

IMPEDIMENTS TO DIFFUSION IN QUANTUM GRAPHS: GEOMETRY-BASED UPPER BOUNDS ON THE SPECTRAL GAP

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ABSTRACT. We derive several upper bounds on the spectral gap of the Laplacian on compact metric graphs with standard or Dirichlet vertex conditions. In particular, we obtain estimates based on the length of a shortest cycle (girth), diameter, total length of the graph, as well as further metric quantities introduced here for the first time, such as the avoidance diameter. Using known results about Ramanujan graphs, a class of expander graphs, we also prove that some of these metric quantities, or combinations thereof, do not deliver any spectral bounds with the correct scaling.

1. INTRODUCTION AND STATEMENT OF THE MAIN RESULTS

Quantum graphs, a common term for differential operators in function spaces defined on metric graphs, often arise as limits or approximations of physical problems on thin structures. They have been used to study evolution of free electrons in molecules [31], light propagation in optical waveguides (both analytically and experimentally) [20, 21], heat and water flow in branched pathways [26, 33], Brownian motions in ramified structures [16], vibration in steel frames [19, 25, 4], and many other applied questions.

The most well-understood operator is the Laplacian with standard (alternatively known as Neumann–Kirchhoff) as well as Dirichlet vertex conditions^[1]. On a connected graph and with no Dirichlet vertices present, relaxation time of a diffusive process to equilibrium is controlled by the first non-zero eigenvalue, which we denote by $\lambda_2^N > \lambda_1^N = 0$. In the presence of at least one Dirichlet vertex^[2] a corresponding role is played by the first eigenvalue $\lambda_1^D > 0$, which controls dissipation of heat from the graph. These are the eigenvalues that we focus

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¹Basic definitions in the theory of Laplacian on metric graphs, as well as some results we use in the proofs of this paper, are collected in Appendix A, where we also fix our notation.

²Here and in the following, in a slight abuse of notation we will sometimes refer to properties of the (Dirichlet or standard) Laplacian as properties of $\mathcal{G}$, e.g. speak of Dirichlet vertices of $\mathcal{G}$.

on in this paper, aiming to give upper bounds in terms of certain metric characteristics of the graph.

This study is motivated by the following question: what (geo)metric feature can, on its own, act as an impediment to diffusion? To illustrate this question, consider the following.

Example 1.1. The simple estimates below only depend on the fact that certain specific metric graphs are (or are not) embedded in the given ambient metric graph $\mathcal{G}$ with vertex set $\mathbf{V}$ and edge lengths ℓ_e , $e \in \mathbf{E}$:

- (1) If $\ell_{\max}$ is the length of the longest edge of $\mathcal{G}$, then

$$(1.1) \quad \lambda_2^N \leq \frac{4\pi^2}{\ell_{\max}^2}.$$

For a graph with Dirichlet vertices, the analogous estimate reads

$$(1.2) \quad \lambda_1^D \leq \frac{\pi^2}{\ell_{\max}^2}.$$

- (2) Assume $\mathcal{G}$ contains neither a complete graph on five vertices ($\mathbf{K}_5$), nor a complete bipartite graph on $3 + 3$ vertices ($\mathbf{K}_{3,3}$), as an induced subgraph³. Then

$$(1.3) \quad \lambda_2^N \leq \frac{16\pi^2}{L} \max_{v \in \mathbf{V}} \sum_{e \in \mathbf{E}_v} \frac{1}{\ell_e},$$

where L is the total length of $\mathcal{G}$ and $\mathbf{E}_v$ is the set of edges incident with v .

- (3) If a cycle $\mathbf{c}$ is included in $\mathcal{G}$ as an induced subgraph, and if (the closure of) each connected component of $\mathcal{G} \setminus \mathbf{c}$ meets $\mathbf{c}$ at *exactly one point*, then

$$(1.4) \quad \lambda_2^N(\mathcal{G}) \leq \frac{4\pi^2}{s^2}$$

where s denotes the length of $\mathcal{S}$. Actually, the same result holds if $\mathbf{c}$ is a so-called *pumpkin graph* (see Figure 1 below), and s is the length of the shortest cycle in it.

The first inequality is standard and will be shown in Section 2.2 below; inequality (1.3) has been proved in [28, Theorem 3.11] and depends on the fact that, by Kuratowski's Theorem, a graph is planar if and only if it does not include any subgraph isomorphic to $\mathbf{K}_5$ or $\mathbf{K}_{3,3}$ (whereas [28, Theorem 4.8] suggests that metric graphs of higher genus have higher λ_2^N); finally, the proof of inequality (1.4) is based on the principle that attaching pendants to a graph lowers its eigenvalues (see [5, Theorem 3.10]), together with an estimate on the eigenvalues of the pumpkin graph. This inequality also has a counterpart for higher eigenvalues.

The above examples suggest that having to cross a long edge, or an “independent” cycle, retards convergence to equilibrium. We are going to make this observation more systematic. Not to be overly ambitious, we can try to use the length of the *shortest cycle*⁴ in place of $\ell_{\max}$ in (1.1): in the case of standard vertex conditions, it is to be expected that the presence of a “minimal” cycle of a given length should, like a long edge, be an obstacle to rapid convergence.

³That is, a subgraph formed from a subset of the vertices of $\mathcal{G}$ and all the edges of $\mathcal{G}$ that connect the vertices in this subset.

⁴This length is known in combinatorial graph theory as the girth, see also [5, Section 6].

In a graph with Dirichlet vertices, which act as heat sinks at any point at which they are placed, the distance to the nearest Dirichlet vertex becomes important, and the shortest distance between two such vertices plays the same role as the minimal cycle length. For this reason, for the purpose of defining girth (and only for this purpose, cf. Remark [A.1](#)), we identify all Dirichlet vertices; this leads to the following modified definition:

Definition 1.2. The *girth* $s = s(\mathcal{G})$ of a compact, connected graph $\mathcal{G}$ shall be given by

$$\min\{|\mathfrak{c}| : \mathfrak{c} \subset \mathcal{G} \text{ is a cycle in } \mathcal{G}'\},$$

where $\mathcal{G}'$ is the metric graph obtained from $\mathcal{G}$ by identifying (or “gluing together”) all Dirichlet vertices of $\mathcal{G}$, if any are present. The girth is defined to be zero if $\mathcal{G}'$ is a tree. Here $|\mathcal{H}|$ denotes the total length of a given subset $\mathcal{H}$ of $\mathcal{G}$.

1.1. Estimates based on girth. If the graph has at least one Dirichlet vertex, girth by itself is indeed enough to yield an upper bound.

Theorem 1.3. *If a compact, connected graph $\mathcal{G}$ has at least one Dirichlet vertex, then*

$$(1.5) \quad \lambda_1^D(\mathcal{G}) \leq \frac{\pi^2}{s^2}.$$

Equality is attained if and only if $\mathcal{G}$ is an equilateral star graph with $n \geq 2$ edges of length $s/2$ with Dirichlet conditions at all degree one vertices.

(The case of a Dirichlet interval of length s corresponds to $n = 2$.)

We believe Theorem [1.3](#) to be new even in the case where $\mathcal{G}$ is a tree equipped with Dirichlet conditions at all leaves. This may be contrasted with [\[29, Eq. \(1.4\)\]](#), which shows that for a tree graph, the diameter alone is enough to control λ_2^N .

The result of Theorem [1.3](#) can also be immediately extended to graphs with a particular reflection symmetry.

Corollary 1.4. *Suppose the compact, connected graph $\mathcal{G}$ is obtained from two copies of another connected graph, $\widehat{\mathcal{G}}$, by pairwise gluing of finitely many pairs of the duplicated vertices. If $\mathcal{G}$ has girth s , then the spectral gap of the Laplacian with standard vertex conditions satisfies*

$$(1.6) \quad \lambda_2^N(\mathcal{G}) \leq \frac{4\pi^2}{s^2}.$$

Equality is attained if $\mathcal{G}$ is an equilateral pumpkin (watermelon) graph (see Figure [1](#)).

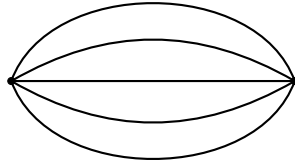


FIGURE 1. An m -pumpkin graph (a.k.a. m -watermelon graph) consists of some number $m \geq 2$ of parallel edges stretched between two vertices; here $m = 5$. It is equilateral if all edges have the same length.

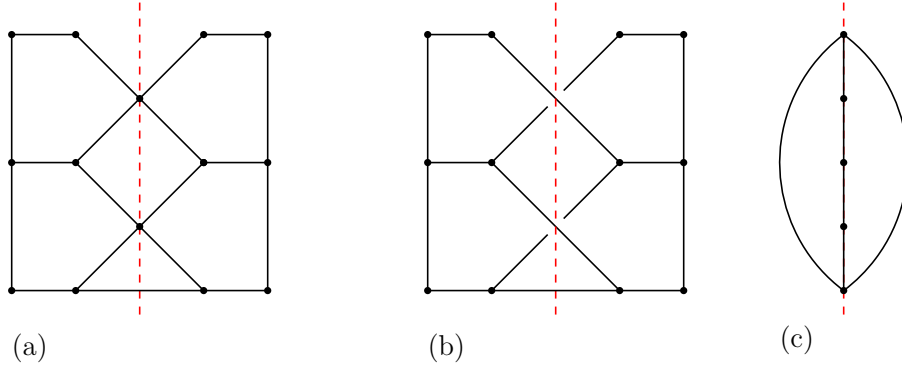


FIGURE 2. (a) An example of a graph that has the symmetry sufficient for (1.6) to hold (note that we can place a dummy vertex in the middle of the lowest edge). (b) A graph with a reflection symmetry that cannot be obtained by gluing pairs of duplicated vertices. (c) A graph with a symmetry that would require gluing along entire edges.

Note that $\mathcal{G}$ does not have any Dirichlet vertices, and so its girth coincides with the length of its shortest cycle, which either comes from a cycle in $\hat{\mathcal{G}}$ or from a cycle created in the gluing process. Figure 2 presents an example of $\hat{\mathcal{G}}$ covered by Corollary 1.4, and examples of symmetric graphs which are not covered.

Even without such symmetry, one could reasonably expect to use bound (1.5) on each of the nodal domains of the second standard Laplacian eigenfunction (generically, there are exactly two!) to obtain (1.6) for a general graph. Furthermore, (1.6) can be shown to hold for many other classes of “highly connected” graphs, including *pumpkin chains* (finite sequences of pumpkin graphs glued together at their vertices to form a chain), equilateral complete graphs on at least three edges (see [14, Section 3]) and also any graphs which contain an “independent” cycle, see Example 1.1(3).

It is thus all the more surprising that the girth alone is *not* always enough to bound λ_2^N from above, as the following examples show.

Example 1.5. We first provide a counterexample to the validity of (1.6) with the symmetry restriction dropped. We consider Tutte’s 12-cage, a 3-regular graph on 126 vertices with girth 12 (cf., e.g., [12, p. 283]): the second largest eigenvalue ν_2 of its adjacency matrix is known to be $\sqrt{6}$. A formula of von Below [2, Theorem, p. 320], which relates the eigenvalues of an equilateral metric graph to the eigenvalues of the normalized Laplacian, can be adapted to the eigenvalues of the adjacency matrix in the k -regular case, giving

$$(1.7) \quad \lambda_2^N(\mathcal{G}) = \left(\arccos(\nu_2/k) \right)^2.$$

We conclude that the spectral gap of the equilateral quantum graph built upon Tutte’s 12-cage is $\left(\arccos(\sqrt{6}/3) \right)^2 \approx 0.379$, whereas the right-hand side of (1.6) is $4\pi^2/144 \approx 0.274$.

We remark that the automorphism group of Tutte’s 12-cage is known to be a semi-direct product of $\text{PSU}(3, 3)$ with the cyclic group $\mathbf{Z}_2$; in particular the 12-cage graph does have a reflection symmetry. It is far from obvious that this symmetry does not satisfy the assumptions of Corollary 1.4.

Example 1.6. Basic scaling arguments show that if an estimate of the form $\lambda_2^N(\mathcal{G}) \leq Cs^\alpha$ is to exist, the power α must be equal to -2 . We now show that such estimate is in fact impossible for any C . A counterexample is given by the class of equilateral metric graphs built out of combinatorial k -regular graphs known as Ramanujan graphs, which were introduced in [22]. The second largest adjacency matrix eigenvalue ν_2 of a Ramanujan graph is, by definition, no larger than $2\sqrt{k-1}$ (the largest one always being k , since the graph is k -regular), therefore

$$(1.8) \quad \lambda_2^N(\mathcal{G}) \geq (\arccos(2\sqrt{k-1}/k))^2,$$

again by (1.7). It is established in [22, 8], that for infinitely many values of k , Ramanujan graphs on arbitrarily many vertices $|\mathbf{V}|$ can be constructed and that the asymptotic equality

$$(1.9) \quad s \sim \frac{4}{3} \log_{k-1}(|\mathbf{V}|) \quad \text{as } |\mathbf{V}| \rightarrow \infty$$

holds for these graphs. Combining (1.8) and (1.9) we see that the estimate $\lambda_2^N(\mathcal{G}) = \mathcal{O}(s^{-2})$ cannot hold in general, and thus no upper bound on λ_2^N in terms of girth alone is possible.

Remark 1.7. A more recent construction of Ramanujan graphs uses the theorem of [23] which, expressed in terms of metric graphs, states that any equilateral k -regular graph $\mathcal{G}$ has a *signing* $\mathcal{G}_S$ such that its lowest eigenvalue satisfies

$$(1.10) \quad \lambda_1^S(\mathcal{G}_S) \geq (\arccos(2\sqrt{k-1}/k))^2.$$

A signing is, in this context, a choice of edges $\{e_j\}$ on which we impose anti-periodic conditions (see (A.2) and Remark A.2). Let ψ be the eigenfunction corresponding to λ_1^S of a graph $\mathcal{G}_S$ satisfying (1.10). It is easy to see that the zeros of the function ψ are located exactly on the anti-periodic cycles of the graph $\mathcal{G}_S$, i.e. the cycles on which an odd number of anti-periodic conditions have been imposed. Imposing Dirichlet conditions at the locations of the zeros we obtain a graph $\mathcal{G}^D$ with only standard and Dirichlet conditions (by gauge invariance). Then $|\psi|$ is a non-negative eigenfunction of $\mathcal{G}^D$ and thus the ground state (cf. Theorem A.3); hence $\lambda_1^D(\mathcal{G}^D) = \lambda_1^S(\mathcal{G}_S)$. The girth s of $\mathcal{G}^D$ is equal to the least of the two quantities: the length of the shortest cycle of $\mathcal{G}$ and the shortest distance between two zeros of ψ . Theorem 1.3 then implies the estimate

$$(1.11) \quad s \leq \frac{\pi}{\arccos(2\sqrt{k-1}/k)}.$$

The right-hand side is less than 10 when $k = 3$ and less than 3 when $k \geq 15$. Intuitively, (1.11) shows that the signing producing (1.10) on a graph with large girth must be fairly dense (to guarantee a dense set of zeros of ψ).

1.2. Estimates based on total length and one further metric quantity. Having seen that the “single metric quantity estimates” of the type given in Theorem 1.3 are rather subtle, we will now present some estimates that use a combination of two metric quantities while having the correct overall scaling $(\text{length})^{-2}$. For similar estimates involving other quantities, we refer, e.g., to [1, 5, 10, 15, 28, 30] and the references therein.

Proposition 1.8. *If the compact, connected metric graph $\mathcal{G}$ has girth s and total length L , then the spectral gap of the Laplacian with standard vertex conditions satisfies*

$$(1.12) \quad \lambda_2^N(\mathcal{G}) < \frac{48L}{s^3}.$$

We remark that s together with L are also sufficient to bound λ_2^N from below, too [5, Corollary 6.7]. The idea behind estimate (1.12) (explained in Section 2.2) is to use a homotopy between two test functions built around a minimal cycle; this idea readily generalizes to combinations of L with other metric quantities.

Recall that the *diameter* D of a metric graph $\mathcal{G}$ is the maximal distance between any two points on the graph,

$$(1.13) \quad D = \max_{x_1, x_2 \in \mathcal{G}} \text{dist}(x_1, x_2).$$

Theorem 1.9. *If the compact, connected metric graph $\mathcal{G}$ has diameter D and total length L , then the spectral gap of the Laplacian with standard vertex conditions satisfies*

$$(1.14) \quad \lambda_2^N(\mathcal{G}) < \frac{24L}{D^3}.$$

Remark 1.10. (1) It has been known since [14] that for a general $\mathcal{G}$ one cannot bound λ_2^N in terms of D alone. The same work [14, Theorem 7.1] established the estimate

$$(1.15) \quad \lambda_2^N(\mathcal{G}) \leq \frac{4\pi^2}{D^2} \left(\frac{L}{D} - \frac{3}{4} \right).$$

We also mention a generalization of Rohleder’s diameter-based estimate [29], observed in [13], namely

$$(1.16) \quad \lambda_2^N(\mathcal{G}) \leq \frac{4\pi^2}{D^2} \left(\frac{1 + \beta}{2} \right)^2,$$

where β is the first Betti number, i.e., $\beta := |E| - |V| + 1$. One can easily construct examples which show that none of the estimates (1.12), (1.14), (1.15) or (1.16) is implied by a combination of the others.

- (2) The Ramanujan graphs encountered in Example 1.6 also show that we cannot in general improve (1.12) to $\lambda_2^N(\mathcal{G}) \lesssim D/s^3$. The conclusion is obtained by combining the girth estimate (1.9) with the estimate $D \leq (2 + \epsilon) \log_{k-1}(|V|)$ established in [22] (see also [32] for more precise diameter asymptotics in subfamilies of the LPS Ramanujan graphs).

We now introduce some generalizations of the diameter, which “interpolate” between D and s (see (1.21) and Table 1). We have not seen these generalization in the existing literature, but they arise naturally from the homotopy argument. First, the *triameter* T of a metric graph $\mathcal{G}$ is

$$(1.17) \quad T := \max_{x_1, x_2, x_3 \in \mathcal{G}} \min_{j \neq k} \text{dist}(x_j, x_k),$$

i.e. the maximal pairwise separation among any *three* points on $\mathcal{G}$.

Theorem 1.11. *If the compact, connected graph $\mathcal{G}$ has triiameter T and total length L , then the spectral gap of the Laplacian with standard vertex conditions satisfies*

$$(1.18) \quad \lambda_2^N(\mathcal{G}) < \frac{12L}{T^3}.$$

Second, we introduce the “avoidance diameter”, which, intuitively, measures how far apart two points can remain while exchanging places. Let $\mathbb{S}^1$ be the unit circle in $\mathbb{C}$ and let Γ

denote the class of injective continuous maps from $\mathbb{S}^1$ to $\mathcal{G}$. Then the *avoidance diameter* is defined as

$$(1.19) \quad A := \max_{\gamma \in \Gamma} \min_{t \in \mathbb{S}^1} \text{dist}(\gamma(-t), \gamma(t)).$$

In the case of trees, $\Gamma = \emptyset$, and we set $A = 0$.

Theorem 1.12. *If the compact, connected graph $\mathcal{G}$ has avoidance diameter A and total length L , then*

$$(1.20) \quad \lambda_2^N(\mathcal{G}) < \frac{6L}{A^3}.$$

Remark 1.13. The metric quantities used in this section satisfy

$$(1.21) \quad \frac{s}{2} \leq A \leq D \quad \text{and} \quad \frac{s}{3} \leq T \leq D.$$

Proposition 1.8 is now an immediate corollary of Theorem 1.12.

Example 1.14. For each inequality in (1.21) one can construct examples of metric graphs where that inequality is strict (see Table 1).

$\mathcal{G}$	s	A	T	D	Best estimate
path graph	0	0	$\frac{L}{2}$	L	(1.14): D
equilateral figure-8 graph	$\frac{L}{2}$	$\frac{L}{4}$	$\frac{L}{4}$	$\frac{L}{2}$	(1.14): D
figure-8 graph with lengths $\ell_1 > \ell_2 \geq \ell_1/2$	ℓ_2	$\frac{\ell_1}{2}$	$\frac{\ell_1}{2}$	$\frac{L}{2}$	(1.20): A
equilateral flower graph on k edges, $k \geq 3$	$\frac{L}{k}$	$\frac{L}{2k}$	$\frac{L}{k}$	$\frac{L}{k}$	(1.18): T
equilateral star graph on k edges, $k \geq 3$	0	0	$\frac{2L}{k}$	$\frac{2L}{k}$	(1.18): T
equilateral pumpkin graph on k edges, $k \geq 3$	$\frac{2L}{k}$	$\frac{L}{k}$	$\frac{L}{k}$	$\frac{L}{k}$	(1.12) and (1.20): s, A

TABLE 1. A comparison of the various metric quantities defined in Section 1.2. We also show which estimate among those presented in Section 1.2 is the sharpest in each case.

Remark 1.15. Let $\mathbf{G}$ be an unweighted combinatorial graph without loops or parallel edges, and consider the corresponding metric graph $\mathcal{G}$ with all edges having length 1. The *normalized Laplacian* associated with $\mathbf{G}$ is the $|\mathbf{V}| \times |\mathbf{V}|$ -matrix whose diagonal entries are 1 and whose off-diagonal $(\mathbf{v}, \mathbf{w})$ -entry is $-(\deg(\mathbf{v}) \deg(\mathbf{w}))^{-1/2}$, where $\deg(\mathbf{v})$ denotes the degree of vertex $\mathbf{v}$; see [11, Section 1.2]. It now follows from [2, Theorem, page 320], already mentioned in Example 1.5, that the lowest positive eigenvalue λ_2 of the standard Laplacian satisfies

$$(1.22) \quad \alpha_2 = 1 - \cos \sqrt{\lambda_2} \quad \text{whenever } \lambda_2 < \pi^2,$$

where α_2 is the lowest positive eigenvalue of the normalized Laplacian. The quantities s, D, T all have a natural version $s_{\mathbf{G}}, D_{\mathbf{G}}, T_{\mathbf{G}}$ for combinatorial graphs, which are no larger than their counterpart on metric graphs. Accordingly, estimates (1.6), (1.12), (1.14), and (1.18) all imply corresponding estimates on α_2 :

- $\alpha_2 \leq 1 - \cos \frac{2\pi}{s_{\mathbf{G}}}$ whenever $\mathbf{G}$ is obtained from two copies of another connected graph, $\hat{\mathbf{G}}$, by pairwise gluing of pairs of the duplicated vertices;

- $\alpha_2 < 1 - \cos \sqrt{\frac{48|E|}{s_G^3}}$ whenever $\frac{48|E|}{s_G^3} < \pi^2$;
- $\alpha_2 < 1 - \cos \sqrt{\frac{24|E|}{D_G^3}}$ whenever $\frac{24|E|}{D_G^3} < \pi^2$;
- $\alpha_2 < 1 - \cos \sqrt{\frac{12|E|}{T_G^3}}$ whenever $\frac{12|E|}{T_G^3} < \pi^2$.

To the best of our knowledge, upper estimates on α_2 based on the total number of edges, on girth, diameter (and of course on triameter, which we have introduced in this paper) were not previously known.

2. PROOFS

2.1. Proof of the estimates in Section 1.1. In this section we prove Theorem 1.3 and Corollary 1.4.

Proof of Theorem 1.3. We want to show that if $\mathcal{G}$ has at least one Dirichlet vertex, then the first non-trivial eigenvalue satisfies the bound (1.5), which we repeat here for convenience,

$$\lambda_1^D(\mathcal{G}) \leq \frac{\pi^2}{s^2}.$$

Due to our definition of the girth, the statement of the theorem is vacuous if $\mathcal{G}$ has no cycles and only one Dirichlet point. Henceforth we exclude such graphs from consideration. Then we may assume that vertices of $\mathcal{G}$ have degree one if and only if they are equipped with the Dirichlet condition. Indeed, we may remove any pendant edges with standard conditions since this operation increases the eigenvalues (see [18, Theorem 2] or [5, Theorem 3.10]); a Dirichlet condition imposed at a vertex of degree d separates the vertex into d copies.

The proof will be based on the notion (see [5]) of *cutting through vertices along the eigenfunction* ψ associated with λ_1^D , that is, finding a simple subgraph $\tilde{\mathcal{G}}$ within $\mathcal{G}$, which, when cut out of $\mathcal{G}$ and equipped with non-positive δ -potentials determined by ψ , will have its first eigenvalue equal to $\lambda_1^D(\mathcal{G})$ (and its eigenfunction will be $\psi|_{\tilde{\mathcal{G}}}$). The graph $\tilde{\mathcal{G}}$ can then be compared directly with an interval or a tadpole (lasso) without δ -potentials, yielding the inequality.

We recall that $\psi \geq 0$ has no local minima and that the maxima are isolated because $\psi(x) > 0$ implies

$$(2.1) \quad \psi''(x) = -\lambda_1^D(\mathcal{G})\psi(x) < 0.$$

For the purpose of this proof all internal (to an edge) local maxima are to be considered vertices. Moreover, without loss of generality we assume there are no other vertices of degree two, see Remark A.1. The process of finding the subgraph $\tilde{\mathcal{G}}$ uses the following notion of *serious points* with respect to the eigenfunction ψ .

Definition 2.1. Given a metric graph $\mathcal{G}$ and a function $0 \leq f \in D(\Delta)$, a vertex $\mathbf{v} \in \mathbf{V}$ of degree $d \geq 2$ shall be called a *serious point* (of the function f) if $f(\mathbf{v}) \neq 0$ and there exist at least two edges $\mathbf{e}_1, \mathbf{e}_2 \sim \mathbf{v}$ such that

$$(2.2) \quad \partial_\nu f|_{\mathbf{e}_i}(\mathbf{v}) \geq 0, \quad i = 1, 2.$$

Here the normal derivatives are taken pointing *into* the vertex.

We remark that by the Kirchhoff condition, see (A.1), every vertex is incident with *at least one* edge satisfying condition (2.2).

Any local maximum of f (as defined in the obvious way) is serious, therefore the set of serious points of ψ is a non-empty finite subset of the compact graph $\mathcal{G}$. Let $\mathbf{v}_0 \in \mathbf{V}(\mathcal{G})$ denote a lowest serious point, that is, $\mathbf{v}_0$ is serious and $0 < \psi(\mathbf{v}_0) \leq \psi(\mathbf{v})$ for every serious point $\mathbf{v} \in \mathbf{V}(\mathcal{G})$ of ψ . Denote by $\mathbf{e}_1, \mathbf{e}_{-1}$ any two edges incident with $\mathbf{v}_0$ such that $\partial_\nu \psi|_{\mathbf{e}_{\pm 1}}(\mathbf{v}_0) \geq 0$.

Now denote by $\mathbf{v}_1$ the other vertex incident with $\mathbf{e}_1$. If it is a Dirichlet vertex, we stop. Otherwise, by concavity (2.1) we have $\psi(\mathbf{v}_1) < \psi(\mathbf{v}_0)$; hence, $\mathbf{v}_1$ is not serious. We denote by $\mathbf{e}_2$ the unique edge $\mathbf{e}_2$ adjacent to $\mathbf{v}_1$ such that $\partial_\nu \psi|_{\mathbf{e}_2}(\mathbf{v}_1) \geq 0$. Repeating the process with $\mathbf{e}_2$ and so on, we obtain a path $\mathbf{e}_1, \mathbf{v}_1, \mathbf{e}_2, \dots, \mathbf{e}_m$ terminating at a Dirichlet vertex. We perform the same for $\mathbf{e}_{-1}$, constructing another path $\mathbf{e}_{-1}, \mathbf{v}_{-1}, \mathbf{e}_{-2}, \dots, \mathbf{e}_{-n}$ through $\mathcal{G}$, also terminating at a Dirichlet vertex. We define the graph $\tilde{\mathcal{G}}$ to be the union of these two paths. It is either a path in $\mathcal{G}$ joining two Dirichlet vertices, or at some point the two paths leading from $\mathbf{e}_1$ and $\mathbf{e}_{-1}$ meet and $\tilde{\mathcal{G}}$ is a tadpole ending at a single Dirichlet point, see Figures 3 and 4.

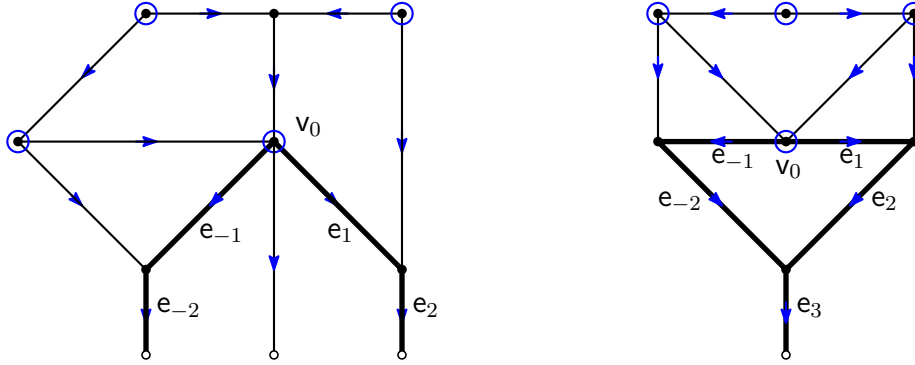


FIGURE 3. Examples of metric graphs with Dirichlet vertices (marked as small empty disks) and with a schematic depiction of the first eigenfunction as a gradient flow (blue arrows). The serious points are now the vertices with at least two outward-pointing arrows; they are circled in blue. The paths that are constructed in the course of the proof of Theorem 1.3 are shown as thicker edges.

In the first case, the path is at least of length s ; in the second, the cycle of the tadpole is of length at least s .

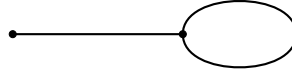


FIGURE 4. A *tadpole* (or *lasso*) consists of a cycle attached to a pendant edge. In the proof the degree one vertex will be equipped with a Dirichlet condition.

Now we wish to cut $\tilde{\mathcal{G}}$ out of $\mathcal{G}$ “along” the eigenfunction ψ : at each non-Dirichlet vertex $\mathbf{v}_i$ of $\tilde{\mathcal{G}}$ ($i = 0, \pm 1, \pm 2, \dots$), we add a δ -condition of the form

$$\sum_{\substack{\mathbf{e} \sim \mathbf{v}_i \\ \mathbf{e} \in \tilde{\mathcal{G}}}} \partial_\nu u|_{\mathbf{e}}(\mathbf{v}_i) + \gamma_{\mathbf{v}_i} u(\mathbf{v}_i) = 0,$$

where

$$(2.3) \quad \gamma_{\mathbf{v}_i} := \frac{1}{\psi(\mathbf{v}_i)} \sum_{\substack{\mathbf{e} \sim \mathbf{v}_i \\ \mathbf{e} \in \mathcal{G} \setminus \tilde{\mathcal{G}}}} \partial_\nu \psi|_{\mathbf{e}}(\mathbf{v}_i) = -\frac{1}{\psi(\mathbf{v}_i)} \sum_{\substack{\mathbf{e} \sim \mathbf{v}_i \\ \mathbf{e} \in \tilde{\mathcal{G}}}} \partial_\nu \psi|_{\mathbf{e}}(\mathbf{v}_i),$$

where the second equality follows from the Kirchhoff condition. The δ -conditions are chosen precisely so that $\psi|_{\tilde{\mathcal{G}}}$ is still an eigenfunction of $\tilde{\mathcal{G}}$. Therefore, $\lambda_1^D(\mathcal{G})$ is still an eigenvalue, and, since ψ is non-negative, $\lambda_1^D(\mathcal{G}) = \lambda_1(\tilde{\mathcal{G}})$ (cf. Theorem [A.3](#)).

We claim that $\gamma_{\mathbf{v}_0} \leq 0$ and $\gamma_{\mathbf{v}_i} < 0$ for $i \neq 0$ (recall that ν points into $\mathbf{v}_i$). For $\mathbf{v}_0$ this follows from the choice of $\mathbf{e}_1$ and $\mathbf{e}_{-1}$. For $i \neq 0$ this follows since $\mathbf{v}_i$ is not serious: $\mathbf{e}_{i+1} \in \tilde{\mathcal{G}}$ is the only edge incident with $\mathbf{v}_i$ in $\mathcal{G}$ for which $\partial_\nu \psi|_{\mathbf{e}}(\mathbf{v}_i) \geq 0$; hence all derivatives in the first sum in [\(2.3\)](#) are strictly negative. Note that the degree of $\mathbf{v}_i$ is at least 3 for all $i \neq 0$ since all degree 2 vertices have been suppressed; thus the sum contains at least one summand.

By Theorem [A.3](#), replacing all $\gamma_{\mathbf{v}_i}$ with 0 can only increase the eigenvalues. Therefore, $\lambda_1^D(\mathcal{G})$ is bounded from above by the first eigenvalue of either the Dirichlet interval of length s or a Dirichlet tadpole with cycle length s . In both cases the eigenvalue is at most $(\pi/s)^2$ by estimate [\(1.2\)](#).

Finally, we discuss the case of equality. The eigenvalue of an equilateral Dirichlet star is well known to be $(\pi/2\ell)^2$, where $\ell = s/2$ is the edge length. To prove necessity, we first observe that $\psi|_{\tilde{\mathcal{G}}}$ is a simple eigenfunction which does not vanish at any point of $\tilde{\mathcal{G}}$ except for the Dirichlet vertices. In particular, in the case of a tadpole the inequality must be strict if the outgrowth is non-trivial. In the case of a path, $\tilde{\mathcal{G}}$ cannot contain any edges other than $\mathbf{e}_1$ or $\mathbf{e}_{-1}$, since $\gamma_{\mathbf{v}_i} < 0$ when $i \neq 0$, and strictly increasing γ strictly increases λ_1 (Theorem [A.3](#)). The same reasoning yields $\partial_\nu \psi|_{\mathbf{e}_{\pm 1}}(\mathbf{v}_0) = 0$.

If the degree of $\mathbf{v}_0$ is larger than 2, the Kirchhoff condition now implies

$$(2.4) \quad \sum_{\mathbf{e} \sim \mathbf{v}_0, \mathbf{e} \neq \mathbf{e}_{\pm 1}} \partial_\nu \psi|_{\mathbf{e}}(\mathbf{v}_0) = 0,$$

and therefore there is another edge $\tilde{\mathbf{e}}_1$ with $\partial_\nu \psi|_{\tilde{\mathbf{e}}_1}(\mathbf{v}_0) \geq 0$. Repeating the proof with $\tilde{\mathbf{e}}_1$ instead of $\mathbf{e}_1$ we can similarly conclude that $\tilde{\mathbf{e}}_1$ leads to a Dirichlet vertex and $\partial_\nu \psi|_{\tilde{\mathbf{e}}_1}(\mathbf{v}_0) = 0$. Proceeding by induction (and applying [\(2.4\)](#) to the sums over fewer and fewer edges), we conclude that every edge incident with $\mathbf{e}_0$ leads to a Dirichlet vertex with no vertices of degree ≥ 3 along the way. Thus $\mathcal{G}$ is a star graph, whose ground state eigenfunction reaches its maximum at the central vertex $\mathbf{v}_0$. Moreover, $\partial_\nu \psi|_{\mathbf{e}}(\mathbf{v}_0) = 0$ for every incident edge $\mathbf{e}$, therefore — since the eigenvalue is π^2/s^2 — the edge length must be $s/2$. $\square$

Proof of Corollary [1.4](#). Let R be the reflection operator on $L^2(\mathcal{G})$ induced by the corresponding reflection operator $\rho : \mathcal{G} \rightarrow \mathcal{G}$ acting on the metric space $\mathcal{G}$. Now, R is a bounded linear operator on $L^2(\mathcal{G})$ that commutes with the standard Laplacian; in particular, the standard Laplacian is reduced by the closed orthogonal subspaces

$$\mathcal{S} := \left\{ \frac{f + Rf}{2} : f \in L^2(\mathcal{G}) \right\} \quad \text{and} \quad \mathcal{A} := \left\{ \frac{f - Rf}{2} : f \in L^2(\mathcal{G}) \right\}$$

of symmetric and anti-symmetric functions in $L^2(\mathcal{G})$, respectively.

Since the ground state of $\mathcal{G}$ clearly belongs to $\mathcal{S}$,

$$(2.5) \quad \lambda_2(\Delta_{\mathcal{G}}) \leq \lambda_1(\Delta_{\mathcal{G}}|_{\mathcal{A}}).$$

It is easy to see that $\mathcal{A}$ is isomorphic to $L^2(\widehat{\mathcal{G}})$, whereas $\text{Dom}(\Delta_{\mathcal{G}}|_{\mathcal{A}})$ is the domain of the standard Laplacian on $\widehat{\mathcal{G}}$ with the exception of Dirichlet conditions at $\partial\widehat{\mathcal{G}} = \{\mathbf{v} \in \mathcal{G} : \rho(\mathbf{v}) = \mathbf{v}\}$, identified as a subset of $\widehat{\mathcal{G}}$. The Dirichlet conditions may decompose $\widehat{\mathcal{G}}$ into several connected components joined together at $\partial\widehat{\mathcal{G}}$. In any case, each connected component of $\widehat{\mathcal{G}}$ necessarily has girth at least $s/2$, while the estimate (1.5) also applies on each connected component. Estimate (1.6) follows immediately. $\square$

2.2. Proof of the estimates in Section 1.2. Throughout this section we assume the graph $\mathcal{G}$ is finite, compact, and connected, and has standard (Neumann–Kirchhoff) conditions at every vertex. All upper bounds in this section are based on the variational characterization of the second eigenvalue,

$$(2.6) \quad \lambda_2^N(\mathcal{G}) = \min \left\{ \frac{\int_{\mathcal{G}} |f'(x)|^2 dx}{\int_{\mathcal{G}} |f(x)|^2 dx} : f \in H^1(\mathcal{G}), \int_{\mathcal{G}} f(x) dx = 0 \right\},$$

where the Sobolev space H^1 of the graph is defined as

$$(2.7) \quad H^1(\mathcal{G}) := \left\{ u \in C(\mathcal{G}) \cap \bigoplus_{e \in E} H^1(0, \ell_e) : \|u'\|_{L^2(\mathcal{G})} < \infty \right\}.$$

Upper bounds can now be obtained by choosing a suitable test function $f \in H^1(\mathcal{G})$ having mean value 0 (i.e. being orthogonal to the constants, which span the eigenspace of the first eigenvalue). For example, using the test function $f(x) = \sin(2\pi x/\ell_{\max})$ on the longest edge, extended by zero to the rest of the graph, we immediately obtain estimate (1.1) from the introduction.

The main difficulty in choosing the test function arises from the requirement that f have mean zero. Our principal tool for satisfying this requirement will be to build a homotopy between a function and its negative in the punctured form domain.

Lemma 2.2. *Let a be a positive, closed quadratic form whose domain $D(a)$ is compactly embedded in a Hilbert space H . Assume the associated positive semi-definite self-adjoint operator A on H to have one-dimensional null space spanned by some function u . If, for a family of functions $\psi : [0, 1] \rightarrow D(a) \setminus \{0\}$,*

- (1) *the mapping $[0, 1] \ni t \mapsto \langle \psi_t, u \rangle_H \in \mathbb{R}$ is continuous, and*
- (2) *$\psi_0 = -\psi_1$,*

then there exists t_0 such that the second lowest eigenvalue of A satisfies

$$(2.8) \quad \lambda_2(A) \leq \frac{a(\psi_{t_0})}{\|\psi_{t_0}\|_H^2}.$$

Proof. Since $\langle \psi_0, u \rangle_H = -\langle \psi_1, u \rangle_H$, by the Intermediate Value Theorem there is at least one $t_0 \in [0, 1]$ such that $\langle \psi_{t_0}, u \rangle_H = 0$. Then we use ψ_{t_0} as a test function in the abstract version of (2.6). $\square$

Taking $H = L^2(\mathcal{G})$, $u = \mathbf{1} \in L^2(\mathcal{G})$ and a the quadratic form associated with the metric graph Laplacian with standard vertex conditions, we immediately obtain the following.

Corollary 2.3. *Let $\psi : [0, 1] \rightarrow H^1(\mathcal{G}) \setminus \{0\}$ be such that $\psi_0 = -\psi_1$ and the mapping $t \mapsto \langle \psi_t, 1 \rangle_{L^2(\mathcal{G})}$ is a continuous function $[0, 1] \rightarrow \mathbb{R}$. Then there exists t_0 such that*

$$(2.9) \quad \lambda_2^N(\mathcal{G}) \leq \frac{\|\psi'_{t_0}\|_{L^2(\mathcal{G})}^2}{\|\psi_{t_0}\|_{L^2(\mathcal{G})}^2}.$$

The proofs of the theorems in Section 1.2 are now reduced to constructing a suitable family of test functions.

Proof of Theorem 1.9. Introduce the “tent” function

$$(2.10) \quad \tau_{y,d}(x) = \begin{cases} d - \text{dist}(x, y), & \text{if } \text{dist}(x, y) \leq d, \\ 0, & \text{otherwise,} \end{cases}$$

let $d = D/2$, and take

$$(2.11) \quad \psi_t := \cos(\pi t)\tau_{x_1,d} + \sin(\pi t)\tau_{x_2,d},$$

where x_1 and x_2 are a pair of points on the graph realizing the diameter. Note that $\tau_{x_1,d}$ and $\tau_{x_2,d}$ have disjoint supports. Then ψ_t satisfies the conditions of Corollary 2.3 and we can estimate

$$\|\tau'_{x_1,d}(x)\|_{L^2(\mathcal{G})}^2 \leq \int_{x: \text{dist}(x, x_1) \leq d} 1 dx \leq L,$$

and

$$(2.12) \quad \|\tau_{x_1,d}(x)\|_{L^2(\mathcal{G})}^2 \geq \int_0^d (d-x)^2 dx = \frac{d^3}{3},$$

where we estimate the L^2 -norm by only integrating along the path realizing the diameter. Combining, we obtain the desired estimate

$$\lambda_2^N \leq \frac{\cos^2(\pi t)L + \sin^2(\pi t)L}{\cos^2(\pi t)\frac{D^3}{24} + \sin^2(\pi t)\frac{D^3}{24}} \leq \frac{24L}{D^3}.$$

Since our test function cannot possibly be an eigenfunction, being piecewise linear, the inequality is strict. $\square$

Proof of Theorem 1.12. We use Corollary 2.3 with

$$(2.13) \quad \psi_t := \tau_{\gamma(e^{i\pi t}),d} - \tau_{\gamma(-e^{i\pi t}),d},$$

where γ is the curve realizing the avoidance diameter and $d = A/2$. The supports are disjoint and the gradient is 1 or 0, therefore $\|\psi'_t\|^2 \leq L$. For the norm, we amend estimate (2.12) to use injectivity of γ and obtain

$$(2.14) \quad \|\psi_t\|^2 \geq 2 \int_{-d}^d (d-|x|)^2 dx = \frac{4d^3}{3} = \frac{A^3}{6}.$$

It is clear that the test function is not an eigenfunction, therefore the inequality is strict. $\square$

Proof of Theorem 1.11. We use Corollary 2.3 with

$$(2.15) \quad \psi_t := h_1(t)\tau_{x_1,d} + h_2(t)\tau_{x_2,d} + h_3(t)\tau_{x_3,d},$$

where $x_1, x_2, x_3 \in \mathcal{G}$ are any three points realizing the triameter, $d = T/2$, and the functions h_j satisfy $h_j(0) = 1$ and $h_j(1) = -1$. Using the disjoint supports, we can estimate

$$\lambda_2^N \leq \max_{t \in [0,1]} \frac{3L \max \{h_1(t)^2, h_2(t)^2, h_3(t)^2\}}{d^3 (h_1(t)^2 + h_2(t)^2 + h_3(t)^2)}.$$

Choosing h_j so that $|h_j(t)| \leq 1$ and only one of them can be different from ± 1 at any given time (in other words, they take turns to go from 1 to -1), yields

$$\lambda_2^N < \frac{3L}{2d^3} = \frac{12L}{T^3}.$$

This concludes the proof. $\square$

APPENDIX A. LAPLACIAN ON METRIC GRAPHS: DEFINITIONS AND USEFUL RESULTS

In this appendix we review the basic definitions and terminology used in this paper. For further information, the reader is invited to consult various surveys and books on the subject [3, 7, 27]. We also formulate a result based on [5, 17] that we use repeatedly in Section 2.1.

Let $\mathcal{G} = (\mathbf{V}, \mathbf{E})$ be a graph with vertex set $\mathbf{V}$ and edge set $\mathbf{E}$. The graph is a metric graph if each edge $\mathbf{e} \in \mathbf{E}$ is identified with an interval $(0, \ell_{\mathbf{e}})$, where $\ell_{\mathbf{e}} > 0$ is regarded as the length of the edge. We shall write $\mathbf{e} \sim \mathbf{v}$ to mean that the edge $\mathbf{e}$ is incident with the vertex $\mathbf{v}$; and denote by $\mathbf{E}_{\mathbf{v}}$ the set of such edges. A graph is *compact*, if it has a finite number of edges, each edge of finite length. We denote by L or $|\mathcal{G}|$ the total length of the graph, i.e. the sum of the lengths of the edges of the graph. $\mathcal{G}$ is allowed to contain loops as well as multiple edges between given pairs of vertices. A cycle in $\mathcal{G}$ is, formally, a map $\gamma : [0, 1] \rightarrow \mathcal{G}$ such that $\gamma(0) = \gamma(1)$ and γ is injective on $[0, 1)$. However, we do not usually distinguish between γ and its image, a closed subset of $\mathcal{G}$.

In this paper we study the spectrum of the Laplacian $-\Delta$ on $\mathcal{G}$. More precisely, the operator acts as $-\frac{d^2}{dx^2}$ on the functions which are in the Sobolev space $H^2(0, \ell_{\mathbf{e}})$ on each edge $\mathbf{e} \in \mathbf{E}$. The domain $D(\Delta)$ of the operator is further restricted to functions that satisfy at any vertex $\mathbf{v} \in \mathbf{V}$ one of the following conditions:

- *Standard*⁵ conditions: at $\mathbf{v}$, we demand continuity of the functions and that the sum of the normal derivatives at each vertex is zero (“Kirchhoff” or “current conservation” condition):

$$(A.1) \quad \sum_{\mathbf{e} \sim \mathbf{v}} \partial_{\nu} f|_{\mathbf{e}}(\mathbf{v}) = 0,$$

where $\partial_{\nu} f|_{\mathbf{e}}(\mathbf{v})$ is the normal derivative of f on $\mathbf{e}$ at $\mathbf{v}$, with $\nu = \nu_{\mathbf{e}}(\mathbf{v})$ pointing *outward* (away from the edge $\mathbf{e}$, towards the vertex);

- *Dirichlet* conditions: at $\mathbf{v}$, any functions in the domain of Δ should take on the value zero. We denote the set of vertices equipped with Dirichlet conditions by $\mathbf{V}_D$.

⁵Also known as Neumann–Kirchhoff, among other names; observe that on a degree-one vertex standard conditions agree with common Neumann ones.

- *Anti-periodic*⁶ conditions: at $\mathbf{v}$ of degree 2,

$$(A.2) \quad f_{\mathbf{e}_1}(\mathbf{v}) = -f_{\mathbf{e}_2}(\mathbf{v}), \quad \partial_\nu f_{\mathbf{e}_1}(\mathbf{v}) = \partial_\nu f_{\mathbf{e}_2}(\mathbf{v}).$$

These conditions are used in Remarks 1.7 of the present paper (see also Remark A.2 below).

- δ (or *Kirchhoff–Robin*) conditions: associated with $\mathbf{v}$ there is a $\gamma = \gamma(\mathbf{v}) \in \mathbb{R}$, $\gamma \neq 0$ such that the functions $f \in D(\Delta)$ are continuous at $\mathbf{v}$ and the derivatives at $\mathbf{v}$ satisfy

$$(A.3) \quad \sum_{\mathbf{e} \sim \mathbf{v}} \partial_\nu f|_{\mathbf{e}}(\mathbf{v}) + \gamma f(\mathbf{v}) = 0,$$

where, again, ν is the outer unit normal to the edge. We sometimes refer to γ as the *strength* of the δ -condition, or as the δ -*potential* at $\mathbf{v}$.

We see immediately that the δ -condition with $\gamma(\mathbf{v}) = 0$ corresponds to the standard condition. Furthermore, Dirichlet conditions correspond formally to δ -conditions of strength $\gamma = \infty$ (this correspondence may be made rigorous [6], and we will use it below).

Remark A.1. Any point in the interior of an edge may be declared to be a vertex of degree two with standard conditions without affecting the spectral properties of the operator. We will refer to this as introducing a “dummy” vertex. Conversely, any vertex v of degree two with standard conditions may be suppressed. Likewise, the operator is not modified if a subset of the elements of V_D are identified to form one single Dirichlet vertex.

Remark A.2. Declaring an arbitrary point $x \in \mathbf{e}$ to be a vertex $\mathbf{v} = \mathbf{v}_x$ of degree two, we can also impose anti-periodic conditions (A.2) there. Due to “gauge invariance”, different choices for the location x within the same edge result in unitarily equivalent operators [7, Section 2.6]; we thus refer to this as imposing anti-periodic conditions on the edge $\mathbf{e} \in \mathbf{E}$.

As is well known, under the above set of assumptions the Laplacian is self-adjoint, semi-bounded, and has trace class resolvent; in particular, its spectrum consists of a sequence of real eigenvalues of finite multiplicity, which we denote by

$$(A.4) \quad \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots,$$

where each is repeated according to its multiplicity. The corresponding eigenfunctions may be chosen to form an orthonormal basis of $L^2(\mathcal{G})$, and may additionally without loss of generality all be chosen real.

The following theorem summarizes properties of the first eigenvalue used extensively in Section 2.1, including an interlacing inequality for the eigenvalues, which in its sharpest form (with a characterization of equality) appeared in [5].

Theorem A.3. *Let $\mathcal{G}$ be a compact graph equipped with a δ -condition of strength $\gamma_i \in (-\infty, \infty]$ at each vertex $\mathbf{v}_i \in \mathbf{V}$. Denote by V_D the set of all Dirichlet vertices,*

$$V_D = \{\mathbf{v}_i \in \mathbf{V} : \gamma_i = \infty\},$$

and suppose that $\mathcal{G} \setminus V_D$ is connected. Then $\lambda_1 = \lambda_1(\mathcal{G})$ is simple and its eigenfunction ψ may be chosen strictly positive in $\mathcal{G} \setminus V_D$.

⁶The name “anti-periodic” goes back to the theory of Hill’s operator, see, e.g., [24]. Some authors use the name “signing conditions” to highlight connections to the construction of combinatorial Ramanujan graphs [9, 23]. For vertices of general degree, the corresponding conditions are often called “anti-Kirchhoff” conditions, as in, e.g., [30, Classification 2.3.II].

Moreover, if $\mathcal{G}'$ is formed by replacing the potential $\gamma_i \in \mathbb{R}$ at $\mathbf{v}_i$ with $\gamma'_i \in (\gamma_i, \infty]$, then

$$(A.5) \quad \lambda_1(\mathcal{G}') > \lambda_1(\mathcal{G}).$$

Proof. For simplicity of λ_1 and strict positivity of ψ , see [17]. For (A.5), since ψ does not satisfy the δ -condition at $\mathbf{v}_i$ in the graph $\mathcal{G}'$, it cannot be an eigenfunction; hence $\lambda_1(\mathcal{G}')$ and $\lambda_1(\mathcal{G})$ have no eigenfunctions in common. The (strict) inequality (A.5) now follows immediately from [5, Theorem 3.4]. $\square$

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