



# Quantum Graphs which Optimize the Spectral Gap

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**Abstract.** A finite discrete graph is turned into a quantum (metric) graph once a finite length is assigned to each edge and the one-dimensional Laplacian is taken to be the operator. We study the dependence of the spectral gap (the first positive Laplacian eigenvalue) on the choice of edge lengths. In particular, starting from a certain discrete graph, we seek the quantum graph for which an optimal (either maximal or minimal) spectral gap is obtained. We fully solve the minimization problem for all graphs. We develop tools for investigating the maximization problem and solve it for some families of graphs.

## 1. Introduction

The spectral gap is a vastly explored quantity due to its importance both for applicative purposes and for theoretic ones. The applicative aspects range from estimates of convergence to equilibrium to behavior of quantum many-body systems. The theoretic study concerns with connecting the shape of an object to a fundamental spectral property. Such relations stand in the heart of spectral geometry and motivate the current work.

A compact quantum graph can be thought of as a threefold object, consisting of a topology, a metric and an operator. The topology is described by an underlying discrete graph and the metric is simply the assignment of a positive length to each of the edges. The operator together with its domain completes this description. In the current work we adopt the most common choice and fix the operator to be the one-dimensional Laplacian acting on functions which satisfy the so-called Neumann conditions at the graph vertices (see [5, 17]). It is then most natural to fix a certain graph topology and explore how the graph spectral properties depend on the choice of edge lengths [6, 13, 16]. In particular, we examine the spectral gap which, in our case, is the first positive eigenvalue of the Laplacian. Picking a particular graph topology, we ask

which edge lengths minimize or maximize the spectral gap. We notice that as our space of edge lengths is not compact, it is possible that there is no maximum or no minimum. The space of edge lengths is thus extended by allowing zero length edges so that the minima (maxima) of this new length space are the infimums (supremums) of the previous. This leads to a most interesting exploration direction: sending edge lengths to zero changes the topology of the original graph and makes us wonder what are the topologies which are obtained as optimizers (either maximizers or minimizers) of other graphs. This is the central question of the current paper.

Already in 1987, Nicaise showed that among all graphs with a fixed length, the minimal spectral gap is obtained for the single-edge graph [29]. In 2005, Friedlander proved a more general result, showing that the minimum of the  $k$ th eigenvalue is uniquely obtained for a star graph with  $k$  edges [15]. More recently, Exner and Jex showed how the change of graph edge lengths may increase or decrease the spectral gap, depending on the graph's topology [13]. In the last couple of years, a series of works on the subject came to light. Kurasov and Naboko [25] treated the spectral gap minimization and together with Malenová they explored how the spectral gap changes with various modifications of the graph connectivity [24]. Kennedy, Kurasov, Malenová and Mugnolo provided a broad survey on bounding the spectral gap in terms of various geometric quantities of the graph [20]. Karreskog, Kurasov and Trygg Kupersmidt generalized the minimization results mentioned above to Schrödinger operators with potentials and  $\delta$ -type vertex conditions [19]. Del Pezzo and Rossi proved upper and lower bounds for the spectral gap of the  $p$ -Laplacian and evaluated its derivatives with respect to change of edge lengths [11]. Rohleder solved the spectral gap maximization problem for all eigenvalues of tree graphs [31]. When this manuscript was accepted for publication, two additional preprints became available online. Ariturk provides some improved upper bounds for all graph eigenvalues [1]. Berkolaiko, Kennedy, Kurasov and Mugnolo further generalize lower and upper bounds of the spectral gap in terms of the edge connectivity [4].

We complement this literature review by mentioning some interesting and recent works on the spectral gap of metric graphs, whose scope is different than ours. Post [30], Kurasov [23], Kennedy and Mugnolo [21] all treated various estimates of the spectral gap in terms of the Cheeger constant (a line of research which already originated in [29] for quantum graphs). Buttazzo, Ruffini and Velichkov optimize over spectral gap of graphs given some prescribed set of Dirichlet vertices embedded in  $\mathbb{R}^d$  [7].

The spectral gap optimization we consider in this paper is close in nature to the first line of works mentioned above. Nevertheless, our point of view is different as we wish to solve the optimization problem for each and every topology. This broad phrasing of the question provides a unified framework for several of the works mentioned above. In particular, it allows to take a step forward and complement those.

### 1.1. Discrete Graphs and Graph Topologies

Let  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$  be a connected graph with finite sets of vertices  $\mathcal{V}$  and edges  $\mathcal{E}$  and we denote  $V := |\mathcal{V}|$ ,  $E := |\mathcal{E}|$ . We allow edges to connect either two distinct vertices or a vertex to itself. In the latter case, this edge is called a loop, or sometimes a petal.

For a vertex  $v \in \mathcal{V}$ , its *degree*,  $d_v$ , equals the number of edges connected to it. Vertices of degree one are called leaves. Furthermore, we abuse this naming and frequently also use the name leaf for an edge which is connected to a vertex of degree one.

An important topological quantity of the graph is

$$\beta := E - V + 1, \tag{1.1}$$

which counts the number of “independent” cycles on the graph (assuming the graph is connected). This is also known as the first Betti number, which is the dimension of the graph’s first homology. In particular, tree graphs are characterized by  $\beta = 0$ .

We consider the following two ways for treating the graph connectivity. The graph’s edge connectivity is the minimal number of edges one needs to remove in order to disconnect the graph. If the graph’s edge connectivity equals one, then an edge whose removal disconnects the graph is called a *bridge*. In particular, leaf edges are bridges. Similarly, the graph’s vertex connectivity is the number of vertices needed to be removed in order to disconnect the graph. In particular, we show the special role played by graphs of edge connectivity one (Theorem 2.1) and of vertex connectivity one (Theorem 2.6).

### 1.2. Spectral Theory of Quantum Graphs

A *metric graph* is a discrete graph for which each edge,  $e \in \mathcal{E}$ , is identified with a one-dimensional interval  $[0, l_e]$  of positive finite length  $l_e$ . We assign to each edge  $e \in \mathcal{E}$  a coordinate,  $x_e$ , which measures the distance along the edge from the starting vertex of  $e$ . We denote a coordinate by  $x$ , when its precise nature is unimportant.

A function on the graph is described by its restrictions to the edges,  $\{f|_e\}_{e \in \mathcal{E}}$ , where  $f|_e : [0, l_e] \rightarrow \mathbb{C}$ . We equip the metric graphs with a self-adjoint differential operator,

$$\mathcal{H} : f|_e(x_e) \mapsto -\frac{d^2}{dx_e^2} f|_e(x_e), \tag{1.2}$$

which in our case is just the one-dimensional negative Laplacian on every edge.<sup>1</sup> It is most common to call this setting of a metric graph and an operator by the name quantum graph.

To complete the definition of the operator we need to specify its domain. We denote by  $H^2(\Gamma)$  the following direct sum of Sobolev spaces

$$H^2(\Gamma) := \bigoplus_{e \in \mathcal{E}} H^2([0, l_e]) . \tag{1.3}$$

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<sup>1</sup> Note that more general operators appear in the literature. See, for example, the book [5] and the survey [17].

In addition, we require the following matching conditions on the graph vertices. A function  $f \in H^2(\Gamma)$  is said to satisfy the Neumann vertex conditions at a vertex  $v$  if

1.  $f$  is continuous at  $v \in \mathcal{V}$ , i.e.,

$$\forall e_1, e_2 \in \mathcal{E}_v \quad f|_{e_1}(0) = f|_{e_2}(0), \tag{1.4}$$

where  $\mathcal{E}_v$  is the set of edges connected to  $v$ , and for each  $e \in \mathcal{E}_v$  we choose the coordinate such that  $x_e = 0$  at  $v$ .

2. The outgoing derivatives of  $f$  at  $v$  satisfy

$$\sum_{e \in \mathcal{E}_v} \left. \frac{df}{dx_e} \right|_e (0) = 0. \tag{1.5}$$

Another common vertex condition is called the Dirichlet condition. Imposing Dirichlet condition at vertex  $v \in \mathcal{V}$  means

$$\forall e \in \mathcal{E}_v \quad f|_e(0) = 0. \tag{1.6}$$

Requiring either of these conditions at each vertex leads to the operator (1.2) being self-adjoint and its spectrum being real and bounded from below [5]. In addition, since we only consider compact graphs, the spectrum is discrete. We number the eigenvalues in the ascending order and denote them with  $\{\lambda_n\}_{n=0}^\infty$  and their corresponding eigenfunctions with  $\{f_n\}_{n=0}^\infty$ . As the operator is both real and self-adjoint, we may choose the eigenfunctions to be real, which we will always do.

In this paper, we almost solely consider graphs whose vertex conditions are Neumann at all vertices. Those are called *Neumann graphs*. For Neumann graphs, we define the Rayleigh quotient

$$\mathcal{R}(f) := \frac{\int_\Gamma |f'(x)|^2 dx}{\int_\Gamma |f(x)|^2 dx}, \tag{1.7}$$

which makes sense whenever  $f \in H^1(\Gamma)$  (see (1.3)). The eigenvalues of a Neumann graph have a nice expression using the Rayleigh quotient. Indeed, denoting  $V_n := \text{Span}\{f_0, \dots, f_n\}$  for  $n \in \mathbb{N}$ , we have

$$\lambda_n = \min_{f \perp V_{n-1}} \mathcal{R}(f). \tag{1.8}$$

In particular, the spectrum of a Neumann graph is nonnegative, which means that we may represent the spectrum by the nonnegative square roots of the eigenvalues,  $k_n = \sqrt{\lambda_n}$ , and say that  $\{k_n\}_{n=0}^\infty$  are the  $k$ -eigenvalues of the graph. For convenience, we express most of our results and proofs in terms of the  $k$ -eigenvalues. This choice makes all expressions of this paper look nicer. A Neumann graph has  $k_0 = 0$  with multiplicity which equals the number of graph components (which is taken to be one throughout this paper). It is  $k_1$  which is in the focus of this paper and is called the spectral gap.<sup>2</sup>

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<sup>2</sup> This terminology is justified, as a spectral gap is a common name for the difference between some trivial eigenvalue (which is  $k_0 = 0$  in our case) and the next eigenvalue. We note that in this sense it is also common to call  $\lambda_1$  the spectral gap.

### 1.3. Graph Optimizers

**Definition 1.1.** Let  $\mathcal{G}$  be a discrete graph with  $E$  edges.

1. Denote by

$$\mathcal{L}_{\mathcal{G}} := \left\{ (l_1, \dots, l_E) \in \mathbb{R}^E \mid \sum_{e=1}^E l_e = 1 \text{ and } \forall e, l_e > 0 \right\} \tag{1.9}$$

the space of all possible lengths we may assign to the edges of  $\mathcal{G}$ . We further denote by  $\overline{\mathcal{L}}_{\mathcal{G}}$  the closure of  $\mathcal{L}_{\mathcal{G}}$  in  $\mathbb{R}^E$  and by  $\partial\mathcal{L}_{\mathcal{G}}$  its boundary.

2. Denote by  $\Gamma(\mathcal{G}; \underline{l})$  the metric graph whose connectivity is the same as  $\mathcal{G}$  and whose edge lengths are given by  $\underline{l} \in \overline{\mathcal{L}}_{\mathcal{G}}$ . We take  $\Gamma(\mathcal{G}; \underline{l})$  to be a Neumann graph. If  $\underline{l} \in \partial\mathcal{L}_{\mathcal{G}}$ , then  $\underline{l}$  has some vanishing entries and in this case the connectivity of  $\Gamma(\mathcal{G}; \underline{l})$  is not the same as  $\mathcal{G}$ . For each vanishing entry,  $l_e = 0$ , the edge  $e$  does not exist in  $\Gamma(\mathcal{G}; \underline{l})$ , but rather the vertices at the endpoints of this edge are identified and form a single vertex when considered in  $\Gamma(\mathcal{G}; \underline{l})$ .

We emphasize that the definition above contains a normalization choice; unless otherwise stated, all the graphs studied in this paper are required to have total metric length one.

This paper studies the spectral gap,  $k_1[\Gamma(\mathcal{G}; \underline{l})]$ , as a function of  $\underline{l} \in \overline{\mathcal{L}}_{\mathcal{G}}$ . A first step is to show that the function  $k_1[\Gamma(\mathcal{G}; \underline{l})]$  is continuous on  $\overline{\mathcal{L}}_{\mathcal{G}}$ , which is done in ‘‘Appendix A.’’ Combining this continuity statement with the compactness of this set  $\overline{\mathcal{L}}_{\mathcal{G}}$ , the existence of a maximum and a minimum of the spectral gap on  $\overline{\mathcal{L}}_{\mathcal{G}}$  (but not necessarily on  $\mathcal{L}_{\mathcal{G}}$ ) follows. Indeed, the focus of the current paper is on the extremal points of  $k_1[\Gamma(\mathcal{G}; \underline{l})]$ . In particular, we investigate whether the extremal points are obtained on  $\mathcal{L}_{\mathcal{G}}$  or on  $\partial\mathcal{L}_{\mathcal{G}}$  and to which metric graphs  $\Gamma(\mathcal{G}; \underline{l})$  they correspond. This motivates the following.

**Definition 1.2.** Let  $\mathcal{G}$  be a discrete graph.

1.  $\Gamma(\mathcal{G}; \underline{l}^*)$  is called a maximizer of  $\mathcal{G}$  if  $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$  and

$$\forall \underline{l} \in \mathcal{L}_{\mathcal{G}} \quad k_1[\Gamma(\mathcal{G}; \underline{l}^*)] \geq k_1[\Gamma(\mathcal{G}; \underline{l})]. \tag{1.10}$$

In this case we call  $k_1[\Gamma(\mathcal{G}; \underline{l}^*)]$  the maximal spectral gap of  $\mathcal{G}$ .

2.  $\Gamma(\mathcal{G}; \underline{l}^*)$  is called a supremizer of  $\mathcal{G}$  if  $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$  and

$$\forall \underline{l} \in \overline{\mathcal{L}}_{\mathcal{G}} \quad k_1[\Gamma(\mathcal{G}; \underline{l}^*)] \geq k_1[\Gamma(\mathcal{G}; \underline{l})]. \tag{1.11}$$

In this case we call  $k_1[\Gamma(\mathcal{G}; \underline{l}^*)]$  the supremal spectral gap of  $\mathcal{G}$ .

3.  $\Gamma(\mathcal{G}; \underline{l}^*)$  is called the unique maximizer of  $\mathcal{G}$  if for all  $\underline{l} \neq \underline{l}^*$ ,  $\Gamma(\mathcal{G}; \underline{l})$  is not a maximizer of  $\mathcal{G}$ . The same definition holds for the unique supremizer.
4. Analogous definitions to the above hold for minimizers and infimizers.
5.  $\Gamma(\mathcal{G}; \underline{l}^*)$  is called an optimizer of  $\mathcal{G}$  if it is either a supremizer, a maximizer, an infimizer or a minimizer of  $\mathcal{G}$ .

Continuing the discussion preceding the definition, we note that there might be graphs which do not have a maximizer or a minimizer. Yet, a supremizer and an infimizer exist for any graph. Let  $\mathcal{G}$  be a discrete graph and  $\Gamma(\mathcal{G}; \underline{l}^*)$

be its supremizer (infimizer), with  $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$ . Denote by  $\mathcal{G}^*$  the discrete graph which corresponds to  $\Gamma(\mathcal{G}; \underline{l}^*)$ . We note that if  $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$  then  $\mathcal{G}^* = \mathcal{G}$  and if  $\underline{l}^* \in \partial\mathcal{L}_{\mathcal{G}}$  then  $\mathcal{G}^*$  is obtained from  $\mathcal{G}$  by contracting all edges which correspond to the zero entries of  $\underline{l}$ .

The questions which motivate this work are the following: What are the metric graphs  $\Gamma(\mathcal{G}; \underline{l}^*)$  which serve as supremizers (or infimizers) and what are all the possible topologies (i.e., the discrete graphs  $\mathcal{G}^*$ ) obtained by these optimizations?

We start by presenting a few examples of topologies which form part of the answer to the questions above.

*Example 1.3* (Star graph). Let  $\mathcal{G}$  be a graph with  $V \geq 3$  vertices, and  $E = V - 1$  edges, where one of the vertices (called the central vertex) is connected by edges to all the  $V - 1$  other vertices (Fig. 1a).  $\mathcal{G}$  is called a star graph. The graph  $\Gamma(\mathcal{G}; \underline{l})$  with  $\underline{l} = (\frac{1}{E}, \dots, \frac{1}{E})$  is called the equilateral star. A simple calculation shows that  $k_1[\Gamma(\mathcal{G}; \underline{l})] = \frac{\pi}{2}E$ . We show (Theorem 2.2) that the equilateral star is the unique maximizer of the star topology and that it is also the unique supremizer of any tree graph with  $E$  leaves. If we choose above  $V = 2$ ,  $E = 1$  we get an interval, which is the unique infimizer of any graph with a bridge (Theorem 2.1).

*Example 1.4* (Flower graph). Let  $\mathcal{G}$  be a graph with a single vertex and  $E \geq 2$  edges, where each edge is a loop (petal) connecting that single vertex to itself (Fig. 1b).  $\mathcal{G}$  is called a flower graph. The graph  $\Gamma(\mathcal{G}; \underline{l})$  with  $\underline{l} = (\frac{1}{E}, \dots, \frac{1}{E})$  is called the equilateral flower. A simple calculation shows that  $k_1[\Gamma(\mathcal{G}; \underline{l})] = \pi E$ . We show (Corollary 2.8) that the equilateral flower is the unique maximizer of the flower topology. If we choose above  $E = 1$  we get a single-loop graph, which is an infimizer for all bridgeless graphs (Theorem 2.1).

*Example 1.5* (Stower graph). Let  $\mathcal{G}$  be a graph with  $V$  vertices and  $E = E_p + E_l \geq 2$  edges.  $E_p$  of the edges are loops which connect a single vertex to itself (the same vertex for all those edges) and, as before, they are called petals. Each of the rest  $E_l = V - 1$  edges connects this single vertex to another graph vertex and they are called dangling edges or just leaves (Fig. 1c). Being a hybrid between a star graph and a flower graph, such  $\mathcal{G}$  is called a stower

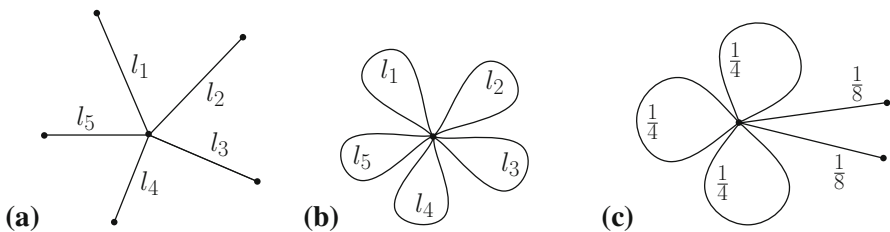


FIGURE 1. A few basic examples. **a** Star graph, **b** flower graph, **c** equilateral stower graph with  $E_p = 3$ ,  $E_l = 2$

graph. We note that a flower graph is a stower (with  $E_l = 0$ ) and a star graph is a stower as well (with  $E_p = 0$ ). The graph  $\Gamma(\mathcal{G}; \underline{l})$  with

$$\underline{l} = \frac{1}{2E_p + E_l} (\underbrace{2, \dots, 2}_{E_p}, \underbrace{1, \dots, 1}_{E_l})$$

is called the equilateral stower. Note that we abuse terminology and call the graph equilateral, even though not all edges of the description above have the same length. A simple calculation shows that  $k_1[\Gamma(\mathcal{G}; \underline{l})] = \frac{\pi}{2}(2E_p + E_l)$ . We show (Corollary 2.8) that the equilateral stower is the unique maximizer of the stower topology, except when  $E_p = E_l = 1$ , for which the supremizer is actually a single loop. Furthermore, spectral gaps of stowers obey a sort of additive property in the following sense: if two graphs whose supremizers are stowers are glued at non-leaf vertices to form a single graph, then this graph's supremizer is a stower graph obtained by adding the petals and the leaves of the two individual stower supremizers (Corollary 2.8).

*Example 1.6* (Mandarin graph). Let  $\mathcal{G}$  be a graph with 2 vertices and  $E$  edges, each connecting those two vertices (Fig. 2a). Such  $\mathcal{G}$  is called a mandarin graph. In the literature it is also called a watermelon or a pumpkin, but we adopt the name mandarin which was used in a thorough exploration of spectral properties of these graphs [2]. The graph  $\Gamma(\mathcal{G}; \underline{l})$  with  $\underline{l} = (\frac{1}{E}, \dots, \frac{1}{E})$  is called the equilateral mandarin. A simple calculation shows that  $k_1[\Gamma(\mathcal{G}; \underline{l})] = \pi E$ . The equilateral mandarin is the unique maximizer of the mandarin topology, as shown recently in [20] (theorem 4.2 there).

*Example 1.7* (Necklace graph). Let  $\mathcal{G}$  be a graph with  $V$  vertices and  $E = 2(V - 1)$  edges, such that every two adjacent vertices,  $v_i, v_{i+1}$  ( $1 \leq i \leq V - 1$ ) are connected by two edges (Fig. 2b). If  $\underline{l}$  is chosen such that every pair of parallel edges connecting two vertices has the same length,  $\Gamma(\mathcal{G}; \underline{l})$  is called a symmetric necklace. Note that the two vertices at the endpoints of the necklace are redundant, being Neumann vertices of degree two (they are merely used here to shorten the graph description). Necklace graphs are the only graphs which may serve as infimizers of bridgeless graphs (Theorem 2.1).

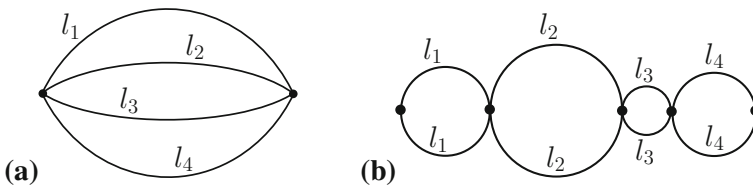


FIGURE 2. **a** Mandarin graph, **b** symmetric necklace graph

## 2. Main Results

The main results of the current paper are stated below, arranged by subjects. In each of the following subsections, we mention which section of the paper contains the relevant proofs and discussions.

### 2.1. Infimizers (Sect. 3)

#### Theorem 2.1.

1. Let  $\mathcal{G}$  be a graph with a bridge. Then the infimal spectral gap of  $\mathcal{G}$  equals  $\pi$ . Moreover, the unique infimizer is the unit interval.
2. Let  $\mathcal{G}$  be a bridgeless graph. Then the infimal spectral gap of  $\mathcal{G}$  equals  $2\pi$ . Moreover, any infimizer is a symmetric necklace graph.

We note that it was already proved in [15, 25, 29] that  $\pi$  is a universal lower bound for the spectral gap, attained only by the interval. In [15] it is even shown that  $\pi n$  is a lower bound for  $k_n$ . The paper [25] proves that the lower bound may be improved to  $2\pi$  if all vertices have even degrees. Theorem 2.1 extends the set of graph topologies whose spectral gap is bounded by  $2\pi$  to all bridgeless graphs (indeed graphs whose all vertices are of even degrees form a particular case). Furthermore, combining Theorem 2.1 with the continuity of eigenvalues with respect to the graphs edge lengths (Appendix A) allows to conclude that our result cannot be improved by imposing further restrictions on the graph topology. For any bridgeless graph  $\mathcal{G}$ , there exists  $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$  for which  $\Gamma(\mathcal{G}; \underline{l}^*)$  is a single-cycle graph with spectral gap  $2\pi$ . As  $k_1[\Gamma(\mathcal{G}; \underline{l})]$  is a continuous function of  $\underline{l}$ , the spectral gap may be as close to  $2\pi$  as we wish, by choosing  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$  close enough to  $\underline{l}^*$ . Similarly, the lower bound  $\pi$  cannot be improved for graphs with a bridge. Therefore, Theorem 2.1 complements the previous results and provides a complete answer to the infimization problem.

### 2.2. Supremizers of Tree Graphs (Sect. 4)

**Theorem 2.2.** *Let  $\mathcal{G}$  be a tree graph with  $E_l \geq 2$  leaves. Then the unique supremizer of  $\mathcal{G}$  is the equilateral star with  $E_l$  edges, whose spectral gap is  $\frac{\pi}{2}E_l$ . In particular, the uniqueness implies that this supremizer is a maximizer if and only if  $\mathcal{G}$  is a star graph.*

Theorem 2.2 completely solves the optimization problem for tree graphs. While writing this paper, we became aware of the recent work, [31], which solves the maximization problem for trees (theorem 3.2 there). In the course of doing so, that work provides the upper bound  $\frac{\pi}{2}E$  on the spectral gap of trees.<sup>3</sup> Our proof is close in spirit to that of theorem 3.4 in [31]. Yet, thanks to a basic geometric observation (Lemma 4.2 here), the better bound  $\frac{\pi}{2}E_l$  is obtained.<sup>4</sup>

Theorem 2.2 allows to deduce the following.

<sup>3</sup> Theorem 3.2 in that paper is actually more general and provides the upper bound  $\frac{\pi n}{2}E$  for  $k_n$ .

<sup>4</sup> Furthermore, the same geometric observation may be used to improve the more general Theorem 3.2 of [31].



**Corollary 2.3.** *Let  $\mathcal{G}$  be a non-tree graph. Then its supremizer is not a tree graph.*

**2.3. Supremizers Whose Spectral Gap is a Simple Eigenvalue (Sect. 5)**

Whenever the spectral gap is a simple eigenvalue, it is differentiable with respect to edge lengths, which allows to search for local maximizers. There are indeed examples for critical values (not just maximizers) of the spectral gap, which we demonstrate in Proposition 5.8. If such a local critical point is actually a supremizer it is possible to prove the following.

**Theorem 2.4.** *Let  $\mathcal{G}$  be a discrete graph and let  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ . Assume that  $\Gamma(\mathcal{G}; \underline{l})$  is a supremizer of  $\mathcal{G}$  and that the spectral gap  $k_1(\Gamma(\mathcal{G}; \underline{l}))$  is a simple eigenvalue. Then  $\Gamma(\mathcal{G}; \underline{l})$  is not a unique supremizer. There exists a choice of lengths  $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$  such that  $\Gamma(\mathcal{G}; \underline{l}^*)$  is an equilateral mandarin and*

$$k_1(\Gamma(\mathcal{G}; \underline{l})) = k_1(\Gamma(\mathcal{G}; \underline{l}^*)). \tag{2.1}$$

**2.4. Supremizers of Vertex Connectivity One (Sects. 6, 7, 8)**

Next, we describe a bottom to top construction which allows to find out a supremizer of a graph by knowing the supremizers of two of its subgraphs. This is possible for graphs of vertex connectivity one. In order to state the result, the following criteria are introduced.

- Definition 2.5.**
1. A Neumann graph  $\Gamma$  obeys the *Dirichlet criterion* with respect to its vertex  $v$  if imposing Dirichlet vertex condition at  $v$  does not change the value of  $k_1$  (comparing to the one with Neumann condition at  $v$ ).
  2. A Neumann graph  $\Gamma$  obeys the *strong Dirichlet criterion* with respect to its vertex  $v$  if it obeys the Dirichlet criterion and if imposing the Dirichlet vertex condition at  $v$  strictly increases the eigenvalue multiplicity of  $k_1$ .

**Theorem 2.6.** *Let  $\mathcal{G}_1, \mathcal{G}_2$  be discrete graphs; let  $v_i$  ( $i = 1, 2$ ) be a vertex of  $\mathcal{G}_i$ . Let  $\mathcal{G}$  be the graph obtained by identifying  $v_1$  and  $v_2$ . Let  $\underline{l}^{(i)} \in \overline{\mathcal{L}}_{\mathcal{G}_i}$  and  $\Gamma_i := \Gamma(\mathcal{G}_i; \underline{l}^{(i)})$  be the corresponding metric graphs. Define  $\underline{l} := (L\underline{l}^{(1)}, (1 - L)\underline{l}^{(2)}) \in \overline{\mathcal{L}}_{\mathcal{G}}$ , for some  $L \in [0, 1]$ . Then the graph  $\Gamma := \Gamma(\mathcal{G}; \underline{l})$  is a supremizer of  $\mathcal{G}$  if all the following conditions are met:*

1.  $L = \frac{k_1(\Gamma_1)}{k_1(\Gamma_1) + k_1(\Gamma_2)}$ .
2.  $\Gamma_i$  is a supremizer of  $\mathcal{G}_i$  ( $i = 1, 2$ ).
3.  $\Gamma_i$  obeys the Dirichlet criterion with respect to  $v_i$  ( $i = 1, 2$ ).

*If we further assume either of the following:*

- (a) For both  $i = 1, 2$ ,  $\Gamma_i$  is a unique supremizer of  $\mathcal{G}_i$  or
- (b) For both  $i = 1, 2$ ,  $\Gamma_i$  obeys the strong Dirichlet criterion and any other supremizer of  $\mathcal{G}_i$  violates the Dirichlet criterion,

*then  $\Gamma$  is the unique supremizer of  $\mathcal{G}$ .*

*Remark.* This theorem may be strengthened by weakening condition (3). Yet, the description of the weaker condition is more technical and we leave its specification, as well as the proof of the stronger version of this theorem, to Sect. 6.

We note that the equilateral stower obeys the Dirichlet criterion with respect to its central vertex. Obviously, this observation also includes the equilateral star and equilateral flower as special cases. This observation together with Theorem 2.6 allows to prove the following corollaries.

**Corollary 2.7.** *Let  $\mathcal{G}_1, \mathcal{G}_2$  be discrete graphs. Denote by  $v_1, v_2$  non-leaf vertices of each of those graphs and let  $\mathcal{G}$  be the graph obtained by identifying  $v_1$  and  $v_2$ . If the (unique) supremizer of  $\mathcal{G}_i$  is the equilateral stower with  $E_p^{(i)}$  petals and  $E_l^{(i)}$  leaves, such that  $E_p^{(i)} + E_l^{(i)} \geq 2$ , then the (unique) supremizer of  $\mathcal{G}$  is an equilateral stower with  $E_p^{(1)} + E_p^{(2)}$  petals and  $E_l^{(1)} + E_l^{(2)}$  leaves.*

We note that as we have shown (Theorem 2.2) that equilateral stars are the unique supremizers of trees, the corollary above implies that gluing a tree (at its internal vertex) to any graph whose (unique) supremizer is a stower gives a graph whose (unique) supremizer is a stower as well.

**Corollary 2.8.** *Let  $\mathcal{G}$  be a stower graph with  $E_p$  petals and  $E_l$  leaves, such that  $E_p + E_l \geq 2$  and  $(E_p, E_l) \neq (1, 1)$ . Then it has a maximizer which is the equilateral stower graph with  $E_p$  petals and  $E_l$  dangling edges and the corresponding spectral gap is  $\frac{\pi}{2}(2E_p + E_l)$ . Furthermore, this maximizer is unique for all cases except  $(E_p, E_l) \in \{(2, 0), (1, 2)\}$ .*

We remark that a partial result of the above was already proved within the proof of theorem 4.2 in [20]. It was shown there that the equilateral flower is the unique maximizer among all flowers.<sup>5</sup> This was used there to prove the global bound  $k_1[\Gamma] \leq \pi E$  (theorem 4.2 in [20]). Having corollary 2.8, it is possible to prove the following improved bound.

**Corollary 2.9.** *Let  $\mathcal{G}$  be a graph with  $E$  edges, out of which  $E_l$  are leaves. Then*

$$\forall \underline{l} \in \mathcal{L}_{\mathcal{G}}, \quad k_1[\Gamma(\mathcal{G}; \underline{l})] \leq \pi \left( E - \frac{E_l}{2} \right), \tag{2.2}$$

*provided that  $(E, E_l) \notin \{(1, 1), (1, 0), (2, 1)\}$ .*

*Assume in addition that  $(E, E_l) \notin \{(2, 0), (3, 2)\}$ . Then an equality above implies that the graph  $\Gamma(\mathcal{G}; \underline{l})$  achieving the inequality is either an equilateral mandarin or an equilateral stower.*

This latter bound is sharp as it is attained by most equilateral stower graphs (see Example 1.5 and Corollary 2.8).

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<sup>5</sup> It is claimed there that the equilateral flower is the unique maximizer for all flowers with  $E \geq 2$ . Actually, the uniqueness does not hold for the  $E = 2$  case, as we show in the proof of Corollary 2.8.

### 3. Infimizers

*Proof of Theorem 2.1.* Let  $\Gamma$  be a metric graph whose total edge length equals one and let  $f$  be an eigenfunction corresponding to the spectral gap  $k_1(\Gamma)$  and normalized such that its  $L^2$  norm equals one. Denote

$$m := \min f < 0 \tag{3.1}$$

$$M := \max f > 0, \tag{3.2}$$

where the inequalities arise as  $f$ , being a Neumann eigenfunction is orthogonal to the constant function. In what follows we bound from below the Rayleigh quotient of  $f$  by using the rearrangement technique in a similar manner to the proof of lemma 3 in [15]. We further define

$$\mu_f(t) := |\{x \in \Gamma \mid f(x) < t\}| \text{ for } t \in [m, M], \tag{3.3}$$

where  $|\cdot|$  denotes the Lebesgue measure of the corresponding set on the graph. This allows to define a continuous, non-decreasing function  $f^*$  on the interval  $[0, 1]$ , such that  $\mu_{f^*} = \mu_f$ . This property gives

$$1 = \int_{\Gamma} |f(x)|^2 dx = \int_m^M t^2 d\mu_f = \int_0^1 |f^*(x)|^2 dx \tag{3.4}$$

and

$$0 = \int_{\Gamma} f(x) dx = \int_m^M t d\mu_f = \int_0^1 f^*(x) dx, \tag{3.5}$$

where the first equality in (3.5) holds since  $f$  is orthogonal to the constant function.

Another ingredient we use in the proof is the co-area formula [8]. Let  $t \in [m, M]$  such that if  $f(x) = t$  then  $x$  is not a vertex and  $f'(x) \neq 0$  and call this  $t$  a regular value. By Sard's theorem, the non-regular values are of zero measure. According to the co-area formula if  $t$  is a regular value then

$$\mu'_f(t) = \sum_{x; f(x)=t} \frac{1}{|f'(x)|}, \tag{3.6}$$

and for any  $L^1$  function  $g$  on the graph

$$\int_{\Gamma} g(x) |f'(x)| dx = \int_m^M \left( \sum_{x; f(x)=t} g(t) \right) dt. \tag{3.7}$$

We now estimate the numerator of the Rayleigh quotient,  $\int_{\Gamma} |f'(x)|^2 dx$ , as follows. Denote by  $x_m, x_M$  two points for which  $f(x_m) = m, f(x_M) = M$  (they are not necessarily unique). Let  $t \in [m, M]$  be a regular value. As  $\Gamma$  is connected there is a path on the graph connecting  $x_m$  with  $x_M$  and by continuity of  $f$  it attains the value  $t$  at least once along this path, say at some point  $x_t$ . By the choice of  $t, x_t$  is not a vertex. If  $\Gamma$  is a bridgeless graph, then cutting the graph at  $x_t$ , the graph is still connected and we can find another path joining  $x_m$  and  $x_M$ . By the same reasoning  $f$  attains the value  $t$  along this path as well, so that  $t$  is attained by  $f$  at least twice on  $\Gamma$ . Denoting by

$n(t)$  the number of times that the value  $t$  is attained by  $f$  on the graph, we get that

$$n(t) \geq \begin{cases} 1 & \text{if } \Gamma \text{ has a bridge,} \\ 2 & \text{if } \Gamma \text{ is bridgeless.} \end{cases} \tag{3.8}$$

We may also bound  $n(t)$  from above

$$(n(t))^2 = \left( \sum_{x; f(x)=t} \frac{1}{\sqrt{|f'(x)|}} \sqrt{|f'(x)|} \right)^2 \tag{3.9}$$

$$\leq \left( \sum_{x; f(x)=t} \frac{1}{|f'(x)|} \right) \left( \sum_{x; f(x)=t} |f'(x)| \right) \tag{3.10}$$

$$= \mu'_f(t) \left( \sum_{x; f(x)=t} |f'(x)| \right), \tag{3.11}$$

by applying the Cauchy–Schwarz inequality and (3.6). Writing (3.7) with  $g(x) = |f'(x)|$  gives

$$\int_{\Gamma} |f'(x)|^2 dx = \int_m^M \left( \sum_{x; f(x)=t} |f'(x)| \right) dt \geq \int_m^M \frac{(n(t))^2}{\mu'_f(t)} dt. \tag{3.12}$$

We may repeat the arguments above for  $f^*$ , which attains each regular value exactly once and obtain that (3.11),(3.12) hold for  $f^*$  as equalities and with  $n^*(t) = 1$ . Therefore,

$$\int_{\Gamma} |f'(x)|^2 dx \geq \operatorname{ess\,inf}_{m \leq t \leq M} (n(t))^2 \int_{\Gamma} |(f^*)'(x)|^2 dx, \tag{3.13}$$

where the infimum above is taken only with respect to regular values. As  $f$  is the eigenfunction corresponding to  $k_1(\Gamma)$  with unit  $L^2$  norm we have  $\int_{\Gamma} |f'(x)|^2 dx = (k_1(\Gamma))^2$ . Considering  $f^*$  as a test function of unit  $L^2$  norm (see (3.4)) and zero mean (see (3.5)) on the unit interval we get that its Rayleigh quotient is no less than the first positive eigenvalue, namely that  $\int_{\Gamma} |(f^*)'(x)|^2 dx \geq \pi^2$ . Combining this with (3.13) and (3.8) we get the lower bounds,

$$k_1(\Gamma) \geq \begin{cases} \pi & \text{if } \Gamma \text{ has a bridge,} \\ 2\pi & \text{if } \Gamma \text{ is bridgeless.} \end{cases} \tag{3.14}$$

All that remains to complete the proof is the characterization of the infimizers.

Assume first that  $\Gamma$  has a bridge. An equality in (3.14) is possible only if  $n(t) = 1$  for all regular  $t \in [m, M]$ . This implies that  $\Gamma$  does not have vertices of degree 3 and above. Otherwise, due to continuity of  $f$ , we would have  $n \neq 1$  in the vicinity of such a vertex.  $\Gamma$  cannot be a single-cycle graph as it has a bridge and is therefore the unit interval,  $[0, 1]$ . Hence, it is the unique candidate for an infimizer. Indeed, its spectral gap is  $\pi$  and starting from any discrete

graph  $\mathcal{G}$  with a bridge,  $\Gamma(\mathcal{G}; \underline{l})$  is the unit interval if  $\underline{l} \in \overline{\mathcal{L}}_{\mathcal{G}}$  is chosen such that all of its entries vanish, except the entry corresponding to the bridge.

Next, the possible minimizers of bridgeless graphs are characterized. By Menger’s theorem [27], a graph is bridgeless if and only if there are at least two edge disjoint paths connecting any pair of points. We use that to deduce that if  $\mathcal{G}$  is bridgeless then  $\Gamma(\mathcal{G}; \underline{l})$  is bridgeless as well. Indeed, any path between a pair of points in  $\Gamma(\mathcal{G}; \underline{l})$  corresponds to at least one path between those points in  $\mathcal{G}$ . Thus, to seek for a possible minimizer, we assume that  $\Gamma$  is bridgeless and  $k_1(\Gamma) = 2\pi$ . As a bridgeless graph is 2-edge-connected, we deduce from Menger’s theorem that there are at least two edge disjoint paths connecting  $x_m$  with  $x_M$ . Pick two such paths and denote them by  $\gamma_1, \gamma_2$ . A necessary condition for  $k_1(\Gamma) = 2\pi$  is that  $n(t) = 2$  for each regular value  $t \in [m, M]$ . By continuity,  $f$  attains each regular value at least once on  $\gamma_1$  and at least once on  $\gamma_2$ . As  $n(t) = 2$  for a regular value  $t$ ,  $f$  attains the value  $t$  exactly once on each of  $\gamma_1$  and  $\gamma_2$ . Hence,  $f$  is strictly increasing on  $\gamma_1$  from  $x_m$  to  $x_M$  and the same holds for  $\gamma_2$ . We further conclude that  $f$  may attain only non-regular values at  $\Gamma \setminus \{\gamma_1 \cup \gamma_2\}$ . In particular, if there exists an edge in  $\Gamma \setminus \{\gamma_1 \cup \gamma_2\}$ ,  $f$  should be constant on that edge and due to  $-f'' = (2\pi)^2 f$  this constant equals zero. Thus, the edges of  $\Gamma \setminus \{\gamma_1 \cup \gamma_2\}$  may be removed from  $\Gamma$ , such that  $f$  still satisfies the Neumann conditions on the remaining graph  $\gamma_1 \cup \gamma_2$  and it is an eigenfunction on that graph. However, by this we find an eigenfunction of  $k$ -eigenvalue  $2\pi$  on a bridgeless graph whose total length smaller than one, which contradicts the lower bound, (3.14). Hence,  $\Gamma$  consists of just the union of the paths  $\gamma_1, \gamma_2$ . As  $\gamma_1, \gamma_2$  are edge disjoint,  $\gamma_1 \cap \gamma_2$  contains only vertices. We denote those vertices by  $v_0, \dots, v_n$ , with  $v_0 = x_m, v_n = x_M$  and the indices are arranged in an increasing order along the path  $\gamma_1$ . As  $f$  is strictly increasing along both  $\gamma_1, \gamma_2$ , the order of those vertices along  $\gamma_2$  is the same:  $v_0, \dots, v_n$ . Consider two adjacent vertices  $v_i, v_{i+1}$  ( $0 \leq i \leq n - 1$ ) and denote the corresponding path segments connecting them by  $\gamma_1(v_i, v_{i+1}), \gamma_2(v_i, v_{i+1})$ . As  $f$  takes the same values on the endpoints of  $\gamma_1(v_i, v_{i+1}), \gamma_2(v_i, v_{i+1})$ , is increasing and satisfies  $-f'' = (2\pi)^2 f$  on both, we conclude  $f|_{\gamma_1(v_i, v_{i+1})} = f|_{\gamma_2(v_i, v_{i+1})}$  and also that  $\gamma_1(v_i, v_{i+1})$  has the same length as  $\gamma_2(v_i, v_{i+1})$ . Hence,  $\Gamma = \gamma_1 \cup \gamma_2$  is a symmetric necklace.  $\square$

*Remark.* A further exploration of symmetric necklace graphs appears in Proposition 5.8. It is shown there that a symmetric necklace graph belongs to a family of graphs in which every graph has a simple spectral gap and its spectral gap  $k_1[\Gamma(\mathcal{G}; \underline{l})]$  is a critical value when considered as a function of  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ .

Theorem 2.1 provides a complete answer to the minimization problem. In particular, it states that any infimizer of a bridgeless graph is a symmetric necklace. A further task would be to classify the entire family of necklace graphs which serve as infimizers of a particular discrete graph. We start treating this by observing that the spectral gap of any symmetric necklace (of total length one) is  $2\pi$ . This follows from noting that  $2\pi$  is an eigenvalue of any symmetric necklace and combining this with Theorem 2.1. Now, let  $\mathcal{G}$  be a bridgeless graph and let  $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$ , such that  $\Gamma(\mathcal{G}; \underline{l}^*)$  is a symmetric necklace

with some  $\beta$  number of cycles. By the observation above and Theorem 2.1 we have that  $\Gamma(\mathcal{G}; \underline{l}^*)$  is an infimizer of  $\mathcal{G}$ . Furthermore, by choosing other values for  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$  we may get  $\Gamma(\mathcal{G}; \underline{l})$  to be any symmetric necklace with at most  $\beta$  cycles, and from the above this  $\Gamma(\mathcal{G}; \underline{l})$  would also serve as an infimizer. Therefore, the answer to the classification problem above would be given once we find what is the maximal number of cycles among all symmetric necklaces that can be obtained from a given discrete graph  $\mathcal{G}$ . Solving this requires some elements from the theory of graph connectivity which we shortly present below. A graph is called  $k$ -edge-connected if it remains connected whenever less than  $k$  edges are removed. In particular, a bridgeless graph is 2-edge-connected. A cactus graph is a graph in which every edge is contained in exactly one cycle. Let  $\mathcal{G}$  be a bridgeless graph. There exists  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$  such that  $\Gamma(\mathcal{G}; \underline{l})$  is a cactus graph with the following property. For every two edges  $e, e'$  which form a 2-edge-cut in  $\mathcal{G}$  (two edges whose removal disconnects the graph), we have  $l_e, l_{e'} \neq 0$ . Namely, those two edges also appear in  $\Gamma(\mathcal{G}; \underline{l})$ . The theory leading to this result appears in [12, 14, 28] for general  $k$ -connected graphs and is very nicely explained for the particular case of 2-edge-connected graphs in section 10 of the recent paper [26]. Now, in order to determine the maximal number of cycles of a necklace obtained from  $\mathcal{G}$  we perform the following procedure. Find all subgraphs of  $\mathcal{G}$  which are 3-edge-connected and contract each of them to a vertex; for example by choosing  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$  such that the corresponding entries vanish and considering  $\Gamma(\mathcal{G}; \underline{l})$ . This yields a cactus graph with the property mentioned above [26]. The cactus graph has a tree-like structure. This can be observed by considering an auxiliary graph  $\Gamma'$ , where each cycle of  $\Gamma(\mathcal{G}; \underline{l})$  is represented by a vertex of  $\Gamma'$  and two vertices of  $\Gamma'$  are connected if the corresponding cycles in  $\Gamma(\mathcal{G}; \underline{l})$  share a vertex (a cactus graph has the property that any two cycles of it, share at most one vertex). The obtained graph,  $\Gamma'$  turns to be a tree graph. Any path of this tree graph then corresponds to a necklace which can be obtained from the cactus  $\Gamma(\mathcal{G}; \underline{l})$  by further setting some edge lengths to zero. The longest possible necklace is found by identifying the longest path of the tree  $\Gamma'$ .

### 4. Supremizers of Tree Graphs

The proof of Theorem 2.2 is based on bounding the graph diameter, as follows.

**Definition 4.1.** Let  $\Gamma$  be a compact metric graph. The diameter of  $\Gamma$  is

$$d(\Gamma) := \max \{ \text{dist} (x, y) \mid x, y \in \Gamma \} . \tag{4.1}$$

**Lemma 4.2.** Let  $\Gamma$  be a metric tree graph of total length 1 and with  $E_l \geq 2$  leaves. Then

$$d(\Gamma) \geq \frac{2}{E_l} \tag{4.2}$$

with equality if and only if  $\Gamma$  is an equilateral star.

*Proof.* Choose two points,  $x_1, x_2$ , in  $\Gamma$  such that the distance between them is exactly  $d(\Gamma)$ . We show that  $x_1, x_2$  are necessarily leaves. Assume by contradiction that (w.l.o.g)  $x_1$  is not a leaf. Then  $\Gamma \setminus \{x_1\}$  has at least two connected components. Let  $\Gamma_1$  be one of these components satisfying  $x_2 \notin \Gamma_1$ . Let  $z$  be a point of  $\Gamma_1$  different from  $x_1$ . As  $\Gamma$  is a tree, any path from  $z$  to  $x_2$  contains  $x_1$ , which yields

$$d(x_2, z) > d(x_2, x_1) = d(\Gamma), \tag{4.3}$$

thus contradicting the definition of  $d(\Gamma)$ . Let now  $\mathcal{P}$  be the shortest path connecting  $x_1$  to  $x_2$  and denote by  $x_0$  its middle, such that

$$d(x_1, x_0) = d(x_2, x_0) = \frac{d(\Gamma)}{2}. \tag{4.4}$$

We cover  $\Gamma$  with  $E_l$  paths, each starting at  $x_0$  and ending at a leaf of  $\Gamma$ . The length of each of these paths is at most  $d(x_1, x_0)$  (otherwise, we may replace  $x_1$  by a different leaf and increase  $d(\Gamma)$ ). As the union of these paths cover  $\Gamma$ , whose total length is 1, we have

$$1 \leq \sum_{v \text{ is a leaf}} d(x_0, v) \leq \sum_{v \text{ is a leaf}} d(x_0, x_1) = E_l \frac{d(\Gamma)}{2}, \tag{4.5}$$

from which the inequality of the lemma follows. The first inequality can be an equality if and only if  $\Gamma$  is a star and  $x_0$  is its central vertex. Assuming this, the second inequality can be an equality if and only if the star is equilateral.  $\square$

Aided with Lemma 4.2, we turn to the proof of the theorem.

*Proof of Theorem 2.2.* We show in the following that there exists a test function  $f$  on  $\Gamma$  such that its Rayleigh quotient satisfies

$$\mathcal{R}(f) \leq \left( \frac{\pi}{d(\Gamma)} \right)^2. \tag{4.6}$$

Indeed, let  $y, z$  be two leaves of  $\Gamma$  such that the distance between them is exactly  $d(\Gamma)$ . Let us denote by  $\mathcal{P}$  a path of  $\Gamma$ , of length  $d(\Gamma)$ , connecting  $y$  and  $z$ . We consider  $\mathcal{P}$  as the interval  $[0, d(\Gamma)]$ , for example by identifying  $y$  with 0 and  $z$  with  $d(\Gamma)$  and define the following function on  $\mathcal{P}$ ,

$$f(x) = \cos \left( \frac{\pi x}{d(\Gamma)} \right) \text{ for } x \in \mathcal{P}. \tag{4.7}$$

We extend  $f$  to be defined on the whole graph,  $\Gamma$ , by setting its value on each connected component of  $\Gamma \setminus \mathcal{P}$  to the unique constant which preserves the continuity of  $f$ . Referring to ‘‘Appendix C’’ and using  $f - \langle f \rangle$  as our test function we have from (C.2),

$$\mathcal{R}(f - \langle f \rangle) = \frac{\int_{\Gamma} |f'(x)|^2 dx}{\int_{\Gamma} |f(x)|^2 dx - \left( \int_{\Gamma} f(x) dx \right)^2} \tag{4.8}$$

$$= \frac{\left( \frac{\pi}{d(\Gamma)} \right)^2 \frac{d(\Gamma)}{2}}{\frac{d(\Gamma)}{2} + \int_{\Gamma \setminus \mathcal{P}} |f(x)|^2 dx - \left( \int_{\Gamma} f(x) dx \right)^2}. \tag{4.9}$$

As the integral of  $f$  on  $\mathcal{P}$  vanishes, using Cauchy–Schwarz inequality we get

$$\left(\int_{\Gamma} f(x)dx\right)^2 = \left(\int_{\Gamma \setminus \mathcal{P}} f(x)dx\right)^2 \leq (1 - d(\Gamma)) \int_{\Gamma \setminus \mathcal{P}} |f(x)|^2 dx. \tag{4.10}$$

Plugging (4.10) in (4.9) gives

$$\mathcal{R}(f - \langle f \rangle) \leq \frac{\left(\frac{\pi}{d(\Gamma)}\right)^2 \frac{d(\Gamma)}{2}}{\frac{d(\Gamma)}{2} + d(\Gamma) \int_{\Gamma \setminus \mathcal{P}} |f(x)|^2 dx} \leq \left(\frac{\pi}{d(\Gamma)}\right)^2. \tag{4.11}$$

Using this and Lemma 4.2 we get

$$k_1(\Gamma) \leq \frac{\pi}{d(\Gamma)} \leq \frac{\pi}{2} E_l. \tag{4.12}$$

Let  $\mathcal{G}$  be a tree graph with  $E_l$  leaves. We may choose  $\underline{l} \in \overline{\mathcal{L}}_{\mathcal{G}}$  such that  $\Gamma(\mathcal{G}; \underline{l})$  is an equilateral star graph with  $E_l$  leaves, so that  $k_1[\Gamma(\mathcal{G}; \underline{l})] = \frac{\pi}{2} E_l$  and from the bound above we get that  $\Gamma(\mathcal{G}; \underline{l})$  is a supremizer. This is a unique supremizer as having equality in the right inequality of (4.12) implies by Lemma 4.2 that  $\Gamma$  is an equilateral star with  $E_l$  leaves.  $\square$

*Remark.* We note that the upper bound  $k_1(\Gamma) \leq \frac{\pi}{d(\Gamma)}$ , which is obtained in the course of the proof above, is a particular case of a result proven recently in [31]. There it was shown that for any  $n$ ,  $k_n(\Gamma) \leq \frac{\pi n}{d(\Gamma)}$ . Applying (4.2) to the latter we may get that for any  $n \geq 1$ ,  $k_n(\Gamma) \leq \frac{\pi n}{2} E_l$ , which improves the bound  $k_n(\Gamma) \leq \frac{\pi n}{2} E$  given in [31].

The theorem above yields the following.

*Proof of Corollary 2.3.* Let  $\mathcal{G}$  be a graph with  $\beta > 0$  cycles and  $E_l$  leaves. We start by observing that for  $(\beta, E_l) \in \{(1, 0), (1, 1)\}$ , the supremizer is the single-cycle graph (see Lemma 8.5), which is not a tree. We continue assuming  $(\beta, E_l) \notin \{(1, 0), (1, 1)\}$ . Choose a maximal spanning tree of  $\mathcal{G} \setminus \mathcal{E}_l$ , where  $\mathcal{E}_l$  is the set of the graph’s  $E_l$  leaves. Choose  $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$  such that all of its entries corresponding to the spanning tree edges are set to zero. This makes  $\Gamma(\mathcal{G}; \underline{l}^*)$  a stower with  $\beta$  petals and  $E_l$  leaves. Furthermore,  $\underline{l}^*$  may be chosen such that  $\Gamma(\mathcal{G}; \underline{l}^*)$  is an equilateral stower. The spectral gap of this graph is  $\frac{\pi}{2} (2\beta + E_l)$  (see Example 1.5). Alternatively, if  $\underline{l} \in \overline{\mathcal{L}}_{\mathcal{G}}$  is such that  $\Gamma(\mathcal{G}; \underline{l})$  is a tree then the number of its leaves is at most  $E_l$  and by Theorem 2.2 its spectral gap is at most  $\frac{\pi}{2} E_l$ . Therefore, the stower graph  $\Gamma(\mathcal{G}; \underline{l}^*)$  obtained above has a greater spectral gap than any tree graph  $\Gamma(\mathcal{G}; \underline{l})$ .  $\square$

### 5. Spectral Gaps as Critical Values

In this section we assume that the spectral gap,  $k_1(\Gamma(\mathcal{G}; \underline{l}))$ , is a simple eigenvalue. This allows to take derivatives of the eigenvalue with respect to the edge lengths,  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ , and to find critical points which serve as candidates for maximizers. We prove here Theorem 2.4 which shows that such local maximizers



do not achieve a spectral gap higher than that achieved by turning the graph into a mandarin or a flower.

**Lemma 5.1.** *Let  $\Gamma$  be a metric graph and  $f$  an eigenfunction corresponding to the eigenvalue  $k^2$  with arbitrary vertex conditions. Then the function  $f'(x)^2 + k^2 f(x)^2$  is constant along each edge.*

*Proof.* The proof is immediate by differentiating the function  $f'(x)^2 + k^2 f(x)^2$  along an edge.  $\square$

The last lemma motivates us to define the energy<sup>6</sup> of an eigenfunction on an edge  $e$  as  $\mathcal{E}_e := f'(x)^2 + k^2 f(x)^2$  for any  $x \in e$ . This energy shows up naturally when differentiating an eigenvalue with respect to an edge length. In order to evaluate such derivatives we extend Definition 1.1 so that  $\Gamma(\mathcal{G}; \underline{l})$  is defined for all  $\underline{l} \in \mathbb{R}^E$  with positive entries and relax the restriction  $\sum_{e=1}^E l_e = 1$ , imposed by  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ . The following lemma appears also as Lemma A.1 in [9] and within the proof of a lemma in [16].

**Lemma 5.2.** *Let  $\mathcal{G}$  be a discrete graph and let  $\underline{l} \in \mathbb{R}^E$  with positive entries. Assume that the spectral gap,  $k_1[\Gamma(\mathcal{G}; \underline{l})]$  is a simple eigenvalue and let  $f$  be the corresponding eigenfunction, normalized to have unit  $L^2$  norm. Then  $k_1[\Gamma(\mathcal{G}; \underline{l})]$  is differentiable with respect to any edge length  $l_{\bar{e}}$  and*

$$\frac{\partial}{\partial l_{\bar{e}}} \left( (k_1[\Gamma(\mathcal{G}; \underline{l})])^2 \right) = -\mathcal{E}_{\bar{e}}. \tag{5.1}$$

*Proof.* In this proof we use the analyticity of the eigenvalues and eigenfunctions with respect to the edge lengths. This is established, for example, in sections 3.1.2, 3.1.3 of [5]. Let  $s \in \mathbb{R}$  and let  $\bar{e}$  be an edge of  $\Gamma(\mathcal{G}; \underline{l})$ . Denote  $\underline{l}(s) := \underline{l} + s\bar{e}$ , with  $\bar{e} \in \mathbb{R}^E$  a vector with one at its  $\bar{e}^{\text{th}}$  position and zeros in all other entries. We use the notation  $\Gamma(s) := \Gamma(\mathcal{G}; \underline{l}(s))$  and denote by  $k_1(s)$  the spectral gap of  $\Gamma(s)$ . By assumption,  $k_1(0)$  is a simple eigenvalue and hence there is a neighborhood of zero for which all  $k_1(s)$  are simple eigenvalues. The corresponding eigenfunctions are denoted by  $f(s; \cdot)$  and we further assume that all those eigenfunctions have unit  $L^2$  norm,

$$\int_{\Gamma(s)} (f(s; x))^2 dx = \sum_{e=1}^E \int_0^{l_e(s)} (f(s; x_e))^2 dx_e = 1, \tag{5.2}$$

where  $l_e(s) = l_e + \delta_{e,\bar{e}}s$  and  $\delta_{e,\bar{e}}$  being the Kronecker delta function.

Taking a derivative of the above with respect to  $s$ ,

$$(f(s; l_{\bar{e}}(s)))^2 + 2 \sum_{e=1}^E \int_0^{l_e(s)} f(s; x_e) \frac{\partial}{\partial s} f(s; x_e) dx_e = 0. \tag{5.3}$$

In addition, evaluating the Rayleigh quotient of  $f$ ,

$$k_1(s)^2 = \mathcal{R}[f(s; \cdot)] = \sum_{e=1}^E \int_0^{l_e(s)} \left( \frac{\partial}{\partial x_e} f(s; x_e) \right)^2 dx_e, \tag{5.4}$$

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<sup>6</sup> A simple harmonic oscillator whose spring constant is  $k$  and whose position is given by  $f(x)$  has a total energy of  $\frac{1}{2}\mathcal{E}_e$ .

using that  $f(s; \cdot)$  has unit norm. Differentiating this with respect to  $s$  gives

$$\begin{aligned} \frac{d}{ds} (k_1(s)^2) &= \left( \frac{\partial}{\partial x_{\bar{e}}} f(s; l_{\bar{e}}(s)) \right)^2 \\ &\quad + 2 \sum_{e=1}^E \int_0^{l_e(s)} \frac{\partial}{\partial x_e} f(s; x_e) \frac{\partial^2}{\partial s \partial x_e} f(s; x_e) dx_e. \end{aligned} \tag{5.5}$$

Integrating by parts in the right-hand side and using the eigenvalue equation, we get for each term in the sum above

$$\begin{aligned} &\int_0^{l_e(s)} \frac{\partial}{\partial x_e} f(s; x_e) \frac{\partial^2}{\partial s \partial x_e} f(s; x_e) dx_e \\ &= \frac{\partial}{\partial x_e} f(s; l_e(s)) \left( \frac{\partial}{\partial s} f \right) (s; l_e(s)) - \frac{\partial}{\partial x_e} f(s; 0) \frac{\partial}{\partial s} f(s; 0) \\ &\quad + k_1(s)^2 \int_0^{l_e(s)} f(s; x_e) \frac{\partial}{\partial s} f(s; x_e) dx_e \\ &= \frac{\partial f}{\partial x_e} \left( \frac{df}{ds} - \delta_{e, \bar{e}} \frac{\partial f}{\partial x_e} \right) \Big|_{(s; l_e(s))} - \frac{\partial f}{\partial x_e} \frac{df}{ds} \Big|_{(s; 0)} \\ &\quad + k_1(s)^2 \int_0^{l_e(s)} f \frac{\partial f}{\partial s} \Big|_{(s; x_e)} dx_e, \end{aligned} \tag{5.6}$$

where the partial derivatives with respect to  $s$  are rewritten in terms of complete derivatives.

Summing the first two terms of the right-hand side of (5.6) over all edges and rewriting it as a sum over all graph vertices we get

$$\begin{aligned} &\sum_{e=1}^E \left\{ \frac{\partial f}{\partial x_e} f \left( \frac{df}{ds} - \delta_{e, \bar{e}} \frac{\partial f}{\partial x_e} \right) \Big|_{(s; l_e(s))} - \frac{\partial f}{\partial x_e} \frac{df}{ds} \Big|_{(s; 0)} \right\} \\ &= \sum_v \left( \sum_{e \sim v} \frac{\partial f}{\partial x_e} \right) \frac{df}{ds} \Big|_{(s; v)} - \left( \frac{\partial f}{\partial x_{\bar{e}}} \Big|_{(s; l_{\bar{e}}(s))} \right)^2 \\ &= - \left( \frac{\partial f}{\partial x_{\bar{e}}} \Big|_{(s; l_{\bar{e}}(s))} \right)^2, \end{aligned} \tag{5.7}$$

where the sum  $e \sim v$  above is taken over all edges adjacent to a chosen vertex  $v$ , the derivatives  $\frac{\partial}{\partial x_e}$  in this sum are all taken toward the vertex  $v$  and  $\sum_{e \sim v} \frac{\partial}{\partial x_e} f(s; v) = 0$ , as  $f$  satisfies Neumann conditions at  $v$ .

Plugging (5.6), (5.7) and (5.3) in Eq. (5.5) we get

$$\frac{d}{ds} (k_1(s)^2) = - \left( \frac{\partial f}{\partial x_{\bar{e}}} \Big|_{(s; l_{\bar{e}}(s))} \right)^2 - (k_1(s))^2 \left( f|_{(s; l_{\bar{e}}(s))} \right)^2 = -\mathcal{E}_{\bar{e}}, \tag{5.8}$$

which finishes the proof once  $s = 0$  is taken. □

We note that the derivative of an eigenvalue with respect to an edge length is derived in [11] (theorem 4.4) for the general case of the  $p$ -Laplacian

on a graph. In the case of the 2-Laplacian, using Lemma 5.1 shows that the integral expression obtained in [11] simplifies to equal  $-\mathcal{E}_{\bar{e}}$ .

The lemma above provides a practical tool for increasing the spectral gap once the corresponding eigenfunction is known. In order to do so, one should increase the length of edges with lower energy on the expense of shortening those with higher energy. In particular, focusing on a particular vertex, one should increase the lengths of the edges for which the eigenfunction derivative is the lowest and vice versa. This method is useful as long as the spectral gap is not a critical point in the edge length space,  $\mathcal{L}_{\mathcal{G}}$ . An equilateral star with an odd number of edges illustrates the importance of simplicity: though we cannot increase the spectral gap, no eigenfunction on this graph will have equal energy at all edges.

The next lemma provides a necessary and sufficient condition for existence of a critical point in the edge length space,  $\mathcal{L}_{\mathcal{G}}$ .

**Lemma 5.3.** *Let  $\mathcal{G}$  be a discrete graph and let  $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$ . Assume that the spectral gap,  $k_1[\Gamma(\mathcal{G}; \underline{l}^*)]$  is a simple eigenvalue and let  $f$  be the corresponding eigenfunction. The function  $k_1[\Gamma(\mathcal{G}; \underline{l})]$  has a critical value at  $\underline{l} = \underline{l}^*$  if and only if both conditions below are satisfied*

1. The derivative of  $f$  vanishes at all vertices of odd degree.
2. The derivative of  $f$  satisfy,  $\left| \frac{\partial}{\partial x_{e_1}} f(v) \right| = \left| \frac{\partial}{\partial x_{e_2}} f(v) \right|$ , for all edges  $e_1, e_2$  adjacent to a vertex of even degree,  $v$ .

*Proof.* We first observe that positivity of the spectral gap yields that  $k_1[\Gamma(\mathcal{G}; \underline{l})]$  has a critical point at  $\underline{l} = \underline{l}^*$  if and only if  $(k_1[\Gamma(\mathcal{G}; \underline{l})])^2$  has a critical point there. From Lemma 5.2 we deduce that a critical point occurs if and only if the corresponding eigenfunction has equal energies on all graph edges. The last deduction comes as this is a critical point under the constraint  $\sum_e l_e = 1$ . Let  $v$  be a graph vertex and  $e_1, e_2$  two edges adjacent to it. Since  $f$  is continuous (i.e., single valued) at  $v$  we conclude

$$\mathcal{E}_e = \mathcal{E}_{\bar{e}} \Leftrightarrow \left( \frac{\partial}{\partial x_e} f(v) \right)^2 = \left( \frac{\partial}{\partial x_{\bar{e}}} f(v) \right)^2, \tag{5.9}$$

which proves the second claim of the lemma. The first claim follows since the Neumann condition gives that the sum of all derivatives at  $v$  vanishes.  $\square$

Obviously, graphs whose spectral gap is a critical point in the space  $\mathcal{L}_{\mathcal{G}}$  serve as good candidates for maximizers. The next lemma characterizes those graphs and their corresponding eigenfunctions.

**Lemma 5.4.** *Let  $\mathcal{G}$  be a discrete graph,  $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$  and denote  $\Gamma := \Gamma(\mathcal{G}; \underline{l}^*)$ . Assume that  $k := k_1[\Gamma]$  is a critical value and let  $f$  be the corresponding eigenfunction. Then we have the following edge disjoint decomposition*

$$\Gamma = \bigcup_{i=1}^P \mathcal{P}_i, \tag{5.10}$$

where

1. All  $\mathcal{P}_i$ 's are graphs which possess an Eulerian path or an Eulerian cycle. Namely, for each  $\mathcal{P}_i$  there is a path (either open path or a cycle), which visits each edge exactly once.
2. Different  $\mathcal{P}_i$ 's may share only vertices, but not edges.
3.  $f|_{\mathcal{P}_i}$  is a Neumann eigenfunction of  $\mathcal{P}_i$ , whose eigenvalue equals  $k$ .
4. Denote by  $\mu_i$  the number of zeros of  $f|_{\mathcal{P}_i}$ , where each zero at a vertex of  $\mathcal{P}_i$  is counted as half the degree of this vertex in  $\mathcal{P}_i$ . Denoting by  $L_i$  the metric length of  $\mathcal{P}_i$ , the following holds

$$kL_i = \pi\mu_i. \tag{5.11}$$

5. In addition,

$$k = \pi\mu, \tag{5.12}$$

where  $\mu$  is the number of zeros of  $f$  on  $\Gamma$ , where each zero at a vertex of  $\Gamma$  is counted as half the degree of this vertex in  $\Gamma$ .

*Proof.* We use the claims of Lemma 5.3 to describe a recursive process, which produces this path decomposition.

- Assume first that  $\Gamma$  has at least one vertex of odd degree,  $v_0$ . Take  $v_0$  to be the starting point of a path  $\mathcal{P}$  and add to  $\mathcal{P}$  any edge,  $e_0$ , which is adjacent to  $v_0$  and the vertex connected at its other end, which we denote by  $v_1$ . If  $v_1$  is of even degree we seek for an edge  $e_1$  connected to  $v_1$  such that  $f'|_{e_1}(v_1) = -f'|_{e_0}(v_1)$  (both derivatives are outgoing from  $v_1$ ). Such edge exists by Lemma 5.3,(2) and as the sum of derivatives of  $f$  at  $v$  vanish. Add  $e_1$  and its other endpoint,  $v_2$  to  $\mathcal{P}$  and repeat the step above until reaching a vertex of odd degree. Once an odd degree vertex is reached, we end the construction of  $\mathcal{P}$  and continue recursively to form the next path on  $\Gamma \setminus \mathcal{P}$ . Note that a certain vertex may be reached more than once during  $\mathcal{P}$ 's construction. Such a vertex would appear in  $\mathcal{P}$  only once, but with a degree greater than two. This process of path constructions continues until we exhaust the whole of  $\Gamma$  or alternatively, until  $\Gamma$  does not have any more odd degree vertices, at which point we continue with performing the next stage.
- If  $\Gamma$  has no vertex of odd degree, the construction of  $\mathcal{P}$  is as follows. We choose an arbitrary vertex,  $v_0$  as the starting point of  $\mathcal{P}$  and choose an arbitrary edge,  $e_0$  which is connected to  $v_0$  and add it to  $\mathcal{P}$  as well, together with its other endpoint,  $v_1$ . Now, just as we did in the first stage, we seek for an edge  $e_1$  connected to  $v_1$  such that  $f'|_{e_1}(v_1) = -f'|_{e_0}(v_1)$ . We keep constructing  $\mathcal{P}$  as above, keeping in mind that all vertices are of even degree. At some point we reach again the vertex  $v_0$ , arriving from some edge denoted  $e_n$ . If  $f'|_{e_0}(v_0) = -f'|_{e_n}(v_0)$  (both derivatives are outgoing from  $v_0$ ) then we end the construction of  $\mathcal{P}$ . Otherwise, continue the construction of  $\mathcal{P}$  until the condition above is satisfied. This will indeed occur, as the graph is finite and  $f$  satisfies Neumann conditions on  $\Gamma$ . Once we finish constructing of  $\mathcal{P}$  we continue recursively to form the next path on  $\Gamma \setminus \mathcal{P}$ .

By construction, each  $\mathcal{P}_i$  either possesses an Eulerian path (first stage above) or an Eulerian cycle (second stage) and  $f|_{\mathcal{P}_i}$  satisfies Neumann conditions on  $\mathcal{P}_i$ . Thus, claims (1) and (3) are valid. Also, as each subgraph  $\mathcal{P}_i$  is removed from  $\Gamma$  once constructed, it is clear that  $\forall i \neq j, \mathcal{P}_i \cap \mathcal{P}_j$  may contain only vertices, which is stated in claim (2). A subgraph  $\mathcal{P}_i$  of the first stage of the construction, where  $\Gamma$  has some odd degree vertices, possesses an Eulerian path and may be identified with an interval  $[0, L_i]$ , where  $L_i$  is the metric length of  $\mathcal{P}_i$ . Also by way of construction,  $f|_{[0, L_i]}$  is a Neumann eigenfunction (notice that this is more restrictive than stating that  $f|_{\mathcal{P}_i}$  is a Neumann eigenfunction, because of possible self-crossings). Hence,  $f|_{[0, L_i]} = \cos\left(\frac{\pi}{L_i}\mu_i x\right)$  for some positive integer,  $\mu_i$ . Clearly,  $\mu_i$  equals the number of zeros of  $f|_{[0, L_i]}$ . Furthermore,  $\mu_i$  also equals the number of zeros of  $f|_{\mathcal{P}_i}$ , where a zero at a vertex is counted as many times as half the degree of that vertex in  $\mathcal{P}_i$ . A subgraph  $\mathcal{P}_i$  of the second construction stage, where all  $\Gamma$  vertices are of even degrees possesses an Eulerian cycle and may be identified with an interval  $[0, L_i]$ , where  $L_i$  is the metric length of  $\mathcal{P}_i$ . Also by way of construction,  $f|_{[0, L_i]}$  is a Neumann eigenfunction which satisfies periodic boundary conditions. Hence,  $f|_{[0, L_i]} = \cos\left(\frac{\pi}{L_i}\mu_i x\right)$  for some positive even integer,  $\mu_i$ . As before,  $\mu_i$  equals the number of zeros of  $f|_{\mathcal{P}_i}$ , counted according to vertex degrees. In both cases, we have that  $k = \frac{\pi}{L_i}\mu_i$ , which shows claim (4) of the theorem.

Finally, claim (5) is deduced from claim (4), by summing over all  $\mathcal{P}_i$ 's. □

Having characterized local critical points, we wish to connect those to supremizers.

**Lemma 5.5.** *Let  $\Gamma(\mathcal{G}; \underline{l})$  be a supremizer of a discrete graph  $\mathcal{G}$ , such that its spectral gap  $k_1[\Gamma(\mathcal{G}; \underline{l})]$  is simple. Then, there exists a discrete graph  $\mathcal{G}^*$  and positive edge lengths  $\underline{l}^* \in \mathcal{L}_{\mathcal{G}^*}$  such that  $\Gamma(\mathcal{G}; \underline{l}) = \Gamma(\mathcal{G}^*; \underline{l}^*)$  and the spectral gap  $k_1[\Gamma(\mathcal{G}^*; \underline{l}^*)]$  is a critical value.*

*Proof.* Start by forming a new discrete graph  $\mathcal{G}^*$  by contracting the edges of  $\mathcal{G}$  which correspond to the vanishing values of  $\underline{l}$ , or setting  $\mathcal{G}^* = \mathcal{G}$  if all entries of  $\underline{l}$  are strictly positive. We get that there exists  $\underline{l}^* \in \mathcal{L}_{\mathcal{G}^*}$  such that  $\Gamma(\mathcal{G}; \underline{l}) = \Gamma(\mathcal{G}^*; \underline{l}^*)$ . In effect,  $\underline{l}^*$  entries are exactly the non-vanishing entries of  $\underline{l}$ . Since  $\Gamma(\mathcal{G}; \underline{l})$  is a supremizer of  $\mathcal{G}$  we get that  $\Gamma(\mathcal{G}^*; \underline{l}^*)$  is a supremizer of  $\mathcal{G}^*$ . Furthermore,  $\Gamma(\mathcal{G}^*; \underline{l}^*)$  is even a maximizer of  $\mathcal{G}^*$  as all of  $\underline{l}^*$  entries are positive. Since  $k_1[\Gamma(\mathcal{G}^*; \underline{l}^*)]$  is a simple eigenvalue, it is analytic with respect to edge lengths and therefore must be a critical value. □

Having Lemma 5.5 allows to conclude that all the claims in Lemmata 5.3 and 5.4 hold for supremizers whose spectral gaps are simple. We use this in proving Theorem 2.4.

*Proof of Theorem 2.4.* We start by noting that the path decomposition of Lemma 5.4 is valid under the assumptions of the theorem. Denote for brevity  $\Gamma := \Gamma(\mathcal{G}; \underline{l})$  and  $k := k_1[\Gamma]$ , with corresponding eigenfunction  $f$ . Denote

$\Gamma_+ := \{x \in \Gamma \mid f(x) > 0\}$ ,  $\Gamma_- := \{x \in \Gamma \mid f(x) < 0\}$  and denote by  $\beta_+, \beta_-$  their corresponding first Betti numbers. The connected components of  $\Gamma_+, \Gamma_-$  are called the nodal domains of  $f$ . As  $k$  is the second eigenvalue of  $\Gamma$ , we deduce from the Courant nodal theorem and the simplicity of  $k$  that  $f$  has only two nodal domains (see [10] for the original proof of Courant, or [3, 18] for its adaptation for graphs). Hence, the sets  $\Gamma_+$  and  $\Gamma_-$  are connected (notice that  $\Gamma_{\pm}$  are not exactly subgraphs, as they do not include the vertices at which  $f$  vanishes).

Next, note that  $f$  cannot completely vanish on an edge. Otherwise, the energy of that edge equals to zero and as  $k$  is a critical value, by the proof of Lemma 5.3 all edge energies are equal to zero which leads to  $f \equiv 0$ . Furthermore, we show that  $f$  cannot vanish more than once on the same edge, including its endpoints. Assume by contradiction that there exists an edge,  $e = [u, v]$  on which  $f$  vanishes at least twice. As  $f$  has only two nodal domains, it can vanish at most twice on  $e$ . For each zero of  $f$  located on the interior of  $e$ , add a dummy vertex of degree two at the position of this zero. Those two zeros now coincide with two vertices of  $\Gamma(\mathcal{G}; \underline{l})$ , which we denote by  $v_1, v_2$  and further denote the degrees of those vertices by  $d_1, d_2$ . We note that both  $d_1$  and  $d_2$  are even and in particular not smaller than two. This holds as a zero at an odd degree vertex implies by Lemma 5.3 that the energy at this vertex vanishes as well. As  $k$  is a critical value, all energies are equal throughout the graph, which implies  $f \equiv 0$ . From Lemma 5.4, (5) we get  $k = \frac{1}{2}(d_1 + d_2)\pi$ . We modify  $\Gamma$  by contracting the edge segment connecting between  $v_1$  and  $v_2$ , turning them into a single vertex which we denote by  $v_0$ . We get that in the new graph, the vertex  $v_0$  has a degree  $d_0 = d_1 + d_2 - 2$ . This new graph is connected and we modify it by contracting all edges except those  $d_0$  edges connected to  $v_0$ . Doing so, we obtain a mandarin graph with  $d_1 + d_2 - 2$  edges. By turning the mandarin into an equilateral mandarin it achieves a spectral gap of  $(d_1 + d_2 - 2)\pi$  (see Example 1.6). As  $\Gamma$  is a supremizer we conclude  $(d_1 + d_2 - 2)\pi \leq \frac{1}{2}(d_1 + d_2)\pi$ , so that  $d_1 + d_2 \leq 4$ . Since we have seen above that  $d_1 \geq 2, d_2 \geq 2$  we deduce  $d_1 = d_2 = 2$ . By the path decomposition in Lemma 5.4, each path must contain at least one zero of  $f$ . Hence, only a single path is possible in the decomposition and  $\Gamma$  must be a single-cycle graph. We arrive at a contradiction, as the spectral gap of this graph is not simple. Hence,  $f$  vanishes at most once on each edge, which includes both the interior of the edge and its two endpoints.

If  $f$  vanishes at points which are not vertices, we turn those points into dummy vertices of degree two. Each zero of  $f$  is now located at some vertex of  $\Gamma$ . We introduce the following notation. Denote by  $V_+ (V_-)$  the number of vertices at which  $f$  is positive (negative), which is just the number of vertices of  $\Gamma_+ (\Gamma_-)$ . Denote by  $V_0$  the number of vertices at which  $f$  vanishes (this includes the additional dummy vertices we added). Similarly, denote by  $E_{++} (E_{--})$  the number of edges which connect two vertices from  $V_+ (V_-)$ . Note that  $f$  does not vanish at all on those edges. Further denote by  $E_{0+} (E_{0-})$  the number of edges which connect a vertex of  $V_0$  to a vertex of  $V_+ (V_-)$ . Note that due to the additional dummy vertices there are no edges which connect a

positive vertex to a negative one. With those notations, the graph's first Betti number is

$$\begin{aligned} \beta &= E - V + 1 \\ &= (E_{++} + E_{--} + E_{0+} + E_{0-}) - (V_+ + V_- + V_0) + 1 \\ &= (E_{++} - V_+ + 1) + (E_{--} - V_- + 1) + (E_{0+} + E_{0-} - V_0) - 1 \\ &= \beta_+ + \beta_- + (E_{0+} + E_{0-} - V_0) - 1, \end{aligned} \tag{5.13}$$

where  $\beta_+ := E_{++} - V_+ + 1$  is the first Betti number of  $\Gamma_+$  and similarly for  $\beta_- := E_{--} - V_- + 1$  and  $\Gamma_-$ . In addition,

$$E_{0+} + E_{0-} = \sum_{v \in V_0} d_v = 2V_0 + 2\delta, \tag{5.14}$$

where  $\delta \geq 0$  is defined by the equality above. The sum above is even by Lemma 5.3 and hence,  $\delta$  is an integer. In addition,  $\delta = 0$  if and only if  $f$  does not vanish on the original vertices of  $\Gamma$  (i.e., it vanishes only on the added dummy vertices which are of degree two). The number of graph zeros, counted with their multiplicities as in Lemma 5.4 (namely, each zero is counted as many times as half the degree of the corresponding vertex) is

$$\mu = \frac{1}{2} \sum_{v \in V_0} d_v = E_{0+} + E_{0-} - V_0 - \delta, \tag{5.15}$$

where we used (5.14). Combining (5.12), (5.13), (5.15) we get

$$k = \pi(\beta + 1 - (\beta_+ + \beta_-) - \delta). \tag{5.16}$$

Let  $v$  be a vertex such that  $f(v) = 0$ . We concluded above such a vertex must be of even degree. Furthermore, from Lemma 5.3 we have that half of  $f$  derivatives at  $v$  are positive and half negative. Hence,  $v$  is connected to the same number of positive values vertices as to negative valued once. We conclude that  $E_{0+} = E_{0-}$  and from the left equalities in (5.14) and (5.15) we get  $\mu = E_{0-}$ . Choose  $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$  such that all of its entries equal zero except those which correspond to the  $E_{0-}$  edges, which we set to be equal  $1/E_{0-}$ . We get that  $\Gamma(\mathcal{G}; \underline{l}^*)$  is an equilateral mandarin graph whose spectral gap equals  $\pi E_{0-} = \pi\mu$ , which finishes the proof of the theorem.  $\square$

The proof above yields the following.

**Corollary 5.6.** *Let  $\mathcal{G}$  be a discrete graph and let  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ . Assume that  $\Gamma(\mathcal{G}; \underline{l})$  is a supremizer of  $\mathcal{G}$  and that the spectral gap  $k_1(\Gamma(\mathcal{G}; \underline{l}))$  is a simple eigenvalue and let  $f$  be the corresponding eigenfunction. Denote  $\Gamma_+ := \{x \in \Gamma \mid f(x) > 0\}$ ,  $\Gamma_- := \{x \in \Gamma \mid f(x) < 0\}$  and further denote by  $\beta_+, \beta_-$  their corresponding first Betti numbers. Then*

1.  $\beta_+ + \beta_- \leq 1$ .
2. If  $\beta_+ + \beta_- = 1$  there exists a choice of lengths  $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$  such that  $\Gamma(\mathcal{G}; \underline{l}^*)$  is an equilateral flower and

$$k_1(\Gamma(\mathcal{G}; \underline{l})) = k_1(\Gamma(\mathcal{G}; \underline{l}^*)) = \beta\pi. \tag{5.17}$$

3. The number of (non-dummy) vertices at which  $f$  vanishes is at most one. Such a vertex may exist only if  $\beta_+ + \beta_- = 0$  and if it exists then this vertex is of degree four.

*Remark.* We note that  $\Gamma_-, \Gamma_+$  defined above are open sets and hence not metric graphs in the sense defined so far in the paper. Nevertheless, we can still define their Betti numbers according to the usual definition for topological spaces.

*Proof.* We start from Eq. (5.16) in the preceding proof. If  $\beta_+ + \beta_- > 1$  we get that  $k < \pi\beta$ , so that the spectral gap of  $\Gamma(\mathcal{G}; \underline{l})$  is strictly smaller than the one we can get by turning it into an equilateral flower ( $\pi\beta$ ) which contradicts it being a supremum. Therefore,  $\beta_+ + \beta_- \leq 1$ , which is claim (1).

If  $\beta_+ + \beta_- = 1$ , then by (5.16), the spectral gap of  $\Gamma(\mathcal{G}; \underline{l})$  equals  $\pi(\beta - \delta)$ . As it cannot be smaller than the one of the equilateral flower we have  $\delta = 0$ , which means that  $f$  does not vanish at vertices (with the exception of the dummy ones) and also that there exists  $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$  for which  $\Gamma(\mathcal{G}; \underline{l}^*)$  is an equilateral flower, hence showing claim (2).

If  $\beta_+ + \beta_- = 0$ , then by (5.16), the spectral gap of  $\Gamma(\mathcal{G}; \underline{l})$  equals  $\pi(\beta + 1 - \delta)$ . As it cannot be smaller than the one of the equilateral flower we have  $\delta \leq 1$ , which means that  $f$  vanishes at most on a single (non-dummy) vertex. In addition, if such a vertex exists its degree equals four. □

Another corollary of the proof of Theorem 2.4 is the following

**Corollary 5.7.** *Let  $\mathcal{G}$  be a discrete graph. Let  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$  and assume that  $\Gamma := \Gamma(\mathcal{G}; \underline{l})$  decomposes as*

$$\Gamma = \Gamma_+ \cup \Gamma_0 \cup \Gamma_-, \tag{5.18}$$

such that

1. The subgraphs  $\Gamma_+, \Gamma_0$  and  $\Gamma_-$  are pairwise edge disjoint.
2. The subgraphs  $\Gamma_+$  and  $\Gamma_-$  do not have any vertex in common.
3. The vertices of  $\Gamma_0$  have an odd degree in  $\Gamma$ .

Then, the spectral gap of  $\Gamma$  cannot be both a simple eigenvalue and a critical value as a function of  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ .

*Proof.* Let  $k$  denote the spectral gap of  $\Gamma$  and assume that it is a simple eigenvalue and a critical value. Let  $f$  be the eigenfunction corresponding to  $k$ . Since  $k$  is simple, Courant’s nodal theorem ([3, 10, 18]) entails that  $f$  has exactly two nodal domains. By Lemma 5.3 and as the vertices of  $\Gamma_0$  are of odd degree, we deduce that  $f$  vanishes on every edge of  $\Gamma_0$ . From the decomposition (5.18), it follows that  $\Gamma_+$  and  $\Gamma_-$  are contained each in a different nodal domain of  $\Gamma$  and also that each is a connected subgraph. Furthermore,  $\Gamma_0$  does not have any interior vertex as otherwise, it would belong to a third nodal domain. It follows that  $\Gamma_0$  consists of edges connecting vertices of  $\Gamma_+$  and  $\Gamma_-$ .

Observe that  $f|_{\Gamma_+}$  is a Neumann eigenfunction on  $\Gamma_+$ . Indeed, it satisfies Neumann conditions at all vertices of  $\Gamma_+ \setminus \Gamma_0$  and its derivative vanishes at each edge connected to a vertex in  $\Gamma_+ \cap \Gamma_0$ . Therefore,  $f|_{\Gamma_+}$  should be orthogonal



to the constant function on  $\Gamma_+$ . As  $f|_{\Gamma_+}$  is positive everywhere, this is possible only if  $\Gamma_+$  consists of a single vertex, which we denote by  $v_+$  (it cannot contain more than a single vertex as we have shown it is connected). The same goes for  $\Gamma_-$  (its vertex denoted by  $v_-$ ) and as we have shown that  $\Gamma_0$  consists of edges connecting vertices of  $\Gamma_+$  and  $\Gamma_-$ , we conclude that  $\Gamma$  is a mandarin graph. As all derivatives of  $f$  at  $v_{\pm}$  vanish and  $f$  cannot vanish more than once on edges connecting them we deduce that all those edges are of equal length. Hence,  $\Gamma$  is an equilateral mandarin, whose spectral gap is not a simple eigenvalue and we get a contradiction.  $\square$

This corollary applies, among other examples, to graphs having a bridge linking two vertices of odd degrees, or to bipartite and  $d$ -regular graphs for some odd  $d$ . All of those cannot have a spectral gap which is both simple and a critical value.

Demonstrating examples of the other side, we next show a family of discrete graphs,  $\mathcal{G}$ , and connected subsets  $\mathcal{L}^* \subset \mathcal{L}_{\mathcal{G}}$ , such that for all  $\underline{l}^* \in \mathcal{L}^*$ ,  $\Gamma(\mathcal{G}; \underline{l}^*)$  satisfies the conditions of Lemma 5.3. This provides a collection of graphs whose spectral gap is both simple and a critical value. Those graphs are essentially chains of mandarins glued serially one to the other and with an optional star glued at either side of this chain. We call those standarin chains (see Fig. 3).

**Proposition 5.8.** *Let  $n \geq 2$ ,  $M \geq 1$  be integers. Take some  $M$  discrete  $n$ -mandarin graphs and glue them serially to form a chain of mandarins. At each end of this chain either glue or not an  $n$ -star graph at its central vertex. Let  $S \in \{0, 1, 2\}$  be the number of star graphs which were glued and assume  $M + S \geq 2$ . Denote the obtained discrete graph by  $\mathcal{G}$ . Set  $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$  to be a vector of edge lengths such that*

1. All edges belonging to the same mandarin have equal length.
2. All edges belonging to the same star graph have equal length, which is in the range  $(0, \frac{1}{2n})$ .

Then for all such  $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$ ,  $\Gamma(\mathcal{G}; \underline{l}^*)$  satisfies the conditions of Lemma 5.3. Namely

1. The spectral gap,  $k_1[\Gamma(\mathcal{G}; \underline{l}^*)]$ , is a simple eigenvalue.
2. The function  $\underline{l} \mapsto k_1[\Gamma(\mathcal{G}; \underline{l})]$  has a critical value at  $\underline{l} = \underline{l}^*$ .

In addition, the corresponding spectral gap  $k = k_1[\Gamma(\mathcal{G}; \underline{l})]$  equals  $n\pi$ .

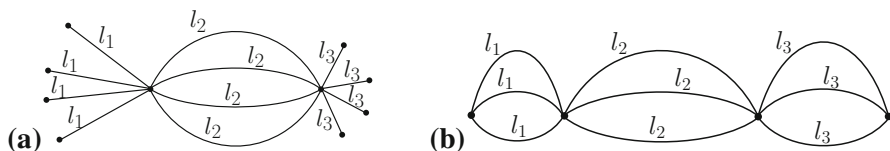


FIGURE 3. Two examples for the standarin chain graphs

*Proof.* Let  $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$  which satisfies the assumptions of the proposition. Denote  $\Gamma := \Gamma(\mathcal{G}; \underline{l}^*)$  and note that we may construct  $\Gamma$  by taking  $n$  intervals,  $\{\gamma_i\}_{i=1}^n$ , of length  $\frac{1}{n}$  each, picking  $M + 1$  points on each interval which are similarly positioned on each of the intervals, and identifying each set of parallel  $n$  points to form a vertex of  $\Gamma$ . We use this decomposition of  $\Gamma$  to describe an eigenfunction which is shown on the sequel to correspond to the spectral gap of  $\Gamma$ . Set  $f|_{\gamma_i}(x) = \cos(n\pi x_i)$  on each  $\gamma_i$ . It is easy to check that  $f$  satisfies Neumann conditions at all vertices and hence it is a valid eigenfunction and its  $k$ -eigenvalue equals  $n\pi$ . We conclude that the spectral gap obeys,  $k_1[\Gamma] \leq n\pi$ , and show in the sequel that this is actually an equality and that the spectral gap is a simple eigenvalue.

Let  $g$  be an eigenfunction corresponding to the spectral gap  $k_1[\Gamma]$ . We may assume that all the restrictions  $g|_{\gamma_i}$  at mentioned intervals are equal. Otherwise, we symmetrize  $g$  by taking

$$\forall 1 \leq i \leq n, \tilde{g}|_{\gamma_i} = \sum_{j=1}^n g|_{\gamma_j}. \tag{5.19}$$

This symmetrized function  $\tilde{g}$  indeed satisfies Neumann conditions at all vertices and we just need to justify that it is different from the zero function. Assume by contradiction that it is the zero function. In particular,  $\tilde{g}$  vanishes at all vertices and hence  $g$  itself vanishes at all vertices which are not leaves. Necessarily, there exists some edge on which  $g$  does not identically vanish. If such an edge,  $e$ , is an inner edge we get that  $k_1[\Gamma] \geq \frac{\pi}{l_e} > n\pi$ , and a contradiction. If this edge is a dangling edge, we get by assumption (2) that  $k_1[\Gamma] \geq \frac{\pi}{2l_e} > n\pi$ , which is again a contradiction. Hence, we continue assuming that  $g$  is an eigenfunction with all  $\{g|_{\gamma_i}\}_{i=1}^n$  equal to each other. From here we conclude that for all  $i$ ,  $g|_{\gamma_i}$  is an eigenfunction of the interval with Neumann condition at both of its ends. This together with  $g$  being an eigenfunction corresponding to the spectral gap implies  $g = f$  and  $k_1[\Gamma] = n\pi$ .

Next, we show the simplicity of  $k_1[\Gamma]$ . Let  $g$  be an eigenfunction of  $k_1[\Gamma]$ , not assuming it is symmetric this time. Take all parallel edges of some mandarin which is a subgraph of  $\Gamma$ . All those edges have a common length  $l < \frac{1}{n}$  and we have  $k_1[\Gamma] \cdot l = n\pi l < \pi$  so that  $\sin(k_1[\Gamma] \cdot l) \neq 0$ . Therefore, the value of  $g$  on each of those parallel edges is given by

$$g|_e(x) = \frac{1}{\sin(k_1[\Gamma] \cdot l)} \{g(u) \sin(k_1[\Gamma] \cdot (l - x)) + g(v) \sin(k_1[\Gamma] \cdot x)\}, \tag{5.20}$$

where  $u, v$  are the vertices of this mandarin and  $e$  any edge connecting them. A similar argument shows that  $g$  is also uniquely determined at the dangling edges. The simplicity of  $k_1[\Gamma]$  follows.

Finally, computing the energy,  $\mathcal{E}_e = (f')^2 + k^2 f^2$ , of  $f$  as defined above, we get that it is equal on all edges. By Lemma 5.2 we conclude that the function  $\underline{l} \mapsto k_1[\Gamma(\mathcal{G}; \underline{l})]$  has a critical value at  $\underline{l} = \underline{l}^*$ . □

We note that the particular case  $n = 2, M = 1, S = 1$  is dealt with in Lemma 8.1. It is stated there that for this particular stower the graphs  $\Gamma(\mathcal{G}; \underline{l})$  not only have the spectral gap as a critical value, but they are also maximizers. Furthermore, those graphs are supremizers and thus satisfy the conditions of Theorem 2.4. Indeed, this stower has a spectral gap of  $2\pi$ , which equals the spectral gap of a single cycle, which is merely a one-petal flower or a two-edge mandarin.

In general, the graphs in the proposition above share the same spectral gap as equilateral  $n$ -mandarin graphs. As such they obey the conclusion of Theorem 2.4 even though they do not satisfy the requirements of the theorem as they are not necessarily supremizers. For example, the graphs  $\Gamma(\mathcal{G}; \underline{l}^*)$  of the proposition above are not supremizers if we take  $n \geq 3$ . In this case, there is a choice of lengths,  $l$ , for which  $\Gamma(\mathcal{G}; \underline{l})$  is a stower graph with  $E_p = M \cdot (n - 1)$  and  $E_l = S \cdot n$ , whose spectral gap is  $\frac{\pi}{2}(2M \cdot (n - 1) + S \cdot n)$  and greater than  $n\pi$ .

### 6. Gluing Graphs

In this section we develop spectral gap inequalities for graphs whose vertex connectivity equals one. Such graphs may be obtained by considering two disjoint graphs and identifying two vertices, one of each graph. We bound the spectral gap of the obtained graph by the sum of spectral gaps of its two subgraphs and provide necessary and sufficient conditions for equality to hold (Proposition 6.5). We use this in order to prove sufficient conditions needed for graphs with vertex connectivity one to be supremizers (Theorem 2.6).

We fix some notations to use throughout this section. Let  $\Gamma$  be a graph and let  $v$  be a vertex of  $\Gamma$ . We say that  $f$  satisfies the  $\delta$ -type conditions at  $v$  with parameter  $\theta$  if

$$\begin{aligned}
 & f \text{ is continuous at } v \\
 & \text{and} \\
 & \cos\left(\frac{\theta}{2}\right) \sum_{e \in \mathcal{E}_v} \frac{df}{dx_e}(v) = \sin\left(\frac{\theta}{2}\right) f(v), \tag{6.1}
 \end{aligned}$$

where  $\theta \in (-\pi, \pi]$  (see Definition B.1). Note that Neumann conditions are obtained as a special case with  $\theta = 0$  and Dirichlet conditions are obtained from  $\theta = \pi$ . We denote by  $k_n(\Gamma; \theta)$  the  $n$ th  $k$ -eigenvalue of  $\Gamma$ , endowed with the  $\delta$ -type condition with parameter  $\theta$  at  $v$  and Neumann at all other vertices. The corresponding  $k$ -spectrum is denoted by

$$\sigma(\Gamma; \theta) := \cup_n \{k_n(\Gamma; \theta)\}. \tag{6.2}$$

It will be understood in the sequel which vertex  $v$  is chosen so that it is not indicated in the notation. In addition, we omit the notation  $\Gamma$  from  $k_n(\Gamma; \theta)$  and  $\sigma(\Gamma; \theta)$  whenever it is clear which graph we refer to. Similarly,  $\theta$  is omitted from these notations whenever  $\theta = 0$  to comply with the notations used so far. At this point, we refer the reader to ‘‘Appendix B,’’ where we quote some

results from [5] on  $\delta$ -type conditions, that are used throughout this section. The structure of the spectrum as it depends on the parameter  $\theta$  (for some chosen vertex  $v$ ) is described in the next lemma, which quotes parts of Theorem 3.1.13 from [5], slightly rephrased for our purpose.

**Lemma 6.1.** *Let  $\Gamma$  be a metric graph and let  $v$  be a vertex of  $\Gamma$ . There exist a bounded from below discrete set,  $\Delta(\Gamma) \subset \mathbb{R}$  and a real smooth function,  $K(\Gamma; \cdot) : (-\pi, \infty) \rightarrow \mathbb{R}$  (called “dispersion relation”) such that*

1. *The function  $\theta \mapsto K(\Gamma; \theta)$  is strictly increasing so that  $\lim_{\theta \rightarrow -\infty} K(\Gamma; \theta) = \infty$ .*
2. *For any  $\theta \in (-\pi, \pi]$ ,  $\sigma(\Gamma; \theta) = \{K(\Gamma; \theta + 2\pi n)\}_{n=0}^\infty \cup \Delta(\Gamma)$ .*

*Remark.* We see from the lemma above that

$$\Delta(\Gamma) = \bigcap_{\theta \in (-\pi, \pi]} \sigma(\Gamma; \theta). \tag{6.3}$$

The values of this discrete set, common to all spectra, are often called flat bands.

A particular value of  $\theta$  which plays a special role is defined below.

**Definition 6.2.** Let  $\Gamma$  be a graph and let  $v$  be a vertex of  $\Gamma$ . A parameter  $\theta^{SG} \in \mathbb{R}$  which satisfies

$$K(\Gamma; \theta^{SG}) = k_1(\Gamma; 0) \tag{6.4}$$

is called the spectral gap parameter (SGP) of  $\Gamma$  (with respect to  $v$ ). See Fig. 4.

In the following we point out some of the SGP properties.

**Lemma 6.3.** 1. *The spectral gap parameter exists and it is unique.*

2.  $\theta^{SG} \in [0, 2\pi]$ .
3. If  $\theta^{SG} \neq 2\pi$  then  $k_1(\Gamma; 0) \in \Delta(\Gamma)$ .
4. If  $\theta^{SG} \in (0, \pi]$  then

$$\begin{cases} k_0(\theta) < k_1(0) & \text{for } \theta \in (0, \theta^{SG}) \\ k_0(\theta) = k_1(0) & \text{for } \theta \in [\theta^{SG}, \pi] \\ k_1(\theta - 2\pi) = k_1(0) & \text{for } \theta \in (\pi, 2\pi]. \end{cases} \tag{6.5}$$

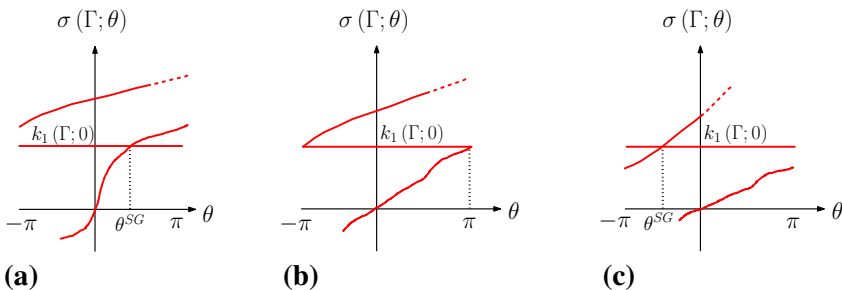


FIGURE 4. Three examples of dispersion relations curves. **a**  $\theta^{SG} \in (0, \pi)$ , **b**  $\theta^{SG} = \pi$ , **c**  $\theta^{SG} \in (\pi, 2\pi)$

5. If  $\theta^{SG} \in (\pi, 2\pi)$  then

$$\begin{cases} k_0(\theta) < k_1(0) & \text{for } \theta \in [0, \pi] \\ k_1(\theta - 2\pi) < k_1(0) & \text{for } \theta \in (\pi, \theta^{SG}) \\ k_1(\theta - 2\pi) = k_1(0) & \text{for } \theta \in [\theta^{SG}, 2\pi]. \end{cases} \tag{6.6}$$

*Proof.* The existence of the spectral gap parameter follows from  $K(\Gamma; 0) = 0$  together with  $K(\Gamma; \cdot)$  being monotonically increasing. This latter argument also shows the uniqueness of the SGP and that  $\theta^{SG} \geq 0$ .

We have that  $K(\Gamma; 2\pi) = k_n(\Gamma; 0)$  for some  $n$  and hence, by continuity and monotonicity of  $K$  we get  $\theta^{SG} \leq 2\pi$ , which shows property (2) above.

If  $\theta^{SG} < 2\pi$  we have  $k_1(\Gamma; 0) \in \sigma(\Gamma; 0) \cap \sigma(\Gamma; \theta^{SG})$  and by Lemma B.5 conclude  $k_1(\Gamma; 0) \in \Delta(\Gamma)$ , which proves property (3). Finally, properties (4) and (5) are straightforward consequences of the strict monotonicity of  $K$  together with the eigenvalue interlacing with respect to the  $\delta$ -type condition parameter (see Lemma B.2).  $\square$

The main construction in this section involves scaling two disjoint graphs and gluing them at a vertex to form a new graph, as defined below.

**Definition 6.4.** Let  $\Gamma_1, \Gamma_2$  be two Neumann graphs of total length 1 each. Let  $v_i$  be a vertex of  $\Gamma_i$  ( $i = 1, 2$ ). Let  $\Gamma$  be the graph obtained by the following process

1. Multiply all edge lengths of  $\Gamma_1$  by some factor  $L \in [0, 1]$ .
2. Multiply all edge lengths of  $\Gamma_2$  by a factor of  $1 - L$ .
3. Identify  $v_1$  and  $v_2$  of the graphs above and endow the new vertex with Neumann vertex conditions.

We call  $\Gamma$  the *gluing* of  $\Gamma_1, \Gamma_2$  (with respect to  $v_1, v_2$  and  $L$ ).

**Proposition 6.5.** Let  $\Gamma_1, \Gamma_2$  be two connected Neumann graphs of total length 1 each. Let  $v_i$  be a vertex of  $\Gamma_i$  ( $i = 1, 2$ ). Let  $\Gamma$  be the gluing of  $\Gamma_1, \Gamma_2$  with respect to  $v_1, v_2$  and some value  $L \in [0, 1]$ . Let  $\theta_1^{SG}, \theta_2^{SG}$  be the spectral gap parameters of  $\Gamma_1, \Gamma_2$  with respect to  $v_1, v_2$ , correspondingly. Then the following inequality holds

$$k_1(\Gamma) \leq k_1(\Gamma_1) + k_1(\Gamma_2), \tag{6.7}$$

with equality if and only if both conditions below are satisfied

1.  $L = \frac{k_1(\Gamma_1)}{k_1(\Gamma_1) + k_1(\Gamma_2)}$ .
2.  $\theta_1^{SG} + \theta_2^{SG} \leq 2\pi$ .

Additional necessary conditions for equality in (6.7) are

- (a) The spectral gaps of the glued graphs obey  $k_1(\Gamma_1) \in \Delta(\Gamma_1)$  and  $k_1(\Gamma_2) \in \Delta(\Gamma_2)$ .
- (b) The spectral gap of the outcome graph,  $k_1(\Gamma)$  is a multiple (i.e., non-simple) eigenvalue.

*Proof.* We start by showing the inequality (6.7).

Let  $L \in [0, 1]$ . If  $L = 0$  ( $L = 1$ ), then  $\Gamma = \Gamma_2$  ( $\Gamma = \Gamma_1$ ) and (6.7) obviously holds as a strict inequality and indeed condition (1) is violated if  $L = 0$  or

$L = 1$ . We therefore assume  $L \in (0, 1)$ . Denote by  $\tilde{\Gamma}_1$  the graph obtained by multiplying all edge lengths of  $\Gamma_1$  by  $L$  and by  $\tilde{\Gamma}_2$  the graph obtained by multiplying all edge lengths of  $\Gamma_2$  by  $1 - L$ . Therefore, identifying the vertices  $v_1, v_2$  of  $\Gamma_1, \Gamma_2$  gives the graph  $\Gamma$ . Applying Lemma B.3 we get

$$k_1(\Gamma) \leq k_2(\tilde{\Gamma}_1 \cup \tilde{\Gamma}_2). \tag{6.8}$$

As the spectrum of  $\tilde{\Gamma}_1 \cup \tilde{\Gamma}_2$  is the union of spectra of both graphs, we have that

$$\begin{aligned} k_0(\tilde{\Gamma}_1 \cup \tilde{\Gamma}_2) &= k_1(\tilde{\Gamma}_1 \cup \tilde{\Gamma}_2) = 0 \\ \text{and} \\ k_2(\tilde{\Gamma}_1 \cup \tilde{\Gamma}_2) &= \min(k_1(\tilde{\Gamma}_1), k_1(\tilde{\Gamma}_2)) \end{aligned} \tag{6.9}$$

and conclude

$$k_1(\Gamma) \leq \min(k_1(\tilde{\Gamma}_1), k_1(\tilde{\Gamma}_2)) = \min\left(\frac{k_1(\Gamma_1)}{L}, \frac{k_1(\Gamma_2)}{1-L}\right). \tag{6.10}$$

We consider the right-hand side of (6.10) as a function of  $L$ . The minimal value of this function is  $k_1(\Gamma_1) + k_1(\Gamma_2)$  and it is obtained at  $L = \frac{k_1(\Gamma_1)}{k_1(\Gamma_1) + k_1(\Gamma_2)}$ , which proves (6.7). In addition, as the minimal value of this function is unique, it also proves that condition (1) is necessary for equality in (6.7) to hold. From now on we assume throughout the proof that condition (1) of the proposition is satisfied, so that  $k_1(\tilde{\Gamma}_1) = k_1(\tilde{\Gamma}_2)$ .

Next, we examine two ranges of  $\theta_1^{SG}, \theta_2^{SG}$  values and show those values make the inequality in (6.7) strict.

1.  $\theta_1^{SG} > \pi$  and  $\theta_1^{SG} > \pi$ .

By (6.6) we have  $k_0(\tilde{\Gamma}_i; \pi) < k_1(\tilde{\Gamma}_i; 0)$  for both  $i = 1, 2$ . Assume first that  $k_0(\tilde{\Gamma}_1; \pi) \neq k_0(\tilde{\Gamma}_2; \pi)$  and without loss of generality that  $k_0(\tilde{\Gamma}_1; \pi) > k_0(\tilde{\Gamma}_2; \pi)$ .

Examine the function

$$h(\theta) := \begin{cases} k_0(\tilde{\Gamma}_1; \theta) - k_1(\tilde{\Gamma}_2; -\theta) & \theta \in [0, \pi) \\ k_0(\tilde{\Gamma}_1; \pi) - k_0(\tilde{\Gamma}_2; \pi) & \theta = \pi. \end{cases} \tag{6.11}$$

By Lemma B.4 we have that  $h$  is a continuous non-decreasing function. In addition,  $h(0) = -k_1(\tilde{\Gamma}_2; 0) < 0$  and by the assumption  $k_0(\tilde{\Gamma}_1; \pi) > k_0(\tilde{\Gamma}_2; \pi)$  we have  $h(\pi) > 0$ . Hence,  $h$  vanishes at some value  $\tilde{\theta} \in (0, \pi)$ , so that we find

$$k_0(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\tilde{\Gamma}_2; -\tilde{\theta}). \tag{6.12}$$

Denote by  $\tilde{f}_1$  the eigenfunction corresponding to  $k_0(\tilde{\Gamma}_1; \tilde{\theta})$  and by  $\tilde{f}_2$  the eigenfunction corresponding to  $k_1(\tilde{\Gamma}_2; -\tilde{\theta})$ . We use  $\tilde{f}_1, \tilde{f}_2$  to construct an eigenfunction on the whole of  $\Gamma$  as follows. First, notice that for both  $i = 1, 2$ ,  $\tilde{f}_i(v_i) \neq 0$ . Assuming otherwise, we obtain that  $\tilde{f}_i$  obeys Dirichlet condition at  $v_i$  and as  $\tilde{\theta} \neq \pi$  we get that  $\tilde{f}_i$  obeys Neumann conditions as

well at  $v_i$ . Since  $\tilde{\theta} < \theta_i^{SG}$ , the corresponding eigenvalue is strictly lower than the spectral gap. As  $\tilde{f}_i(v_i) \neq 0$  for  $i = 1, 2$ , we may normalize the  $\tilde{f}_i$ 's so that  $\tilde{f}_1(v_1) = \tilde{f}_2(v_2)$ . Now form an eigenfunction  $f$  on  $\Gamma$  by setting

$$f(x) := \begin{cases} \tilde{f}_1(x) & x \in \tilde{\Gamma}_1, \\ \tilde{f}_2(x) & x \in \tilde{\Gamma}_2. \end{cases} \tag{6.13}$$

where we consider  $\tilde{\Gamma}_1, \tilde{\Gamma}_2$  as subgraphs of  $\Gamma$ . The normalization  $\tilde{f}_1(v_1) = \tilde{f}_2(v_2)$  gives that  $f$  is continuous at the glued vertex  $v$ . In addition, its sum of derivatives there equals

$$\sum_{e \in \mathcal{E}_{v_1}} \tilde{f}'_1|_e(v_1) + \sum_{e \in \mathcal{E}_{v_2}} \tilde{f}'_2|_e(v_2) = \tan\left(\frac{\tilde{\theta}}{2}\right) \tilde{f}_1(v_1) + \tan\left(\frac{-\tilde{\theta}}{2}\right) \tilde{f}_2(v_2) = 0. \tag{6.14}$$

We conclude that  $f$  is a Neumann eigenfunction on  $\Gamma$  whose eigenvalue equals  $k_0(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\tilde{\Gamma}_2; -\tilde{\theta})$ . However, this eigenvalue is strictly smaller than  $k_1(\tilde{\Gamma}_i)$ , for both  $i = 1, 2$ , as shows the following chain of inequalities

$$k_0(\tilde{\Gamma}_1; \tilde{\theta}) \leq k_0(\tilde{\Gamma}_1; \pi) < k_1(\tilde{\Gamma}_1; 0) = k_1(\tilde{\Gamma}_2; 0), \tag{6.15}$$

where the first inequality is due to eigenvalue monotonicity, the second is by (6.6) and the last equality results since our current working assumption is the validity of condition (1), as discussed above. Therefore, we have found an eigenvalue of  $\Gamma$  strictly smaller than both  $k_1(\tilde{\Gamma}_i)$ , so that there is a strict inequality in (6.10) and therefore strict inequality in (6.7).

We now assume  $k_0(\tilde{\Gamma}_1; \pi) = k_0(\tilde{\Gamma}_2; \pi)$ . Denote by  $\tilde{f}_1, \tilde{f}_2$  as above the corresponding eigenfunctions. By (6.6)  $k_0(\tilde{\Gamma}_i; \pi) < k_1(\tilde{\Gamma}_i; 0)$  for both  $i = 1, 2$  and therefore  $\tilde{f}_i$  does not obey Neumann conditions at  $v_i$  (as otherwise, its eigenvalue would be the spectral gap). Using that the sum of derivatives of  $\tilde{f}_i$  at  $v_i$  differs from zero, we may normalize both  $\tilde{f}_1, \tilde{f}_2$  so that their sums of derivatives are opposite. Now, constructing a function  $f$  on  $\Gamma$  as in (6.13) shows just as above (see (6.15) and the argument which follows) that inequality (6.10) is strict in this case as well. We conclude that the inequality in (6.7) is strict if  $\theta_1^{SG} > \pi$  and  $\theta_1^{SG} > \pi$ .

- 2.  $\theta_1^{SG} + \theta_2^{SG} > 2\pi$  and  $\{\theta_1^{SG} \leq \pi < \theta_2^{SG} \text{ or } \theta_2^{SG} \leq \pi < \theta_1^{SG}\}$ .

Assume without loss of generality that  $\theta_1^{SG} < \theta_2^{SG}$ . We have the following chain of inequalities

$$k_0(\tilde{\Gamma}_2; \pi) < k_1(\tilde{\Gamma}_2; 0) = k_1(\tilde{\Gamma}_1; 0) = k_0(\tilde{\Gamma}_1; \pi), \tag{6.16}$$

where the first inequality comes from (6.6) (keeping in mind that  $\theta_2^{SG} > \pi$ ), the first equality is our working assumption (assuming the validity of condition (1)) and the second equality comes from (6.5) (keeping in mind that  $\theta_1^{SG} \leq \pi$ ). Therefore, defining the function  $h$  as in (6.11) we find that  $h(0) < 0$  and  $h(\pi) > 0$ . As before we conclude that  $h$  vanishes for some value  $\tilde{\theta} \in (0, \pi)$  and hence  $k_0(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\tilde{\Gamma}_2; -\tilde{\theta})$ . Similarly

to the previous case, we may use this equality to construct a Neumann eigenfunction on  $\Gamma$  whose eigenvalue equals  $k_0(\tilde{\Gamma}_1; \tilde{\theta})$  and to show that strict inequality happens in (6.7) for this case.

Notice that condition (2) of the proposition forms the complement of the two cases examined above. Therefore, we have proven so far that this condition is necessary for the equality in (6.7) to hold. We proceed to show that conditions (1), (2) are sufficient as well. Recall that assuming condition (1) implies  $k_1(\tilde{\Gamma}_1; 0) = k_1(\tilde{\Gamma}_2; 0)$ . We further assume by contradiction that  $k_1(\Gamma) < k_1(\tilde{\Gamma}_1; 0)$ , and consider the following two cases for the  $\theta_1^{SG}, \theta_2^{SG}$  values:

1.  $\theta_1^{SG} \leq \pi$  and  $\theta_2^{SG} \leq \pi$ .

First, we note that by (6.5) we have  $k_1(\tilde{\Gamma}_i; 0) = k_0(\tilde{\Gamma}_i; \pi)$  for both  $i = 1, 2$ .

Let  $f$  be the eigenfunction corresponding to  $k_1(\Gamma)$ . Denote  $\tilde{f}_i = f|_{\tilde{\Gamma}_i}$  for  $i = 1, 2$ . We find that there exists some  $\tilde{\theta}$  such that  $k_{n_1}(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\Gamma)$ , for some  $n_1$ . We cannot have  $\tilde{\theta} = \pi$ , as otherwise we get

$$k_{n_1}(\tilde{\Gamma}_1; \pi) = k_1(\Gamma) < k_1(\tilde{\Gamma}_1; 0) = k_0(\tilde{\Gamma}_1; \pi) \tag{6.17}$$

and contradiction. We find that as  $\tilde{f}_1$  satisfies the  $\delta$ -type condition at  $v_1$  with the parameter  $\tilde{\theta}$ ,  $\tilde{f}_2$  satisfies the  $\delta$ -type condition at  $v_2$  with the parameter  $-\tilde{\theta}$  (since the total sum of derivatives is zero and see (6.14)). Assume without loss of generality that  $\tilde{\theta} > 0$ . We get that

$$k_{n_2}(\tilde{\Gamma}_2; -\tilde{\theta}) = k_1(\Gamma) < k_1(\tilde{\Gamma}_2; 0), \tag{6.18}$$

which implies either  $n_2 = 0$  or  $n_2 = 1$ . We rule out  $n_2 = 0$  as it renders the left-hand side of (6.18) negative, while  $k_1(\Gamma) > 0$ . We also rule out  $n_2 = 1$ , as by (6.5) the left- and right-hand sides of (6.18) are equal. Hence, in this case, we get a contradiction to the assumption  $k_1(\Gamma) < k_1(\tilde{\Gamma}_1; 0)$ .

2.  $\theta_1^{SG} + \theta_2^{SG} \leq 2\pi$  and  $\{\theta_1^{SG} \leq \pi < \theta_2^{SG}$  or  $\theta_2^{SG} \leq \pi < \theta_1^{SG}\}$ .

We repeat the construction of  $\tilde{f}_1, \tilde{f}_2$  as in the previous case to get that there exists some  $\tilde{\theta} \neq \pi$  such that  $k_{n_1}(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\Gamma)$ , for some  $n_1$  and  $k_{n_2}(\tilde{\Gamma}_2; -\tilde{\theta}) = k_1(\Gamma)$ , for some  $n_2$ . Assume without loss of generality  $\theta_1^{SG} < \theta_2^{SG}$ . Combining

$$k_{n_1}(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\Gamma) < k_1(\tilde{\Gamma}_1; 0) \tag{6.19}$$

with (6.5) shows that  $n_1 = 0$  and  $0 < \tilde{\theta} < \theta_1^{SG}$ . Similarly, we have for  $\tilde{\Gamma}_2$ ,

$$k_{n_2}(\tilde{\Gamma}_2; -\tilde{\theta}) = k_1(\Gamma) < k_1(\tilde{\Gamma}_2; 0), \tag{6.20}$$

where the positivity of the left-hand side implies  $n_2 = 1$ . Together with (6.6) we get  $-\tilde{\theta} < \theta_2^{SG} - 2\pi$ . Combining that with  $\tilde{\theta} < \theta_1^{SG}$  gives  $\theta_1^{SG} + \theta_2^{SG} > 2\pi$  and contradiction to the assumption in this case.

Thus, we have shown that conditions (1), (2) of the proposition are also sufficient for equality in (6.7) to hold.



Finally, we show the necessity of conditions (a), (b) of the proposition. We have seen that necessary conditions for equality in (6.7) are  $\{\theta_1^{SG} \leq \pi$  and  $\theta_2^{SG} \leq \pi\}$  or  $\{\theta_1^{SG} + \theta_2^{SG} \leq 2\pi$  and  $\{\theta_1^{SG} \leq \pi < \theta_2^{SG}$  or  $\theta_2^{SG} \leq \pi < \theta_1^{SG}\}$ . Under those conditions we have both  $\theta_1^{SG} \neq 2\pi$  and  $\theta_2^{SG} \neq 2\pi$  and by Lemma 6.3, (3) we get  $k_1(\tilde{\Gamma}_i) \in \Delta(\tilde{\Gamma}_i)$  for both  $i = 1, 2$ , which is condition (a). Now, in order to show that  $k_1(\Gamma)$  is a non-simple eigenvalue we construct two linearly independent eigenfunctions. As  $k_1(\tilde{\Gamma}_i) \in \Delta(\tilde{\Gamma}_i)$ , by Lemma B.5 there exists an eigenfunction corresponding to  $k_1(\tilde{\Gamma}_i)$  which vanishes at  $v_i$  and its sum of derivatives vanishes there as well. Extend this function to an eigenfunction of  $\Gamma$ , whose eigenvalue is  $k_1(\tilde{\Gamma}_i) = k_1(\Gamma)$  by setting it to be equal zero on the complementary subgraph,  $\tilde{\Gamma}_{3-i}$ . Performing this for both  $i = 1$  and  $i = 2$  we get two linearly independent eigenfunctions on  $\Gamma$ , which shows the necessity of condition (b).  $\square$

We use Proposition 6.5 to study the supremizers of graphs whose vertex connectivity equals one. Let  $\mathcal{G}$  be such a graph which is obtained by taking two graphs  $\mathcal{G}_1, \mathcal{G}_2$  and identifying two of their vertices  $v_1, v_2$ . An immediate guess is that a supremizer of  $\mathcal{G}$  may be obtained by taking the supremizers of  $\mathcal{G}_1, \mathcal{G}_2$  and identifying their vertices corresponding to  $v_1, v_2$ . This holds under some conditions, as stated in Theorem 2.6 and proved below.

*Proof of Theorem 2.6.* We start by formulating the Dirichlet criterion in terms of the SGP,  $\theta^{SG}$ , used in the conditions of Proposition 6.5. Let  $\Gamma$  be a graph which obeys the Dirichlet criterion. This means that  $k_0(\Gamma; \pi) = k_1(\Gamma; 0)$  and by Lemma 6.3 we deduce  $\theta^{SG} \leq \pi$ . Hence, condition (3) of Theorem 2.6 implies condition (2) of Proposition 6.5.

Assuming conditions (1), (3) of the theorem we may now apply Proposition 6.5 and get

$$k_1(\Gamma) = k_1(\Gamma_1) + k_1(\Gamma_2). \tag{6.21}$$

Let  $\hat{\Gamma}$  be a supremizer of  $\mathcal{G}$ . In particular,  $k_1(\Gamma) \leq k_1(\hat{\Gamma})$ . Denote by  $\hat{\Gamma}_1, \hat{\Gamma}_2$  the subgraphs of  $\hat{\Gamma}$  corresponding to  $\mathcal{G}_1, \mathcal{G}_2$  and rescaled such that the total length of each of them equals 1. By Proposition 6.5

$$k_1(\hat{\Gamma}) \leq k_1(\hat{\Gamma}_1) + k_1(\hat{\Gamma}_2). \tag{6.22}$$

Hence, we get

$$k_1(\hat{\Gamma}) \leq k_1(\hat{\Gamma}_1) + k_1(\hat{\Gamma}_2) \leq k_1(\Gamma_1) + k_1(\Gamma_2) = k_1(\Gamma), \tag{6.23}$$

where the second inequality holds as  $\Gamma_1, \Gamma_2$  are supremizers. We therefore get that  $k_1(\Gamma) = k_1(\hat{\Gamma})$ , so that  $\Gamma$  is a supremizer of  $\mathcal{G}$  as  $\hat{\Gamma}$  is a supremizer of  $\mathcal{G}$  (and possibly  $\Gamma = \hat{\Gamma}$ ).

We now further assume that either for both  $i = 1, 2$   $\Gamma_i$  is the unique supremizer of  $\mathcal{G}_i$  or that both  $\Gamma_1, \Gamma_2$  obey the strong Dirichlet criterion and any other supremizer violates the Dirichlet criterion. Assume that  $\hat{\Gamma}$  is a supremizer of  $\mathcal{G}$  so that  $k_1(\Gamma) = k_1(\hat{\Gamma})$ . From (6.21), (6.22) we get

$$k_1(\Gamma_1) + k_1(\Gamma_2) \leq k_1(\hat{\Gamma}_1) + k_1(\hat{\Gamma}_2). \tag{6.24}$$

As  $\Gamma_1, \Gamma_2$  are supremizers of  $\mathcal{G}_1, \mathcal{G}_2$ , we have an equality in (6.24) and get that for both  $i = 1, 2$ ,  $k_1(\Gamma_i) = k_1(\hat{\Gamma}_i)$ , so that  $\hat{\Gamma}_1, \hat{\Gamma}_2$  are supremizers of  $\mathcal{G}_1, \mathcal{G}_2$  as well. If both  $\Gamma_1, \Gamma_2$  are unique supremizers of  $\mathcal{G}_1, \mathcal{G}_2$  then  $\Gamma_i = \hat{\Gamma}_i$  for both  $i = 1, 2$ . Hence,  $\hat{\Gamma} = \Gamma$ .

We carry on by assuming that both  $\Gamma_1, \Gamma_2$  obey the strong Dirichlet criterion and any other supremizer violates the Dirichlet criterion. From Lemma 6.3 we deduce that a graph violates the Dirichlet criterion if and only if its spectral gap parameter satisfies  $\theta^{SG} \in (\pi, 2\pi]$ . If for both  $i = 1, 2$ ,  $\hat{\Gamma}_i$  is different than  $\Gamma_i$ , then we have  $\theta_1^{SG}, \theta_2^{SG} \in (\pi, 2\pi]$  and by Proposition 6.5 we have the strict inequality

$$k_1(\hat{\Gamma}) < k_1(\hat{\Gamma}_1) + k_1(\hat{\Gamma}_2), \tag{6.25}$$

which together with

$$k_1(\hat{\Gamma}_1) + k_1(\hat{\Gamma}_2) = k_1(\Gamma_1) + k_1(\Gamma_2) = k_1(\Gamma) \tag{6.26}$$

contradicts  $\hat{\Gamma}$  being a supremizer. From Lemma 6.6 which follows this proof we deduce that a graph obeys the strong Dirichlet criterion if and only if its SGP equals  $\pi$ . Therefore, if  $\hat{\Gamma}_i = \Gamma_i$  for either  $i = 1$  or  $i = 2$ , say  $\hat{\Gamma}_1 = \Gamma_1$ , then we have  $\theta_1^{SG} = \pi$  and  $\theta_2^{SG} \in (\pi, 2\pi]$  and once again we get by Proposition 6.5 the inequality (6.25) which contradicts  $\hat{\Gamma}$  being a supremizer.  $\square$

**Lemma 6.6.** *Let  $k \in \Delta(\Gamma)$ . Let  $n \in \mathbb{N}$  and  $\theta \in (-\pi, \pi]$  such that  $k = K(\theta + 2n\pi)$ . Assume that  $k$  has multiplicity  $m + 1$  in the spectrum  $\sigma(\Gamma; \theta)$ . Then, for any  $\theta' \neq \theta$ ,  $k$  has a multiplicity  $m$  as an eigenvalue in the spectrum  $\sigma(\Gamma; \theta')$ .*

*Proof.* Since  $\Delta(\Gamma)$  is a discrete set, for  $k' < k$  sufficiently close to  $k$ ,  $k'$  does not belong to  $\Delta(\Gamma)$ . Thus, for  $\theta' < \theta$  sufficiently close to  $\theta$ ,  $K(\theta' + 2n\pi)$  is not in  $\Delta(\Gamma)$ . We define  $a \in \mathbb{N}$  as the unique integer satisfying  $K(\theta' + 2n\pi) = k_a(\Gamma, \theta')$  for all  $\theta' < \theta$  sufficiently close to  $\theta$ . Since  $K(\cdot + 2n\pi)$  and  $k(\Gamma, \cdot)$  are continuous functions of their arguments (see Lemmas 6.1 and B.4), letting  $\theta'$  go to  $\theta$  gives

$$k = k_a(\Gamma, \theta). \tag{6.27}$$

If  $\theta \neq \pi$ , we may argue similarly with  $\theta' > \theta$  sufficiently close to  $\theta$  to find that

$$k = k_b(\Gamma, \theta) < k_b(\Gamma, \theta'). \tag{6.28}$$

Notice that since  $a$  and  $b$  are, respectively, minimal and maximal integers such that  $k = k_a(\Gamma, \theta) = k_b(\Gamma, \theta)$ , the multiplicity assumption on  $k$  in  $\sigma(\Gamma; \theta)$  entails  $b = a + m$ . As  $K$  is strictly increasing and by Lemma B.2, we get

$$\begin{aligned} \forall \theta' \in (-\pi, \theta), \quad k_a(\Gamma; \theta') < k = k_{a+1}(\Gamma; \theta') \\ = \dots = k_b(\Gamma; \theta') < k_{b+1}(\Gamma; \theta') \end{aligned} \tag{6.29}$$

and

$$\begin{aligned} \forall \theta' \in (\theta, \pi], \quad k_{a-1}(\Gamma; \theta') < k = k_a(\Gamma; \theta') \\ = \dots = k_{b-1}(\Gamma; \theta') < k_b(\Gamma; \theta'). \end{aligned} \tag{6.30}$$

We conclude from these inequalities that  $k$  has multiplicity  $m$  in  $\sigma(\Gamma; \theta')$  for all  $\theta' \neq \theta$ .

If  $\theta = \pi$ , we have

$$\forall \theta' \neq \pi, \quad k = k_b(\Gamma, \pi) < k_{b+1}(\Gamma, \theta'), \tag{6.31}$$

and once again

$$\begin{aligned} \forall \theta' \neq \pi, \quad k_a(\Gamma; \theta') < k = k_{a+1}(\Gamma; \theta') \\ = \dots = k_b(\Gamma; \theta') < k_{b+1}(\Gamma; \theta'), \end{aligned} \tag{6.32}$$

from which the result follows. □

### 7. Symmetrization of Dangling Edges and Loops

**Proposition 7.1.** *Let  $\mathcal{G}$  be a graph with  $E \geq 3$  edges. Let  $v$  be a vertex of  $\mathcal{G}$  and  $e_1, e_2$  either two dangling edges or two loops connected to  $v$ . Let  $l_1, l_2$  be the lengths of those edges and denote their average by  $\ell := \frac{1}{2}(l_1 + l_2)$ .*

*Denoting  $\tilde{\Gamma} := \Gamma(\mathcal{G}; (l_1, l_2, l_3, \dots, l_E))$ ,  $\Gamma := \Gamma(\mathcal{G}; (\ell, \ell, l_3, \dots, l_E))$ , we have*

$$k_1(\tilde{\Gamma}) \leq k_1(\Gamma). \tag{7.1}$$

*Moreover, if either  $k_1(\Gamma) = \frac{\pi}{2\ell}$  in the dangling edges case (respectively,  $k_1(\Gamma) = \frac{\pi}{\ell}$  in the loops case) or alternatively both the following conditions are satisfied*

1.  $\Gamma$  is a supremizer of some graph.
2.  $k_1(\tilde{\Gamma})$  is a simple eigenvalue.

*then equality above holds if and only if  $l_1 = l_2$ .*

*Proof.* Let  $f$  be an eigenfunction of  $\Gamma$  corresponding to  $k_1(\Gamma)$ . The proof for both cases—dangling edges and loops—is by constructing a test function  $\tilde{f}$  on  $\tilde{\Gamma}$ , whose Rayleigh quotient obeys  $\mathcal{R}(\tilde{f}) \leq \mathcal{R}(f) = k_1(\Gamma)^2$ , from which (7.1) follows.

We start with the dangling edges case. First, we get a bound on  $k_1(\Gamma)$  using a test function,

$$g|_{e_1 \cup e_2} = \cos\left(\frac{\pi x}{2\ell}\right), \quad g|_{\Gamma \setminus (e_1 \cup e_2)} = 0, \tag{7.2}$$

where  $e_1 \cup e_2$  is considered as single interval. We have  $\mathcal{R}(g) = \left(\frac{\pi}{2\ell}\right)^2$  and hence  $k_1(\Gamma) \leq \frac{\pi}{2\ell}$ .

Assume that  $k_1(\Gamma) = \frac{\pi}{2\ell}$ . Let  $\tilde{f}$  be the following test function on  $\tilde{\Gamma}$ .

$$\tilde{f}|_{\tilde{e}_1 \cup \tilde{e}_2} = \cos\left(\frac{\pi x}{2\ell}\right), \quad \tilde{f}|_{\tilde{\Gamma} \setminus (\tilde{e}_1 \cup \tilde{e}_2)} = \tilde{f}(v), \tag{7.3}$$

where  $\tilde{f}(v)$  in the right equation is determined from the value  $\tilde{f}|_{\tilde{e}_1 \cup \tilde{e}_2}$  on the left attains at  $v$ . As  $\tilde{f}$  is not necessarily orthogonal to the constant function,

we actually take  $\tilde{f} - \langle \tilde{f} \rangle$  to be the test function, where  $\langle \tilde{f} \rangle := \int_{\tilde{\Gamma}} \tilde{f} dx$ . By Lemma C.1

$$\mathcal{R} \left( \tilde{f} - \langle \tilde{f} \rangle \right) = \frac{\left(\frac{\pi}{2\ell}\right)^2 \ell}{\ell + \left| \tilde{f}(v) \right|^2 2\ell(1 - 2\ell)} < \left(\frac{\pi}{2\ell}\right)^2 = (k_1(\Gamma))^2, \tag{7.4}$$

where we use that  $l_1 \neq l_2 \Rightarrow \tilde{f}(v) = \cos(\frac{\pi l_1}{2\ell}) \neq 0$  to get the inequality.

Next, assume  $k_1(\Gamma) < \frac{\pi}{2\ell}$  and also that  $f(v) = 0$ . Then  $f$  has to identically vanish on both  $e_1$  and  $e_2$ . We may then choose the test function  $\tilde{f} = f$  and get  $\mathcal{R}(\tilde{f}) = \mathcal{R}(f)$ , as required.

Finally, assume  $k_1(\Gamma) < \frac{\pi}{2\ell}$  and  $f(v) \neq 0$ . This results in  $f|_{e_1} = f|_{e_2}$ . Assume without loss of generality that  $l_1 < l_2$ . We define the test function  $\tilde{f}$  on  $\tilde{\Gamma}$  as follows.

$$\tilde{f}|_{\tilde{\Gamma} \setminus (\tilde{e}_1 \cup \tilde{e}_2)} = f|_{\Gamma \setminus (e_1 \cup e_2)}, \quad \tilde{f}|_{\tilde{e}_1} = f|_{e_1(0, l_1)}, \tag{7.5}$$

where  $e_1(0, l_1)$  denotes a subset of  $e_1$  in  $\Gamma$  whose origin is  $v$ . On  $\tilde{e}_2$  we set

$$\tilde{f}|_{\tilde{e}_2}(x) = \begin{cases} f|_{e_2}(x) & x \in (0, \ell) \\ f|_{e_1}(l_1 + l_2 - x) & x \in (\ell, l_2). \end{cases} \tag{7.6}$$

This is a valid continuous test function and by construction,  $\mathcal{R}(\tilde{f}) = \mathcal{R}(f)$ .

We have therefore shown inequality (7.1) and also that assuming  $k_1(\Gamma) = \frac{\pi}{2\ell}$  assures equivalence between  $l_1 = l_2$  and equality in (7.1). It is therefore left to show that under assumptions (1), (2) of the proposition,  $l_1 \neq l_2$  implies  $k_1(\tilde{\Gamma}) < k_1(\Gamma)$ . Assume by contradiction that  $l_1 \neq l_2$  and also  $k_1(\tilde{\Gamma}) = k_1(\Gamma)$ . As  $\Gamma$  is a supremizer of some graph,  $\tilde{\Gamma}$  is also a supremizer of the same graph. Since  $k_1(\tilde{\Gamma})$  is simple we deduce from Lemma 5.5 that its spectral gap is a critical value and by Lemma 5.3 we get  $\left| \frac{\partial}{\partial x_{\tilde{e}_1}} \tilde{f}(v) \right| = \left| \frac{\partial}{\partial x_{\tilde{e}_2}} \tilde{f}(v) \right|$ , where  $\tilde{f}$  is the eigenfunction corresponding to  $k_1(\tilde{\Gamma})$ . If  $\tilde{f}(v) = 0$  we get that  $\tilde{f}$  has at least three nodal domains (at least one nodal domain on each of  $\tilde{e}_1$ ,  $\tilde{e}_2$  and  $\tilde{\Gamma} \setminus \{\tilde{e}_1 \cup \tilde{e}_2\}$ ), which contradicts Courant’s nodal theorem ([3, 10, 18]). Assume without loss of generality  $\tilde{f}(v) > 0$ . As  $l_1 \neq l_2$  and as the derivative of  $\tilde{f}$  vanishes at the endpoints of  $\tilde{e}_1$ ,  $\tilde{e}_2$ , we get that at least one of  $\tilde{e}_1$ ,  $\tilde{e}_2$  should contain two nodal domains of  $\tilde{f}$ . In addition, by Courant’s bound it is not possible for both derivatives,  $\frac{\partial}{\partial x_{\tilde{e}_1}} \tilde{f}(v)$ ,  $\frac{\partial}{\partial x_{\tilde{e}_2}} \tilde{f}(v)$  to be negative as this results in a total of at least three nodal domains. If one derivative is positive and the second is negative, i.e.,  $\frac{\partial}{\partial x_{\tilde{e}_1}} \tilde{f}(v) = -\frac{\partial}{\partial x_{\tilde{e}_2}} \tilde{f}(v)$ , we get that  $f|_{\tilde{e}_1 \cup \tilde{e}_2}$  is proportional to  $\cos(\frac{\pi}{2\ell}x)$ , so that  $k_1(\tilde{\Gamma}) = \frac{\pi}{2\ell}$ , which is a contradiction, to what we have shown above [see (7.4)]. If both derivatives are positive,  $\frac{\partial}{\partial x_{\tilde{e}_1}} \tilde{f}(v) = \frac{\partial}{\partial x_{\tilde{e}_2}} \tilde{f}(v)$ , then we get contradiction as  $\langle \tilde{f} \rangle \neq 0$ . Indeed, assuming without loss of generality  $l_1 < l_2$ , the restriction of  $\tilde{f}$  on an interval of length  $l_2 - l_1$  at the end of edge  $\tilde{e}_2$  is of zero mean, but the  $\tilde{f}$ ’s restriction to the rest of the graph is positive, as  $\tilde{f}$  has only two nodal domains and therefore.

We turn to deal with the loops case. Just as above, we start by getting an upper bound on the spectral gap. Choose the following test function on  $\Gamma$

$$g|_{e_1 \cup e_2} = \cos\left(\frac{\pi x}{\ell}\right) \quad g|_{\Gamma \setminus (e_1 \cup e_2)} = 0, \tag{7.7}$$

where  $e_1 \cup e_2$  is considered as single cycle (self-intersecting itself at its middle).

In this case,  $\mathcal{R}(g) = \left(\frac{\pi}{\ell}\right)^2$  so that  $k_1(\Gamma) \leq \frac{\pi}{\ell}$ .

The proof now splits into three cases exactly as it was for the dangling edges:

1. If  $k_1(\Gamma) = \frac{\pi}{\ell}$ , we may construct a test function  $\tilde{f}$  on  $\tilde{\Gamma}$ , such that  $\mathcal{R}(\tilde{f}) \leq \mathcal{R}(f)$  and with equality only if  $l_1 = l_2$ .
2. If  $k_1(\Gamma) < \frac{\pi}{\ell}$  and  $f(v) = 0$ , we conclude that  $f$  identically vanishes on the edges  $e_1, e_2$  and we may construct a test function  $\tilde{f}$  on  $\tilde{\Gamma}$ , such that  $\mathcal{R}(\tilde{f}) = \mathcal{R}(f)$ .
3. If  $k_1(\Gamma) < \frac{\pi}{\ell}$  and  $f(v) \neq 0$ , we conclude that both  $f|_{e_1}$  and  $f|_{e_2}$  are symmetric functions and write

$$f|_{e_i} = A_i \cos(k_1(\Gamma) \cdot x), \tag{7.8}$$

for  $x \in \left(-\frac{\ell}{2}, \frac{\ell}{2}\right)$  and  $A_i \in \mathbb{R}$ . Construct a test function  $\tilde{f}$  on  $\tilde{\Gamma}$  by setting

$$\tilde{f}|_{\tilde{\Gamma} \setminus (\tilde{e}_1 \cup \tilde{e}_2)} = f|_{\Gamma \setminus (e_1 \cup e_2)}, \tag{7.9}$$

and

$$\tilde{f}|_{\tilde{e}_i}(x) = A_i \cos\left(k_1(\Gamma) \left|x - \frac{l_i - \ell}{2}\right|\right) \quad \text{for } x \in \left(-\frac{l_i}{2}, \frac{l_i}{2}\right). \tag{7.10}$$

This last relation pictorially means that if  $\tilde{e}_1$  is the shorter edge,  $\tilde{f}|_{\tilde{e}_1}$  is a symmetric function which equals  $f|_{e_1}$  up to a piece of length  $\ell - l_1$  around the middle of the edge  $e_1$  which is glued to the middle of the edge  $e_2$ . Overall,  $\tilde{f}$  has zero mean and  $\mathcal{R}(\tilde{f}) = \mathcal{R}(f)$ , as required.

Just as above, assumptions (1), (2) of the proposition together with assuming  $l_1 \neq l_2$  and  $k_1(\tilde{\Gamma}) = k_1(\Gamma)$ , enable to use Lemmata 5.3 and 5.5 together with Courant’s bound to arrive at a contradiction. □

An immediate generalization of this proposition is the following.

**Corollary 7.2.** *Let  $\mathcal{G}$  be a graph with  $E \geq 3$  edges. Let  $n \geq 2$  be an integer. Let  $v$  be a vertex of  $\mathcal{G}$  and  $e_1, \dots, e_n$  be either  $n$  dangling edges or  $n$  loops connected to  $v$ . Denote by  $l_1, \dots, l_n$  the lengths of those edges and by  $l_{n+1}, \dots, l_E$  the lengths of all other edges. Defining*

$$\ell := \frac{1}{n} \sum_{i=1}^n l_i, \tag{7.11}$$

and denoting

$$\tilde{\Gamma} := \Gamma(\mathcal{G}; (l_1, \dots, l_n, l_{n+1}, \dots, l_E)), \quad \Gamma := \Gamma(\mathcal{G}; (\ell, \dots, \ell, l_{n+1}, \dots, l_E)),$$

we have

$$k_1(\tilde{\Gamma}) \leq k_1(\Gamma). \tag{7.12}$$

Moreover, if either  $k_1(\Gamma) = \frac{\pi}{2\ell}$  in the dangling edges case (respectively,  $k_1(\Gamma) = \frac{\pi}{\ell}$  in the loops case) or alternatively both the following conditions are satisfied

1.  $\Gamma$  is a supremizer of some graph;
2.  $k_1(\tilde{\Gamma})$  is a simple eigenvalue,

then equality above holds if and only if  $l_j = \ell$ , for all  $1 \leq j \leq n$ .

*Proof.* Denote by  $\vec{L}$  the vector of lengths  $(l_1, \dots, l_n)$ , and by  $k_1(l_1, \dots, l_n)$  the corresponding spectral gap, keeping all the other  $E - n$  edge lengths fixed. Assume without loss of generality that  $l_1 \geq \dots \geq l_n$ . If  $l_1 > l_n$ , we replace these two lengths by  $\frac{1}{2}(l_1 + l_n)$  and get by Proposition 7.1 that

$$k_1(l_1, \dots, l_n) \leq k_1\left(\frac{1}{2}(l_1 + l_n), l_2, \dots, l_{n-1}, \frac{1}{2}(l_1 + l_n)\right). \tag{7.13}$$

Repeating this process infinitely many times, we get a sequence of vectors

$$\left\{ \vec{L}^{(m)} \right\}_{m=1}^{\infty} := \left\{ (l_1^{(m)}, \dots, l_n^{(m)}) \right\}_{m=1}^{\infty} \tag{7.14}$$

such that

- $l_1^{(m)} \geq \dots \geq l_n^{(m)}$  (up to reordering the lengths),
- $\frac{1}{n} \sum_{i=1}^n l_i^{(m)} = \ell$ ,
- $l_1^{(m)} - l_n^{(m)} \rightarrow 0$  as  $m \rightarrow \infty$ ,
- the sequence  $\left\{ k_1(l_1^{(m)}, \dots, l_n^{(m)}) \right\}_{m=1}^{\infty}$  is non-decreasing.

From the first three claims we deduce that,  $l_j^{(m)} \rightarrow \ell$  as  $m \rightarrow \infty$ , for any  $1 \leq j \leq n$ . Therefore, the continuity of eigenvalues with respect to edge lengths (see ‘‘Appendix A’’) gives

$$k_1(l_1^{(m)}, \dots, l_n^{(m)}) \rightarrow k_1(\ell, \dots, \ell) \text{ as } m \rightarrow \infty. \tag{7.15}$$

As the sequence  $\left\{ k_1(l_1^{(m)}, \dots, l_n^{(m)}) \right\}_{m=1}^{\infty}$  is non-decreasing it follows that

$$k_1(l_1, \dots, l_n) \leq k_1(\ell, \dots, \ell), \tag{7.16}$$

as desired.

We now turn to the strict inequality conditions. In the dangling edge case, if the spectral gap satisfies  $k_1(\ell, \dots, \ell) = \frac{\pi}{2\ell}$ , then particular eigenfunctions are given by that of the equilateral star with  $n$  edges and total length  $n\ell$ . Among them, we choose one supported only on two edges and repeat the argument given in Proposition 7.1 to deduce the strict inequality if  $l_i \neq l_j$  for some  $i \neq j$ . We argue similarly if  $k_1(\ell, \dots, \ell) = \frac{\pi}{\ell}$  in the dangling loops case. Alternatively, we may assume by contradiction that there exist  $i \neq j$  such that  $l_i \neq l_j$  and  $k_1(\tilde{\Gamma}) = k_1(\Gamma)$ . This together with assumptions (1), (2) enables to proceed exactly as in the proof of Proposition 7.1 in order to get a contradiction.  $\square$

## 8. Applications of Graph Gluing and Symmetrization

This section applies the techniques of graph gluing and edge symmetrization developed in the previous two sections in order to prove the next few corollaries.

*Proof of Corollary 2.7.* This proof is a direct application of Theorem 2.6 once we observe the following

1. The glued vertices,  $v_1, v_2$  become the central vertices of the supremizing stowers.
2. Every equilateral stower obeys the Dirichlet criterion with respect to its internal vertex, assuming the numbers of its petals and leaves obey  $E_p + E_l \geq 2$ .
3. Denoting the supremizing stowers by  $\Gamma_1, \Gamma_2$ , their spectral gaps are

$$k_1(\Gamma_i) = \frac{\pi}{2} \left( 2E_p^{(i)} + E_l^{(i)} \right). \tag{8.1}$$

4. Gluing  $\Gamma_1, \Gamma_2$  with the length parameter

$$L = \frac{k_1(\Gamma_1)}{k_1(\Gamma_1) + k_1(\Gamma_2)} = \frac{2E_p^{(1)} + E_l^{(1)}}{2E_p^{(1)} + E_l^{(1)} + 2E_p^{(2)} + E_l^{(2)}} \tag{8.2}$$

results in an equilateral stower whose all petals are of length  $\frac{2}{2E_p^{(1)} + E_l^{(1)} + 2E_p^{(2)} + E_l^{(2)}}$  and all dangling edges are of length  $\frac{1}{2E_p^{(1)} + E_l^{(1)} + 2E_p^{(2)} + E_l^{(2)}}$ . □

*Remark.* We note that an equilateral stower obeys the strong Dirichlet criterion. Therefore, by Theorem 2.6, if we assume for  $\mathcal{G}_1, \mathcal{G}_2$  that all their supremizers other than the stower violate the Dirichlet criterion, we also get uniqueness in Corollary 2.7.

*Proof of Corollary 2.8.* We show that equilateral stars and flowers (with  $E \geq 2$ ) satisfy condition (b) of Theorem 2.6, when considered as supremizers of the corresponding stowers. This allows to employ Theorem 2.6 in order to glue a star with a flower and to show the statement of the Corollary for all stowers with  $E_l \geq 2$  and  $E_p \geq 2$  (note that when gluing an equilateral flower and equilateral star according to condition (1) of Theorem 2.6, the stower obtained is equilateral). The rest of the stowers will be dealt with, at the end of the proof.

Start by noting that Theorem 2.2 implies that the statement of the corollary holds for all star graphs, which are stowers with  $E_p = 0, E_l \geq 2$ . The spectral gap of equilateral star is  $\frac{E\pi}{2}$  and it remains the same after imposing Dirichlet condition at their central vertex, so that it obeys the Dirichlet criterion. Furthermore, the multiplicity of its spectral gap is  $E - 1$  and it increases to  $E$  after imposing Dirichlet condition, so that it obeys the strong Dirichlet criterion. As equilateral stars are unique maximizers of stars, we conclude that they obey condition (b) of Theorem 2.6.

Among the flower graphs, we start with the two-petal and three-petal flowers. An easy calculation reveals that the spectral gap of a flower with two petals equals  $2\pi$ . Note that this spectral gap is independent of the edge lengths, so that this give a continuous family of (trivial) maximizers. In particular, the equilateral flower with two petals is a non-unique maximizer. Yet, this equilateral two-petal flower is the only maximizer in this family which obeys the Dirichlet criterion and it further obeys the strong Dirichlet criterion, as

we show next. Consider a two-petal flower whose edge lengths are  $l_1 \neq l_2$  and assume  $l_1 > l_2$ . Imposing Dirichlet condition at the vertex lowers the spectral gap of the graph from  $2\pi$  to  $\pi/l_1$ , so that it does not obey the Dirichlet criterion. The equilateral flower, on the other hand, maintains the spectral gap of  $2\pi$  even after imposing a Dirichlet condition at its vertex. In addition, its spectral gap with Neumann condition at the vertex is a simple eigenvalue, but once imposing Dirichlet at the vertex, the spectral gap becomes of multiplicity two. By this we have shown that the two-petal flower satisfies condition (b) of Theorem 2.6.

Let  $\Gamma$  be a flower with three petals and denote its vertex by  $v$ . Let  $\tilde{\Gamma}$  be the two-petal subgraph which consists of the largest two petals of  $\Gamma$ . Denote the total length of  $\tilde{\Gamma}$  by  $\tilde{l}$  (so that  $\tilde{l} \geq \frac{2}{3}$ ). Let  $\tilde{f}$  be the first non-constant eigenfunction on  $\tilde{\Gamma}$ . Construct the following test function on  $\Gamma$

$$f|_{\tilde{\Gamma}} = \tilde{f}, \quad f|_{\Gamma \setminus \tilde{\Gamma}} = \tilde{f}(v). \tag{8.3}$$

By Lemma C.1

$$\mathcal{R}(f - \langle f \rangle) = \frac{\left(\frac{2\pi}{\tilde{l}}\right)^2 \frac{\tilde{l}}{2}}{\frac{\tilde{l}}{2} + |\tilde{f}(v)|^2 \tilde{l} (1 - \tilde{l})} \leq \left(\frac{2\pi}{\tilde{l}}\right)^2 \leq (3\pi)^2, \tag{8.4}$$

where equality holds if and only if  $\tilde{l} = 2/3$  and  $\tilde{f}(v) = 0$ . Conversely, it is easy to show that the spectral gap of the equilateral three-petal flower equals  $3\pi$ . Hence, the equilateral three-petal graph is a unique maximizer. In addition, imposing a Dirichlet condition at the vertex maintains a spectral gap of  $3\pi$ , so that the three-petal equilateral flower obeys the Dirichlet criterion. It further obeys the strong Dirichlet criterion as the multiplicity of its spectral gap is 2 and it increases to 3 after imposing Dirichlet condition at central vertex. Therefore, a three-petal flower satisfies condition (b) of Theorem 2.6.

From the above, we may glue two flowers of those types (each either with two petals or three petals) and get a four-, five- or six-petal flower. Applying Theorem 2.6 shows that the equilateral version of each of these graphs serves as the unique maximizer. Furthermore, it is easy to show that any equilateral flower obeys the strong Dirichlet criterion (as shown for the two-petal and three-petal flower above). This together with the uniqueness of four-, five- and six-petal flowers implies that they obey condition (b) of Theorem 2.6. Repeating this gluing process as many times as needed shows that any equilateral flower is both a unique maximizer (except for  $E = 2$ ) and obeys condition (b) of Theorem 2.6 (which holds also for  $E = 2$ ).

By this, we have both proved the corollary for all stars and flowers with  $E \geq 2$  and also conclude the validity of the corollary for all stowers with  $E_l \geq 2$  and  $E_p \geq 2$ , as claimed in the beginning of this proof. It is left to treat stowers with either  $E_p = 1$  or  $E_l = 1$ . In order to do that, we state in Lemmata 8.1, 8.2, 8.3, 8.4 (which follow this proof) that the current corollary is valid for the following small stowers  $(E_p, E_l) \in \{(1, 2), (1, 3), (2, 1), (3, 1)\}$  and that in addition, the equilateral versions of those stowers all obey condition (b) of Theorem 2.6. Hence, each stower with either  $E_p = 1$  or  $E_l = 1$  may be



obtained by gluing one of those small stowers with an appropriate flower or star and applying Theorem 2.6 for such a gluing finishes the proof.  $\square$

*Remark.* We note that the proof above might have been simplified if we were after a weaker result. Namely, using the more elementary methods of Rayleigh quotient calculations one can prove the statement in the Corollary for all stowers except those with  $E_p = 1$  or  $E_l = 1$  and without the uniqueness part of the result.

*Proof of Corollary 2.9.* Let  $\mathcal{G}$  be a graph with  $E$  edges out of which  $E_l$  are leaves and  $E - E_l$  are internal edges. Let  $\underline{l} \in \mathcal{L}_{\mathcal{G}}$  and denote  $\Gamma := \Gamma(\mathcal{G}; \underline{l})$ . Identifying all internal (i.e., non-leaf) vertices of  $\Gamma$  we get a stower graph with  $E_l$  leaves and  $E - E_l$  petals which we denote by  $\tilde{\Gamma}$  and by Lemma B.3 we get

$$k_1(\Gamma) \leq k_1(\tilde{\Gamma}). \tag{8.5}$$

From Corollary 2.8 we have

$$k_1(\tilde{\Gamma}) \leq \pi \left( (E - E_l) + \frac{E_l}{2} \right) = \pi \left( E - \frac{E_l}{2} \right) \tag{8.6}$$

if  $E \geq 2$  and  $(E, E_l) \neq (2, 1)$  which are exactly the conditions in this corollary and this proves its first part.

Assuming equality in (2.2) we have equality in (8.6). If we further assume  $(E, E_l) \notin \{(2, 0), (3, 2)\}$ , we satisfy the uniqueness conditions in Corollary 2.8. Namely, we conclude that equality in (8.6) is possible only if  $\tilde{\Gamma}$  is equilateral in the stower sense: leaves are of half length than petals. We conclude that  $\Gamma$  is also equilateral in the following sense: all of its leaves are of length  $\frac{1}{2E - E_l}$  each and all the rest (inner) edges are of length  $\frac{2}{2E - E_l}$  each. We carry on by conditioning on the number of internal (i.e., non-leaf) vertices of  $\Gamma$  and keeping in mind that  $k_1(\Gamma) = \pi \left( E - \frac{E_l}{2} \right)$ .

If  $\Gamma$  has a single internal vertex then it is a stower graph and we are done. Assume that  $\Gamma$  has at least two internal vertices. Choose two such internal vertices. In the following we described a recursive process which marks some set of edges of the graphs, to be denoted by  $\mathcal{E}_0$ . Choose a path on  $\Gamma$  connecting  $v_+$  with  $v_-$  without going through graph leaves. This is possible as  $\Gamma$  is connected. Choose an arbitrary edge,  $e$ , on this path and add it to  $\mathcal{E}_0$ . Next, if  $\Gamma \setminus e$  is connected repeat the step above on  $\Gamma \setminus e$ . Namely, choose a path on  $\Gamma \setminus e$  connecting  $v_+$  and  $v_-$  not going through graph leaves (with the exception of  $v_+, v_-$  which might have now turned themselves into leaves). Repeat this process until  $\Gamma \setminus \mathcal{E}_0$  is a disconnected graph. We may then write  $\Gamma = \Gamma_+ \cup \Gamma_- \cup \mathcal{E}_0$ , where  $\Gamma_+$  is a connected subgraph of  $\Gamma$  containing  $v_+$ , and similarly for  $\Gamma_-$  and  $v_-$ . Set the following test function on  $\Gamma$ :

$$f(x) = \begin{cases} 1 & x \in \Gamma_+ \\ -1 & x \in \Gamma_- \\ \cos(k_1(\Gamma) \cdot x) & x \in e \text{ s.t. } e \in \mathcal{E}_0. \end{cases} \tag{8.7}$$

By construction, this test function is continuous. It is easy to verify by (C.2) (alternatively, by an easy extension of Lemma C.1) that  $\mathcal{R}(f) < k_1(\Gamma)$  if

$\Gamma_+ \cup \Gamma_- \neq \emptyset$ . As  $\mathcal{R}(f) < k_1(\Gamma)$  contradicts the equality in (2.2) we conclude that  $\Gamma_+ \cup \Gamma_- \neq \emptyset$ , which implies that  $\Gamma = \mathcal{E}_0$  and hence  $\Gamma$  is a mandarin graph. It is actually an equilateral mandarin, as we have shown above.  $\square$

The lemmata needed in the proof of Corollary 2.8 are now stated. Their proofs involve some technical computations and appear in “Appendix D.”

**Lemma 8.1.** *Let  $\mathcal{G}$  be a stower with  $E_p = 1$  petal and  $E_l = 2$  leaves. Then  $\mathcal{G}$  has a continuous family of maximizers whose spectral gap is  $2\pi$ . Those are all the stowers with both leaf lengths equal and not greater than  $1/4$ . Furthermore, the equilateral stower obeys condition (b) of Theorem 2.6.*

**Lemma 8.2.** *Let  $\mathcal{G}$  be a stower graph with  $E_p = 1$  petal and  $E_l = 3$  leaves. Then the equilateral stower graph is the unique maximizer of  $\mathcal{G}$ , and the corresponding spectral gap equals  $\frac{5\pi}{2}$ . Furthermore, the equilateral stower obeys condition (b) of Theorem 2.6.*

**Lemma 8.3.** *Let  $\mathcal{G}$  be a stower graph with  $E_l = 1$  and  $E_p = 2$ . Then  $\mathcal{G}$  has a unique maximizer, which is the equilateral stower graph with spectral gap equal to  $\frac{5\pi}{2}$ . Furthermore, the equilateral stower obeys condition (b) of Theorem 2.6.*

**Lemma 8.4.** *Let  $\mathcal{G}$  be a stower graph with  $E_l = 1$  and  $E_p = 3$ . Then  $\mathcal{G}$  has a unique maximizer, which is the equilateral stower graph with spectral gap equal to  $\frac{7\pi}{2}$ . Furthermore, the equilateral stower obeys condition (b) of Theorem 2.6.*

The stower with  $E_p = E_l = 1$  was not mentioned in the theorem above, as it is not maximized by the equilateral stower. Its unique supremizer is the single-loop graph ( $E_p = 1$ ,  $E_l = 0$ ), as we state in the following in order to complete the picture.

**Lemma 8.5.** *Let  $\mathcal{G}$  be a stower graph with one leaf and one petal. Then  $\mathcal{G}$  has a unique maximizer, which is the unit circle, with spectral gap equal to  $2\pi$ .*

## 9. Summary

This work investigates the problem of optimizing a graph’s spectral gap in terms of its edge lengths. We start by providing a natural formulation of this problem (Definitions 1.1, 1.2 and adjacent discussion). Our formalism allows both to state the optimization questions in utmost generality (for all graph topologies and all edge length values) and, moreover, to determine when such a question is fully answered. For example, this is the case with the infimization problem for which both the optimal bounds and all the possible infimizing topologies are found, with no more room for improvement (see the discussion which follows Theorem 2.1). Contrary to the infimization problem, we point out that the supremization problem is not solved in full generality. We show its complete solution for tree graphs and for a family of graphs whose vertex connectivity equals one. In addition, a global upper bound is provided (Corollary 2.9), improving the upper bound known so far, by taking into account the number of graph leaves. Furthermore, we provide a set of techniques to tackle

the supremization problem. Among those are the gluing graphs approach, the symmetrization of dangling edges and loops and the characterization of local maximizers. Those tools are applicable in the current work and might assist in further exploration of the problem. The techniques and the results of the current work lead to forming a few conjectures regarding the maximization problem.

First, the supremizer graph families known so far are stower graphs (including stars and flowers as particular cases) and mandarin graphs. The spectral gap of these graphs is highly degenerate due to their large symmetry groups. The symmetry groups corresponding to the stower and the mandarin are correspondingly  $S_{E_p} \times S_{E_l}$  and  $S_E$ , where  $E$  is the number of mandarin edges and  $E_p, E_l$  numbers of stower petals and leaves. The corresponding spectral gap multiplicity of both a stower and a mandarin is  $E - 1$ , which is indeed high. In the other extreme of spectral gaps which are simple eigenvalues, we show that those are unlikely to be supremizers. In Theorem 2.4 we prove that a supremizer whose spectral gap is simple can never have a spectral gap higher than a mandarin and in some cases than a flower (Corollary 5.6). In Proposition 6.5 we prove that if a supremizer is obtained by the gluing method then its spectral gap is necessarily a multiple eigenvalue. As high multiplicities of eigenvalues is related to large-order symmetry groups (or even to large dimension of their representations), the discussion above leads to the following two conjectures:

1. A supremizer of a graph is obtained by choosing edge lengths which maximize the order of the symmetry group of the resulting graph.<sup>7</sup>
2. A supremizer of a graph is obtained by choosing edge lengths which maximize the multiplicity of the spectral gap.

We note that the conjectures above are not necessarily correlated. We demonstrate this by mandarin chains, which are  $M$  copies of  $n$ -mandarin graphs glued serially, as presented in Proposition 5.8. The symmetry group of those graphs is  $(S_n)^M$  whose order is  $(n!)^M$ . Yet, a mandarin chain with  $n \geq 2$ ,  $M \geq 2$  always has a simple spectral gap, as proved in Proposition 5.8. Hence, the large order of the symmetry group does not guarantee large multiplicity of the spectral gap. Seeking for supremizers for those graphs, we observe that turning such a graph into an equilateral flower with  $m(n - 1)$  petals, increases its spectral gap from  $n\pi$  to  $M(n - 1)\pi$ . The symmetry group of this flower is  $S_{M(n-1)}$ , which is of order  $(M(n - 1))!$ . For most values of  $n, M$ , the flower's symmetry group is of larger order than that of the mandarin chain, which is correlated to its spectral gap being of higher multiplicity. However, for  $n = 3$ ,  $M = 2$ , the symmetry group of the flower is of order 24, while that of the mandarin chain is of order 36. This flower possesses a higher spectral gap ( $3\pi$ ) than the mandarin chain ( $4\pi$ ) despite its lower-order symmetry group. On the one hand, this example serves in the favor of the second conjecture over the first one. On the other hand, we still do not know what is the supremizer in this example and feel that at this stage, both conjectures are equally appealing.

<sup>7</sup> We thank Gregory Berkolaiko for raising this conjecture in a private communication.

Finally, we state a more explicit conjecture: the supremizer of a certain graph is either a stower graph (in its generalized sense) or a mandarin. These are indeed the only supremizers this work revealed. Given a certain graph, the maximal spectral gap among all stowers which may be obtained from that graph equals  $\pi(\beta + \frac{E_l}{2})$ , where  $\beta$  is the graph's first Betti number and  $E_l$  is the number of its dangling edges. The maximal spectral gap among all possible mandarins has a less explicit expression, and we describe it next. Let  $\mathcal{G}$  be a graph and let  $\mathcal{G}_1, \mathcal{G}_2$  be two connected subgraphs, sharing neither an edge nor a vertex and such that each vertex of  $\mathcal{G}$  belongs to  $\mathcal{G}_1 \cup \mathcal{G}_2$ . Let  $E(\mathcal{G}_1, \mathcal{G}_2)$  be the number of edges connecting a vertex of  $\mathcal{G}_1$  to a vertex of  $\mathcal{G}_2$ . Contracting all edges of  $\mathcal{G}_1$  and  $\mathcal{G}_2$  we get a mandarin of  $E(\mathcal{G}_1, \mathcal{G}_2)$  edges. The maximal spectral gap among all mandarins is therefore given by

$$\pi \cdot \max_{\mathcal{G}_1, \mathcal{G}_2} E(\mathcal{G}_1, \mathcal{G}_2). \quad (9.1)$$

We note that the expression above is curiously related to the Cheeger constant, but do not further elaborate on that. For the allowed  $(\mathcal{G}_1, \mathcal{G}_2)$  partitions among which we maximize we may also write  $E(\mathcal{G}_1, \mathcal{G}_2) = \beta + 1 - (\beta_1 + \beta_2)$ , where  $\beta_i$  is the first Betti number of  $\mathcal{G}_i$ . This expression allows for a comparison with the optimal stower spectral gap,  $\pi(\beta + \frac{E_l}{2})$ . For example, it is seen that for a graph with at most one dangling edge, the mandarin achieves a strictly higher spectral gap than the stower (or flower in this case) only if there is a partition where both  $\mathcal{G}_1, \mathcal{G}_2$  are tree graphs. On the other hand, if the graph has at least three dangling edges, any mandarin has a lower spectral gap than the optimal stower. Does the conjecture above hold or are there supremizers other than stowers and mandarins? This question remains open.

## Acknowledgements

We acknowledge Richard Maynes for taking part in the preliminary examination of the problem. We thank Gregory Berkolaiko and Uzy Smilansky for their stimulating feedback. We thank Adam Sawicki and his student, Oskar Słowik, for some fruitful discussions regarding graph connectivity. We thank Sebastian Egger and Lior Alon, as well as the anonymous referees for a careful reading and useful comments. R.B. was supported by ISF (Grant No. 494/14), Marie Curie Actions (Grant No. PCIG13-GA-2013-618468) and the Taub Foundation (Taub Fellow). G.L. thanks the Mathematics faculty of the Technion for their kind hospitality, without which the current collaboration would not have been possible.

## Appendix A: Eigenvalue Continuity with Respect to Edge Lengths

In this section we sketch a proof for the continuity of all the graph's eigenvalues (not only the spectral gap) with respect to the graph's edge lengths. The continuity (and even differentiability) of eigenvalues with respect to edge lengths

is proven in [5, 11]. Yet, those proofs deal only with positive edge lengths,<sup>8</sup> whereas in the current work we are interested in particular in  $l \in \partial\mathcal{L}_{\mathcal{G}}$ , when we distinguish between supremizers and maximizers (see Definition 1.2). We claim that eigenvalue continuity indeed carries over to the zero edge length case. We do not prove this in full rigor, but rather point out the general lines for forming a proof for this statement. We start by introducing the scattering approach for quantum graphs (see also [5, 17]).

### A.1. The Scattering Approach to the Graph Spectrum

Let  $\Gamma$  be a Neumann graph. The eigenvalue equation,

$$-\frac{d^2 f}{dx^2} = k^2 f(x), \quad (\text{A.1})$$

has a solution on each directed edge  $e$ , written as (assuming  $k \neq 0$ )

$$f_e(x_e) = a_e^{\text{in}} e^{-ikx_e} + a_e^{\text{out}} e^{ikx_e}. \quad (\text{A.2})$$

We may consider the edge  $\hat{e}$ , which is the same as  $e$ , but with a reverse direction (resulting in different parametrization of the coordinate,  $x_{\hat{e}} = l_e - x_e$ ) and write the same function as above in the following form

$$f_{\hat{e}}(x_{\hat{e}}) = a_{\hat{e}}^{\text{in}} e^{-ikx_{\hat{e}}} + a_{\hat{e}}^{\text{out}} e^{ikx_{\hat{e}}}. \quad (\text{A.3})$$

Comparing both expressions above we arrive at

$$a_e^{\text{in}} = e^{ikl_e} a_e^{\text{out}} \quad \text{and} \quad a_{\hat{e}}^{\text{in}} = e^{ikl_e} a_e^{\text{out}}. \quad (\text{A.4})$$

Fixing a vertex  $v$  and using the Neumann vertex conditions to relate solutions  $f_e$  for all edges whose origin is  $v$  one arrives at

$$\vec{a}_v^{\text{out}} = \sigma^{(v)} \vec{a}_v^{\text{in}}, \quad (\text{A.5})$$

where  $\vec{a}_v^{\text{out}}$  and  $\vec{a}_v^{\text{in}}$  are vectors of the outgoing and incoming coefficients ( $a_e^{\text{in}}$ ,  $a_e^{\text{out}}$ ) at  $v$  and  $\sigma^{(v)}$  is a  $d_v \times d_v$  unitary matrix,  $d_v$  being the degree of the vertex  $v$ . The matrix  $\sigma^{(v)}$  is called the vertex-scattering matrix and its entries were first calculated in [22]:

$$\sigma_{e,e'}^{(v)} = \frac{2}{d_v} - \delta_{e,e'}. \quad (\text{A.6})$$

We collect all coefficients  $a_e^{\text{in}}$  from the whole graph into a vector  $\vec{a}$  of size  $2E$  such that the first  $E$  entries correspond to edges which are the inverses of the last  $E$  entries. We can then define the matrix  $J$  acting on  $\vec{a}$  by requiring that it exchanges  $a_e^{\text{in}}$  and  $a_{\hat{e}}^{\text{in}}$  for all  $e$  such that,

$$J = \begin{pmatrix} 0 & \mathbf{I} \\ \mathbf{I} & 0 \end{pmatrix}. \quad (\text{A.7})$$

Then, collecting equations (A.5) for all vertices into one system and using (A.4) we have,

$$J e^{-ikL} \vec{a} = \Sigma \vec{a}, \quad (\text{A.8})$$

<sup>8</sup> It is possible that the proof in Sect. 4 of [11], which is based on test functions, may be adapted for the zero edge length case. Nevertheless, we provide here a different argument based on the scattering approach.

where  $L = \text{diag}\{l_1, \dots, l_E, l_1, \dots, l_E\}$  is a diagonal matrix of edge lengths and  $\Sigma$  is block-diagonalizable with individual  $\sigma^{(v)}$  as blocks. This can be rewritten as (note that  $J^{-1} = J$ ),

$$\vec{a} = e^{ikL} J \Sigma \vec{a}, \tag{A.9}$$

and hence all the nonzero eigenvalues of the graph are the solutions of

$$\det(\mathbf{I} - U(k)) = 0, \tag{A.10}$$

where  $U(k) := e^{ikL} J \Sigma$ .

**A.2. Continuity of Eigenvalues via Scattering Approach**

The scattering approach allows for a reduction in the dimensions of the matrix  $U(k)$  by reducing a subgraph into a single composite vertex with some (non-trivial) vertex conditions (see Sect. 3.3 in [17]). We pick a certain edge,  $e$ , to be the mentioned subgraph and turn it into a single (composite) vertex by shrinking it to zero length.

The length of this edge,  $l_e$ , will show up only in the scattering matrix of this composite vertex and will allow to examine how the eigenvalues depend on this length. We carry on with an explicit computation. Let  $e$  be an edge connecting two vertices,  $v_1, v_2$ , of degrees  $d_1, d_2$ . Hence, the new composite vertex,  $v$ , would be of degree  $d_1 + d_2 - 2$ . We calculate a reflection coefficient of this vertex (i.e., an on-diagonal entry of its vertex-scattering matrix). The calculation may be done by summing infinitely many trajectories on the original graph all starting by entering  $v_1$  from some edge  $e_1$  (different than  $e$ ) and eventually leaving  $v_1$  along the same edge,  $e_1$  (see section 3.3 in [17], for further details).

$$\begin{aligned} \sigma_{e_1, e_1}^{(v)} &= \frac{2 - d_1}{d_1} + \frac{2}{d_1} \cdot e^{ik2l_e} \cdot \frac{2 - d_2}{d_2} \cdot \sum_{n=0}^{\infty} \left( e^{ik2l_e} \frac{2 - d_2}{d_2} \frac{2 - d_1}{d_1} \right)^n \cdot \frac{2}{d_1} \\ &= -1 + \frac{2}{d_1} \left( 1 + \frac{4 - 2d_2}{e^{-ik2l_e} d_1 d_2 - (2 - d_1)(2 - d_2)} \right) \\ &\xrightarrow{l_e \rightarrow 0} -1 + \frac{2}{d_1 + d_2 - 2}. \end{aligned} \tag{A.11}$$

where the continuity of the expression above in  $l_e$  is apparent and allows to take the limit  $l_e \rightarrow 0$ . We calculate just another entry of the composite vertex-scattering matrix—the entry which corresponds to entering at vertex  $v_1$  and leaving at  $v_2$ . The calculation is similar to the one above and gives

$$\begin{aligned} \sigma_{e_1, e_2}^{(v)} &= \frac{2}{d_1} \cdot e^{ikl_e} \cdot \sum_{n=0}^{\infty} \left( e^{ik2l_e} \frac{2 - d_2}{d_2} \frac{2 - d_1}{d_1} \right)^n \cdot \frac{2}{d_2} \\ &= \frac{4}{e^{-ikl_e} d_1 d_2 - e^{ikl_e} (2 - d_1)(2 - d_2)} \xrightarrow{l_e \rightarrow 0} \frac{2}{d_1 + d_2 - 2}. \end{aligned} \tag{A.12}$$

There is just another computation which is similar in nature and will not be repeated here. All the rest of the composite vertex-scattering matrix entries may be obtained by symmetry. We hence get that the resulting scattering matrix when taking the limit  $l_e \rightarrow 0$  is the same as the one obtained by

considering Neumann conditions at the composite vertex. As the scattering matrix continuously determines the graph’s eigenvalues (see (A.10)) we get the desired continuity result.

### Appendix B: $\delta$ -Type Conditions and Interlacing Theorems

We present here the so-called  $\delta$ -type conditions, of which both Neumann and Dirichlet conditions form special cases.

**Definition B.1.** We say that  $f$  satisfies the  $\delta$ -type condition with the coefficient  $\alpha \in \mathbb{R}$  at vertex  $v$  if

1.  $f$  is continuous at  $v$ :

$$f_{e_1}(v) = f_{e_2}(v), \tag{B.1}$$

for all edges  $e_1, e_2 \in \mathcal{E}_v$ , where  $\mathcal{E}_v$  is the set of edges incident to  $v$ .

2. The derivatives of  $f$  at  $v$  satisfy

$$\sum_{e \in \mathcal{E}_v} \frac{df}{dx_e}(v) = \alpha f(v). \tag{B.2}$$

We consider the following transformations

$$\alpha \mapsto \theta = \arg \left( \frac{i + \alpha}{i - \alpha} \right), \tag{B.3}$$

and

$$\theta \mapsto \alpha = i \frac{1 - \exp(i\theta)}{1 + \exp(i\theta)} = \tan \left( \frac{\theta}{2} \right). \tag{B.4}$$

The transformations (B.3), (B.4) are the inverses one of the other and allow to write the condition (B.2) in the form (6.1), which is the one used throughout the paper. We denote by  $k_n(\Gamma; \theta)$  the  $n^{\text{th}}$   $k$ -eigenvalue of such a graph and possibly omit either  $\Gamma$  or  $\theta$  from this notation whenever it is clear what they are from the context. Similarly, the spectrum is denoted  $\sigma(\Gamma; \theta)$  (see (6.2)).

We quote below some useful results from [5] as lemmata.

The following lemma is a slight rephrasing of Theorem 3.1.8 from [5].

**Lemma B.2.** *Let  $\Gamma$  be a compact (not necessarily connected) graph. Let  $v$  be a vertex of  $\Gamma$  endowed with the  $\delta$ -type condition and arbitrary self-adjoint vertex conditions at all other vertices of  $\Gamma$ . If  $-\pi < \theta < \theta' \leq \pi$ , then*

$$k_n(\theta) \leq k_n(\theta') \leq k_{n+1}(\theta). \tag{B.5}$$

*If the eigenvalue  $k_n(\theta')$  is simple and its eigenfunction  $f$  is such that either  $f(v)$  or  $\sum f'(v)$  is nonzero, then the inequalities above are strict,*

$$k_n(\theta) < k_n(\theta') < k_{n+1}(\theta). \tag{B.6}$$

The following lemma is a slight rephrasing of Theorem 3.1.10 from [5].

**Lemma B.3.** *Let  $\Gamma$  be a compact (not necessarily connected) graph. Let  $v_1$  and  $v_2$  be vertices of  $\Gamma$  endowed with the  $\delta$ -type conditions with corresponding coefficients  $\alpha_1, \alpha_2$  and arbitrary self-adjoint vertex conditions at all other vertices of  $\Gamma$ . Let  $\Gamma'$  be the graph obtained from  $\Gamma$  by gluing the vertices  $v_1$  and  $v_2$  together into a single vertex  $v$ , so that  $\mathcal{E}_v = \mathcal{E}_{v_1} \cup \mathcal{E}_{v_2}$  and endowed with  $\delta$ -type condition at  $v$ , with the coefficient  $\alpha_1 + \alpha_2$ .*

*Then the eigenvalues of the two graphs satisfy the inequalities*

$$k_n(\Gamma) \leq k_n(\Gamma') \leq k_{n+1}(\Gamma). \tag{B.7}$$

*We apply the lemma above in the case  $\alpha_1 = -\alpha_2$ , for which  $\Gamma'$  satisfies Neumann conditions at  $v$ .*

The following lemma is a rephrasing of part of lemma 3.1.14 from [5] and the discussion which precedes it.

**Lemma B.4.**  *$k_n(\theta)$  is a continuous non-decreasing function of  $\theta \in (-\pi, \pi]$  and obeys the following continuity relation*

$$k_n(\pi) = \lim_{\theta \rightarrow -\pi^+} k_{n+1}(\theta). \tag{B.8}$$

The following lemma contains a statement which is proved in the course of the proof of Lemma 3.1.15 in [5]. We state here the lemma we need and its proof for completeness.

**Lemma B.5.** *Let  $\Gamma$  be a graph and let  $v$  be a vertex of  $\Gamma$ . Let  $\theta_1 \neq \theta_2$  and let  $k \in \sigma(\Gamma; \theta_1) \cap \sigma(\Gamma; \theta_2)$ . Then there exists an eigenfunction corresponding to  $k$  which vanishes at  $v$  and its sum of derivatives vanish at  $v$ . Therefore, this eigenfunction satisfies the  $\delta$ -type condition at  $v$  for every  $\theta \in (-\pi, \pi]$ . Hence,  $k \in \Delta(\Gamma)$ .*

*Proof.* Let  $f_1, f_2$  the eigenfunctions corresponding to  $k \in \sigma(\Gamma; \theta_1) \cap \sigma(\Gamma; \theta_2)$ , with coefficients  $\theta_1, \theta_2$ , respectively. Assume first that either  $k \in \sigma(\Gamma; \theta_1)$  or  $k \in \sigma(\Gamma; \theta_2)$  is a multiple eigenvalue. Assume without loss of generality that it is  $k \in \sigma(\Gamma; \theta_1)$ . Further assume that  $\theta_1 \neq \pi$ . As the eigenvalue is multiple, we can choose a corresponding eigenfunction which vanishes at  $v$  and denote it by  $f_1$ . We deduce from the  $\delta$ -type condition that the sum of derivatives of  $f_1$  at  $v$  vanishes as well and conclude that  $f_1$  satisfies  $\delta$ -type condition at  $v$  for any value of  $\theta$ . If we assume  $\theta_1 = \pi$ , then we may use the multiplicity of the eigenvalue to choose an eigenfunction  $f_1$  whose sum of derivatives at  $v$  vanishes and once again conclude that  $f_1$  satisfies  $\delta$ -type condition at  $v$  for any value of  $\theta$ . We have shown that the lemma holds if one of the eigenvalues is multiple. Otherwise, assume that  $k \in \sigma(\Gamma; \theta_1)$  and  $k \in \sigma(\Gamma; \theta_2)$  are simple eigenvalues. Assume without loss of generality that  $\theta_1 \neq \pi$ . Let  $f_1$  be the eigenfunction corresponding to  $k$  and satisfying the  $\delta$ -type condition with  $\theta_1$ . If  $f_1(v) \neq 0$ , then the strict eigenvalue interlacing (Lemma B.2) contradicts  $k \in \sigma(\Gamma; \theta_1) \cap \sigma(\Gamma; \theta_2)$ . Therefore,  $f_1(v) = 0$  and the sum of derivatives of  $f_1$  vanishes at  $v$ , due to the  $\delta$ -type condition.  $\square$



### Appendix C: A Basic Rayleigh Quotient Computation

In the current section, we develop a basic but useful bound on the Rayleigh quotient, which is used throughout the paper. We define the mean of a function on a graph as

$$\langle f \rangle := \int_{\Gamma} f \, dx, \tag{C.1}$$

and observe that

$$\mathcal{R}(f - \langle f \rangle) = \frac{\int_{\Gamma} |f'|^2 \, dx}{\int_{\Gamma} f^2 \, dx - \langle f \rangle^2}, \tag{C.2}$$

which is useful as the test functions for which the Rayleigh quotient is computed ought to be of zero mean.

**Lemma C.1.** *Let  $\Gamma$  be a graph of length 1. Assume that  $\Gamma = \Gamma_1 \cup \Gamma_2$  where  $\Gamma_{1,2}$  are subgraphs of  $\Gamma$  such that  $\Gamma_1 \cap \Gamma_2$  is a single vertex, denoted by  $v$ . Choose an eigenfunction  $f$  on  $\Gamma_1$  corresponding to  $k_1(\Gamma_1)$  and extend it to  $\Gamma_2$  by the constant  $f(v)$ . The resulting test function on  $\Gamma$ , denoted  $\tilde{f}$ , satisfies*

$$\mathcal{R}(\tilde{f} - \langle \tilde{f} \rangle) = \frac{k_1(\Gamma_1)^2 \left( \int_{\Gamma_1} f^2 \, dx \right)}{\left( \int_{\Gamma_1} f^2 \, dx \right) + |f(v)|^2 l_2 (1 - l_2)}, \tag{C.3}$$

where  $l_2$  denotes the total length of  $\Gamma_2$ .

*Proof.* We compute the mean and the  $L^2$  norm of  $\tilde{f}$ :

$$\langle \tilde{f} \rangle = \int_{\Gamma_2} f(v) \, dx = f(v) l_2 \tag{C.4}$$

and

$$\int_{\Gamma} |\tilde{f}|^2 \, dx = \left( \int_{\Gamma_1} f^2 \, dx \right) + \int_{\Gamma_2} |f(v)|^2 \, dx = \left( \int_{\Gamma_1} f^2 \, dx \right) + |f(v)|^2 l_2. \tag{C.5}$$

As  $\tilde{f}$  is constant on  $\Gamma_2$  and  $f$  is an eigenfunction on  $\Gamma_1$ , we have

$$\int_{\Gamma} |\tilde{f}'(x)|^2 \, dx = \int_{\Gamma_1} |f'(x)|^2 \, dx = k_1(\Gamma_1)^2 \left( \int_{\Gamma_1} f^2 \, dx \right). \tag{C.6}$$

Plugging the above in (C.2) gives the desired result. □

An immediate corollary of Lemma C.1 is the following.

**Corollary C.2.** *With the notations above we have  $k_1(\Gamma) \leq k_1(\Gamma_1)$ . This inequality is strict if there exists an eigenfunction of  $k_1(\Gamma_1)$  not vanishing at  $v$ .*

In the decomposition discussed above,  $\Gamma = \Gamma_1 \cup \Gamma_2$ , we call  $\Gamma_1$  the *main subgraph* of  $\Gamma$  and  $\Gamma_2$  the *attached subgraph*. Note that when the main subgraph is a single loop, we may rotate its eigenfunction so that it achieves its maximal value at  $v$ . We exploit this in the sequel when applying Lemma C.1, since this choice leads to a low value of the Rayleigh quotient.

### Appendix D: Proofs for Small Stowers (Lemmata 8.1–8.5)

In this more technical appendix, we extensively use Lemma C.1. Namely, we consider the decomposition  $\Gamma = \Gamma_1 \cup \Gamma_2$  and refer to  $\Gamma_{1,2}$  as either the main or the attached subgraph of  $\Gamma$  (see “Appendix C”).

*Proof of Lemma 8.1.* Let us denote by  $l_1, l_2$  and  $l_p$  the lengths of the two leaves and the petal, respectively, and by  $v$  the vertex of degree three. Denote by  $k_1(l_1, l_2, l_p)$  the spectral gap corresponding to these edge lengths. First, if  $l_1 + l_2 > \frac{1}{2}$ , we use the interval made of the two leaves as the main subgraph and the petal as the attached subgraph. We thus get, in this case, the inequality  $k_1(l_1, l_2, l_p) < 2\pi$ . Now, if  $l_1 + l_2 \leq \frac{1}{2}$  and  $l_1 = l_2$ , explicit calculations show that the spectral gap is equal to  $2\pi$ . Applying the symmetrization principle on the leaves (Proposition 7.1) shows that whenever  $l_1 + l_2 \leq \frac{1}{2}$  and  $l_1 \neq l_2$ , we have  $k_1(l_1, l_2, l_p) \leq 2\pi$ . We further wish to prove that this inequality is strict and do so by checking the assumptions in Proposition 7.1. Assumption (1) is valid as we have shown above that the stower with  $l_1 = l_2 \leq \frac{1}{4}$  is a supremizer. We now check assumption (2) that whenever  $0 \leq l_1 < l_2$  and  $l_1 + l_2 \leq \frac{1}{2}$  the corresponding spectral gap is simple. In turn, thanks to Proposition 7.1, we will get the strict inequality  $k_1(l_1, l_2, l_p) < 2\pi$  for  $l_1 \neq l_2$  and  $l_1 + l_2 \leq \frac{1}{2}$ . Assume by contradiction that there exist  $0 \leq l_1 < l_2$  with  $l_1 + l_2 \leq \frac{1}{2}$  such that the spectral gap  $k_1(l_1, l_2, l_p)$  is not simple. Thanks to the multiplicity, we may choose an eigenfunction vanishing at  $v$ . Since  $l_1 < \frac{1}{4}$ , such an eigenfunction has to vanish on the whole edge  $e_1$  for otherwise, the spectral gap would satisfy  $k_1(l_1, l_2, l_p) \geq \frac{\pi}{2l_1} > 2\pi$ . Furthermore, the eigenfunction does not identically vanish neither on  $e_2$  (again, this would contradict the bound on  $k_1$ ) nor on  $e_p$  (because of the Neumann condition at  $v$ ). Thus, there exist two integers  $\alpha, \beta$  with  $\alpha$  odd such that  $k_1(l_1, l_2, l_p) = \frac{\alpha\pi}{2l_2} = \frac{\beta\pi}{l_p}$ . From the bound on  $k_1(l_1, l_2, l_p)$  and the conditions on the lengths, we get  $\alpha = \beta = 1$ . But as  $k_1(l_1, l_2, l_p) = \frac{\pi}{2l_2}$  and  $l_1 \neq l_2$ , all eigenfunctions should vanish at  $v$ . Using again multiplicity, we may choose another eigenfunction which vanishes at  $v$  and at another point on  $e_2$ , call it  $w$ . But this contradicts the equality  $k_1(l_1, l_2, l_p) = \frac{\pi}{2l_2}$ , hence the simplicity. We have therefore found a continuous family of maximizers - all stowers with  $l_1 = l_2 \leq \frac{1}{4}$ . It is easy to check that among all those, only the equilateral stower satisfies the Dirichlet criterion. In addition, the multiplicity of the spectral gap increases from two to three when imposing the Dirichlet condition at the central vertex, which is exactly the strong Dirichlet criterion. Hence, the equilateral stower satisfies condition (b) of Theorem 2.6.  $\square$

*Proof of Lemma 8.2.* Denote by  $\Gamma$  the metric graph corresponding to  $\mathcal{G}$ , whose length of the petal is  $l_p$  and lengths of the leaves are  $l_1, l_2, l_3$  (so that  $l_p + l_1 + l_2 + l_3 = 1$ ). Assume, for instance, that  $l_1 \geq l_2 \geq l_3$  and denote  $\ell := \frac{l_1 + l_2 + l_3}{3}$ . Using the three leaves a main subgraph and the petal as an attached subgraph, we get the inequality

$$k_1(\Gamma) \leq \frac{\pi}{2\ell}. \tag{D.1}$$

On the other hand, using the petal and the longest two leaves as a main subgraph and the shortest leaf as an attached subgraph, we use Lemma 8.1 to get

$$k_1(\Gamma) \leq \frac{2\pi}{1-l_3}. \tag{D.2}$$

Combining these two inequalities,

$$k_1(\Gamma) \leq \min\left(\frac{\pi}{2\ell}, \frac{2\pi}{1-l_3}\right) \leq \min\left(\frac{\pi}{2\ell}, \frac{2\pi}{1-\ell}\right). \tag{D.3}$$

This immediately yields, for any choice of  $l_i$ ,

$$k_1(\Gamma) \leq \frac{5\pi}{2}, \tag{D.4}$$

with equality possible only if  $\ell = \frac{1}{5}$  and  $l_3 = \ell$ . These two conditions together imply  $l_1 = l_2 = l_3 = \frac{1}{5}$  and  $l_p = \frac{2}{5}$ . Conversely, for this specific choice of lengths, it is straightforward to point out the eigenfunction whose  $k$ -eigenvalue equals  $\frac{5\pi}{2}$ . Furthermore, it is also easy to check that in this case, the spectral gap indeed equals  $\frac{5\pi}{2}$ , with multiplicity three. Furthermore, imposing the Dirichlet condition at the central vertex increases the multiplicity of the spectral gap from three to four. Hence, the equilateral stower satisfies the strong Dirichlet criterion and is a unique supremizer, which proves that the equilateral stower satisfies condition (b) of Theorem 2.6.  $\square$

*Proof of Lemma 8.3.* Let us denote by  $l_1, l_2$  and  $l_l$  the lengths of the two petals and the leaf, respectively. Denote  $\ell := \frac{l_1+l_2}{2}$ . From Proposition 7.1, we have the inequality  $k_1(l_1, l_2, l_l) \leq k_1(\ell, \ell, l_l)$ . We now focus on the case where  $l_1 = l_2 = \ell$ . Let  $v$  be the central vertex of the stower. Using the two petals as a main subgraph and the leaf as an attached subgraph, we get

$$k_1(\ell, \ell, l_l) \leq \frac{2\pi}{1-l_l}. \tag{D.5}$$

Thus, for  $0 \leq l_l \leq \frac{1}{5}$ , we have  $k_1(\ell, \ell, l_l) \leq \frac{5\pi}{2}$ , with equality possible only if  $l_l = \frac{1}{5}$ . Now, using the leaf as a main subgraph and the two loops as an attached subgraph, we get

$$k_1(\ell, \ell, l_l) \leq \frac{\pi}{2l_l\sqrt{3-l_l}}. \tag{D.6}$$

In particular, we have  $k_1(\ell, \ell, l_l) < \frac{5\pi}{2}$  for  $0.26 \leq l_l \leq 1$ . To cover the remaining values of  $l_l$ , we construct the following test function. Take the function  $x \mapsto \cos(\frac{\pi x}{l_l})$  on the leaf, so that it vanishes at  $v$ . On each petal, take the function  $x \mapsto \frac{l_l}{1-l_l} \sin(\frac{2\pi x}{1-l_l})$ . Denoting the resulting function by  $h$ , we have

$$\mathcal{R}(h) = \pi^2 \frac{(1-l_l)^3 + 16l_l^3}{4l_l^2(1-l_l)^2}. \tag{D.7}$$

In particular, we have  $k_1(\ell, \ell, l_l) \leq \frac{5\pi}{2}$  for  $\frac{1}{5} \leq l_l \leq \frac{2}{5}$ , with equality possible only if  $l_l = \frac{1}{5}$ . Gathering the information given by these three test functions, we

conclude that for all  $l_i$  values we have  $k_1(\ell, \ell, l_i) \leq \frac{5\pi}{2}$ , with equality possible only if  $l_i = \frac{1}{5}$ .

Moreover, it is easy to show that  $k_1(\frac{2}{5}, \frac{2}{5}, \frac{1}{5}) = \frac{5\pi}{2}$  with multiplicity two. This multiplicity increases to three when imposing the Dirichlet condition at the central vertex, so that the equilateral stower satisfies the strong Dirichlet criterion. It only remains to show that if  $l_i = \frac{1}{5}$  and  $l_1 \neq l_2$ , we have  $k_1(l_1, l_2, l_i) < \frac{5\pi}{2}$ . This is obtained by applying Corollary C.2 to the two loops as the main subgraph and the leaf as the attached subgraph. Thus, the equilateral stower is a unique maximizer and satisfies in particular condition (b) of Theorem 2.6.  $\square$

*Proof of Lemma 8.4.* Denote by  $l_1, l_2, l_3$  and  $l_l$  the lengths of the three petals and the leaf. Assume without loss of generality that  $l_1 \geq l_2 \geq l_3$  and define  $\ell := \frac{l_1+l_2+l_3}{3}$ . Using the three petals as a main subgraph and the leaf as an attached subgraph, we have  $k_1(l_1, l_2, l_3, l_p) \leq \frac{\pi}{2\ell}$ . Moreover, equality is possible only if  $l_1 = l_2 = l_3 = \ell$ . Using the longest two petals and the leaf as a main subgraph and the shortest petal as an attached subgraph we further have

$$k_1(l_1, l_2, l_3, l_l) \leq \frac{5\pi}{2(1-l_3)} \leq \frac{5\pi}{2(1-\ell)}. \tag{D.8}$$

Combining the two bounds we got on  $k_1$ , it follows that  $k_1(l_1, l_2, l_3, l_p) \leq \frac{7\pi}{2}$ , with an equality possible only if  $\ell = \frac{2}{7}$  and  $l_3 = \ell$ . These two equalities together entail that  $l_1 = l_2 = l_3 = \frac{2}{7}$  and  $l_l = \frac{1}{7}$ . With this choice of lengths, it is easy to show that the spectral gap equals  $\frac{7\pi}{2}$  and of multiplicity three. This multiplicity increases to four when imposing the Dirichlet condition at the central vertex, which means that the equilateral stower satisfies the strong Dirichlet criterion. As the equilateral stower is a unique supremizer, it also satisfies condition (b) of Theorem 2.6.  $\square$

*Proof of Lemma 8.5.* Let  $\ell \in [0, 1]$  be the length of the leaf and  $1-\ell$  the length of the petal. Using the leaf as a main subgraph and the petal as an attached subgraph, we get

$$k_1(\ell, 1-\ell) \leq \frac{2\pi}{2\ell\sqrt{3-2\ell}}. \tag{D.9}$$

In particular, we have  $k_1(\ell, 1-\ell) \leq 2\pi$  as long as  $2\ell\sqrt{3-2\ell} \geq 1$ . This is satisfied for  $\ell \geq \frac{1}{3}$ , and in this case the inequality is strict. Next, we refer to the scattering approach described in ‘‘Appendix A’’ and more precisely to Eq. (A.10), whose zeros are the graph’s eigenvalues. This equation is equivalent, in our case, to  $F(k, \ell) = 0$ , where

$$F(k, \ell) := 2 \cos(k\ell) \sin\left(k \frac{1-\ell}{2}\right) + \sin(k\ell) \cos\left(k \frac{1-\ell}{2}\right). \tag{D.10}$$

Substituting  $k = 2\pi$ , and using basic trigonometric identities, we get

$$F(2\pi, \ell) = 2 \cos(2\pi\ell) \sin(\pi(1-\ell)) + \sin(2\pi\ell) \cos(\pi(1-\ell)) \tag{D.11}$$

$$= 2 \sin(\pi\ell) (\cos(2\pi\ell) - \cos^2(\pi\ell)) = 2 \sin(\pi\ell) (\cos^2(\pi\ell) - 1). \tag{D.12}$$

We notice that  $F(k, \ell) > 0$  for small positive values of  $k$  and that  $F(2\pi, \ell) < 0$  for  $\ell \in (0, \frac{1}{3}]$ . As  $F$  is continuous in  $k$ , we deduce that there exists some  $k < 2\pi$  such that  $F(k, \ell) = 0$ . This means that for  $\ell \in (0, \frac{1}{3}]$ , the spectral gap is strictly below  $2\pi$ . As we have seen above that this is also the case for  $\ell > \frac{1}{3}$  and since the spectral gap is  $2\pi$  for  $\ell = 0$  (single-cycle graph), the result follows.  $\square$

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Communicated by Jan Dereziński.

Received: August 6, 2016.

Accepted: May 11, 2017.