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Signless Laplacians of finite graphs ☆

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Abstract

We survey properties of spectra of signless Laplacians of graphs and discuss possibilities for developing a spectral theory of graphs based on this matrix. For regular graphs the whole existing theory of spectra of the adjacency matrix and of the Laplacian matrix transfers directly to the signless Laplacian, and so we consider arbitrary graphs with special emphasis on the non-regular case. The results which we survey (old and new) are of two types: (a) results obtained by applying to the signless Laplacian the same reasoning as for corresponding results concerning the adjacency matrix, (b) results obtained indirectly via line graphs. Among other things, we present eigenvalue bounds for several graph invariants, an interpretation of the coefficients of the characteristic polynomial, a theorem on powers of the signless Laplacian and some remarks on star complements.

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1. Introduction

Let G be a simple graph with n vertices. The characteristic polynomial $\det(\lambda I - A)$ of a (0, 1)-adjacency matrix A of G is called the *characteristic polynomial of* G and denoted by $P_G(\lambda)$. The eigenvalues of A (i.e. the zeros of $\det(\lambda I - A)$) and the spectrum of A (which consists of the n eigenvalues) are also called the *eigenvalues* and the *spectrum* of G, respectively. The eigenvalues of G are usually denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$; they are real because A is symmetric. Graphs with the same spectrum are called *isospectral* or *cospectral* graphs. The term "(unordered) pair of isospectral non-isomorphic graphs" will be denoted by PING.

An overview of basic results on graph spectra is given in [4].

Together with the spectrum of the adjacency matrix of a graph we shall consider the spectrum of another matrix associated with the graph.

Let n, m, R be the number of vertices, the number of edges and the vertex-edge incidence matrix of a graph G. The following relations are well-known:

$$RR^{\mathrm{T}} = A + D, \quad R^{\mathrm{T}}R = A_L + 2I, \tag{1}$$

where D is the diagonal matrix of vertex degrees and A_L is the adjacency matrix of the line graph $L(G)$ of G.

Since non-zero eigenvalues of RR^{T} and $R^{\mathrm{T}}R$ are the same, from the relations (1) we immediately obtain

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

where $Q_G(\lambda)$ is the characteristic polynomial of the matrix $Q = A + D$.

Remark. If $m < n$, the matrix Q must have eigenvalue 0 with multiplicity at least $n - m$. This will be verified later (see Corollary 2.2).

The polynomial $Q_G(\lambda)$ will be called the *Q-polynomial* of the graph G. The spectrum and the eigenvalues of Q will be called the *Q-spectrum* and *Q-eigenvalues*, respectively.

The matrix $L = D - A$ is known as the *Laplacian* of G and is studied extensively in the literature (see, e.g., [4]). The matrix $A + D$ is called the *signless Laplacian* in [15] and appears very rarely in published papers (see [4]), the paper [10] being one of the very few research papers concerning this matrix.

Graphs with the same spectrum of an associated matrix M are called *cospectral* graphs with respect to M. 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 an associated matrix M. The ratio $|\mathcal{G}'|/|\mathcal{G}|$ is called the *spectral uncertainty* of $\mathcal{G}$ (with respect to M).

The papers [8,15] provide spectral uncertainties r_n with respect to the adjacency matrix and q_n with respect to the signless Laplacian 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
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 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 spectra perform better also in comparison to spectra of other commonly used graph matrices (Laplacian, the Seidel matrix), an idea was expressed in [8] 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.

The relation (2) provides a direct link between the spectra of line graphs and the Q-spectra of graphs.

It is well known that if G and H are connected graphs such that $L(G) = L(H)$ then $G = H$ unless $\{G, H\} = \{K_3, K_{1,3}\}$. This result opens the possibility of studying graphs in terms of their line graphs, at least in principle. One could consider whether it would be more efficient to consider the spectrum of $L(G)$ instead of describing a graph G by its own spectrum.

The computational evidence that Q-spectra perform better than the adjacency spectra supports the idea of using the spectrum of $L(G)$ instead of the spectrum of G.

On the other hand, the well developed theory of graphs with least eigenvalue -2 (see [7]) provides additional motivation to study Q-spectra of graphs.

These arguments have been developed in detail in the paper [3].

As usual, K_n, C_n and P_n denote respectively the *complete graph*, the *cycle* and the *path* on n vertices. Further, $K_{m,n}$ denotes the *complete bipartite* graph on $m + n$ vertices. A unicyclic graph containing an odd cycle is called *odd-unicyclic*. A bicyclic graph consisting of two disjoint odd cycles connected by a path is called an *odd dumb-bell*. 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 plan of the present paper is as follows. In Section 2 we discuss some basic properties of the characteristic polynomial of the signless Laplacian. Section 3 explains how the Q-spectra of regular graphs are reduced to adjacency and Laplacian spectra. In Section 4 we have collected results which can be transferred easily from spectra to Q-spectra. Section 5 contains some results specific to the signless Laplacian. The largest eigenvalue is considered in Section 6, while in Section 7 star complements are discussed in the context of the signless Laplacian. The Appendix contains the Q-spectra of connected graphs up to 5 vertices.

2. Basic properties of Q-spectra

Almost all known 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. 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. Concerning the least eigenvalue we have the following proposition.

Proposition 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 $\mathbf{x}^{\mathrm{T}} = (x_1, x_2, \ldots, x_n)$. For a non-zero vector $\mathbf{x}$ we have $Q\mathbf{x} = \mathbf{0}$ if and only if $R^{\mathrm{T}}\mathbf{x} = \mathbf{0}$. 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, **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 [7], 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. *In any graph the multiplicity of the eigenvalue* 0 *of the signless Laplacian is equal to the number of bipartite components.*

The least eigenvalue of the signless Laplacan is studied in [10] as a measure of non-bipartiteness of a graph and Proposition 2.1 was obtained there as a corollary of a more general theorem (see Section 5).

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.

The proof of the following proposition can be found in many places (see, for example, [13]).

Proposition 2.3. *In bipartite graphs the Q-polynomial is equal to the characteristic polynomial of the Laplacian.*

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.

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

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 2.1) whether G is bipartite and go on to calculate $P_{L(G)}(\lambda)$ using (2).

Proposition 2.4. *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 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 005 and 006 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 [4, p. 157]) are not Q-PINGs. The paper [15] 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 *L-cospectral* if their line graphs are cospectral.

Proposition 2.5. *If two graphs are Q-cospectral, then they are L-cospectral.*

Proof. Since Q-cospectral graphs have the same number of vertices and the same number of edges, their L-cospectrality follows from formula (2). □

However, two L-cospectral graphs need not be Q-cospectral. This is because two cospectral line graphs need not have the same number of vertices in their root graph. (Such an example of cospectral line graphs is given in Fig. 1.)

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 in this direction (See [3] for more comments on this example.)

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 [7] a regular line graph could be cospectral with another line graph for which the root graph has a different number of vertices (see [3] for an example), and this fact would cause additional problems if the polynomial $P_{L(G)}(\lambda)$ alone were given.

Now for a graph G we 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.

Fig. 1. Cospectral line graphs.

3. Regular graphs

Regular graphs can be recognized, and their degree and the number of components calculated, from $Q_G(\lambda)$, as noticed in [8]. In particular, we have the following proposition.

Proposition 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. [4], Theorems 3.8, 3.22 and 3.23). In fact, one should compare the value of the Rayleigh quotient in (5) 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 3.1.

Of course, in regular graphs we can calculate the characteristic polynomial of the adjacency matrix and of the Laplacian 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

$$P_G(\lambda) = Q_G(\lambda + r).$$

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

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

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

Recall that for bipartite graphs we have $L_G(\lambda) = Q_G(\lambda)$. Hence, for non-regular non-bipartite graphs the Q-polynomial really plays an independent role; for other graphs it can be reduced to either $P_G(\lambda)$ or $L_G(\lambda)$ or to both.

4. Results related to the adjacency matrix

In this section we consider graphs in general with special emphasis on the non-regular case. The results which we survey are of two types: results of *type a* are obtained by applying to the signless Laplacian the same reasoning as for corresponding results concerning the adjacency matrix, and results of *type b* are obtained indirectly via line graphs.

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 $\mathbf{u} = R^{\mathrm{T}}\mathbf{x}$ 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 $\mathbf{x}^{\mathrm{T}} = (x_1, x_2, \ldots, x_n)$ and $\mathbf{u}^{\mathrm{T}} = (u_1, u_2, \ldots, u_m)$. If the edge k of G joins vertices i and j, then from the relation $\mathbf{u} = R^{\mathrm{T}}\mathbf{x}$ 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 $v_1, e_1, v_2, e_2, \ldots, v_k, e_k, v_{k+1}$ of vertices $v_1, v_2, \ldots, v_{k+1}$ 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 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 [4, p. 44] has the following counterpart for the signless Laplacian.

Theorem 4.1. *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. $\square$

Remark. The proof can also be carried out by applying the theorem concerning the powers of the adjacency matrix to the multigraph obtained by adding d_i loops to the vertex i for $i = 1, 2, \ldots, n$, where d_i is the degree of the vertex i.

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

Corollary 4.2. *The spectral moment T_k is equal to the number of closed semi-edge walks of length k.*

Corollary 4.3. *Let G be a graph with n vertices, m edges, t triangles and vertex degrees $d_1, d_2, \ldots, d_n$. 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. 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 2.4.

Let G be a connected graph with n vertices and m edges where $m \geqslant n$. 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 4.4. *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 [4, p. 60], and then we obtain (3) by induction, as noted in [14].)

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 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 [7]).

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, [5]). 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. $\square$

This result appeared in [9]; here we have given a new proof.

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 2.4. 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 4.5. *$p_1 = -2m$ and $p_2 = a + \frac{3}{2}m(m - 1)$, where a is the number of pairs of non-adjacent edges in G.*

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., [12], vol. II, p. 63, or [4], p. 83).

Theorem 4.6. *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*

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

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.

Theorem 4.7. *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*

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

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

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

which proves the theorem. □

A version of this theorem appears in [20]. See also [16,17]. Theorem 4.6 can be classified as a result of type a while Theorem 4.7 is of type b.

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.

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 [4])

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

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 [4] 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

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

from which the following assertion follows:

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

This assertion, a result of type b, is very weak although the initial inequalities are known to be good. In fact, we have $d_{\max} \leqslant \chi'(G) \leqslant d_{\max} + 1$ where $d_{\max}$ is the maximal vertex degree; these bounds are much better than those obtained from the assertion in conjunction with Theorem 4.6 (a result of type a).

5. Other results

This section contains results based essentially on characteristic features of the signless Laplacian. It appears that the only papers which contain substantive results of this sort are [9–11].

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 [10] 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,

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

where $d_{\max}$ is the maximal vertex degree.

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 [11] 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).

The paper [9] was already mentioned in connection with the coefficient theorem (Theorem 4.4). It contains also some results on the reconstructibility of the Q-polynomial from vertex-deleted subgraphs of G.

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

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

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

6. The largest eigenvalue

When applying the Perron–Frobenius theory of non-negative matrices (see, for example, Section 0.3 of [4]) 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 [4]. The interlacing theorem holds in a specific way, namely the 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.

Proposition 6.1. *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 $2\cos\frac{\pi}{n}j$ $(j = 1, 2, \dots, n-1)$ and by (2) the Q-eigenvalues of P_n are $2 + 2\cos\frac{\pi}{n}j$ $(j = 1, 2, \dots, n)$. 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. □

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

$$q_1 = \sup_{\mathbf{x}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\mathbf{x}^{\mathrm{T}}Q\mathbf{x}}{\mathbf{x}^{\mathrm{T}}\mathbf{x}} = \max_{\|\mathbf{x}\|=1} \mathbf{x}^{\mathrm{T}}Q\mathbf{x}. \tag{5}$$

(see, for example, [6]). 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 (5) we obtain:

$$q_1' - q_1 = \max_{\|\mathbf{y}\|=1} \mathbf{y}^{\mathrm{T}}Q'\mathbf{y} - \mathbf{x}^{\mathrm{T}}Q\mathbf{x} \geqslant \mathbf{x}^{\mathrm{T}}(A'-A)\mathbf{x} + \mathbf{x}^{\mathrm{T}}(D'-D)\mathbf{x}, \tag{6}$$

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

On basis of this observation, we obtain:

Lemma 6.2. *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 $\mathbf{x} = (x_1, x_2, \ldots, x_n)^{\mathrm{T}}$ be the principal eigenvector of G. If $x_t \geqslant x_s$ then $q_1' > q_1$.*

Proof. From (6) we immediately obtain

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

Since x_r, x_s and x_t are positive and $x_t \geqslant x_s$ we obtain $q_1' \geqslant q_1$. 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. □

The following theorem can be proved in the same way as Theorem 2.4 from [19].

Theorem 6.3. *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 (cf. Theorem 2.4′) from [19]).

Theorem 6.3′. *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.*

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 $i = 1, 2, \ldots, k-1$.

From Theorems 6.3. and 6.3$'$ 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.

In addition, we can prove:

Proposition 6.4. *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 $\mathbf{x} = (x_1, x_2, \ldots, x_n)^{\mathrm{T}}$ be a principal eigenvector of G. If $(x_a - x_c)(x_b - x_d) \geqslant 0$ then $q_1' \geqslant q_1$, with equality if and only if $x_a = x_c$ and $x_b = x_d$.*

Proof. From (6) we have

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

and the first assertion follows. The second assertion follows from the eigenvalue equations for G and G'. $\square$

7. Star complements

The theory of star complements of graphs is presented in [18] and in the book [7], Chapter 5. We offer here a few observations indicating possibilities to extend the theory to signless Laplacians.

For a graph G we describe the relation between the eigenspaces $\mathscr{E}_L(\lambda)$ $(\lambda \neq -2)$ of an eigenvalue λ of the line graph $L(G)$ and the eigenspaces $\mathscr{E}_{D+A}(\lambda)$ $(\lambda \neq 0)$ 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 7.1. (i) *The map $\mathbf{x} \mapsto R\mathbf{x}$ is an isomorphism $\mathscr{E}_L(\lambda) \to \mathscr{E}_{D+A}(\lambda+2)(\lambda \neq -2)$.*

(ii) *If P represents the orthogonal projection $\mathbb{R}^m \to \mathscr{E}_L(\lambda)$ and P' denotes the orthogonal projection $\mathbb{R}^n \to \mathscr{E}_{D+A}(\lambda+2)$ $(\lambda \neq -2)$ then $RP = P'R$.*

Proof. (i) See [6, Theorem 2.6.1].

(ii) Let $\mathbf{y}$ be an arbitrary element of $\mathbb{R}^m$, say $\mathbf{y} = \mathbf{w} + \mathbf{z}$, where $\mathbf{w} \in \mathscr{E}_L(\lambda)$ and $\mathbf{z} \in \mathscr{E}_L(\lambda)^{\perp}$. 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 $R\mathbf{z} \in \mathscr{E}_{D+A}(\lambda+2)^{\perp}$. But if $\mathbf{v} \in \mathscr{E}_{D+A}(\lambda+2)$ then $\mathbf{v} = R\mathbf{x}$ for some $\mathbf{x} \in \mathscr{E}_L(\lambda)$, and we have $\mathbf{v}^{\mathrm{T}}(R\mathbf{z}) = \mathbf{x}^{\mathrm{T}}R^{\mathrm{T}}R\mathbf{z} = (\lambda+2)\mathbf{x}^{\mathrm{T}}\mathbf{z} = 0$. $\square$

We note in passing that in Proposition 7.1, we have $\lambda > -2$ and the map $\mathbf{x} \mapsto (\lambda+2)^{-\frac{1}{2}}R\mathbf{x}$ is an isometry $\mathscr{E}_L(\lambda) \to \mathscr{E}_{D+A}(\lambda+2)$ $(\lambda \neq -2)$.

Next let $\mathbb{R}^m$ have standard basis $\{\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_m\}$ and let $\mathbb{R}^n$ have standard basis $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\}$. From [6, Theorem 7.2.9] we know that X is a star set for λ in $L(G)$ if and only if $\{P\mathbf{f}_j : j \in X\}$ is a basis for $\mathscr{E}_L(\lambda)$. In this situation, $\mathscr{E}_{D+A}(\lambda+2)$ has basis $\{RP\mathbf{f}_j : j \in X\}$. By Proposition 7.1, $\{P'R\mathbf{f}_j : j \in X\}$ is a basis for $\mathscr{E}_{D+A}(\lambda+2)$. Now $R\mathbf{f}_j$ is the jth column of R, i.e. $R\mathbf{f}_j = \mathbf{e}_u + \mathbf{e}_v$, where uv is the jth edge of G. It follows that $\mathscr{E}_{D+A}(\lambda+2)$ has basis $\{P'\mathbf{e}_u + P'\mathbf{e}_v : uv \in X\}$, where now the vertices in X are labelled as edges. Hence $\mathscr{E}_{D+A}(\lambda+2) \subseteq \mathrm{span}\{P'\mathbf{e}_u : u \in X^*\}$, where X^* denotes the set of end-vertices of edges in X. We may select a basis for $\mathscr{E}_{D+A}(\lambda+2)$ from this spanning set to obtain the following result.

Corollary 7.2. *If X is a star set for λ in $L(G)$ $(\lambda \neq -2)$ then there exists $Y \subseteq \cup X$ such that $\{P'\mathbf{e}_u : u \in Y\}$ is a basis for $\mathscr{E}_{D+A}(\lambda+2)$.*

We note in passing that $|Y| = |X|$, and the vectors $P'\mathbf{e}_u (u \in Y)$ are necessarily linearly independent. Thus if $|X| = d$ then the d edges in X cannot be chosen from a subgraph of G with fewer than d vertices. Also, the vectors $\mathbf{e}_u + \mathbf{e}_v$ $(uv \in X)$ are linearly independent and so X cannot include the set of edges of an even cycle or of an odd dumb-bell, an observation which follows from stronger results in [7, Section 5.2]. Indeed, such edges (called *strong* edges) cannot belong to any star complement for -2 in $L(G)$, while by [6, Theorem 7.4.5] X lies in some such star complement. The *L-core* of a graph G is the subgraph induced by its strong edges. The L-core can be characterized by spectral properties of $L(G)$ (cf. [2, Section 4]), but it remains to find a satisfactory non-spectral characterization.

If Y is any set of vertices in G for which $\{P'\mathbf{e}_u : u \in Y\}$ is a basis for $\mathscr{E}_{D+A}(\lambda)$ (cf. Corollary 7.2) then we may refer to Y as a star set for λ with respect to $D + A$. In this situation, we have

$$D + A = \begin{pmatrix} D_1 + A_Y & B^{\mathrm{T}} \\ B & D_2 + C \end{pmatrix}, \quad \text{where } D = \begin{pmatrix} D_1 & O \\ O & D_2 \end{pmatrix}.$$

The arguments of [7, Proposition 5.1.1] carry over to show that λ is not an eigenvalue of $D_2 + C$, and we have the following analogue of the Reconstruction Theorem (cf. [6], Theorem 5.1.7):

$$\lambda I - D_1 - A_Y = B^{\mathrm{T}}(\lambda I - D_2 - C)^{-1}B.$$

It follows that if $K = G - Y$ then G is determined by λ, K and the K-neighbourhoods of vertices in Y, since D_2 can be reconstructed from the row sums of $[B|C]$. However we cannot say that λ is not an eigenvalue of the signless Laplacian of K because this matrix differs from $D_2 + C$.

Appendix

We have computed Q-spectra of graphs on up to 5 vertices.

The graphs are ordered in the same way as in the book [4] and the reader is referred to this book for drawings of the graphs.

For each graph the first line contains eigenvalues while Q-eigenvalues are contained in the second line.

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

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

001    1.0000  -1.0000
       2.0000   0.0000
```

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

001   2.0000  -1.0000  -1.0000
      4.0000   1.0000   1.0000

002   1.4142   0.0000  -1.4142
      3.0000   1.0000   0.0000

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

001   3.0000  -1.0000  -1.0000  -1.0000
      6.0000   2.0000   2.0000   2.0000

002   2.5616   0.0000  -1.0000  -1.5616
      5.2361   2.0000   2.0000   0.7639

003   2.1701   0.3111  -1.0000  -1.4812
      4.5616   2.0000   1.0000   0.4384

004   2.0000   0.0000   0.0000  -2.0000
      4.0000   2.0000   2.0000   0.0000

005   1.7321   0.0000   0.0000  -1.7321
      4.0000   1.0000   1.0000   0.0000

006   1.6180   0.6180  -0.6180  -1.6180
      3.4142   2.0000   0.5858   0.0000

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

001   4.0000  -1.0000  -1.0000  -1.0000  -1.0000
      8.0000   3.0000   3.0000   3.0000   3.0000

002   3.6458   0.0000  -1.0000  -1.0000  -1.6458
      7.3723   3.0000   3.0000   3.0000   1.6277

003   3.3234   0.3579  -1.0000  -1.0000  -1.6813
      6.8284   3.0000   3.0000   2.0000   1.1716

004   3.2361   0.0000   0.0000  -1.2361  -2.0000
      6.5616   3.0000   3.0000   2.4384   1.0000
```

005	3.0861	0.4280	-1.0000	-1.0000	-1.5141
	6.3723	3.0000	2.0000	2.0000	0.6277
006	3.0000	0.0000	0.0000	-1.0000	-2.0000
	6.3723	3.0000	2.0000	2.0000	0.6277
007	2.9354	0.6180	-0.4626	-1.4728	-1.6180
	6.1249	3.0000	2.6367	1.2384	1.0000
008	2.8558	0.3216	0.0000	-1.0000	-2.1774
	5.7785	3.0000	2.7108	2.0000	0.5107
009	2.6855	0.3349	0.0000	-1.2713	-1.7491
	5.7785	2.7108	2.0000	1.0000	0.5107
010	2.6412	0.7237	-0.5892	-1.0000	-1.7757
	5.4679	2.9128	2.0000	1.2011	0.4182
011	2.5616	1.0000	-1.0000	-1.0000	-1.5616
	5.5616	3.0000	1.4384	1.0000	1.0000
012	2.4812	0.6889	0.0000	-1.1701	-2.0000
	5.1149	2.7459	2.6180	1.1392	0.3820
013	2.4495	0.0000	0.0000	0.0000	-2.4495
	5.0000	3.0000	2.0000	2.0000	0.0000
014	2.3429	0.4707	0.0000	-1.0000	-1.8136
	5.3234	2.3579	1.0000	1.0000	0.3187
015	2.3028	0.6180	0.0000	-1.3028	-1.6180
	4.9354	2.6180	1.5374	0.5272	0.3820
016	2.2143	1.0000	-0.5392	-1.0000	-1.6751
	4.6412	2.7237	1.4108	1.0000	0.2243
017	2.1358	0.6622	0.0000	-0.6622	-2.1358
	4.4812	2.6889	2.0000	0.8299	0.0000
018	2.0000	0.6180	0.6180	-1.6180	-1.6180
	4.0000	2.6180	2.6180	0.3820	0.3820
019	2.0000	0.0000	0.0000	0.0000	-2.0000
	5.0000	1.0000	1.0000	1.0000	0.0000
020	1.8478	0.7654	0.0000	-0.7654	-1.8478
	4.1701	2.3111	1.0000	0.5188	0.0000

```
021   1.7321   1.0000   0.0000  -1.0000  -1.7321
      3.6180   2.6180   1.3820   0.3820   0.0000
```

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