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ON THE SPECTRAL GAP OF A QUANTUM GRAPH

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Abstract. We consider the problem of finding universal bounds of "isoperimetric" or "isodiametric" type on the spectral gap of the Laplacian on a metric graph with natural boundary conditions at the vertices, in terms of various analytical and combinatorial properties of the graph: its total length, diameter, number of vertices and number of edges. We investigate which combinations of parameters are necessary to obtain non-trivial upper and lower bounds and obtain a number of sharp estimates in terms of these parameters. We also show that, in contrast to the Laplacian matrix on a combinatorial graph, no bound depending only on the diameter is possible. As a special case of our results on metric graphs, we deduce estimates for the normalised Laplacian matrix on combinatorial graphs which, surprisingly, are sometimes sharper than the ones obtained by purely combinatorial methods in the graph theoretical literature.

1. Introduction

A classical question in spectral theory consists in determining for which bodies – among all those with prescribed volume, or surface measure, or perhaps another relevant geometric quantity – the associated Laplacian has the smallest or greatest k^{th} eigenvalue, say with Dirichlet or Neumann boundary conditions. In the case of domains, this goes back as far as 1870 to a now-famous conjecture of Lord Rayleigh, answered in the affirmative by G. Faber in 1923 in the planar case and E. Krahn in 1926 in the general case, that the first eigenvalue λ_1 of the Laplacian on $\Omega \subset \mathbb{R}^d$ with Dirichlet boundary conditions is always at least as large as that of a ball in $\mathbb{R}^d$ with the same volume, with equality being attained if and only if Ω is in fact a d-dimensional ball. This result was arguably the starting point of spectral geometry. Analogous results for the first positive eigenvalue λ_1 of the Laplacian with Neumann boundary conditions were proved by G. Szegő and H.F. Weinberger in 1954 and 1956, respectively: in the Neumann case, it turns out that the first (non-trivial) eigenvalue is *maximal* if Ω is a d-dimensional sphere. We refer to [Hen06] for a survey of such *isoperimetric inequalities* for differential operators.

The importance of the first positive eigenvalue cannot be overestimated. For example, in the theory of parabolic equations λ_1 gives the speed of convergence of the system towards equilibrium. In mathematical physics it is the energy level associated with the ground state of the system, or the first excited state, if Neumann conditions are imposed; in the latter case λ_1 is therefore often referred to as the *spectral gap*.

In recent years it has become increasingly clear that there exist parallel differential geometrical theories in the continuous setting of manifolds and in the discrete setting of graphs, see e.g. the survey [Kel15]. In the case of graphs, however, there are several competing notions which can be considered as generalisations of the Laplacian, including the *discrete Laplacian* $\mathcal{L}$ and the *normalised Laplacian* $\mathcal{L}_{\text{norm}}$; moreover, it is not quite indisputable which geometric quantities should be chosen in order to impose meaningful restrictions on the class of sets under consideration. For instance, it was already proved by M. Fiedler in [Fie73] that among all connected graphs on a given number of vertices, the first positive eigenvalue of the discrete Laplacian $\mathcal{L}$ is maximal (resp., minimal) in the case of the complete (resp., path) graph. A more delicate analysis is needed to discuss the cases of graphs whose

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number of vertices *and* edges, or else whose number of vertices of degree one, is prescribed, see [LPS11, BL12]. Comparable results are known for the normalised Laplacian $\mathcal{L}_{\rm norm}$, cf. Remark 8.1 below.

In the present paper we are going to focus on quantum graphs: roughly speaking, a (compact) *quantum graph* is a (finite, connected) graph each of whose edges e is identified with an interval of $\mathbb{R}$ of (finite) length $|\mathsf{e}|$. Then, the usual Euclidean distance on each edge induces in a natural way a metric space structure on a quantum graph – we refer the reader to the monographs [BK13, Mug14, Kuron] for more details. It is thus possible to define on each such interval a differential operator (which plays the role of a Hamiltonian in the framework of quantum mechanics on graphs): Here we will only focus on the case of (1-dimensional) Laplacians. Gluing all these operators together by means of suitable boundary conditions yields a new Laplacian-type operator, the subject of our investigations.

It is mathematical folklore that quantum graph Laplacians "interpolate" between Laplace–Beltrami operators on compact manifolds and normalised Laplacians on combinatorial graphs; indeed, interesting relations have been proved using these interplays. It is perhaps then surprising that only few results are known in the area of spectral geometry for graphs: possibly the only Faber–Krahn-type result for quantum graphs says that the lowest non-trivial eigenvalue λ_1, i.e. the spectral gap, of the Neumann (or Kirchhoff) Laplacian on a quantum graph is *minimised* (not maximised!) among all graphs of given total length by the path, cf. [Fri05, KN14, Nic87b].

Our principal aim here is to undertake a more systematic investigation of universal eigenvalue inequalities for the Laplacian with natural conditions in the vertices of quantum graphs. We will restrict ourselves to the prototype problem of the spectral gap and to four quantities (see below for precise definitions):

- the total length L of a graph,
- its diameter D,
- the number V of its vertices and
- the number E of its edges.

Even in the most elementary case it turns out to be a surprisingly subtle question as to which problems are well posed, as we shall attempt to show below, quantum graphs can in fact display types of behaviour that are in a sense more complex than those of manifolds and combinatorial graphs. For up-to-date and fairly comprehensive overviews of the currently known estimates for the spectral gap of the discrete and normalised Laplacians of a combinatorial graph, we refer to [Mol12] and in [Chu97], respectively.

If all edges of a quantum graph are identified with an interval of unit length, the problem of describing the spectrum of the Laplacian was completely settled by J. von Below in [Bel85, Theorem, page 320]. Von Below's approach shows that all spectral problems concerning the Laplacian on an equilateral quantum graph with edges of unit length can be reduced to corresponding spectral problems for the normalised Laplacian $\mathcal{L}_{\rm norm}$ (rather than the discrete Laplacian $\mathcal{L}$) on the underlying combinatorial graph. In particular, the lowest non-zero eigenvalue of the quantum graph Laplacian agrees with

$$\lambda_1 = \arccos^2(1-\alpha_1) \qquad \text{provided } \alpha_1 \in [0,2)\ , \tag{1.1}$$

where α_1 is the lowest non-zero eigenvalue of $\mathcal{L}_{\rm norm}$, cf. [BM13, Fig. 1]. And indeed abundant information is available on the spectrum of $\mathcal{L}_{\rm norm}$, see e.g. [Chu97, BC13]. However, the setting of [Bel85] is a very special case of general quantum graphs: the topic of this paper will be the far more challenging case of quantum graphs with different edge lengths. A variant of (1.1) for non-equilateral graphs was obtained by S. Nicaise in [Nic87a, Theoreme 2.1] by introducing a weighted version of $\mathcal{L}_{\rm norm}$. All our results can be translated into analogous, equivalent bounds on the spectral gap of such a weighted normalised Laplacian $\mathcal{L}^w_{\rm norm}$. One may argue that investigating the spectrum of a differential operator is less convenient than working with a matrix. In fact, we maintain that our approach based on quantum graphs has some advantages that come from the flexibility offered by the continuous setting.

In Sections 2 and 3 we summarise the elementary properties of quantum graphs which we will need in the sequel: in particular, in Section 2, we state a number of basic principles showing how the spectral gap depends on structural properties of the graph (see Lemma 2.3); in Section 3 we list a number of classes of graphs with natural extremising properties. Section 4 is devoted to proving an upper bound on the spectral gap in terms of L, E that complements the known lower bound (4.1) – an old result of S. Nicaise that has been rediscovered several time since [Nic87b].

In Section 5 we will prove that fixing the diameter D of a graph alone is not enough to yield estimates on the spectral gap. This is in our opinion the most surprising result of this paper. In particular, in order to show that D alone cannot bound the spectral gap from above we will introduce a special class of graphs: the so-called *pumpkin chains*, see Definition 5.3. They have a large spectral gap for given diameter and will allow us to reduce our problem to a Sturm–Liouville one: this new method of reduction to Sturm–Liouville theory is one of the main points of interest of this article and is probably amenable to further developments. These pumpkin chains will also allow us to prove various upper bounds in conjunction with other quantities such as V or L in Sections 6 and 7. We will briefly summarise the bounds for the normalised Laplacian which can be deduced from our results in Section 8, see Remark 8.1.

While our graphs will always have finitely many edges and vertices, in some cases we are going to prove bounds that cannot be attained by such finite graphs, but are approximated by suitable families of finite graphs with increasingly many edges.

We can represent the outcome of our investigations in a schematic form; two tables in Section 8 summarise the corresponding bounds and whether optimal graphs realising the bounds exist:

parameter(s) \ λ_1	upper estimate?	lower estimate?
V, E	✗ (Remark 2.4)	✗ (Remark 2.4)
L	✗ (Eq. (4.1))	✓ (Eq. (3.2))
L, V	✗ (Eq. (3.2))	✓ (Eq. (4.1), Example 4.1)
L, E	✓ (Theorem 4.2)	✓ (Eq. (4.1), Example 4.1)
D	✗ (Theorem 5.10)	✗ (Example 5.1)
D, V	✓ (Theorem 6.1)	✗ (Example 5.1)
D, E	✓ (Remark 6.3)	✓ (Remark 6.3)
D, L	✓ (Theorem 7.1)	✓ (Theorem 7.2)

2. Notation and basic techniques

Throughout this paper we are going to adopt the usual notation of graph theory: graphs will be denoted by G, their edge and vertex sets will be denoted by E and V, respectively, then again we will adopt the notation e and v for edges and vertices, respectively. In graph theory it is customary to denote by n (resp., m) the cardinality of V (resp., E), but in this case we prefer to adopt the alternative notation

$$V(\mathsf{G}) := |\mathsf{V}| \qquad \text{and} \qquad E(\mathsf{G}) := |\mathsf{E}|,$$

since we wish to perform analysis on graphs. We will denote by

$$L(\mathsf{G}) := \sum_{\mathsf{e}\in\mathsf{E}} |\mathsf{e}|$$

the total length of G, i.e., the sum of the lengths of all edges of G, and the diameter of G by

$$D(\mathsf{G}) := \sup\left\{\operatorname{dist}(x,y) : x,y \in \mathsf{G}\right\}, \tag{2.1}$$

where the distance between two points of a graph is as usual defined to be the length of the shortest path within G connecting them (Cf. [Mug14, § 3.2]). Note that here we take the supremum over *all* points $x, y \in \mathsf{G}$. If we restrict ourselves to considering $x, y \in \mathsf{V}$, then we have a "weaker" notion of diameter, which we shall call the *combinatorial diameter* D_{V} of G; see Remark 5.5. This is consistent with the classical notion of diameter from combinatorial graph theory.

We will also impose the following standing assumption on all the graphs we consider to ensure simultaneously the non-triviality and the finiteness of all the quantities we consider.

Assumption 2.1. The metric graph G is connected. It is compact and finite, i.e., it consists of finitely many edges of finite length.

The object of our investigations is a realisation of the operator that acts as a second derivative on the intervals associated with each edge of G. The most common choice in the literature is to define a Laplacian Δ on a quantum graph by imposing two conditions in each vertex of G: functions in the domain of Δ

- are continuous across the vertices and
- their normal derivatives about each vertex sum up to 0.

Under Assumption 2.1 and with this choice of "natural" (i.e. continuity and Kirchhoff) boundary conditions, $-\Delta$ is a self-adjoint, positive semi-definite operator with compact resolvent on the Hilbert space $L^2(\mathsf{G})$ of square integrable functions supported on the intervals associated with the edges of the graph. Thus, $-\Delta$ has pure point spectrum $\sigma(-\Delta) \subset [0, \infty)$; we will call its elements simply the eigenvalues of G, since the operator is uniquely determined by the metric graph G.

The value $\lambda_0 = 0$ is an eigenvalue of multiplicity one (since G is connected) with eigenfunction $u_0 \equiv 1$. Thus the spectral gap coincides with the lowest non-trivial eigenvalue $\lambda_1 > 0$, which can be obtained by minimising the Rayleigh quotient subject to the constraint of L^2-orthogonality to the eigensubspace corresponding to $\lambda_0 = 0$:

$$\lambda_1(\mathsf{G}) = \inf \left\{ \frac{\int_{\mathsf{G}} |u'(x)|^2 \, \mathrm{d}x}{\int_{\mathsf{G}} |u(x)|^2 \, \mathrm{d}x} : u \in H^1(\mathsf{G}), \int_{\mathsf{G}} u(x) \, \mathrm{d}x = 0 \right\} . \tag{2.2}$$

Here $H^1(\mathsf{G})$ – the form domain of $-\Delta$ – is the space consisting of those functions defined on the intervals associated with the edges of the graph, belonging to the first Sobolev space H^1 thereon, and satisfying continuity conditions in the vertices, cf. [BK13, § 1.3] or [Mug14, § 3.2].

Remark 2.2. (a) Unlike in combinatorial graph theory, for the purposes of quantum graph theory vertices of degree two are unessential objects that can be inserted or removed without changing either the space $H^1(\mathsf{G})$ or the domain of Δ, and in particular without affecting the spectrum.

(b) In general, we are not going to assume graphs to be simple. Indeed, for our purposes it is always possible to add dummy vertices in the middle of an edge e – thus replacing an edge of length $|\mathsf{e}|$ by two edges of length $|\tilde{\mathsf{e}}|$ and $|\mathsf{e}| - |\tilde{\mathsf{e}}|$, respectively – turning a non-simple graph into a simple one without changing the spectrum of the Laplacian.

From (2.2) follow a handful of elementary but very useful principles, of which we will make extensive use; we note that many of these have already appeared or been proved in [EJ12, KMN13].

Lemma 2.3. *Suppose G and G' are quantum graphs satisfying Assumption 2.1.*

(1) If G' is formed by attaching a pendant edge, or more generally a pendant graph, to one vertex of G, then $\lambda_1(\mathsf{G}) \geq \lambda_1(\mathsf{G}')$.

(2) If G' is formed from G by identifying two vertices of G (say, $\mathsf{v}_1, \mathsf{v}_2$ are replaced with a new vertex v_0 and each edge having v_1 or v_2 as an endpoint is replaced with a new edge having v_0 as an endpoint, and in particular the edges between v_1 and v_2 are replaced with loops around v_0), then $\lambda_1(\mathsf{G}) \leq \lambda_1(\mathsf{G}')$.

(3) If we add an edge $\mathsf{e} = \mathsf{v}_1\mathsf{v}_2$ between two already existing vertices of a quantum graph G, producing the new quantum graph G', then $\lambda_1(\mathsf{G}) \geq \lambda_1(\mathsf{G}')$ provided *there is an eigenfunction corresponding to $\lambda_1(\mathsf{G})$ attaining the same value on both $\mathsf{v}_1, \mathsf{v}_2$.*

(4) If G' is formed from G by lengthening a given edge, then $\lambda_1(\mathsf{G}) \geq \lambda_1(\mathsf{G}')$.

(5) If G' is obtained from G by scaling each edge with the factor $1/c \in \mathbb{R}$, then the corresponding eigenvalues scale as c^2, that is, for all $n \in \mathbb{N}$, we have

$$\lambda_n(\mathsf{G}) = c^{-2} \lambda_n(\mathsf{G}').$$

Proof of Lemma 2.3. We will merely sketch a proof of the statements; details can in most cases be found in [KMN13]. (1) Let ψ be any eigenfunction associated with $\lambda_1(\mathsf{G})$, and suppose that we obtain G' by attaching a pendant graph to a vertex $\mathsf{v} \in \mathsf{G}$. We extend ψ to a function $\tilde{\psi} \in H^1(\mathsf{G}')$ by setting $\tilde{\psi} = \psi(\mathsf{v})$ on $\mathsf{G}' \setminus \mathsf{G}$. Then the function $\varphi = \tilde{\psi} - \int_{\mathsf{G}' \setminus \mathsf{G}} \tilde{\psi}$ is a valid test function for $\lambda_1(\mathsf{G}')$, and it may be checked that the Rayleigh quotient of φ is not larger than $\lambda_1(\mathsf{G})$.

(2) This follows immediately from the fact that $H^1(\mathsf{G}')$ may be identified with a subspace of $H^1(\mathsf{G})$, since the continuity conditions imposed on functions in the former space are more restrictive; but the Rayleigh quotient is given by the same formula.
(3) The proof is similar to (1): extending the eigenfunction ψ_1 minimising the Rayleigh quotient for G by a constant on the new edge (equal to the common value $\psi_1(\mathsf{v}_1) = \psi_1(\mathsf{v}_2)$) yields a trial function for G' whose Rayleigh quotient can be no larger, even after a possible orthogonalisation.
(4) Let us denote by $\mathsf{e}_1 \subset \mathsf{G}$ the edge to be lengthened, which we identify with the interval $(0, a)$, identify the lengthened interval with $(0, a')$, $a' > a$, and let ψ_1 be the eigenfunction on G. Consider the function $\tilde{\psi} \in H^1(\mathsf{G}')$ which is equal to ψ_1 on $\mathsf{G} \setminus \mathsf{e}_1$ (identified canonically with a subset of G') and on $(0, a)$, and which is extended by $\psi_1(a)$ on (a, a'). As in (1), the function $\varphi = \tilde{\psi} - \int_{\mathsf{G}'} \tilde{\psi} = \tilde{\psi} - (a' - a)\psi(a)$ is a valid test function for $\lambda_1(\mathsf{G}')$, and as in (1), its Rayleigh quotient is not larger than $\lambda_1(\mathsf{G})$. Alternatively, this may be viewed as a special case of (3).
(5) The proof follows essentially (4). One needs to take into account that all edges are scaled with the same factor and no orthogonalisation is needed. □

Remark 2.4. (a) Statement (3) can be interpreted as saying that diffusion processes in quantum graphs may in some cases actually converge to equilibrium faster upon *removing* edges. (An analogous assertion does not hold in the case of the discrete Laplacian on combinatorial graphs, cf. [Moh91b, Thm. 3.2].) This paradox seems to have been first explicitly remarked in [KMN13] and may be solved by realising that the edges whose removal increases the spectral gap are in some way redundant.

(b) In particular, quantum graphs cannot be recursively pruned, getting sequences of connected graphs with lower and lower spectral gaps, until a spanning tree is reached. We can however see Statement (2) as the quantum graph version of the assertion that each spanning tree of a combinatorial graph G has lower spectral gap (for the discrete Laplacian) than G itself, cf. [Moh91b, Cor. 3.4].

(c) Statement (5) implies the obvious fact that spectral estimates cannot be obtained without taking into account any metric parameter like the total length or the length of one of the edges. In particular estimates based solely on the number of vertices and/or edges are impossible. This is in sharp contrast with the theory of Laplacians on combinatorial graphs. For instance, the second lowest eigenvalue β_1 of the discrete Laplacian $\mathcal{L}$ on a combinatorial graph satisfies the bounds

$$2e(\mathsf{G})\left(1 - \cos\frac{\pi}{V}\right) \le \beta_1 \le \frac{V}{V-1}\deg_{\min}(\mathsf{G}) \ ,$$

cf. [Fie73], whence the bounds

$$\frac{2e(\mathsf{G})}{\deg_{\max}(\mathsf{G})}\left(1 - \cos\frac{\pi}{V}\right) \le \alpha_1 \le \frac{V}{V-1} \ , \tag{2.3}$$

on the second lowest eigenvalue α_1 of the normalised Laplacian $\mathcal{L}_{\mathrm{norm}}$; if G is planar, then the upper bounds may be improved to

$$\beta_1 \le \frac{8}{V}\deg_{\max}(\mathsf{G}) \qquad \text{and} \qquad \alpha_1 \le \frac{8}{V}\frac{\deg_{\max}(\mathsf{G})}{\deg_{\min}(\mathsf{G})} \ ,$$

cf. [ST07]. Here $\deg_{\min}(\mathsf{G}), \deg_{\max}(\mathsf{G}), e(\mathsf{G})$ denote the minimal degree, the maximal degree, and the edge connectivity of G, respectively.

3. Extremal graphs and special classes of graphs

In the process of studying optimisation problems, it is natural to look for classes of potential optimisers, and the following special classes of graphs seem at various times to play an important role. In order to obtain effective estimates it is important to be able to calculate the spectrum of an optimiser explicitly, which is possible only for graphs with very special choice of the edge lengths. If all edges of a quantum graph have the same length, then we call it *equilateral*: unless otherwise stated, we will always assume flower, star, pumpkin, and complete graphs to be equilateral.

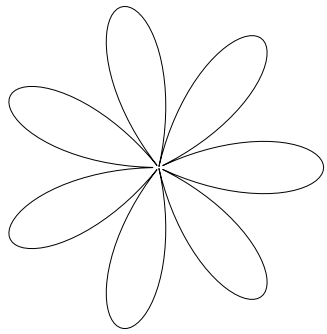

FIGURE 1. A flower graph $\mathsf{F}(L,7)$ on seven edges (petals).

- *Path* graphs $\mathsf{I}(L)$ are intervals of length L viewed as quantum graphs. Because on a path graph the imposed boundary conditions boil down to continuity of a function and its derivative on the internal vertices and Neumann on the extremal ones, the spectral gap of a path graph of total length L clearly agrees with that of an interval of length L, i.e.,

$$\lambda_1(\mathsf{I}(L)) = \frac{\pi^2}{L^2} \ . \tag{3.1}$$

- *Flower* graphs $\mathsf{F}(L,E)$ are quantum graphs built upon non-simple combinatorial graphs consisting of one vertex and E loops attached to it, which we shall call *petals*. A direct computation shows that the spectral gap of a flower graph of total length L on $E \geq 2$ edges is

$$\lambda_1(\mathsf{F}(L,E)) = \frac{\pi^2 E^2}{L^2} \ ; \tag{3.2}$$

  if $E = 1$, then we have a loop of length L, which has $\lambda_1 = 4\pi^2/L^2$.
- *Star* graphs $\mathsf{S}(L,E)$ are quantum graphs consisting of a central vertex v and $E \geq 2$ edges radiating out from v. If we take all edges to have equal length L/E (as we shall always do), then

$$\lambda_1(\mathsf{S}(L,E)) = \frac{\pi^2 E^2}{4L^2}. \tag{3.3}$$

- *Pumpkin* graphs $\mathsf{P}(L,E)$, sometimes also called *dipole* or *banana* graphs in the literature, are quantum graphs built upon non-simple combinatorial graphs consisting of two vertices and E parallel edges, which we shall call *slices*, having both vertices as endpoints. The spectral gap of a pumpkin graph of total length L on E edges is also

$$\lambda_1(\mathsf{P}(L,E)) = \frac{\pi^2 E^2}{L^2} \ , \tag{3.4}$$

  since one can see directly that there is a corresponding eigenfunction having the form $\sin(\frac{\pi E \cdot}{L})$ on each edge, where we identify each edge with the interval $(0, \frac{L}{E})$.
- *Complete* graphs K_V are quantum graphs built upon simple combinatorial graphs consisting of V vertices and exactly one edge joining any pair of vertices, meaning $E = \frac{V(V-1)}{2}$ edges in total. By (1.1) the spectral gap of a complete graph of total length L on E edges is

$$\lambda_1(\mathsf{K}_V) = \left(\arccos\frac{1}{1-V}\right)^2 \frac{V^2(V-1)^2}{4L^2} \ . \tag{3.5}$$

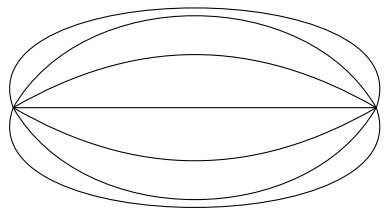

FIGURE 2. A pumpkin graph $\mathsf{P}(L, 7)$ on seven edges (slices).

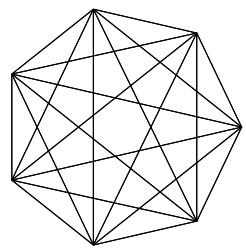

FIGURE 3. A complete graph K_7 on seven vertices.

Remark 3.1. The expressions in (3.2) and (3.4) imply in particular that adding to an (equilateral) flower or pumpkin graph arbitrarily many petals or slices (in the case of flowers and pumpkins, respectively) does not change the spectral gap, instead increasing the multiplicity of λ_1, as long as each of the new edges has the same length as the original ones.

In several cases we will also perform graph surgery to produce examples. A distinguished class consists of what we call *dumbbell graphs*, which are obtained by joining two quantum graphs (ideally, two "massive ones") by only one edge. Naturally, dumbbell graphs are the analogue of dumbbell domains.

Remarkably, we are going to see that in most cases the correct quantum graph equivalents of balls are not complete graphs, as one may naively think (and – as a rule of thumb – as is actually the case when *discrete* graphs are investigated [Fie73]), but rather flower graphs.

4. Estimates involving the length

Perhaps the most natural quantity of a graph G to consider is its total length L, which is the equivalent of the volume of a domain. However, quantum graphs lack a natural (continuous) notion of perimeter, and in some sense V and E might be thought of as discrete counterparts thereof; so it is also natural to consider V and/or E in combination with L. This section is thus devoted to estimates on the spectral gap in terms of the total length L and possibly V and E; first we will consider lower bounds, and then upper bounds.

We remark at this juncture that a graph on E edges can have at most $V = E + 1$ vertices, so that bounding E from above automatically also bounds V from above; put differently, controlling E is in a certain sense a stronger restriction on the graph than controlling V. Moreover, using standard matching conditions allows one to increase the number of vertices and edges without actually changing the metric graph (by introducing new vertices at inner points on the edges), so in general we expect controlling E and V from above to lead to both better upper *and* lower bounds, since this is a restriction on the degree of complexity of the graph.

4.1. **Lower estimates.** The first and fundamental lower estimate was obtained by S. Nicaise [Nic87b, Théorème 3.1] and later independently re-proved by L. Friedlander [Fri05, Theorem 1] and by S. Naboko and one of the present

authors [KN14, Theorem 1]:

$$\lambda_1(\mathsf{G}) \geq \frac{\pi^2}{L^2}\ , \tag{4.1}$$

where G is any graph having total length $L > 0$. The minimiser is essentially unique: it is simply a path graph, which is a one-dimensional ball. This estimate is easy to understand intuitively: the diffusion in a quantum graphs of total length L can be at most as slow as on the interval $[0, L]$.

The lower estimate cannot be improved without taking into account new parameters, since we have a minimiser. However, neither E nor V can be used in combination with L to give a refined lower bound on $\lambda_1(\mathsf{G})$ any better than (4.1), as we show next. The idea behind this is that perturbing a graph in a small but rather complicated way does not affect the spectral gap in a serious way, although it can have an arbitrarily large effect on the graph's combinatorics.

Example 4.1. Given any natural numbers $E \geq 2$ and $V \geq 2$ with $V \leq E+1$ and any positive numbers $L > 0$ and $\varepsilon > 0$, we can find a connected graph G having E edges, V vertices and total length L, such that

$$\lambda_1(\mathsf{G}) \leq \frac{\pi^2}{L^2} + \varepsilon\ .$$

To do so, we take an arbitrary connected graph $\tilde{\mathsf{G}}$ having $V-1$ vertices and $E-1$ edges (if $V \geq 3$ this is always possible to do by starting with a tree with $V-1$ vertices and $V-2 \leq E-1$ edges, and adding extra edges between vertices in an arbitrary fashion until there are $E-1$; if $V = 2$, we take a flower with $E-1$ petals), rescale $\tilde{\mathsf{G}}$ to have total length $\delta > 0$ and form G by taking a Vth vertex v and joining v to an arbitrary vertex w of $\tilde{\mathsf{G}}$ by an Eth edge $\mathsf{e} = \mathsf{vw}$ of length $L - \delta$. It follows from Lemma 2.3.(1) that $\lambda_1(\mathsf{G}) \leq \lambda_1(\mathsf{e}) = \pi^2/(L-\delta)^2$ ("adding" the graph $\tilde{\mathsf{G}}$ to the edge e can only decrease the eigenvalue); choosing $\delta > 0$ small enough proves the claim. ■

4.2. **Upper estimates.** The explicit examples considered in Section 3 show that no upper estimate is possible in terms of L alone: by (3.2), λ_1 can be made arbitrarily large by considering flower graphs on more and more edges of smaller and smaller length. Moreover, the same example shows that fixing just L and V together is not enough to bound λ_1 from above.

However, if we fix L and E, then we obtain a sharp upper bound on λ_1 in terms of the arithmetic mean value $\mathcal{A} = L/E$ of the edge length. An interesting question is to characterise the class of optimisers, which appears to be very large, including but not limited to equilateral flowers and pumpkins.

Theorem 4.2. *Let G be a quantum graph having length $L > 0$ and $E \geq 2$ edges. Then*

$$\lambda_1(\mathsf{G}) \leq \frac{\pi^2 E^2}{L^2} \equiv \frac{\pi^2}{\mathcal{A}^2}, \tag{4.2}$$

with equality if and only if

(1) G is equilateral and

(2) there exists an eigenfunction corresponding to $\lambda_1(\mathsf{G})$ which takes on the value zero at all vertices of G.

If $E = 1$, then

$$\lambda_1(\mathsf{G}) = \begin{cases} 4\pi^2/L^2 & \text{if } \mathsf{G} \text{ is a loop,} \\ \pi^2/L^2 & \text{if } \mathsf{G} \text{ is a path.} \end{cases}$$

Proof of Theorem 4.2. Assume G is any quantum graph as in the statement of the theorem, with $L > 0$ and $E \geq 2$ given, and denote by $\tilde{\mathsf{G}}$ the corresponding flower graph having the same number of edges with the same lengths as G, i.e., $\tilde{\mathsf{G}}$ is the graph which may be formally obtained from G by identifying all vertices of the latter. Then $H^1(\tilde{\mathsf{G}})$ may be canonically identified with the subset of $H^1(\mathsf{G})$ consisting of all functions $u \in H^1(\mathsf{G})$ such that $u(\mathsf{v}_1) = \ldots = u(\mathsf{v}_n)$ for all vertices $\mathsf{v}_1, \ldots, \mathsf{v}_n$ of G. It follows from Lemma 2.3.(3) that $\lambda_1(\mathsf{G}) \leq \lambda_1(\tilde{\mathsf{G}})$.

We now show that the equilateral flower graph $\mathsf{F}(L, E)$ is the (unique) maximiser of λ_1 among all flower graphs of fixed total length $L > 0$ and number of edges $E \geq 2$, which will then complete the proof of (4.2), since

$\lambda_1(\mathsf{F}(L,E)) = \pi^2E^2/L^2$ by (3.2). To that end, let e_1, e_2 be the longest two edges of the arbitrary flower graph $\tilde{\mathsf{G}}$ (or any two longest edges if these are not uniquely determined); by the pigeonhole principle, $M := |\mathsf{e}_1| + |\mathsf{e}_2| \geq 2L/E$. Denote by G_{12} the flower graph consisting of these two longest edges. By Lemma 2.3.(1),

$$\lambda_1(\tilde{\mathsf{G}}) \leq \lambda_1(\mathsf{G}_{12}) \ .$$

But we see immediately that $\lambda_1(\mathsf{G}_{12}) \leq 4\pi^2/M^2 \leq \pi^2E^2/L^2$, since we may use any eigenfunction belonging to the first eigenvalue of a circle of length M as a test function on G_{12}, provided it is rotated appropriately so as to satisfy the continuity condition at the points corresponding to the vertex of G_{12}. This establishes the inequality.

To prove the case of equality, we first note that this is only possible if $M = 2L/E$, that is, if the two longest edges (and all other edges) have length L/E each, and so $\tilde{\mathsf{G}}$ must already be equilateral in this case.

Moreover, equality requires that the identification of all the vertices of G not affect $\lambda_1(\mathsf{G})$. This is only possible if there is already an eigenfunction $\psi \in H^1(\mathsf{G})$ corresponding to $\lambda_1(\mathsf{G})$ for which $\psi(\mathsf{v}_1) = \ldots = \psi(\mathsf{v}_n)$, since otherwise $H^1(\mathsf{F}(L,E))$ – which may be canonically identified with a subspace of $H^1(\mathsf{G})$ – does not contain any minimiser achieving (2.2), so that the infimum in $H^1(\mathsf{F}(L,E))$ must be larger. But since ψ corresponds to an eigenfunction on the flower graph $\mathsf{F}(L,E)$, and any eigenfunction of $\lambda_1(\mathsf{F}(L,E))$ must take on the value zero at the unique vertex of $\mathsf{F}(L,E)$, it follows that $\psi(\mathsf{v}_1) = \ldots = \psi(\mathsf{v}_n) = 0$.

The case $E = 1$ is trivial. □

Remark 4.3. Theorem 4.2 can be regarded as a counterpart to the value of the spectral gap of the second derivative with Neumann conditions on an interval, given that L/E is the arithmetic mean of all edge lengths. A similar assertion for another problem, the first eigenvalue of the Laplacian with a Dirichlet condition on at least one node, was recently proved in [DPR14, Thm. 3.8]. There are other, weaker estimates on λ_1 in terms of the arithmetic, geometric and harmonic means of the sequence of edge lengths of the graph, which we denote by $\mathcal{A}, \mathcal{G}, \mathcal{H}$, respectively: [Kuron, Thm. 2] states that

$$\lambda_1(\mathsf{G}) \leq \frac{4\pi^2}{\mathcal{A}\mathcal{H}} = \frac{4\pi^2}{\mathcal{G}^2};$$

the factor of four may even be dropped if G is bipartite. Observe that this estimate is still sharp, as it is attained in the case of (equilateral) flowers and pumpkins, although (4.2) is better, including in the case where G is bipartite.

An estimate of a similar flavour in terms of the maximal edge length M of G can be obtained via a trivial test function argument, by placing a suitable sine function on the longest edge, extended elsewhere by zero: $\lambda_1(\mathsf{G}) \leq 4\pi^2/M^2$. This is however in general far worse than (4.2). This may be the natural counterpart to the usual estimate in terms of in-radii in the case of domains.

As mentioned above, we leave as an open problem the question of identifying the class of all minimisers – equality is in particular achieved by both equilateral flower graphs and equilateral pumpkin graphs, and it is not hard to construct other examples. An obvious *necessary* condition on a potential maximiser has to do with the possibility of colouring the graph with three colours (in a non-standard way): blue/red edges are those where the sine function attains value +1/-1, whereas green ones are edges where eigenfunctions vanish identically; and additionally every vertex should be balanced in the sense that the same number of red and blue edges should be adjacent to it; cf. the notion of $\mathbb{Z}_3$-*circulation* [Die05, Sec. 6.1].

5. Estimates in terms of the diameter alone: negative results

Another natural choice of metric quantity is the graph diameter D (see (2.1)). Diameter has been regarded as a natural quantity in spectral optimisation of (convex) domains at least since van den Berg's formulation of the Gap Conjecture in 1983.

In this section we will prove that fixing the diameter of a graph alone is not in fact enough to yield upper or lower estimates on the spectral gap. Finding examples showing the impossibility of lower bounds is fairly straightforward; the question of an upper bound is however far more subtle. To that end we will introduce the *pumpkin chains* referred to in the introduction (see Definition 5.3 below), which are an extremising class of graphs for diameter

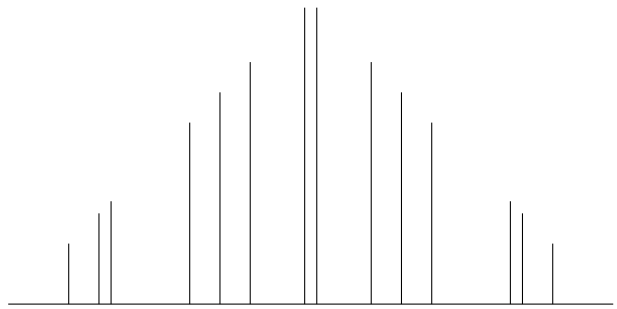

FIGURE 4. A comb graph on fourteen prongs.

(Lemma 5.4). We will not need this extremising property in order to prove that no estimate is possible, but we will use it in Sections 6 and 7 to obtain various upper bounds in conjunction other quantities such as V or L. We also present it in this section to try to give a better insight into how to generate graphs with large spectral gaps. The same types of examples will allow us to show certain other quantities alone also do not control the spectral gap; see Sec. 5.3.

5.1. **Lower bounds are impossible.** We will start with the easier case: proving that no lower bound on λ_1 is possible in terms of the diameter alone. Again, this is in contrast with the theory of Laplacians on combinatorial graphs, whose lowest non-trivial eigenvalue is not less than $\frac{4}{VD}$, see e.g. [Mol12, § 5.3].

Example 5.1. Given $D > 0$, we construct a sequence of dumbbell graphs G_n satisfying Assumption 2.1, all having diameter D, such that $\lambda_1(\mathsf{G}_n) \to 0$: all these graphs will be flower-dumbbells.

More precisely, we start with an edge e_0 of length $D/2$ with endpoints $\mathsf{v}_{-1} \neq \mathsf{v}_1$ and attach to each of these vertices one flower on n edges $\mathsf{e}_{\pm 1}, \dots, \mathsf{e}_{\pm n}$ each of length $D/2$, so that the diameter of G_n is D for all $n \in \mathbb{N}$. Then of course the number of edges of G_n becomes arbitrarily large as $n \to \infty$.

However, $\lambda_1(\mathsf{G}_n) \to 0$: to see this we use a simple test function argument. Identifying e_0 with the interval $(-D/4, D/4)$, we set

$$\psi_n(z) := \begin{cases} 1 & \text{if } z \in \mathsf{e}_k,\ 1 \le k \le n\ , \\ \sin(2\pi x/D) & \text{if } z \in (-D/4, D/4) \simeq \mathsf{e}_0\ , \\ -1 & \text{if } z \in \mathsf{e}_k,\ -n \le k \le -1\ . \end{cases}$$

Then $\psi_n \in H^1(\mathsf{G}_n)$ and by symmetry $\int_{\mathsf{G}_n} \psi_n = 0$; moreover, $\int_{\mathsf{G}_n} |\psi_n'|^2$ is constant in $n \ge 1$, being supported on the fixed edge e_0, while clearly $\int_{\mathsf{G}_n} |\psi_n|^2 \to \infty$ as $n \to \infty$. It follows immediately from the variational characterisation (2.2) that $\lambda_1(\mathsf{G}_n) \to 0$ as $n \to \infty$. ■

Remark 5.2. Making our graphs *flower* dumbbells allows us to keep the number of vertices of G_n equal to two. One can of course attach more general graphs of small diameter but large total length to achieve the same result. One can also find fundamentally different (i.e. non-dumbbell) types of graphs; for example, consider a sequence of "comb graphs" as in Figure 5.2. We take a sequence of graphs by adding more and more "prongs" (the vertical edges) to the comb, keeping it symmetric and making sure that its diameter remains constant. We then build a test function by constructing a stretched cosine along the lower edge, and extending it by a constant along the prongs; by symmetry, this function is orthogonal to the constant functions and it is easy to check that the corresponding Rayleigh quotient goes to zero provided the prongs do not accumulate too rapidly in the middle.

5.2. **Upper bounds are also impossible.** To produce a counterexample we follow the natural line of reasoning one would use to attempt to prove that an upper bound exists. We first show that searching of a graph with the largest spectral gap it is enough to consider so-called pumpkin chains (defined below). Then we prove that spectral

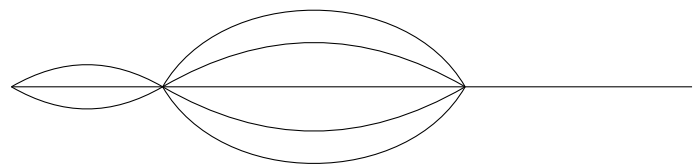

FIGURE 5. A pumpkin chain on nine edges and four vertices.

problem for a pumpkin chain is equivalent to a Sturm–Liouville one-dimensional problem with an integer weight. This analogy allows us to construct a sequence of pumpkin chains of fixed diameter with arbitrarily large gap.

Pumpkin chains maximise the spectral gap. The following class of finite graphs is going to play an important role in our constructions:

Definition 5.3. We call a metric graph G on V vertices satisfying Assumption 2.1 a *pumpkin chain* if

$$\#\{\mathsf{v} \in \mathsf{V} : \mathsf{v} \text{ is adjacent to exactly two other vertices}\} = V - 2,$$
$$\#\{\mathsf{v} \in \mathsf{V} : \mathsf{v} \text{ is adjacent to exactly one other vertex}\} = 2,$$

and if additionally the lengths of any two edges connecting v, w is the same for any pair of adjacent vertices v, w.

In other words, G consists of a chain of vertices, each one connected to a predecessor and a successor, all connecting two "end vertices", call them v_0 and v_D. Every path from v_0 to v_D (of which there may be many) must pass through each of the $V-2$ interior vertices. Alternatively, a pumpkin chain may be thought of as a connected chain of pumpkin graphs; hence the name. See Figure 5.2. Any two edges connecting the same pair of vertices (i.e. belonging to the same pumpkin) will be called *parallel*.

The diameter of a pumpkin chain G is given by $D(\mathsf{G}) = \operatorname{dist}(\mathsf{v}_0, \mathsf{v}_D)$, and, if G has at least three vertices, then the two end vertices are the only points realising D. Moreover, there is a canonical mapping $S : \mathsf{G} \to [0, D]$ such that $S(\mathsf{v}_0) = 0$, $S(\mathsf{v}_D) = D$, given by $S(z) = \operatorname{dist}(\mathsf{v}_0, z)$. We shall call $S(z)$ the *level* of a point $z \in \mathsf{G}$.

The next result shows that for the purpose of estimating the spectral gap from above in terms of V or L, we do not have to bother about any graphs other than pumpkin chains – or, to put it in another way, no spectral information that is relevant to us is lost whenever we prune a quantum graph by deleting all edges that are not crossed by paths that realise the diameter.

Lemma 5.4. *Given any compact, connected, non-empty metric graph G, there exists a pumpkin chain $\tilde{\mathsf{G}}$ such that*

(1) $D(\tilde{\mathsf{G}}) = D(\mathsf{G})$, $L(\tilde{\mathsf{G}}) \le L(\mathsf{G})$ and $V(\tilde{\mathsf{G}}) \le V(\mathsf{G}) + 2$;
(2) $\lambda_1(\tilde{\mathsf{G}}) \ge \lambda_1(\mathsf{G})$.

Proof. We will give an algorithm which constructs $\tilde{\mathsf{G}}$ out of G (note that we do not claim $\tilde{\mathsf{G}}$ to be unique).
Step 1. Choose any two points $x, y \in \mathsf{G}$ such that $\operatorname{dist}(x, y) = D := D(\mathsf{G})$ and relabel them as $\mathsf{v}_0, \mathsf{v}_D$, i.e., relabel them as (artificial) vertices of G. Denote by Γ_1 any shortest path through G connecting v_0 and v_D, that is, Γ_1 is a subgraph of G with $L(\Gamma_1) = D(\mathsf{G})$, and any $\mathsf{v} \in V(\mathsf{G}) \cap \Gamma_1 \setminus \{\mathsf{v}_0, \mathsf{v}_D\}$ has degree two when considered as a vertex of Γ_1. Without loss of generality, Γ_1 may be considered as a directed path from v_0 to v_D, where no part of Γ_1, be it edge or vertex, is counted twice.
Step 2. Assuming such a path to exist, denote by Γ_2 any (directed) shortest path from v_0 to v_D such that $\Gamma_2 \not\subset \Gamma_1$ (as sets), and no point of G is counted twice by Γ_2 (in particular Γ_2 does not contain any loops). Since G is compact, if there is any such path, there will be one of minimal length. Repeat this process inductively to obtain n such paths $\Gamma_1, \dots, \Gamma_n \subset \mathsf{G}$, that is, Γ_k is a directed path from v_0 to v_D without passing through any point twice, with

$$\mathsf{G}_k \not\subset \bigcup_{j=1}^{k-1} \mathsf{G}_j$$

for all $k \geq 2$, and $D = L(\Gamma_1) \leq \ldots \leq L(\Gamma_k) \leq \ldots$. Since G is compact, this process will terminate after $n \geq 1$ steps, that is, no further path $\Gamma \subset \mathsf{G}$ can be found without either being contained in $\bigcup_{k \leq n} \Gamma_k$ or passing through at least one point of G at least twice.

Step 3. Set

$$\hat{\mathsf{G}} := \bigcup_{k=1}^{n} \Gamma_k,$$

taking the vertex set of $\hat{\mathsf{G}}$ to be

$$\mathsf{V}(\hat{\mathsf{G}}) := \{\mathsf{v}_0, \mathsf{v}_D\} \cup \{\mathsf{v} \in \mathsf{V} : \mathsf{v} \text{ has degree} \geq 2 \text{ in } \hat{\mathsf{G}}\} .$$

Then clearly $D(\hat{\mathsf{G}}) = D(\mathsf{G})$, $L(\hat{\mathsf{G}}) \leq L(\mathsf{G})$ and $V(\hat{\mathsf{G}}) \leq V(\mathsf{G}) + 2$. We also see directly that $\lambda_1(\hat{\mathsf{G}}) \geq \lambda_1(\mathsf{G})$, as follows from Lemma 2.3.(1): since any connected component of $\mathsf{G} \setminus \hat{\mathsf{G}}$ is connected to $\hat{\mathsf{G}}$ at a single vertex (otherwise we could find another path not contained in $\Gamma_1, \ldots, \Gamma_n$ as in step two), adding this component to $\hat{\mathsf{G}}$ can only decrease λ_1. Since $\mathsf{G} \setminus \hat{\mathsf{G}}$ can only consist of finitely many connected components, it follows that $\lambda_1(\hat{\mathsf{G}}) \geq \lambda_1(\mathsf{G})$.

Step 4. We shorten the paths $\Gamma_2, \ldots, \Gamma_n$ inductively to obtain new paths $\tilde{\Gamma}_2, \ldots, \tilde{\Gamma}_n$ so that (with $\tilde{\Gamma}_1 = \Gamma_1$) $L(\tilde{\Gamma}_1) = L(\tilde{\Gamma}_2) = \ldots = L(\tilde{\Gamma}_3) = D$, without changing the topology of $\hat{\mathsf{G}}$ (although some edges may contract to a point).

More precisely, we form a new graph $\tilde{\mathsf{G}}_2$ from $\hat{\mathsf{G}}$ by shortening $\Gamma_2 \setminus (\Gamma_1 \cup \mathsf{V})$ by length $L(\Gamma_2) - D \geq 0$; then $\lambda_1(\tilde{\mathsf{G}}_2) \geq \lambda_1(\hat{\mathsf{G}})$ by Lemma 2.3.(4). Note that this may also shorten (a subset of) the other paths $\Gamma_3, \ldots, \Gamma_n$, but each will still have length at least D, and they will still be ordered by increasing length. We then proceed inductively, creating a graph $\tilde{\mathsf{G}}_k$ out of $\tilde{\mathsf{G}}_{k-1}$ by shortening $\Gamma_k \setminus \bigcup_{j \leq k-1} \tilde{\Gamma}_j$ to have length D. We end up with a graph $\tilde{\mathsf{G}}_n$ consisting of n possibly overlapping paths $\tilde{\Gamma}_1, \ldots, \tilde{\Gamma}_n$ from v_1 to v_2, such that $L(\tilde{\Gamma}_k) = D$ for all $k = 1, \ldots, n$, with $D(\tilde{\mathsf{G}}_n) = D$, $L(\tilde{\mathsf{G}}_n) \leq L(\mathsf{G})$, $V(\tilde{\mathsf{G}}_n) \leq V(\mathsf{G}) + 2$ and $\lambda_1(\tilde{\mathsf{G}}_n) \geq \lambda_1(\mathsf{G})$.

Step 5. Finally, we obtain a pumpkin chain $\tilde{\mathsf{G}}$ out of $\tilde{\mathsf{G}}_n$ by identifying all points at a given level where (at least) two of the paths have a common vertex. For each k, there exists a mapping $S_k : \tilde{\Gamma}_k \to [0, D]$ given by $S_k(z) = d_{\tilde{\Gamma}_k}(z, \mathsf{v}_0)$ for all $z \in \tilde{\Gamma}_k$, where $d_{\tilde{\Gamma}_k}$ denotes (Euclidean) distance measured along the path $\tilde{\Gamma}_k$. The vertices $\mathsf{v} \in \mathsf{V}(\tilde{\mathsf{G}}_n) \cap \tilde{\Gamma}_k$ along the path $\tilde{\Gamma}_k$ have the form $\mathsf{v}_0 = S_k^{-1}(0)$, $\mathsf{v}_k^1 = S^{-1}(x_k^1)$, $\ldots$, $\mathsf{v}_k^{n_k} = S^{-1}(x_k^{n_k})$, $\mathsf{v}_D = S_k^{-1}(D)$ for certain levels $x_k^1, \ldots, x_k^{n_k} \in (0, D)$, for each $k = 1, \ldots, n$.

For every x_k^j, for all $j = 1, \ldots, n_k$ and all $k = 1, \ldots, n$, we insert an artificial vertex at each point $S_i^{-1}(x_k^j)$ for all $i = 1, \ldots, n$, and then form $\tilde{\mathsf{G}}$ out of $\tilde{\mathsf{G}}_n$ by identifying for every fixed pair j, k the vertices $S_i^{-1}(x_k^j)$ for all $i = 1, \ldots, n$. The graph $\tilde{\mathsf{G}}$ is then a pumpkin chain with the same diameter, length and number of vertices as $\tilde{\mathsf{G}}_n$, in particular satisfying condition (1) of the lemma, and $\lambda_1(\tilde{\mathsf{G}}) \geq \lambda_1(\tilde{\mathsf{G}}_n)$ (cf. Lemma 2.3.(3)), so that (2) is satisfied as well. □

Remark 5.5. It is clear that $V(\tilde{\mathsf{G}})$ will be equal to $V(\mathsf{G})$ if the diameter is realised as a distance between certain two vertices – there will be no need to introduce artificial vertices in Step 1. For some estimates it will be sensible to use another notion of diameter, weaker but in practice easier to compute, the *combinatorial diameter* of a graph G introduced at the beginning of Section 2, which is given by

$$D_{\mathsf{V}}(\mathsf{G}) := \sup\{\mathrm{dist}(\mathsf{v}, \mathsf{w}) : \mathsf{v}, \mathsf{w} \in \mathsf{V}(\mathsf{G})\},$$

the maximal distance within G of any two *vertices* of G; then clearly $D_{\mathsf{V}}(\mathsf{G}) \leq D(\mathsf{G})$. Moreover, an inspection of the proof of Lemma 5.4 reveals that it can be trivially modified to allow one to prove the existence, for any given G, of a corresponding pumpkin chain $\tilde{\mathsf{G}}$ with

(1) $D_{\mathsf{V}}(\tilde{\mathsf{G}}) = D_{\mathsf{V}}(\mathsf{G})$, $L(\tilde{\mathsf{G}}) \leq L(\mathsf{G})$ and $V(\tilde{\mathsf{G}}) \leq V(\mathsf{G})$, and
(2) $\lambda_1(\tilde{\mathsf{G}}) \geq \lambda_1(\mathsf{G})$.

All of our statements involving the diameter – at least, all the negative statements as well as all the upper bounds in Section 6 below – also hold for D_{V}, as is easy to see.

Note that if G is e.g. a pumpkin chain, a tree, a (higher dimensional) cube or a complete bipartite graph, see e.g. [Die05, Chapter 1], then $D = D_{\mathsf{V}}$, but this is not the case if G is a complete graph.

Reduction to a Sturm–Liouville problem. Next we prove that we can find an eigenfunction ψ_1 of $\lambda_1(\mathsf{G})$ (where G is a pumpkin chain) which only depends on the level $S(z)$ of any $z \in \mathsf{G}$, that is, ψ_1 takes on the same value on all parallel edges: this is the crucial argument that will allow us to study our problem by Sturm–Liouville arguments.

Lemma 5.6. *Suppose G is a pumpkin chain. There exists an eigenfunction ψ_1 associated with $\lambda_1(\mathsf{G})$ and a function $\varphi : [0, D] \to \mathbb{R}$ such that $\psi_1(z) = \varphi(S(z))$ for all $z \in \mathsf{G}$.*

Proof. If there exists an eigenfunction ψ which does not vanish on at least one vertex of G, then we may construct a new eigenfunction ψ_1 by averaging the value of ψ at each fixed level. It is easily checked that $\psi_1 \not\equiv 0$ created in this way is an eigenfunction for $\lambda_1(\mathsf{G})$, as a linear combination of eigenfunctions on each edge, which also satisfies the Kirchhoff condition at the vertices, and which by construction only depends on the level. So we merely need to ensure the existence of such an eigenfunction ψ.

Denote the vertices of G by $\mathsf{v}_0, \mathsf{v}_1, \dots, \mathsf{v}_V = \mathsf{v}_D$ ($V \geq 2$) and the $V - 1$ pumpkin subgraphs of G by $\mathsf{G}_1, \dots, \mathsf{G}_{V-1}$, G_k running from vertex v_{k-1} to v_k. If there *exists* an eigenfunction ψ such that $\psi(\mathsf{v}_k) = 0$ for all $k = 0, \dots, V$, then, since ψ cannot vanish identically on any pumpkin, ψ is in particular an eigenfunction of the Dirichlet Laplacian on each G_k. Denoting by $\mu_n(\mathsf{G}_k)$ the nth Dirichlet eigenvalue of G_k, it follows that for each k there exists $n \geq 1$ with $\lambda_1(\mathsf{G}) = \mu_n(\mathsf{G}_k) \geq \mu_1(\mathsf{G}_k) \geq \lambda_1(\mathsf{G})$, the last inequality following by an easy monotonicity argument. This implies G must necessarily be equilateral, and ψ restricted to each edge, identified with $(0, a) \subset \mathbb{R}$, is either identically 0 or of the form $\pm \sin(\sqrt{\lambda_1} x) = \pm \sin(\pi x/a)$, $x \in (0, a)$. It follows that each G_k has another eigenfunction taking on the value ± 1 at v_{k-1} and ∓ 1 at v_k (i.e., of the form $\pm \cos(\pi x/a)$ on each of its corresponding edges); we may therefore build another eigenfunction on G taking on the alternate values 1 and -1 at successive vertices. This proves the claim. (Note that it also follows that $\mathsf{V} = 2$ in this case, since for $\mathsf{V} \geq 3$ one can see directly that any such eigenfunction cannot be associated with λ_1, but we do not need this.) □

Let ψ_1 be such an eigenfunction as in the lemma, corresponding to $\lambda_1(\mathsf{G})$. We denote by

$$\rho(x) = \#S^{-1}\{x\} \tag{5.1}$$

the counting function for the number of parallel edges of G at the level $x \in [0, D]$, and by $\varphi(x) := \psi_1(S^{-1}(x))$ the well-defined composite function (in a slight abuse of notation) in $H^1(0, D)$; since $S'(z) = 1$ almost everywhere, it follows that

$$\begin{aligned} \lambda_1(\mathsf{G}) &= \frac{\int_0^D \varphi'(x)^2 \rho(x) \mathrm{d}x}{\int_0^D \varphi(x)^2 \rho(x) \mathrm{d}x} \\ &= \inf \left\{ \frac{\int_0^D u'(x)^2 \rho(x) \mathrm{d}x}{\int_0^D u(x)^2 \rho(x) \mathrm{d}x} : u \in H^1(0, D), \int_0^D u(x) \rho(x) \mathrm{d}x = 0 \right\}; \end{aligned} \tag{5.2}$$

for the second equality, "$\geq$" is clear, and "$\leq$" follows since every such function $u \in H^1(0, D)$ can be mapped canonically onto a function $g \in H^1(\mathsf{G})$ via $g(z) = u \circ S(z)$ for $z \in \mathsf{G}$ (so that we may use the minimisation property of ψ on G). We see in particular that looking for a pumpkin chain with the largest spectral gap it is enough to study a one-dimensional problem.

We shall now introduce a principle which allows us to pass from pumpkin chains to actual one-dimensional weighted eigenvalue problems. The central argument here is that the set of possible weights ρ corresponding to pumpkin graphs, $\{\rho \in L^\infty(0, D; \mathbb{N} \setminus \{0\})\}$, is large enough within $L^\infty(0, D)$ in a sense relevant for our eigenvalue problems.

Proposition 5.7. *Given any function $\omega \in C^1[0, D]$ such that $\min_{x \in [0,D]} \omega(x) > 0$, there exists a sequence of pumpkin chains G_n of diameter D such that $\lambda_1(\mathsf{G}_n) \to \lambda_1(\omega)$.*

Here we have denoted by $\lambda_1(\omega) > 0$ the first non-trivial eigenvalue of the Sturm–Liouville problem

$$\begin{cases} -(\omega(x)u'(x))' = \lambda\omega(x)u(x), & x \in (0,D), \\ u'(0) = u'(D) = 0\ , \end{cases} \tag{5.3}$$

i.e.,

$$\lambda_1(\omega) = \inf\left\{ \frac{\int_0^D u'(x)^2\omega(x)\,\mathrm{d}x}{\int_0^D u(x)^2\omega(x)\,\mathrm{d}x} : u \in H^1(0,D),\ \int_0^D u(x)\omega(x)\mathrm{d}x = 0 \right\}, \tag{5.4}$$

as is easy to see by the usual means.

Remark 5.8. We note that (5.4) makes sense when $\omega \in L^\infty(0,D)$ with $\operatorname{ess\,inf}\omega(x) > 0$, and in this case it is still possible to find pumpkin chains G_n with $\lambda_1(\mathsf{G}_n) \to \lambda_1(\omega)$ – as our proof shows, although we will not go into details. Hence, it follows from (5.2), Lemma 5.4 and Proposition 5.7 that

$$\begin{aligned} \sup\{\lambda_1(\mathsf{G}) : D(\mathsf{G}) = D\} &= \sup\{\lambda_1(\mathsf{G}) : \mathsf{G} \text{ pumpkin chain},\ D(\mathsf{G}) = D\} \\ &= \sup\{\lambda_1(\omega) : \omega \in L^\infty(0,D;\mathbb{N}\setminus\{0\})\}\ . \end{aligned}$$

We can in fact further refine the class of functions that are relevant to us: it follows directly from (5.4) that $\lambda_1(\alpha\omega) = \lambda_1(\omega)$ for any $\alpha > 0$, which leads us finally to consider

$$W = \{\rho \in L^\infty(0,D) : \varepsilon_\rho := \operatorname{ess\,inf}\rho > 0,\ \ \rho(0,D) \text{ is a finite subset of } \varepsilon_\rho\,\mathbb{N}\setminus\{0\}\}\,,$$

the set of all weights which can be obtained by multiplying the weight associated with a pumpkin chain by an arbitrary positive constant. In this way, our original spectral problem on a graph has been reduced to a suitable Sturm–Liouville-like problem with possibly discontinuous elliptic coefficients. We consider this transference principle to be the largest point of interest of this article, which can likely be applied to different investigations in the theory of quantum graphs.

The proof of Proposition 5.7 relies on the following lemma, whose proof is standard and hence omitted.

Lemma 5.9. *Given $\omega_n, \omega \in L^\infty(0,D)$ with $\operatorname{ess\,inf}\omega(x), \operatorname{ess\,inf}\omega_n(x) \geq \varepsilon > 0$ for all $n \in \mathbb{N}$, if $\omega_n \to \omega$ in $L^\infty(0,D)$, then $\lambda_1(\omega_n) \to \lambda_1(\omega)$ (with $\lambda_1(\omega_n), \lambda_1(\omega)$ defined as in (5.4)).*

In fact we can expect convergence in a much stronger sense, but this is all we will need.

Proof of Proposition 5.7. Every finite step function $\rho \in L^\infty(0,D)$ taking on only positive integer values corresponds to a pumpkin chain; hence the proposition reduces to showing that we can find a sequence of functions $\rho_n \in W$ with $\lambda_1(\rho_n) \to \lambda_1(\omega)$, with ω as in the statement of the proposition, since the closure of W in the L^∞-norm contains $\{\omega \in C^1[0,D] : \min\omega > 0\}$, as an elementary (and omitted) approximation argument shows. But this follows from Lemma 5.9. □

Counterexample. We are finally in a position to show that no upper estimate on the spectral gap is possible in terms of the diameter alone. Our result is non-constructive, but it should not be hard to write down a family of examples explicitly based on our proof: a sequence of pumpkin chains, where the pumpkins become increasingly small, and in each pumpkin chain the number of slices of the successive pumpkins increases exponentially from v_0 to v_D.

Theorem 5.10. *Given $D > 0$, there exists a sequence of pumpkin chains G_n with $D(\mathsf{G}_n) = D$ for all $n \in \mathbb{N}$, but $\lambda_1(\mathsf{G}_n) \to \infty$.*

Proof. Proposition 5.7 together with a diagonal argument shows that this follows from the existence of a sequence of weights $\omega_n \in C^1[0,D]$ with $\lambda_1(\omega_n) \to \infty$. We make the explicit choice $\omega_n(x) := e^{nx}$, then it follows from (5.3) and a short calculation that $\lambda_1(\omega_n)$ is the lowest non-zero eigenvalue of

$$\begin{cases} -u''(x) - nu'(x) = \lambda u(x), & x \in (0,D), \\ u'(0) = u'(D) = 0. \end{cases} \tag{5.5}$$

We claim that all non-trivial eigenvalues $\lambda_k(\omega_n)$ of the above problem are bounded from below by $n^2/4$, from which the assertion of the theorem will follow. To see this we use the substitution $w(x) := e^{\frac{n}{2}x}u(x)$ to transform (5.5) into

$$\begin{cases} -w''(x) = \mu w(x), \qquad \mu = \lambda - \dfrac{n^2}{4}, \qquad x \in (0, D), \\ \quad w'(0) = \dfrac{n}{2}w(0),\ w'(D) = \dfrac{n}{2}w(D). \end{cases}$$

An elementary calculation shows that the spectrum of this problem $\mu \geq -\frac{n^2}{4}$; the unique eigenfunction corresponding to $\mu_0 = -\frac{n^2}{4}$ is $w(x) = e^{\frac{n}{2}x}$. The next eigenvalue μ_1 is positive, meaning $\lambda_1(\omega_n) \geq n^2/4$. □

Remark 5.11. The property $\lambda_1(\mathsf{G}_n) \to \infty$ is a global property of the sequence of graphs, as can be seen as follows: create a new graph $\tilde{\mathsf{G}}_n$ out of the graph G_n from Theorem 5.10 by attaching to its end vertex v_D a single edge of fixed length $\ell > 0$ (a *handle*). Then $D(\tilde{\mathsf{G}}_n) = D + \ell$ and the spectral gap does not blow up any more; in fact $\lambda_1(\tilde{\mathsf{G}}_n) \leq \pi^2/\ell^2$ for all $n \in \mathbb{N}$ by Lemma 2.3.(1) and (3.1).

5.3. **Applications: the radius and the longest cycle of a graph.** One could say that the principles set out in the preceding section are more general than simply applying to the quantity diameter. For example, in a natural analogy with the radius of a combinatorial graph, cf. [Die05, § 1.3], we may define the *radius* of a quantum graph G by

$$R(\mathsf{G}) := \inf_{x\in\mathsf{G}} \sup_{y\in\mathsf{G}} \operatorname{dist}(x, y),$$

where as usual dist denotes the shortest (Euclidean) distance between points along paths within the graph, and as with diameter, infimum and supremum are taken over all points in the graph, not just vertices. This is fairly closely related to diameter, and indeed for the flower dumbbells in Example 5.1, the combs in Remark 5.2 and all pumpkin chains, we have that $R(\mathsf{G}) = D(\mathsf{G})/2$. In particular, radius alone leads to neither a lower nor an upper bound on $\lambda_1(\mathsf{G})$.

As another example, the *length of the longest cycle* of a graph G also yields neither a lower nor an upper bound on $\lambda_1(\mathsf{G})$ (unlike the length of the longest edge). For the lower bound, if we take the sequence of graphs G_n from Example 5.1 and modify each by inserting a second edge e_{00} of length $D/2$ between v_1 and v_{-1}, then we obtain a sequence of graphs having a longest cycle of length D and spectral gap tending to zero, as we can see by extending ψ_n by another sine curve in the obvious way on e_{00}. For the upper bound, take a sequence of pumpkin chains G_n as in Theorem 5.10 and identify for each n the two end vertices v_0 and v_D to form a new graph G'_n having a longest cycle of length D and $\lambda_1(\mathsf{G}'_n) \geq \lambda_1(\mathsf{G}_n)$ by Lemma 2.3.(3).

6. Estimates involving the diameter

If beyond the diameter we place additional restrictions on our graphs, we can recover bounds. An interesting fact is that, unlike in the case of length (Example 4.1), bounding V from above is now, in conjunction with D, enough to obtain an upper bound.

Theorem 6.1. *Let G be a quantum graph having diameter $D > 0$ and $V \geq 2$ vertices. Then*

$$\lambda_1(\mathsf{G}) \leq \frac{\pi^2}{D^2}(V+1)^2\ , \tag{6.1}$$

and even

$$\lambda_1(\mathsf{G}) \leq \frac{\pi^2}{D_{\mathsf{V}}^2}(V-1)^2 \tag{6.2}$$

where D_{V} is the combinatorial diameter of G introduced in Remark 5.5.

Proof. In order to prove (6.1) it suffices to prove that

$$\sup\{\lambda_1(\mathsf{G}) : \mathsf{G} \text{ is a pumpkin chain, } D(\mathsf{G}) = D \text{ and } V(\mathsf{G}) \le V\} \le \frac{\pi^2}{D^2}(V-1)^2, \tag{6.3}$$

since by Lemma 5.4 for any graph G we can find a pumpkin chain $\tilde{\mathsf{G}}$ with $D(\tilde{\mathsf{G}}) = D(\mathsf{G})$, $V(\tilde{\mathsf{G}}) \le V(\mathsf{G}) + 2$ and $\lambda_1(\mathsf{G}) \le \lambda_1(\tilde{\mathsf{G}})$; (6.2) will follow from the same statement, appealing to Remark 5.5. We establish this via a somewhat crude test function argument. By the pigeonhole principle, at least two vertices v, w of G, say at levels $a = S(\mathsf{v}) < b = S(\mathsf{w}) \in [0, D]$, must satisfy $\operatorname{dist}(\mathsf{v}, \mathsf{w}) = b - a \ge D/(V-1)$. Roughly speaking, we build a scaled cosine function on (a, b) and extend this by ± 1 to the rest of the graph. More precisely, we set

$$\psi(z) := \begin{cases} \alpha & \text{if } x = S(z) \in [0, a) \\ \alpha \cos(\pi(x-a)/(b-a)) & \text{if } x = S(z) \in [a, (a+b)/2] \\ \beta \cos(\pi(x-a)/(b-a)) & \text{if } x = S(z) \in [(a+b)/2, b] \\ -\beta & \text{if } x \in (b, D] \end{cases}$$

for all $z \in \mathsf{G}$, where $x = S(z)$ throughout, and the constants $\alpha, \beta > 0$ are chosen so that $\int_{\mathsf{G}} \psi = 0$. It is easy to check that ψ has Rayleigh quotient no larger than $\pi^2/(b-a)^2 \le \pi^2(V-1)^2/D^2$, establishing (6.3) and hence (6.1). □

Remark 6.2. (a) A bound on the diameter D is stronger than one on the total length L (as $D \le L$), but on the other hand a bound on the number V of vertices is weaker than one on the number E of edges, as an upper bound on E implies one on V. Comparing Theorem 6.1 with Theorem 4.2 seems therefore to be interesting. We recall (Example 5.1) that D and V together are not enough for a lower bound.

(b) We do not expect the bounds in Theorem 6.1 to reflect the optimal growth of λ_1 with respect to V; for example, we conjecture that $\{\lambda_1(\mathsf{G}) : D_{\mathsf{V}}(\mathsf{G}) = D_{\mathsf{V}} \text{ and } V(\mathsf{G}) \le 4\}$ is equal to $4\pi^2/D_{\mathsf{V}}^2$. We also expect that in general such optima can only be approximated and never attained, since (roughly speaking) one can always add more edges to such a graph without altering D and V, but if added between the right vertices they should speed up diffusion on the graph.

(c) The bounds

$$\frac{4}{VD_{\mathsf{V}}} \le \beta_1 \le \frac{1}{\deg_{\max}} \frac{4\log_2^2 V}{D_{\mathsf{V}}^2} \tag{6.4}$$

on the spectral gap β_1 of the Laplacian of a combinatorial graph in terms of combinatorial diameter D_{V} and number of vertices were obtained in [AM85, Thm. 2.7] and [Moh91a, Thm. 4.2]; as to be expected, and like our upper bound, the bound in [AM85] depends positively on V and inversely on D_{V}. For the lower bound the situation is different: we recall from Example 5.1 that a lower bound in terms of D_{V} (or D) and V alone cannot hold in the context of quantum graphs.

Remark 6.3. Fixing the diameter D and bounding the number of edges E from above is enough to yield non-trivial upper and lower bounds on $\lambda_1(\mathsf{G})$. Indeed, since at least one edge must have length greater than or equal to D/E, we obtain the crude upper bound

$$\lambda_1(\mathsf{G}) \le \frac{4\pi^2 E^2}{D^2},$$

while since $L \le DE$, (4.1) implies the lower bound

$$\lambda_1(\mathsf{G}) \ge \frac{\pi^2}{D^2 E^2},$$

with equality if G is a loop in the first case and a path in the second. Both these bounds are however in general probably far from optimal. Since $\lambda_1(\mathsf{G})$ depends continuously on changes in the length of any given edge of G, even as the edge length tends to zero, it seems likely that there should exist maximisers and minimisers for each $D > 0$ and $E \ge 1$ (as opposed to only a maximising sequence as in Theorem 6.1); we expect that our current bounds

are only sharp if $E = 1$. However, we leave this as an open problem, together with the much harder problem of determining the optimal constants and optimisers for each $E \geq 2$.

7. Estimates in terms of both the total length and the diameter

We will now prove bounds on the eigenvalue in terms of D and L. We will start with the upper bound, which is the easier case.

7.1. An upper bound in terms of D and L.

Interesting in the following upper bound is the *positive* dependence on L, a consequence of L representing a finiteness condition on G as a counterpart to D; it is entirely possible that there could be another upper bound on λ_1 which depends inversely on L and positively on D.

Note that our upper estimate is again probably far from optimal, as we obtain it using another somewhat course test function argument, although it is "sharp" in the sense that we have equality when $L = D$, i.e., when G is a path.

Theorem 7.1. *Any quantum graph G satisfying Assumption 2.1 and having diameter $D > 0$ and total length $L \geq D$ satisfies*

$$\lambda_1(\mathsf{G}) \leq \frac{\pi^2}{D^2}\,\frac{4L - 3D}{D}\,. \tag{7.1}$$

Proof. Since the dependence of the right-hand side of (7.1) on L is positive, the claim will follow from Lemma 5.4 if we can prove the corresponding statement for pumpkin chains. So assume that G is indeed a pumpkin chain. Denoting as usual by v_0 and v_D the terminal vertices of G, and by $S(z) = \operatorname{dist}(z, \mathsf{v}_0)$ the level of the point $z \in \mathsf{G}$, we construct a test function on G by setting

$$\psi(z) := \begin{cases} A\cos\left(\frac{\pi S(z)}{D}\right) & \text{if } S(z) \leq D/2 \\ B\cos\left(\frac{\pi S(z)}{D}\right) & \text{if } S(z) > D/2 \end{cases}$$

for all $z \in \mathsf{G}$, where A, $B > 0$ are chosen to ensure $\int_{\mathsf{G}} \psi = 0$. Denote by

$$\ell_{\mathscr{L}} := |\{z \in \mathsf{G} : S(z) \leq D/2\}| - D/2$$

and

$$\ell_{\mathscr{R}} := |\{z \in \mathsf{G} : S(z) > D/2\}| - D/2$$

the total extra length of G not accounted for by the first path Γ_1 in G realising the diameter in the left and the right half of G, respectively. Then $\ell_{\mathscr{L}} + \ell_{\mathscr{R}} = L - D$ by definition, and, estimating ψ^2 from below by zero and $(\psi')^2$ from above by A^2 and B^2 on the corresponding part(s) of G, we have

$$\begin{aligned} \lambda_1(\mathsf{G}) &\leq \frac{\pi^2}{D^2}\,\frac{A^2\int_0^{D/2}\sin^2(\pi x/D)\,\mathrm{d}x + A^2\ell_{\mathscr{L}} + B^2\int_{D/2}^{D}\sin^2(\pi x/D)\,\mathrm{d}x + B^2\ell_{\mathscr{R}}}{A^2\int_0^{D/2}\cos^2(\pi x/D)\,\mathrm{d}x + B^2\int_{D/2}^{D}\cos^2(\pi x/D)\,\mathrm{d}x} \\ &= \frac{\pi^2}{D^2}\,\frac{(A^2+B^2)\frac{D}{4} + A^2\ell_{\mathscr{L}} + B^2\ell_{\mathscr{R}}}{(A^2+B^2)\frac{D}{4}}. \end{aligned}$$

Estimating both $\ell_{\mathscr{L}}$ and $\ell_{\mathscr{R}}$ from above by $L - D$ and rearranging yields (7.1). □

7.2. A lower bound in terms of D and L.

Finally, we will give a lower bound. It would appear that the minimum is given by the solution of a transcendental equation, which represents the first non-zero eigenvalue of a second-order problem on an interval with a non-standard boundary condition, in which the operator itself appears. This is often called a generalised Wentzell, or Wentzell–Robin, condition in the literature; see for example [AMPR03, MR07].

Theorem 7.2. *For any quantum graph* G *satisfying Assumption 2.1 and having diameter* $D > 0$ *and total length* $L \geq 2D$*, the first eigenvalue* $\lambda_1(\mathsf{G})$ *is at least as large as* κ^2*, where* $\kappa > 0$ *is the smallest positive solution of the transcendental equation*

$$\cos(2\kappa D) = (L - 2D)\kappa \sin(2\kappa D). \tag{7.2}$$

In particular,

$$\lambda_1(\mathsf{G}) \geq \frac{1}{2DL - 2D^2} > \frac{1}{2DL}. \tag{7.3}$$

Remark 7.3. (a) It is not clear if (7.2) is optimal. It follows from Lemma 7.6 below that the optimal bound is not larger than the square of the first positive solution $\tilde{\kappa} > 0$ of

$$\cos\left(\tilde{\kappa}\frac{D}{2}\right) = \tilde{\kappa}\frac{L-D}{2}\sin\left(\tilde{\kappa}\frac{D}{2}\right), \tag{7.4}$$

and it is not hard to show that

$$\frac{1}{DL} < \frac{1}{DL - \frac{D^2}{2}} \leq \tilde{\kappa}^2 \leq \frac{3}{3DL - 2D^2} < \frac{3}{DL}$$

(for the upper bound, use the estimate $\cot x \leq 1/x - x/3$ for $x \in (0, \pi)$; for the lower bound, argue as in the proof of Theorem 7.2, with D in place of $2D$). In particular, the dependence in Theorem 7.2 on D and L is of the correct form.

(b) If $D \geq L/2$, then it follows from (4.1) that

$$\lambda_1(\mathsf{G}) \geq \frac{\pi^2}{L^2} \geq \frac{\pi^2}{2DL}.$$

We see that lower bounds involving L and D are of most interest when D is much smaller than L, and in this case Theorem 7.2 is applicable.

(c) Both equations (7.2) and (7.4) arise by reducing a graph to a path graph of length D with "mass" equal to $L - D$ concentrated at the two vertices, and correspond to a one-dimensional Laplacian with Wentzell boundary conditions at one endpoint. More precisely, consider the problem

$$\begin{aligned} -u''(x) &= \kappa^2 u(x) \qquad \text{in } (0, D) \\ u''(0) - \frac{2}{L-D}u'(0) &= 0 \\ u''(D) + \frac{2}{L-D}u'(D) &= 0. \end{aligned}$$

The first antisymmetric eigenfunction corresponds to the problem on the half interval

$$\begin{aligned} -u''(x) &= \kappa^2 u(x) \qquad \text{in } (0, D/2) \\ u''(D/2) + \frac{2}{L-D}u'(D/2) &= 0 \\ u(0) &= 0. \end{aligned}$$

Then any eigenfunction has the form $\psi(x) = \sin(\kappa x)$, and a short computation using the condition at $x = D$ shows that κ satisfies (7.4) if and only if it solves this problem. (For (7.2) consider the same problem on $(0, 2D)$.)

Important for the proof will be the following class of graphs.

Definition 7.4. A *symmetric star dumbbell* graph (or SSD graph for short) G of diameter D and star size ℓ is a graph consisting of an edge e_0 (the handle) of length $D - 2\ell$ between two vertices v_1 and v_2, with identical star graphs S_1, S_2, each consisting of $m \geq 2$ edges each of length ℓ attached to v_1 and v_2, respectively.

FIGURE 6. A symmetric star dumbbell graph on twenty-two rays.

The next lemma shows that these graphs have a small first eigenvalue for given D and L. Our graphs do not need to be *star* dumbbells; it is merely important that as much mass as possible be concentrated as near the endpoints as possible. However, stars have the advantage that their eigenvalues can be more easily computed.

Lemma 7.5. *Given any quantum graph* G *satisfying Assumption 2.1, there is an SSD graph* T *with* $L(\mathsf{T}) \le L(\mathsf{G})$, $D(\mathsf{T}) \le \min\{2D(\mathsf{G}), L(\mathsf{G})\}$, *and* $\lambda_1(\mathsf{T}) \le \lambda_1(\mathsf{G})$.

An inspection of our proof shows that if the graph G is symmetric about a path representing the diameter, then one can find an SSD graph having the same diameter as G, with the other conclusions of Lemma 7.5. One can also find another graph T' with $D(\mathsf{T}') \le D(\mathsf{G})$, $L(\mathsf{T}') \le 2L(\mathsf{G})$ and $\lambda_1(\mathsf{T}') \le \lambda_1(\mathsf{G})$. Moreover, if G is already an SSD graph, then we can find an SSD graph T'' with $D(\mathsf{T}'') = D(\mathsf{G})$, $L(\mathsf{T}'') = L(\mathsf{G})$ and $\lambda_1(\mathsf{T}'') \le \lambda_1(\mathsf{G})$.

Proof. Given G with length L and diameter D, we take any eigenfunction ψ corresponding to $\lambda_1(\mathsf{G})$. If ψ vanishes identically on an edge, or a collection of edges, then we may remove them from G, decreasing D and L, and leaving λ_1 unchanged. So we may assume that the set where $\psi = 0$ consists of finitely many points. We turn these into (artificial) vertices and identify them, which cannot increase D. By Lemma 2.3.(2), this can only increase λ_1, but since ψ remains an eigenfunction, which is obviously still associated with the first non-trivial eigenvalue, as the new graph cannot have a smaller one, λ_1 remains in fact unchanged.

Hence we may assume that G consists of two subgraphs G^+ and G^-, joined at a single vertex v_0, with a first eigenfunction ψ satisfying $\psi > 0$ on G^+ and $\psi < 0$ on G^-. In particular, ψ is also a first eigenfunction (with λ_1 the corresponding first eigenvalue) of the mixed Dirichlet–Neumann/Kirchhoff problem on G^+ and G^-, i.e., where we impose a Dirichlet condition at v_0 and the usual continuity and Kirchhoff conditions on all other vertices. Moreover, it is immediate that

$$\sup\{\mathrm{dist}(x, \mathsf{v}_0) : x \in \mathsf{G}^+\}, \sup\{\mathrm{dist}(x, \mathsf{v}_0) : x \in \mathsf{G}^-\} \le D \ ,$$

and at least one of these graphs, say G^+, has total length not more than $L/2$. (Of course, one of them will also have this supremum at most $D/2$, but its length may then be large. Choosing this graph would lead to the comparison with T'.) Set

$$d := \sup\{\mathrm{dist}(x, \mathsf{v}_0) : x \in \mathsf{G}^+\} \le \min\{D, L/2\} \ .$$

Denote by T an SSD graph having total length L and diameter $2d$, where the length of the edges of the star graphs will be fixed later. Identify the midpoint (with respect to which T is symmetric) with 0, and the end vertices – i.e., the vertices of degree one in S_1 and S_2, cf. Definition 5.3 – with $-d$ and d, respectively. Denote the right half of the graph by T^+.

We will now construct a test function φ on T out of ψ. Let $z \in \mathsf{G}^+$ be such that ψ reaches its maximum $M > 0$ in G^+ at z; then in particular $s := \mathrm{dist}(z, \mathsf{v}_0) \le d$. Denote by Γ any shortest path from v_0 to z. Now we map the values of ψ on Γ onto T: for $x \in [0, s] \subset [0, d]$ let $\varphi(x) = \psi(w)$, where $\mathrm{dist}(w, \mathsf{v}_0) = x$, so that $\varphi(0) = 0$ and $\varphi(s) = M$. If $s < d$, then extend φ by M on $(s, d]$, and on the star graph S_2 let φ take on the value it takes on at v_2. We then take φ to be symmetric on T; it is clear that $\varphi \in H^1(\mathsf{T})$.

Now fix $\varepsilon > 0$, to be specified later. We assume that v_2 is near enough to d that $\varphi(\mathsf{v}_2) \ge M - \varepsilon$. It remains to show that the Rayleigh quotient of φ is not larger than that of ψ on G; note that we only have to consider G^+, as it follows from the fact that ψ is an eigenfunction and that G^+ is one of its nodal domains that

$$\lambda_1(\mathsf{G}) = \frac{\int_{\mathsf{G}^+} |\psi'|^2}{\int_{\mathsf{G}^+} |\psi|^2}.$$

By symmetry, we also only have to consider φ on T^+. Now it is clear from the construction that

$$\int_{\mathsf{T}^+} |\varphi'|^2 = \int_{(0,s)} |\varphi'|^2 = \int_\Gamma |\psi'|^2 \leq \int_{\mathsf{G}^+} |\psi'|^2.$$

We claim that

$$\int_{\mathsf{T}^+} |\varphi|^2 \geq \int_{\mathsf{G}^+} |\psi|^2$$

if $\varepsilon > 0$ is small enough. If $d = L/2$, then G^+ and T^+ are both just path graphs, and it is clear there is equality between the corresponding eigenvalues. If $d < L/2$, then $L(\mathsf{G}^+) \leq L(\mathsf{T}^+) = L/2$; moreover, since ψ reaches its maximum M on a finite set of points, there exists $\delta > 0$ such that

$$\int_{\mathsf{G}^+\setminus\Gamma} |\psi|^2 \leq (M-\delta)^2 L(\mathsf{G}^+ \setminus \Gamma) \leq (M-\delta)^2(\frac{L}{2} - s).$$

If we choose $\varepsilon \in (0,\delta)$, then, since $L(\mathsf{S}_2 \cup (s,d)) = L/2 - s$,

$$\int_{\mathsf{T}^+\setminus(0,s)} |\varphi|^2 = \int_{\mathsf{S}_2\cup(s,d)} |\varphi|^2 \geq (M-\varepsilon)^2 \left(\frac{L}{2} - s\right) > (M-\delta)^2 \left(\frac{L}{2} - s\right).$$

Since clearly

$$\int_{(0,s)} |\varphi|^2 = \int_\Gamma |\psi|^2,$$

our claim follows, and we have shown that $\lambda_1(\mathsf{T}) \leq \lambda_1(\mathsf{G})$. Since T has total length L and diameter $2d \leq 2D$, we are done. □

We now show that the spectral gap of a sequence T_n of SSD graphs of fixed diameter and total length converges to the claimed equation as the stars become smaller and more concentrated.

Lemma 7.6. *Suppose that T_n is a sequence of SSD graphs with $D(\mathsf{T}_n) = D$ and $L(\mathsf{T}_n) = L$ for all n, such that $\ell_n \to 0$. Then $\lambda_1(\mathsf{T}_n)$ is greater than and converges to κ^2, where κ is the first positive solution of*

$$\cos\left(\kappa\frac{D}{2}\right) = \kappa\frac{L-D}{2}\sin\left(\kappa\frac{D}{2}\right).$$

Proof. Assume that the SSD graph is formed by one edge of length d_n and $2n$ "short" edges of lengths ℓ_n attached to two vertices as shown in Figure 6. Elementary calculations allow one to determine d_n and ℓ_n through D and L

$$\begin{cases} D &= 2\ell_n + d_n \\ L &= 2n\ell_n + d_n \end{cases} \Rightarrow \begin{cases} \ell_n &= \dfrac{L-D}{2(n-1)} \\ d_n &= \dfrac{nD-L}{n-1} \end{cases}.$$

We are interested in the case of large n, when $d_n \gg \ell_n$. The lowest eigenvalue is $\lambda_0 = 0$ with the eigenfunction $\psi_0 \equiv 1$; for sufficiently large n the first nontrivial eigenfunction is antisymmetric with respect to the reflection in the middle point of the dumbbell, and hence zero at that point. By symmetry, it will also attain the same values on all smaller edges attached to each of the vertices, and the Kirchhoff condition implies its normal derivative is zero at every boundary vertex. Taking into account that the function is continuous and the sum of normal derivatives at the inner vertices is zero, we derive the following dispersion equation

$$k\cot\left(k\frac{nD-L}{2(n-1)}\right) = nk\tan\left(k\frac{L-D}{2(n-1)}\right).$$

We are interested in its solution in the interval $0 < k < \dfrac{\pi}{D}$. Multiplying the equation by $\sin\left(k\frac{nD-L}{2(n-1)}\right)\cdot\cos\left(k\frac{L-D}{2(n-1)}\right)$ and using trigonometric identities, this equation can be written in an equivalent form

$$g^n(k) := (1+n)\cos\left(k\frac{D}{2}\right) - (n-1)\cos\left(k\left(\frac{D}{2} - \frac{L-D}{n-1}\right)\right) = 0.$$

The function $g^n(k)$ is obviously positive when $k = 0$ and k_1 is its first zero on the positive semi-axis. Using the fact that the graph of the cosine function on the interval $(0, \pi/2)$ lies below its tangent line, we have

$$\cos\left(k\left(\frac{D}{2} - \frac{L-D}{n-1}\right)\right) \leq \cos\left(k\frac{D}{2}\right) + k\frac{L-D}{n-1}\sin\left(k\frac{D}{2}\right)\cdot,$$

which in turn implies that

$$\begin{aligned} g^n(k) &\geq (1+n)\cos\left(k\frac{D}{2}\right) - (n-1)\left(\cos\left(k\frac{D}{2}\right) + k\frac{L-D}{n-1}\sin\left(k\frac{D}{2}\right)\right) \\ &= 2\left(\cos\left(k\frac{D}{2}\right) - k\frac{L-D}{2}\sin\left(k\frac{D}{2}\right)\right). \end{aligned}$$

It follows that k_1 lies to the right of the lowest positive solution to the equation

$$g^\infty(k) := \cos\left(k\frac{D}{2}\right) - k\frac{L-D}{2}\sin\left(k\frac{D}{2}\right) = 0.$$

On the other hand k_1 approaches the first zero of $g^\infty(k)$ as $n \to \infty$, since g^n converges to g^∞ pointwise. □

Proof of Theorem 7.2. The proof of (7.2) follows directly from combining Lemmata 7.5 and 7.6. To see that (7.3) follows from (7.2), we merely note that since $\cos x \geq 1 - x^2/2$ and $\sin x \leq x$ for all $x \geq 0$, it follows from (7.2) that $2D(L-2D)\kappa^2 \geq 1 - (2\kappa D)^2/2$; rearranging yields $\kappa^2 \geq 1/(2DL - 2D^2)$. □

8. Concluding remarks

It is easy to find perturbations of a graph which have an arbitrarily small effect on the first eigenvalue but which change the combinatorics of the graph enormously; we saw this phenomenon in action in Example 4.1. This is an easy but essential consequence of the principle that the eigenvalues depend continuously on changes in length of a given edge, including when that edge is contracted to a point, cf. the results in [DPR14, § 4]. The moral is that, at least on a small or local scale, the analytic properties of a graph are far more important for determining λ_1 than its combinatorial ones; in particular, quantum and combinatorial graphs can be expected to diverge considerably in their heuristic behaviour. This intuitive rule has been – we believe – underpinned by our results throughout this article. Nevertheless, we expect that other global structural properties of quantum graphs are also essential, even though our investigations have only touched on these aspects peripherally.

Let us summarise the best bounds we currently have:

parameter(s) \ λ_1	available upper bound	is it sharp?
L, E	$\dfrac{\pi^2 E^2}{L^2}$	yes, attained on a pumpkin graph (3.4)
D, V	$\dfrac{\pi^2}{D^2}(V+1)^2$	only if $V = 1$, on a loop
D, E	$\dfrac{4\pi^2 E^2}{D^2}$	only if $E = 1$, on a loop
D, L	$\dfrac{\pi^2(4L-3D)}{D^3}$	yes, attained on a path graph (3.1)

and

parameter(s) \ λ_1	available lower bound	is it sharp?
L	$\dfrac{\pi^2}{L^2}$	yes, attained on a path graph (3.1); V, E cannot improve it (Example (4.1))
D, E	$\dfrac{\pi^2}{D^2E^2}$	only if $E = 1$, on a path graph
D, L	$\dfrac{1}{DL}$	unknown, but cf. Remark 7.3

Of course, this should be viewed as being only a starting point: apart from the question of finding the optimal bounds and optimisers in many of the above cases, there are many other natural properties of a graph one could consider, as well as the higher eigenvalues, and the spectral problems which arise if one replaces the natural (Kirchhoff) boundary conditions with more general conditions on the vertices, such as more general δ or perhaps δ' couplings, cf. [BK13], or impose Dirichlet condition on the vertices of degree one.

Remark 8.1. In the introduction we observed that our estimates on λ_1 can be turned into estimates on the spectral gap α_1 of the normalised Laplacian, and vice versa, by the formula (1.1). Remarkably, some estimates obtained by studying quantum graphs turn into estimates on α_1 that currently seem to be unavailable by purely combinatorial methods.

Let us write such estimates down for the case of the *unweighted* normalised Laplacian, which corresponds to equilateral quantum graphs with edges of unit length (in which case we have $L = E$). It follows from (1.1) that

$$\alpha_1 = 1 - \cos\sqrt{\lambda_1} \qquad \text{whenever } \lambda_1 < \pi^2 \ ,$$

hence α_1 is a monotonically increasing function of λ_1 in the range $\lambda_1 \in [0, \pi^2)$.

For instance, from our first upper bound $0 \le \lambda_1 \le \frac{\pi^2 E^2}{L^2} = \pi^2$ we deduce the well-known fact that α_1 always lies in $[0, 2]$ – in fact, so do *all* eigenvalues of the normalised Laplacian. Furthermore, from our results in Sections 6 and 7, we can obtain the following upper bounds:

parameters \ α_1	available upper bound	holds if
D_{V}, V	$1 - \cos\dfrac{\pi}{D_{\mathsf{V}}}(V+1)$	$V + 1 \le D_{\mathsf{V}}$
D_{V}, E	$1 - \cos\left(\dfrac{\pi}{D_{\mathsf{V}}}\sqrt{\dfrac{4E}{D_{\mathsf{V}}} - 3}\right)$	$\sqrt{\dfrac{4E}{D_{\mathsf{V}}} - 3} \le D_{\mathsf{V}}$

The former bound can only hold for paths, for which however the second bound is sharper (and in fact tight). Here we need the combinatorial diameter $D_{\mathsf{V}} \le D$ of Remark 5.5, since the diameter D is meaningless in the case of combinatorial graphs.

For equilateral quantum graphs with unit side length, which are the only ones we need to consider, we necessarily have $D \le D_{\mathsf{V}} + 1$, since points realising the diameter can be at distance no more than $1/2$ from a vertex. Hence we have the following estimates, which are valid for all graphs:

parameter \ α_1	available lower bound
E	$1-\cos\frac{\pi}{E}$
D_{V}, E	$1-\cos\frac{\pi}{(D_{\mathsf{V}}+1)E}$
D_{V}, E	$1-\cos\frac{1}{\sqrt{(D_{\mathsf{V}}+1)E}}$

The first bound is always better than the second (and in fact tight for paths), while the third – which can be improved slightly by using (7.2) rather than the simpler (7.3) – is better than the first if $E/(D_{\mathsf{V}}+1)\geq\pi^2$ (e.g., for all complete graphs on more than six vertices). Both the first and the third bound are asymptotically (in E) tight for cycles and hypercube graphs, cf. [Chu97, Examples 1.4–1.6].

By estimating cos by a truncated power series expansion, we can summarise our bounds as follows:

$$\left.\begin{array}{r}\frac{\pi^2}{2E^2}-\frac{\pi^4}{24E^4}<1-\cos\frac{\pi}{E}\\ \frac{1}{2(D_{\mathsf{V}}+1)E}-\frac{1}{24(D_{\mathsf{V}}+1)^2E^2}<1-\cos\frac{1}{\sqrt{(D_{\mathsf{V}}+1)E}}\end{array}\right\}\leq\alpha_1\leq 1-\cos\left(\frac{\pi}{D_{\mathsf{V}}}\sqrt{\frac{4E}{D_{\mathsf{V}}}-3}\right)<\frac{\pi^2}{D_{\mathsf{V}}^2}\frac{4E-3D_{\mathsf{V}}}{D_{\mathsf{V}}}\ .$$

They can be compared e.g. with the estimates

$$\left.\begin{array}{r}\frac{1}{2D_{\mathsf{V}}E}\\ \frac{1}{(\deg_{\max}+1)\deg_{\max}^{\lceil\deg_{\max}/2\rceil-1}}\end{array}\right\}\leq\alpha_1\leq\left\{\begin{array}{l}\frac{V}{V-1}\\ 1-2\sqrt{\frac{\deg_{\max}-1}{\deg_{\max}}}\left(1-\frac{2}{D_{\mathsf{V}}}\right)+\frac{2}{D_{\mathsf{V}}}\end{array}\right.$$

in (2.3), [Chu97, Lemma 1.9 and Lemma 1.14] and [BC13]: the first upper bound being tight for complete graphs and asymptotically (in V) tight for stars and complete bipartite graphs, cf. [Chu97, Examples 1.1–1.3].

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