e. everything what can be proved for a graph in Q_c can also be proved in Q_Γ.

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

The proof can be carries 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 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 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_Γ.

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 components some cycles and stars $K_{1,3}$. The vertices belonging to these components are identified by non-zero angles of 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 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 in Part II or [48]).

7 Other recent results

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 the 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] (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 proved for some narrow class of graphs (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 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].

8 Conclusion

Our survey in [11], [12] and in 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. Important tool is also 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 extensively studied.

[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 $K_{n-1} + v$.*

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 appeared 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]).

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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.