MAXIMA OF THE Q-INDEX: FORBIDDEN 4-CYCLE AND 5-CYCLE[*]

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Abstract. This paper gives tight upper bounds on the largest eigenvalue $q(G)$ of the signless Laplacian of graphs with no 4-cycle and no 5-cycle.

If n is odd, let F_n be the friendship graph of order n; if n is even, let F_n be F_{n-1} with an extra edge hung to its center. It is shown that if G is a graph of order $n \geq 4$, with no 4-cycle, then
$$q(G) < q(F_n),$$
unless $G = F_n$.

Let $S_{n,k}$ be the join of a complete graph of order k and an independent set of order $n - k$. It is shown that if G is a graph of order $n \geq 6$, with no 5-cycle, then
$$q(G) < q(S_{n,2}),$$
unless $G = S_{n,k}$.

It is shown that these results are significant in spectral extremal graph problems. Two conjectures are formulated for the maximum $q(G)$ of graphs with forbidden cycles.

Key words. Signless Laplacian, Spectral radius, Forbidden cycles, Extremal problem.

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1. Introduction. Given a graph G, the Q-index of G is the largest eigenvalue $q(G)$ of its signless Laplacian $Q(G)$. In this note we determine the maximum Q-index of graphs with no cycles of length 4 and 5. These two extremal problems turn out to have particular meaning, so before getting to the new theorems, we give an introductory discussion.

Recall that the central problem of the classical extremal graph theory is of the following type:

PROBLEM A. *Given a graph F, what is the maximum number of edges of a graph of order n, with no subgraph isomorphic to F?*

Such problems are fairly well understood nowadays; see, e.g., [2] for comprehensive discussion and [19] for some newer results. Let us mention only two concrete results,

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which will be used for case study later in the paper. Write $T_2(n)$ for the complete bipartite graph with parts of size $\lfloor n/2 \rfloor$ and $\lceil n/2 \rceil$, and note that $T_2(n)$ contains no odd cycles. First, Mantel's theorem [12] reads as: *if G is a graph of order n and $e(G) > e(T_2(n))$, then G contains a triangle.* This theorem seems as good as one can get, but Bollobás in [2], p. 150, was able to deduce a stronger conclusion from the same premise: *if G is a graph of order n and $e(G) > e(T_2(n))$, then G contains a cycle of length t for every $3 \le t \le \lceil n/2 \rceil$.* Below we study similar problems for spectral parameters of graphs.

During the past two decades, subtler versions of Problem A have been investigated, namely for the spectral radius $\mu(G)$, i.e., the largest eigenvalue of the adjacency matrix of a graph G. In this new class of problems the central question is the following one.

PROBLEM B. *Given a graph F, what is the maximum $\mu(G)$ of a graph G of order n, with no subgraph isomorphic to F.*

In fact, in recent years, much of the classical extremal graph theory, as known from [2], has been recast for the spectral radius with an astonishing preservation of detail; see [19] for a survey and discussions. In particular, Mantel's theorem has been translated as: *if G is a graph of order n and $\mu(G) > \mu(T_2(n))$, then G contains a triangle.* Moreover, as shown in [16], the result of Bollobás can be recovered likewise: *if G is a graph of sufficiently large order n and $\mu(G) > \mu(T_2(n))$, then G contains a cycle of length t for every $3 \le t \le n/320$.* The constant $1/320$ undoubtedly can be improved, but its best value is yet unknown.

However, not all extremal results about the spectral radius are similar to the corresponding edge extremal results. The most notable known exceptions are for the spectral radius of graphs with forbidden even cycles. Thus, it has been long known (see [14] and [20]) that the number of edges in a graph G of order n, with no 4-cycle, satisfies

$$e(G) \le \frac{1}{4}n\left(1 + \sqrt{4n-3}\right),$$

and Füredi [10] proved that, for n sufficiently large, equality holds if and only if G is a the polarity graph of Erdős and Renyi [8]. By contrast, it has been shown in [15], [17] and [21], that the spectral radius of a graph G of order n, with no 4-cycle, satisfies

$$\mu(G) \le \mu(F_n),$$

where for n odd, F_n is a union of $\lfloor n/2 \rfloor$ triangles sharing a single common vertex, and for n even, F_n is obtained by hanging an edge to the center of F_{n-1}. Note that for odd n the graph F_n is known also as the *friendship* or *windmill* graph.

For longer even cycles the results for edges and the spectral radius deviate even further. Indeed, if G is a graph of order n, with no cycle of length $2k$, finding the maximum number of edges in G is one of the most difficult problems in extremal graph theory, unsolved for any $k \geq 4$. By contrast, the maximum spectral radius is known within $1/2$ of its best possible value, although the problem is not solved completely - see Conjecture 3.3 at the end of this paper.

The present paper contributes to an even newer trend in extremal graph theory, namely to the study of variations of Problem A for the Q-index of graphs, where the central question is the following one.

PROBLEM C. *Given a graph F, what is the maximum Q-index a graph G of order n, with no subgraph isomorphic to F?*

This question has been resolved for forbidden K_r, $r \geq 3$ in [1] and [11], thereby obtaining stronger versions of the Turán theorem. In general, extremal problems about the Q-index turn out to be more difficult than for the spectral radius and show greater deviation from their edge versions. For example, Mantel's theorem for the Q-index reads as: *if G is a graph of order n and $q(G) > q(T_2(n))$, then G contains a triangle*. While this result is expected, here $T_2(n)$ is not the only extremal graph, unlike the case for $e(G)$ and $\mu(G)$. An even greater rift is observed when we try to translate the result of Bollobás: now the premise $q(G) > q(T_2(n))$ by no means implies the existence of cycles other than triangles. Indeed, write $S_{n,1}^+$ for the star of order n with an additional edge. Clearly $S_{n,1}^+$ contains no cycles other than triangles, although $q(S_{n,1}^+) > q(T_2(n))$. In fact, to guarantee existence of an odd cycle of length k, we need considerably larger $q(G)$. Below, we find the precise lower bound for 5-cycles, and we state a conjecture for general k in the concluding remarks.

For even cycles, $q(G)$ and $\mu(G)$ seem to behave alike, although we are able to prove this fact only for the 4-cycle; we state a general conjecture at the end of the paper.

THEOREM 1.1. *Let G be a graph of order $n \geq 4$. If G contains no C_4, then*

$$q(G) < q(F_n),$$

unless $G = F_n$.

The following proposition adds some numerical estimates to Theorem 1.1.

PROPOSITION 1.2. *If n is odd, then*

$$q(F_n) = \frac{n + 2 + \sqrt{(n-2)^2 + 8}}{2},$$

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and satisfies

$$n + \frac{2}{n-1} < q\left(F_n\right) < n + \frac{2}{n-2}. \tag{1.1}$$

If n is even, then $q\left(F_n\right)$ is the largest root of the equation

$$x^3 - (n+3)\,x^2 + 3nx - 2n + 4 = 0,$$

and satisfies

$$n + \frac{2}{n} < q\left(F_n\right) < n + \frac{2}{n-1}. \tag{1.2}$$

Now let $S_{n,k}$ be the graph obtained by joining each vertex of K_k, the complete graph of order k, to each vertex of an independent set of order $n-k$; in other words, $S_{n,k} = K_k \vee \overline{K}_{n-k}$.

THEOREM 1.3. *Let $n \geq 6$ and let G be a graph of order n. If G contains no C_5, then*

$$q\left(G\right) < q\left(S_{n,2}\right),$$

unless $G = S_{n,2}$.

Note that for $n = 5$, there are two graphs without C_5 and with maximal Q-index: one is $S_{5,2}$, and the other is K_4 with a dangling edge.

The remaining part of the paper is organized as follows. In the next section, we give the proofs of Theorems 1.1, 1.3 and Proposition 1.2. In the concluding remarks, we round up the general discussion and state two conjectures.

2. Proofs. For graph notation and concepts undefined here, we refer the reader to [3]. For introductory material on the signless Laplacian see the survey of Cvetković [4] and its references. In particular, let G be a graph, and X and Y be disjoint sets of vertices of G. We write:

- $V\left(G\right)$ for the set of vertices of G, and $e\left(G\right)$ for the number of its edges;

- $G\left[X\right]$ for the graph induced by X, and $e\left(X\right)$ for $e\left(G\left[X\right]\right)$;

- $e\left(X, Y\right)$ for the number of edges joining vertices in X to vertices in Y;

- $\Gamma\left(u\right)$ for the set of neighbors of a vertex u, and $d\left(u\right)$ for $\left|\Gamma\left(u\right)\right|$.

Write P_k for a path of order k, and recall that Erdős and Gallai [7] have shown that if G is a graph of order n with no P_{k+2}, then $e\left(G\right) \leq kn/2$, with equality holding if and only if G is a union of complete graphs of order $k+1$.

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Proof of Proposition 1.2. If n is odd, then by definition

$$F_n = K_1 \vee \left(\frac{n-1}{2} \right) K_2.$$

Then the Q-index of F_n (see [9]) is the largest root of the equation

$$x^2 - (n+2)\,x + 2\,(n-1) = 0,$$

that is,

$$q\,(F_n) = \frac{n+2+\sqrt{(n-2)^2+8}}{2}.$$

An easy check shows that

$$\left(n - 2 + \frac{4}{n-1} \right)^2 < (n-2)^2 + 8 < \left(n - 2 + \frac{4}{n-2} \right)^2,$$

proving (1.1).

If n is even, then by definition

$$F_n = K_1 \vee \left(K_1 \cup \left(\frac{n-2}{2} \right) K_2 \right).$$

Then, its Q-index (see [9]) is the largest root of the polynomial

$$
\begin{aligned}
p(x) &= x^3 - (n+3)x^2 + 3nx - 2n + 4 \\
&= (x-n)^3 + (2n-3)(x-n)^2 + (n^2 - 3n)(x-n) - 2n + 4.
\end{aligned}
$$

Since $p(x)$ is an increasing function for $x \geq n$, we find that

$$p\left(n + \frac{2}{n} \right) = \frac{-2}{n^3}\left(n^2(n-4) + 2(3n-2) \right) < 0$$

and so,

$$q(F_n) > n + \frac{2}{n}.$$

On the other hand,

$$p\left(n + \frac{2}{n-1} \right) = \frac{4}{(n-1)^2}\left(n - 2 + \frac{2}{n-1} \right) > 0,$$

and it follows that

$$q(F_n) < n + \frac{2}{n-1},$$

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completing the proof of (1.2). □

The proofs of Theorem 1.1 and Theorem 1.3 will be based on a careful analysis of the following bound on $q(G)$, which can be traced back to Merris [13],

$$q(G) \leq \max_{u \in V(G)} d(u) + \frac{1}{d(u)} \sum_{v \in \Gamma(u)} d(v). \tag{2.1}$$

Let us also note that for every vertex $u \in V(G)$,

$$\sum_{v \in \Gamma(u)} d(v) = 2e(\Gamma(u)) + e(\Gamma(u), V \backslash \Gamma(u)). \tag{2.2}$$

Proof of Theorem 1.1. Suppose that G is a graph of order $n \geq 4$, with no C_4, and let Δ be the maximum degree of G. Note first that if $\Delta = n - 1$, then G is a connected subgraph of F_n, hence, $q(G) < q(F_n)$, unless $G = F_n$. Thus, hereafter we shall assume that $\Delta \leq n - 2$.

Let u be a vertex for which the maximum in the right-hand side of (2.1) is attained, and set for short $N = \Gamma(u)$. If $d(u) = 1$, then

$$q(G) \leq d(u) + \frac{1}{d(u)} \sum_{v \in N} d(v) \leq 1 + \frac{\Delta}{1} \leq n - 1 < q(F_n),$$

proving the assertion in this case. Thus, hereafter we shall assume that $d(u) \geq 2$.

Note that every vertex $v \in V \backslash \{u\}$ has at most one neighbor in N because G has no C_4. Therefore,

$$e(N, V \backslash N) = d(u) + |V \backslash (N \cup \{u\})| = d(u) + n - d(u) - 1 = n - 1,$$

and so,

$$\sum_{v \in N} d(v) \leq d(u) + e(N, V \backslash N) \leq d(u) + n - 1,$$

implying that,

$$q(G) \leq d(u) + \frac{1}{d(u)} \sum_{v \in N} d(v) \leq 1 + d(u) + \frac{n - 1}{d(u)}.$$

Since the function

$$f(x) = x + \frac{n - 1}{x}$$

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is convex for $x > 0$, its maximum in any closed interval is attained at one of the ends of this interval. In our case, $2 \leq d(u) \leq n - 2$, and so,

$$q(G) \leq d(u) + \frac{1}{d(u)} \sum_{v \in N} d(v)$$

$$\leq 1 + \max\left\{ 2 + \frac{n-1}{2}, n - 2 + \frac{n-1}{n-2} \right\}$$

$$\leq n + \frac{1}{n-2} < q(F_n),$$

completing the proof of Theorem 1.1. ☐

To simplify the proof of Theorem 1.3, we shall prove two auxiliary statements. First, note the following relations.

PROPOSITION 2.1. *If $n \geq 4$, then*

$$q(S_{n,2}) = \frac{n + 2 + \sqrt{n^2 + 4n - 12}}{2} > n + 2 - \frac{4}{n+1}. \tag{2.3}$$

Proof. Since $S_{n,2} = K_2 \vee \overline{K}_{n-2}$, its Q-index is the largest root of equation

$$x^2 - (n+2)x + 4 = 0,$$

and so,

$$q(S_{n,2}) = \frac{n + 2 + \sqrt{n^2 + 4n - 12}}{2}.$$

Since $n \geq 4$, we find that

$$\sqrt{n^2 + 4n - 12} = \sqrt{(n+2)^2 - 16} > \sqrt{(n+2)^2 - 16\left(1 + \frac{n-3}{(n+1)^2}\right)}$$

$$= n + 2 - \frac{8}{n+1},$$

implying (2.3). ☐

In the following proposition, we prove a crucial case of Theorem 1.3.

PROPOSITION 2.2. *Let G be a graph of order $n \geq 6$, with no C_5. If G has a vertex of degree $n - 1$, then*

$$q(G) < q(S_{n,2}),$$

unless $G = S_{n,2}$.

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Proof. Let u be a vertex of degree $n-1$ and write N for the set of its neighbors. As proved by Chang and Tam [5], if a graph G has a dominating vertex and $4 \le e(N) \le n-2$, then the maximum $q(G)$ is attained uniquely for $G = S_{n,2}$. So it remains to consider the cases $e(N) \le 3$ and $e(N) \ge n-1$. Assume for a contradiction that $q(S_{n,2}) \le q(G)$ and $G \ne S_{n,2}$. By the inequality of Das [6], we have

$$q(S_{n,2}) \le q(G) \le \frac{2e(G)}{n-1} + n - 2,$$

and (2.3) implies that

$$n + 2 - \frac{4}{n+1} \le \frac{2e(G)}{n-1} + n - 2.$$

After some rearrangement we get

$$e(N) \ge n - 1 - 2 + \frac{4}{n+1}$$

and so $e(N) \ge n - 2 \ge 4$. Since $C_5 \nsubseteq G$, the graph $G[N]$ contains no P_4, and so $e(N) \le n-1$, implying that $e(N) = n-1$. By the theorem of Erdős and Gallai, this is only possible if $G[N]$ is a union of disjoint triangles, that is to say,

$$G = K_1 \vee \left(\frac{n-1}{3} \right) K_3.$$

Now, an easy calculation gives

$$q(G) = \frac{n + 4 + \sqrt{(n-4)^2 + 16}}{2} < q(S_{n,2}),$$

a contradiction completing the proof of Proposition 2.2. □

Proof of Theorem 1.3. Let G be a graph of order $n \ge 6$, with no C_5 and with

$$q(G) \ge q(S_{n,2}) \ge n + 2 - \frac{4}{n+1}. \tag{2.4}$$

Assume for a contradiction that $G \ne S_{n,2}$, and so, in view of Proposition 2.2, we can assume that $\Delta(G) \le n - 2$.

Let u be a vertex for which the maximum in the right-hand side of (2.1) is attained and set $N = \Gamma(u)$. Note that (2.1) and (2.4) give

$$n + 2 - \frac{4}{n+1} \le d(u) + \frac{1}{d(u)} \sum_{v \in N} d(v). \tag{2.5}$$

First we deduce that

$$e(N) \ge d(u) - 1. \tag{2.6}$$

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Indeed, a crude estimate gives

$$\frac{e\left(N, V\backslash N\right)}{d\left(u\right)} \leq \frac{d\left(u\right)\left(n - d\left(u\right)\right)}{d\left(u\right)} \leq n - d\left(u\right),$$

and (2.2) implies that

$$d\left(u\right) + \frac{1}{d\left(u\right)} \sum_{v \in N} d\left(v\right) \leq d\left(u\right) + \frac{2e\left(N\right)}{d\left(u\right)} + n - d\left(u\right) = n + \frac{2e\left(N\right)}{d\left(u\right)}.$$

Hence, in view of (2.5), we get

$$e\left(N\right) \geq d\left(u\right) - \frac{2d\left(u\right)}{n+1} \geq d\left(u\right) - \frac{2\left(n-1\right)}{n+1} > d\left(u\right) - 2,$$

and (2.6) follows.

Consider first the case that $G\left[N\right]$ contains no cycles, and so $G\left[N\right]$ is a tree; moreover, since $C_5 \nsubseteq G$, the graph $G\left[N\right]$ contains no P_4, and so it is a star. Note that to avoid C_5, every vertex in $V\backslash\left(N \cup \{u\}\right)$ may be joined to at most one vertex of N. Therefore,

$$e\left(N, V\backslash N\right) \leq n - d\left(u\right) - 1 + d\left(u\right) = n - 1,$$

implying that

$$n + 2 - \frac{4}{n+1} \leq d\left(u\right) + \frac{1}{d\left(u\right)} \sum_{v \in N} d\left(v\right) \leq d\left(u\right) + \frac{2\left(d\left(u\right)-1\right)+n-1}{d\left(u\right)}$$
$$= d\left(u\right) + 2 + \frac{n-3}{d\left(u\right)}.$$

Since the function

$$f\left(x\right) = x + \frac{n-3}{x}$$

is convex for $x > 0$, its maximum in any closed interval is attained at the ends of this interval. In our case, $1 \leq d\left(u\right) \leq n - 2$, and so,

$$d\left(u\right) + 2 + \frac{n-3}{d\left(u\right)} \leq 2 + \max\left\{1 + \frac{n-3}{1}, n - 2 + \frac{n-3}{n-2}\right\} \leq n + 2 - \frac{4}{n+1} < q\left(S_{n,2}\right),$$

which contradicts (2.5). Hence, $G\left[N\right]$ contains cycles. However, since $C_5 \nsubseteq G$, all cycles of $G\left[N\right]$ are triangles. Let say, x, y, z are the vertices of a triangle in $G\left[N\right]$. Clearly, to avoid C_5, every vertex in $V\backslash\left(N \cup \{u\}\right)$ may be joined to at most one of the vertices x, y, z. This requirement reduces the bound on $e\left(N, V\backslash N\right)$ as follows

$$e\left(N, V\backslash N\right) \leq \left(n - d\left(u\right)\right)d\left(u\right) - 2\left(n - d\left(u\right) - 1\right).$$

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Hence, in view of (2.4),

$$n + 2 - \frac{4}{n+1} \leq d(u) + \frac{1}{d(u)} \sum_{v \in N} d(v) = d(u) + \frac{2e(N)}{d(u)} + \frac{e(N, V \setminus N)}{d(u)}$$

$$\leq d(u) + \frac{2e(N)}{d(u)} + n - d(u) - \frac{2(n - d(u) - 1)}{d(u)}$$

$$= n + 2 + \frac{2e(N)}{d(u)} - \frac{2(n-1)}{d(u)}.$$

After some rearrangement, we see that

$$e(N) \geq n - 1 - \frac{2d(u)}{n+1} \geq n - 1 - \frac{2(n-2)}{n+1} = n - 3 + \frac{6}{n+1},$$

which implies that

$$e(N) \geq n - 2.$$

Since $G[N]$ contains no P_4, the Erdős-Gallai theorem says that

$$d(u) = v(G[N]) \geq e(N),$$

with equality holding if an only if $G[N]$ is a union of disjoint triangles. Therefore, we have $d(u) = n - 2$ and $e(N) = n - 2$, and so $G[N]$ is a union of disjoint triangles. As above, we see that every vertex in $V \setminus (N \cup \{u\})$ may be joined to at most one vertex of each triangle, and so

$$e(N, V \setminus N) \leq d(u) + \frac{d(u)}{3} < \frac{4(n-2)}{3}.$$

Hence,

$$\frac{n + 2 + \sqrt{n^2 + 4n - 12}}{2} \leq d(u) + \frac{1}{d(u)} \sum_{v \in N} d(v) \leq d(u) + \frac{2e(N)}{d(u)} + \frac{e(N, V \setminus N)}{d(u)}$$

$$\leq n - 2 + \frac{2(n-2) + \frac{4(n-2)}{3}}{n-2} = n + \frac{4}{3}$$

which is a contradiction for $n \geq 5$. Theorem 1.3 is proved. □

3. Concluding remarks. We have started the study of the maximum Q-index of graphs with forbidden cycles. These questions are very different from the corresponding problems about edges and spectral radius. The main peculiarity for the Q-index is that it seems to behave similarly for odd and even forbidden cycles. Here is a general conjecture for odd cycles.

CONJECTURE 3.1. *Let $k \geq 2$ and let G be a graph of sufficiently large order n. If G has no C_{2k+1}, then*

$$q(G) < q(S_{n,k}),$$

unless $G = S_{n,k}$.

To state the conjecture for even cycles, define $S_{n,k}^+$ as the graph obtained by adding an edge to $S_{n,k}$.

CONJECTURE 3.2. *Let $k \geq 2$ and let G be a graph of sufficiently large order n. If G has no C_{2k+2}, then*

$$q\left(G\right) < q\left(S_{n,k}^+\right),$$

unless $G = S_{n,k}^+$.

For comparison, we would like to reiterate the corresponding conjecture for the spectral radius, stated in [18].

CONJECTURE 3.3. *Let $k \geq 2$ and let G be a graph of sufficiently large order n. If G has no C_{2k+2}, then*

$$\mu\left(G\right) < \mu\left(S_{n,k}^+\right),$$

unless $G = S_{n,k}^+$.

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