

LAPLACIANS ON METRIC GRAPHS: METHODS OF SPECTRAL GEOMETRY

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ABSTRACT. We offer an invitation to the spectral geometry of quantum graphs, with a strong focus on free Laplacians with standard vertex conditions on finite, compact metric graphs. We discuss the fundamental properties of the spectrum of these operators and present the state of the art of upper and lower bounds for their eigenvalues. We introduce a selection of the main tools that have been invented and developed over the last 20 years in this area, and how they can be used in spectral analysis.

This is a preliminary version of our text.

CONTENTS

1. Introduction	2
2. A toy model: the second derivative on bounded interval	4
2.1. Eigenvalues of distinguished realizations	4
3. Metric graphs and function spaces	10
3.1. Metric graph	10
3.2. Functions on graphs	12
3.3. The standard Laplacian	13
3.4. Examples of standard Laplacians	15
3.5. Dirichlet Laplacians	20
3.6. Eigenvalue asymptotics	22
3.7. First results in spectral geometry	24
4. Basic properties of the spectrum	26
4.1. Discreteness	26
4.2. Analyticity	26
4.3. Secular manifold	26
4.4. Setting edge lengths to zero	28

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4.5. Simplicity of the spectrum	29
5. Global methods	30
5.1. Symmetrization	30
5.2. Test functions	33
5.3. Graph decomposition	35
6. Local Methods	40
6.1. Elementary surgery methods	41
6.2. Further interlacing techniques	50
6.3. Pumpkin chains, Sturm–Liouville problems, and diameter	52
6.4. Cutting along eigenfunctions	55
7. M-functions	60
7.1. Definition of the M-function	61
7.2. Elementary examples	62
7.3. Explicit formulas for the M-function	63
7.4. M-function and spectral estimates	65
7.5. M-function and isospectrality	68
8. Generalizations, applications and further topics	70
8.1. Geometry of eigenfunctions: nodal domains and hot spots	70
8.2. Spectral correspondence with difference operators	71
8.3. Infinite metric graphs	73
8.4. Heat kernels	73
8.5. Torsional geometry	74
8.6. Spectral Minimal Partitions	75
8.7. Symmetrization and NLS equations	75
8.8. p -Laplacians	76
8.9. Other self-adjoint realizations of the Laplacian	77
References	77

1. INTRODUCTION

Graphs are fascinating mathematical objects: they have a rigorous mathematical description, yet they can faithfully capture the interaction among agents in models from physics, biology, chemistry, economics, social sciences, and more. Over the last 50 years, graphs have been an abundant source of challenging problems not only in discrete mathematics, but also in spectral theory; many relevant questions about combinatorial graphs have been directly motivated by applications, including computer science and theoretical neuroscience.

Along with combinatorial graphs, another class of objects has become a popular toy model in mathematics and applied sciences: metric graphs – the main topic of this article – have been discovered several times in history: in topology of infinite combinatorial graphs [96], quantum chemistry [196, 103], neuroscience [189, 68], potential theory [99], and algebraic geometry [197, 210] among others. For our purposes, the main role was played by Lumer, who was the first

one [157, 159] who provided a precise mathematical framework of evolution equations on metric graphs (which he called *networks*). Pavlov and Faddeev in [182], and independently Nicaise in [175], observed that the Laplacian becomes self-adjoint in a natural Hilbert space, under what we are going to refer to as *standard vertex conditions*, see Section 3.3: They thus paved the way for the development of a spectral theory.

In particular, Lumer introduced in mathematical analysis a notion of ramified structure: his construction turns enriches the combinatorial structure of a graph by associating each edge with an interval – a metric edge, upon which Laplacians can be defined. Metric graphs are metric measure spaces intuitively defined by suitably gluing the endpoints of intervals $(0, \ell_e)_{e \in E}$, indexed by the edge set E of a combinatorial graph; one identifies such equivalence classes of endpoints with the graph’s vertices. They are currently known under the name of *quantum graphs*, a name coined in [132].

Through his work, his students and his influence on his scientific environment, Lumer was the driving force towards the development of the “first wave” of operator theory on metric graphs. The spectrum of Laplacians with standard vertex conditions on metric graphs: spectral geometric issues have been discussed since [37, 194, 81, 176].

Physics has been the driving force behind the dynamic development of quantum graph theory in the last 20 years. The discreteness of this vertex set allows for easy parametrization of self-adjoint extensions of Laplacian-type operators, making metric graphs to favourite model objects in mathematical physics; at the same time, the convergence of metric graph Laplacians towards Laplace–Beltrami operators on manifolds has been exploited in differential geometry since [81]. Relevant properties of partial differential operators that typically only arise in rough environments can be translated to a more benign setting and then studied by easier means: 1D Sobolev spaces, Sturm–Liouville theory, and elementary combinatorics, to name a few.

This survey is devoted to provide a comprehensive overview of the main results that have been obtained over the last 40 years in the spectral theory of Laplacians on metric graphs; and to present different results and various mathematical tools in a unified framework: we hope that this will foster the discourse between different communities.

At the same time, there are many topics we have not even touched upon: we have summarized the most important ones in Section 8. Further outgrowths of the theory of Laplacians on metric graphs are treated in the monographs [49, 167, 141] as well as in the surveys [107, 25, 41, 92].

Some motivations to study spectral geometry of metric graphs include the following:

- Counterpart of spectral geometry for manifolds
- Rate of convergence to equilibrium of the heat equations
- Applications to beam equations, buckling problems
- Spectral clustering
- Stability of nonlinear waves

2. A TOY MODEL: THE SECOND DERIVATIVE ON BOUNDED INTERVAL

2.1. Eigenvalues of distinguished realizations. As a warm up for our study of Laplacians on metric graphs, let us consider five very simple realizations one may consider on one interval of length L , say $[0, L]$.

Neumann conditions. The Laplacian $\Delta_{\mathbf{N}}$ has domain

$$\{u \in H^2(0, L) : u'(0) = u'(L) = 0\}.$$

The associated form is

$$a(u) := \int_0^L |u'(x)|^2 dx$$

with form domain

$$D_{\mathbf{N}}(a) = H^1(0, L) :$$

the fact that it is positive and the embedding of $D_{\mathbf{N}}(a)$ in $L^2(0, L)$ is compact shows that $\Delta_{\mathbf{N}}$ must have countably many eigenvalues, all of them nonnegative¹. (The fact that the spectrum is discrete will extend to all Laplacian realizations whose form domain is embedded in $H^1(0, L)$, of course, and in particular to all realizations considered in the remainder of this section.)

Indeed, the eigenvalues of $\Delta_{\mathbf{N}}$ are

$$(2.1) \quad \frac{k^2 \pi^2}{|\mathcal{G}|^2}, \quad k = 0, 1, 2, \dots,$$

and all of them are simple. To see this, first observe that constant functions clearly lie in the null space of $\Delta_{\mathbf{N}}$; furthermore, any solution of the eigenvalue equation

$$-u''(x) = \lambda u(x), \quad x \in (0, L),$$

for $\lambda > 0$, is necessarily of the form

$$u(x) = A \cos(\sqrt{\lambda}x) + B \sin(\sqrt{\lambda}x), \quad x \in (0, L).$$

Deriving this formula yields

$$u'(x) = -\sqrt{\lambda}A \sin(\sqrt{\lambda}x) + B\sqrt{\lambda} \cos(\sqrt{\lambda}x), \quad x \in (0, L).$$

and imposing the Neumann condition at $x = 0$ shows that $B = 0$. Hence, all eigenfunctions are of the form

$$u(x) = A \cos(\sqrt{\lambda}x), \quad x \in (0, L).$$

Imposing the second boundary condition thus means that we require the function u to complete a half-integer number of oscillations between 0 and L . (Of course, there are infinitely many λ that enforce this property, but in fact only countably many: this explains again why the point spectrum is discrete.) Because

$$u''(x) = -A\lambda \cos(\sqrt{\lambda}x),$$

¹Technically speaking, these are the eigenvalues of *minus* the Laplacian. Following a common convention in spectral geometry, we will hitherto with an abuse of terminology refer to these nonnegative numbers, obtained by the Courant–Fischer min-max method, as *Laplacian eigenvalues*.

we see that λ is an eigenvalue if and only if $\sqrt{\lambda L}$ is a root of \cos , i.e., if and only if λ is of the form in (2.1). Also, the associated eigenfunctions are either constant functions, for the eigenvalue $\lambda = 0$; or, for higher eigenvalues, multiples of the function

$$\cos\left(\frac{k\pi}{L}x\right), \quad x \in (0, L), \quad k = 1, 2, \dots$$

Dirichlet conditions. The Laplacian Δ_D has domain

$$H^2(0, L) \cap H_0^1(0, L) = \{u \in H^2(0, L) : u(0) = u(L) = 0\}$$

and form domain

$$D_D(a) := H_0^1(0, L) = \{u \in H^1(0, L) : u(0) = u(L) = 0\}.$$

Its eigenvalues, all of them simple, are

$$(2.2) \quad \frac{k^2\pi^2}{|\mathcal{G}|^2}, \quad k = 1, 2, \dots$$

This can be seen with a reasoning similar to that described in the Neumann case, but also by means of a more abstract one: indeed, the second derivative with Dirichlet conditions admits the factorization

$$-\Delta_D = dd^*,$$

where

$$(2.3) \quad df = if', \quad D(d) = H^1(0, L);$$

accordingly,

$$d^*f = if', \quad D(d^*) = H_0^1(0, L);$$

and we observe that the second derivative with Neumann conditions can be written as

$$-\Delta_N = d^*d.$$

Accordingly, by a well-known operator theoretical property, Δ_D, Δ_N must have same eigenvalues, except perhaps 0. But because integrating u'' against u shows that the ordinary differential equation

$$-u''(x)z = 0, \quad x \in (0, L),$$

has constant functions as its sole solution (which must clearly be the constant *zero* function in view of the Dirichlet conditions) we conclude that 0 is not an eigenvalue after all. The associated eigenfunctions are multiples of

$$d \cos\left(\frac{k\pi}{L}x\right) = -\sin\left(\frac{k\pi}{L}x\right), \quad x \in (0, L),$$

d being the operator in (2.3).

Mixed Dirichlet/Neumann conditions. The Laplacian has, in this case, domain

$$\{u \in H^2(0, L) : u(0) = u'(L) = 0\}$$

and form domain

$$D_{D/N}(a) := \{u \in H^1(0, L) : u(0) = 0\}.$$

In order to determine the eigenvalues, consider the reflection operator

$$J : u \mapsto \tilde{u},$$

with

$$\tilde{u}(x) := \begin{cases} u(x), & \text{if } x \in (0, L), \\ u(2 - x), & \text{if } x \in (L, 2L), \end{cases}$$

Now, if \tilde{u} is an eigenfunction for the Dirichlet Laplacian on $(0, 2L)$ associated with the lowest eigenvalue, i.e.,

$$\tilde{u}(x) = B \sin\left(\frac{\pi}{4L}x\right), \quad x \in (0, 2L),$$

then $J^{-1}\tilde{u} = \tilde{u}|_{(0, L)}$ satisfies a Neumann condition at L and is, thus, an eigenfunction for the Laplacian with mixed conditions.

The second eigenfunction for the Dirichlet Laplacian on $(0, 2L)$, corresponding to the eigenvalue $\frac{4\pi^2}{4|\mathcal{G}|^2}$, is a full sine wave, so it vanishes at L : therefore, it does not induce an eigenfunction for the Laplacian with mixed conditions, nor do any eigenfunctions associated with the eigenvalue $\frac{k\pi^2}{4|\mathcal{G}|^2}$ of the Dirichlet Laplacian on $(0, 2L)$, for any *even* k . However, the set of eigenfunctions on $(0, L)$ for the Laplacian with mixed Dirichlet/Neumann conditions and the set of eigenfunctions for the Laplacian with Dirichlet conditions $(0, 2L)$ and associated with $\frac{k\pi^2}{4|\mathcal{G}|^2}$ for *odd* k are indeed bijective.

We conclude that the eigenvalues of the Laplacian with mixed Dirichlet/Neumann conditions are

$$(2.4) \quad \frac{(2k-1)^2\pi^2}{4|\mathcal{G}|^2}, \quad k = 1, 2, \dots$$

each of them with multiplicity one. The associated eigenfunctions are, accordingly, multiples of

$$\sin\left(\frac{(2k-1)\pi}{2L}x\right), \quad x \in (0, L), \quad k = 1, 2, \dots$$

(Clearly, by the same factorization trick as above, the eigenpairs for the mixed Neumann/Dirichlet conditions $u'(0) = u(L) = 0$ display the same behaviour.)

Periodic conditions. The domain of the Laplacian Δ_{per} is

$$\{u \in H^2(0, L) : u(0) = u(L) \text{ and } u'(0) = u'(L)\}$$

and the form domain is

$$D_{\text{per}}(a) := H_{\text{per}}^1(0, L) = \{u \in H^1(0, L) : u(0) = u(L)\}.$$

In order to determine the eigenpairs, we will make use of the decomposition² of $L^2(0, L)$ -functions into their symmetric and anti-symmetric parts,

$$\begin{aligned} L^2(0, L) &= L^2_{\text{sym}}(0, L) \oplus L^2_{\text{anti}}(0, L) \\ &:= \{f \in L^2(0, L) : f(x) = f(L - x) \text{ for a.e. } x \in (0, L)\} \\ &\quad \oplus \{f \in L^2(0, L) : f(x) = -f(L - x) \text{ for a.e. } x \in (0, L)\}, \end{aligned}$$

which is invariant under the Laplacian with periodic conditions. Now, take the part of the Laplacian with periodic conditions in each of these two spaces: their domains are

$$\{u \in H^2(0, L) \cap L^2_{\text{sym}}(0, L) : u(0) = u(L) \text{ and } u'(0) = u'(L)\}$$

and

$$\{u \in H^2(0, L) \cap L^2_{\text{anti}}(0, L) : u(0) = u(L) \text{ and } u'(0) = u'(L)\}$$

respectively. Observe that any continuous anti-symmetric function must vanish at $\frac{L}{2}$, and also at 0 if it additionally satisfies the periodicity conditions. Likewise, the derivative of any symmetric function satisfying periodic conditions vanishes both at 0 and $\frac{L}{2}$.

In other words, the domains of the part of the Laplacian with periodic conditions in $L^2_{\text{sym}}(0, L)$ and $L^2_{\text{anti}}(0, L)$ are isomorphic to

$$\left\{ u \in H^2\left(0, \frac{L}{2}\right) : u'(0) = u'\left(\frac{L}{2}\right) = 0 \right\}$$

and

$$\left\{ u \in H^2\left(0, \frac{L}{2}\right) : u(0) = u\left(\frac{L}{2}\right) = 0 \right\},$$

respectively: therefore, the set of eigenvalues of the Laplacian with periodic conditions on $(0, L)$ is the union of all eigenvalues of the Neumann Laplacian on $(0, \frac{L}{2})$ and all eigenvalues of the Dirichlet Laplacian on $(0, \frac{L}{2})$. We conclude that the eigenvalues are

$$(2.5) \quad \frac{(2k)^2\pi^2}{|\mathcal{G}|^2}, \quad k = 0, 1, 2, \dots :$$

the lowest one is a simple eigenvalue, all further ones have multiplicity two. The associated eigenfunctions are obtained taking the eigenfunctions of the Neumann and Dirichlet Laplacians on $(0, \frac{L}{2})$ and suitably extending them to the whole interval $(0, L)$: any constant function is an eigenfunction for the eigenvalue 0, whereas any higher eigenvalue is associated with both eigenfunctions

$$(2.6) \quad \sin\left(\frac{2k\pi}{L}x\right) \quad \text{and} \quad \cos\left(\frac{2k\pi}{L}x\right), \quad x \in (0, L), \quad k = 1, 2, \dots$$

²Further development of this technique using representation theory of finite groups can be found in [23] and references therein.

Let us apply the factorization trick described above to determine the eigenvalues of a further operator: upon introducing

$$(2.7) \quad df = if', \quad D(d) = H_{\text{per}}^1(0, L),$$

a direct computation shows that d is self-adjoint, see also [91, Proposition A.3], hence

$$-\Delta_{\text{per}} = dd^* = d^*d.$$

Anti-periodic conditions. In this case, the operator Δ_{antiper} has domain

$$\{u \in H^2(0, L) : u(0) + u(L) = 0 \text{ and } u'(0) + u'(L) = 0\}$$

and the form domain is

$$D_{\text{antiper}}(a) := H_{\text{antiper}}^1(0, L) = \{u \in H^1(0, L) : u(0) + u(L) = 0\}.$$

All its eigenvalues have multiplicity two: they are given by

$$(2.8) \quad \frac{(2k-1)^2\pi^2}{|\mathcal{G}|^2}, \quad k = 1, 2, \dots$$

To justify this, we start again from the formula

$$u(x) = A \cos(\sqrt{\lambda}x) + B \sin(\sqrt{\lambda}x), \quad x \in (0, L),$$

for the generic solution of the eigenvalue equation (the possibility that 0 is an eigenvalue can be ruled out, since non-zero constant functions do not satisfy anti-periodic boundary conditions.) Imposing the boundary conditions on u and u' we find the system

$$\begin{cases} A + A \cos(\sqrt{\lambda}L) + B \sin(\sqrt{\lambda}L) = 0, \\ B - A \sin(\sqrt{\lambda}L) + B \cos(\sqrt{\lambda}L) = 0, \end{cases}$$

i.e.,

$$\begin{pmatrix} 1 + \cos(\sqrt{\lambda}L) & \sin(\sqrt{\lambda}L) \\ -\sin(\sqrt{\lambda}L) & 1 + \cos(\sqrt{\lambda}L) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = 0 :$$

the determinant of this matrix vanishes if and only if

$$(1 + \cos(\sqrt{\lambda}L))^2 + \sin^2(\sqrt{\lambda}L) = 2 + 2 \cos(\sqrt{\lambda}L) = 0,$$

i.e., precisely for those $\lambda > 0$ such that

$$\cos(\sqrt{\lambda}L) = -1,$$

which implies that λ is of the form (2.8) and that both

$$\cos\left(\frac{(2k-1)\pi}{L}x\right) \quad \text{and} \quad \sin\left(\frac{(2k-1)\pi}{L}x\right), \quad x \in (0, L), \quad k = 1, 2, \dots$$

are eigenfunctions associated with this eigenvalue.

Kreĩn–von Neumann conditions. The operator Δ_{KN} has domain

$$\{u \in H^2(0, L) : u'(L) = u'(0) = L^{-1}(u(L) - u(0))\};$$

in this case, the associated quadratic form

$$\tilde{a}(u) := \int_0^L |u'(x)|^2 dx - \frac{1}{L} (u(L) - u(0))^2,$$

and the form domain is

$$D_{\text{KN}}(\tilde{a}) := H^1(0, L).$$

Even though the lower order perturbation is induced by a negative semi-definite matrix, the form $(\tilde{a}, D_{\text{KN}}(\tilde{a}))$ is accretive: indeed, Δ_{KN} is the smallest (in the sense of quadratic forms³) positive semi-definite self-adjoint realization of the Laplacian.

It is easy to see that $H^1(0, L) = \text{Har}(0, L) \oplus H_0^1(0, L)$, where $\text{Har}(0, L)$ is the two-dimensional space of harmonic functions on $(0, L)$ (i.e., polynomials of degree ≤ 1). Accordingly, 0 is an eigenvalue of Δ_{KN} with multiplicity 2. Because \tilde{a} acts on $H_0^1(0, L)$ as a_{D} , one may think that the remaining eigenvalues of Δ_{KN} agree with those of the Dirichlet Laplacian: but this is not true, because the relevant Hilbert space on which the operator associated with this form acts is now $L^2(0, L) \ominus \text{Har}(0, L)$. The remaining spectrum of Δ_{KN} has been computed in [12, Example 5.1]: the eigenvalues are given by two sequences

$$\frac{4k^2\pi^2}{|\mathcal{G}|^2} \quad \text{and} \quad j_k^2, \quad k = 1, 2, \dots,$$

with associated eigenfunctions

$$\sin\left(\frac{2k\pi}{L}x\right) \quad \text{and} \quad \sin\left(\frac{j_k}{L}\left(x - \frac{1}{2}\right)\right), \quad x \in (0, L), \quad k = 1, 2, \dots,$$

respectively. Here, (j_k) is the monotonically growing sequence of the zeros of the transcendent equation

$$\frac{j}{2} = \tan\left(\frac{j}{2}\right) :$$

they satisfy

$$\frac{j_k}{2} \in \left(\pi(k-1), \pi\left(k - \frac{1}{2}\right)\right), \quad k = 1, 2, \dots,$$

Apart from 0, all eigenvalues are simple.

Let us stress that all Laplacian realizations discussed above satisfy a one-dimensional Weyl asymptotics, i.e., the eigenvalue sequence $(\lambda_j)_{j \in \mathbb{N}}$, counted with multiplicity, satisfies

$$(2.9) \quad \lambda_j = \frac{\pi^2}{|\mathcal{G}|^2} j^2 + \mathcal{O}(j) \quad \text{as } j \rightarrow \infty.$$

This property is obviously satisfied by both the Dirichlet and the Neumann realizations of the Laplacian on $(0, L)$, and thus extend to all realizations that are sandwiched, in the sense of

³Given two quadratic forms b, c we write $b \preceq c$ – and we say that c is smaller than b in the sense of quadratic forms – if

$$D(b) \supset D(c) \quad \text{and} \quad b(u) \leq c(u) \quad \text{for all } u \in D(c).$$

quadratic forms, between them. The explicit computation of the eigenvalues of Δ_{KN} allows to check that (2.9) holds for the Kreĭn–von Neumann extension as well.

Remark 2.1. We have seen that the eigenvalues $(\mu_k)_{k \in \mathbb{N}}$ and $(\lambda_k)_{k \in \mathbb{N}^*}$ of the Laplacian with Neumann and Dirichlet conditions, respectively, satisfy

$$(2.10) \quad \mu_k = \lambda_k, \quad k = 1, 2, \dots$$

We have stressed that this is due to a suitable factorization of the Laplacian that is not available in higher dimension: for open bounded domains of \mathbb{R}^d we generally only have the inequality

$$(2.11) \quad \mu_k \leq \lambda_k, \quad k = 1, 2, \dots$$

discovered in [97].

Remark 2.2. The boundary conditions discussed above are by no means the only ones that induce a self-adjoint Laplacian realization: it is a well-known fact of Sturm–Liouville theory [112] that such conditions can be, with a more modern formalism, parametrized as follows:

$$\begin{pmatrix} u(0) \\ u(L) \end{pmatrix} \in Y, \quad \begin{pmatrix} -u'(0) \\ u'(L) \end{pmatrix} + R \begin{pmatrix} u(0) \\ u(L) \end{pmatrix} \in Y^\perp$$

for any subspace Y of \mathbb{C}^2 and any Hermitian 2×2 -matrix. The special realizations discussed above arise taking $R = 0$ and considering

- $Y = \mathbb{C}^2$ for Neumann conditions,
- $Y = \{0\}^2$ for Dirichlet conditions,
- $Y = \{0\} \oplus \mathbb{C}$ for mixed Dirichlet/Neumann conditions,
- $Y = \left\langle \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right\rangle$ for periodic conditions,
- $Y = \left\langle \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right\rangle$ for antiperiodic conditions.

Remark 2.3. We have in particular seen that two sets coincide, counting multiplicity: the union of the spectra of $\Delta_{\text{N}}, \Delta_{\text{D}}$ as well as the union of the spectra of $\Delta_{\text{per}}, \Delta_{\text{antiper}}$. The reason for this behaviour has been explained, in the more general setting presented in Remark 2.2, in [38].

3. METRIC GRAPHS AND FUNCTION SPACES

3.1. Metric graph. The current review will be devoted to so-called standard Laplacians only on connected finite compact metric graphs, therefore introducing metric graphs and defining differential operators we shall simplify common definitions to serve our purposes.

Let \mathbf{E} be a finite set of compact intervals $e \in \mathbf{E}$, which we will henceforth call *edges* upon associating with each of them a length $\ell_e \in (0, \infty)$. Then, \mathcal{E} is their disjoint union

$$\mathcal{E} := \bigsqcup_{e \in \mathbf{E}} [0, \ell_e].$$

Consider any partition of the set of interval's endpoints into equivalence classes \mathbf{v} with respect to some equivalence relation \sim : we call such \sim and the associated equivalence classes a *wiring*

and the resulting *vertices*, respectively. The set of all vertices will be denoted by $V \ni v$. Then the *metric graph* \mathcal{G} is the quotient metric space,

$$\mathcal{G} = \mathcal{E}/\sim,$$

that is, the set \mathcal{E} upon identifying some of the edges' endpoints. For a given \mathcal{E} , different equivalence relations \sim lead to different metric graphs which may be seen as mutual "rewirings".

More formal equivalent definitions of metric graphs can be found in [152, 49, 165, 141].

Informally, a metric graph can be visualized as a combinatorial graph each of whose edges is seen as a compact interval. Orientation of the intervals plays no role in the definition – only the lengths of the edges and the way the intervals are connected play a role. But this analogy is not universal since we allow *loops* – edges connected by both endpoints to the same vertex, – and *parallel edges* – several edges connecting the same vertices.

If the vertex v contains an endpoint of the edge e , we will often use the notation

$$e \sim v,$$

and say e is *incident* in v . Likewise, if v, w are endpoints of the same edge, or if a given vertex is an endpoint of two different edges e, f , then we say that the vertices v, w are *adjacent*, and that the edges e, f are *adjacent*, respectively. The set of all edges that are incident in V will be denoted by E_v . The degree of a vertex v , denoted $\deg v$, is the number of elements in the equivalent class v . It coincides with the number of incident edges E_v if no loops are involved.

The *total length*, or *volume*, of the metric graph \mathcal{G} is the sum of the lengths of the edges:

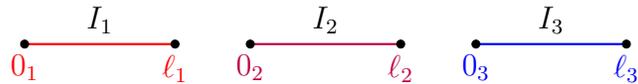
$$(3.1) \quad |\mathcal{G}| := \sum_{e \in E} \ell_e.$$

(We stress that the total length does not change upon rewiring.)

The total length is always finite since we consider only metric graphs formed by a finite set of compact intervals: this class is traditionally referred to in the literature as *compact metric graphs*. Unless explicitly stated, we will in this article always assume \mathcal{G} to be compact.

All abstract notions – especially, *(path) connectedness* – that can be defined for metric spaces carry over to metric graphs. We will, however, sometimes need to introduce new refined notions that have no direct counterpart in the theory of general metric spaces, see e.g. Theorem 5.1 below.

Example 3.1. Let $E = 3$ and take $I_k = [0_k, \ell_k]$, $k = 1, 2, 3$, then $S = \{0_1, 0_2, 0_3, \ell_1, \ell_2, \ell_3\}$.



If we set $v_1 = \{0_1\}$, $v_2 = \{0_2\}$, $v_3 = \{\ell_1\}$, $v_4 = \{\ell_1, \ell_2, 0_3\}$, then we generate a *star graph* on three edges: see Figure 1.

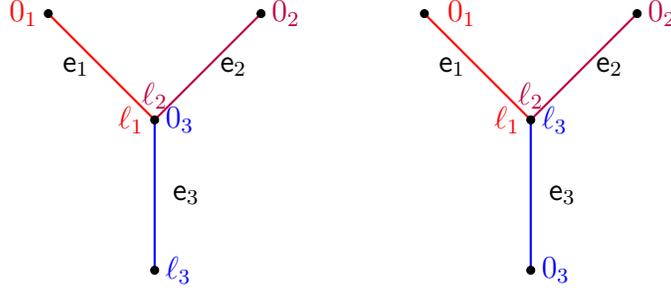


FIGURE 1. The 3-star graph of Example 3.1 with the first-mentioned choice of coordinates (left) and the alternative coordinates (right).

Choosing, for example, $v_1 = \{0_1\}$, $v_2 = \{0_2\}$, $v_3 = \{0_1\}$, $v_4 = \{\ell_1, \ell_2, \ell_3\}$ would lead to the same graph, but the orientation of e_3 in the chosen “local coordinates” would be reversed.

By joining v_2, v_3 , thus producing the three vertices $v_1 = \{0_1\}$, $\tilde{v}_2 = \{0_2\}$, $v_4 = \{\ell_1, \ell_2, \ell_3\}$, we would obtain a so-called *lasso-graph*.

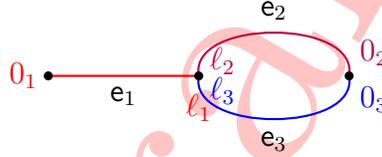


FIGURE 2. The lasso graph obtained identifying two vertices of the right 3-star in Figure 1.

3.2. Functions on graphs. Since our goal is to study differential operators on metric graphs, we need to consider functions defined on \mathcal{G} .

Because \mathcal{G} is a metric space, the notion of continuity is canonically defined and allows us to consider the space

$$C(\mathcal{G})$$

of scalar-valued continuous functions supported on \mathcal{G} ; we can, likewise, define the spaces $C^\alpha(\mathcal{G})$ or $\text{Lip}(\mathcal{G})$ of Hölder or Lipschitz continuous functions on \mathcal{G} . Furthermore, a metric graph can be canonically turned into a metric measure space by endowing it with the measure given by the direct sum of Lebesgue measures on all edges: in particular, this allows for the introduction of the Hilbert space

$$L^2(\mathcal{G}) := \bigoplus_{e \in E} L^2(e), \quad L^2(e) \approx L^2(0, \ell_e).$$

Interval endpoints form a set of measure zero and therefore can be ignored in the definition.

Introducing the Sobolev spaces H^j we shall with slight abuse of terminology require that the functions are continuous at the vertices:

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

The functions from H^j are those functions which j -th weak derivatives are square summable on each edge and therefore are continuous inside the edges. The definition of $H^j(\mathcal{G})$ requires in addition that the functions are continuous at the vertices, which is natural if we want the functions to be defined everywhere on the metric graph \mathcal{G} including the vertices. In what follows we are going to use the function values at the vertices $u(\mathbf{v})$, $\mathbf{v} \in V$.

It is inappropriate to require for functions from H^j with $j \geq 2$ any additional continuity condition on the derivatives since the definition of $H^j(\mathcal{G})$ should be independent of the orientation of the edges. We introduce instead the *sum of normal derivatives* at a vertex \mathbf{v} :

$$(3.2) \quad \partial u(\mathbf{v}) := \sum_{\mathbf{e} \sim \mathbf{v}} \frac{\partial u_{\mathbf{e}}}{\partial n}(\mathbf{v}),$$

where the sum is taken over all edges \mathbf{e} connected at the vertex \mathbf{v} and $\frac{\partial u_{\mathbf{e}}}{\partial n}(\mathbf{v})$ denotes the limiting value as x approaches \mathbf{v} of the first derivative of $u_{\mathbf{e}}$ taken in the direction inside the edge \mathbf{e} . Note that in the case of loops, both endpoints contribute into the sum, but the derivatives are taken in the opposite directions.

3.3. The standard Laplacian. These few ingredients are already sufficient to start developing an operator theory of Laplacians on metric graphs: indeed, we can introduce the *quadratic form*

$$(3.3) \quad a_{\mathcal{G}}(u) := \int_{\mathcal{G}} |u'(x)|^2 dx = \sum_{\mathbf{e} \in E} \int_0^{\ell_{\mathbf{e}}} |u'_{\mathbf{e}}(x)|^2 dx.$$

With an abuse of notation, we denote by $a_{\mathcal{G}}$ the *sesquilinear form* associated with the quadratic form, too. Taking $D(a_{\mathcal{G}}) = H^1(\mathcal{G})$ as its form domain leads us to the following.

Proposition 3.2. *The self-adjoint operator $-\Delta_{\mathcal{G}}$ associated with $a_{\mathcal{G}}$ by means of*

$$\begin{aligned} D(-\Delta_{\mathcal{G}}) &:= \{u \in H^1(\mathcal{G}) : a_{\mathcal{G}}(u, v) = (w, v)_{L^2(\mathcal{G})} \text{ for all } v \in H^1(\mathcal{G}) \text{ and some } w \in L^2(\mathcal{G})\}, \\ -\Delta_{\mathcal{G}}u &:= w \end{aligned}$$

is explicitly given by

$$(3.4) \quad \begin{aligned} D(-\Delta_{\mathcal{G}}) &= \left\{ u \in \bigoplus_{\mathbf{e} \in E} H^2(\mathbf{e}) \text{ for all } \mathbf{e} \in E : u \in C(\mathcal{G}), \partial u(\mathbf{v}) = 0 \text{ for all } \mathbf{v} \in V \right\}, \\ -\Delta_{\mathcal{G}}u &= -u''. \end{aligned}$$

The operator $-\Delta_{\mathcal{G}}$ in (3.4) is called the *Laplacian with standard vertex conditions*, or simply *standard Laplacian*. We are going to refer to the spectrum of the standard Laplacian on \mathcal{G} as the *spectrum of \mathcal{G}* .

It is easy to see that $-\Delta_{\mathcal{G}}$ is closed; therefore, $D(-\Delta_{\mathcal{G}})$ is also a Hilbert space whenever equipped with the graph norm.

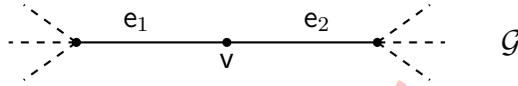
Remark 3.3. Note that $D(-\Delta_{\mathcal{G}}) \subset H^2(\mathcal{G})$, but the functions from the domain satisfy additional condition

$$(3.5) \quad \partial u(\mathbf{v}) \equiv \sum_{\mathbf{e} \sim \mathbf{v}} \frac{\partial u_{\mathbf{e}}}{\partial n}(\mathbf{v}) = 0$$

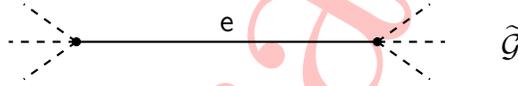
which is often referred to as *Kirchhoff condition* in the literature, since it reminds of the Kirchhoff's law for electrical networks and at the same time guarantees that the total flux through the vertex is zero. On the other hand any other Hermitian vertex condition (not considered here) ensures conservation of the quantum flux.

We stress that (3.5) is fully determined by the quadratic form (including its domain, in particular, by the continuity at the vertices) and by the requirement that its associated operator is self-adjoint in $L^2(\mathcal{G})$.

Suppose $\deg \mathbf{v} = 2$, with $\mathbf{v} \sim \mathbf{e}_1, \mathbf{e}_2$.



Then orienting the two edges appropriately, the continuity and zero normal derivative conditions imply that the function and its first derivative are continuous at the vertex. Create a new graph $\tilde{\mathcal{G}}$ by replacing \mathbf{e}_1 and \mathbf{e}_2 with a single edge \mathbf{e} of length $\ell_{\mathbf{e}} = \ell_{\mathbf{e}_1} + \ell_{\mathbf{e}_2}$, preserving all other incidence and adjacency relations. This “deletes” the vertex \mathbf{v} .



Conversely, we speak of *inserting* a degree two vertex at a point x whenever we replace $x \in \mathbf{e}$ with a dummy vertex, thus “dividing” \mathbf{e} into two edges.

Such degree two vertices will be useful in some of our constructions and will be called *dummy vertices*. All vertices with $\deg \mathbf{v} = 2$ are called *essential*. In the case of cycle graph – the graph made of one interval with both endpoints identified into one vertex – the vertex of degree two cannot be removed.

Theorem 3.4. *Let \mathcal{G} be a metric graph. If $\tilde{\mathcal{G}}$ is obtained from \mathcal{G} by inserting a dummy vertex at any $x \in \mathcal{G}$, then there is an isometry between the graphs \mathcal{G} and $\tilde{\mathcal{G}}$, which induces an isometric isomorphism between the spaces $L^2(\mathcal{G})$ and $L^2(\tilde{\mathcal{G}})$, $C(\mathcal{G})$ and $C(\tilde{\mathcal{G}})$, $H^1(\mathcal{G})$ and $H^1(\tilde{\mathcal{G}})$, as well as $D(-\Delta_{\mathcal{G}})$ and $D(-\Delta_{\tilde{\mathcal{G}}})$ and the operators $-\Delta_{\mathcal{G}}$ and $-\Delta_{\tilde{\mathcal{G}}}$ are unitarily equivalent.*

Inserting or deleting a dummy vertex does not “change” the graph at a metric or measure-theoretic level. Any point $x \in \mathcal{G}$ may thus be treated as a vertex if it is convenient to do so.

Proposition 3.5. *The spectrum of the standard Laplacian $-\Delta_{\mathcal{G}}$ is pure discrete and consists of infinitely many non-negative eigenvalues λ_n tending to $+\infty$. Its lowest eigenvalue is 0 and its multiplicity agrees with the number of connected components of \mathcal{G} .*

Because the spectrum of the standard Laplacian on a disconnected metric graph is merely the union of the spectra of the standard Laplacian on each connected component, we will

for simplicity always assume the metric graph \mathcal{G} to be connected. We adopt throughout the following notations: the spectrum of the standard Laplacian will be denoted by

$$(3.6) \quad 0 = \mu_1(\mathcal{G}) < \mu_2(\mathcal{G}) \leq \mu_3(\mathcal{G}) \leq \dots \mu_n(\mathcal{G}) \rightarrow \infty;$$

or by

$$(3.7) \quad 0 = \mu_1 < \mu_2 \leq \mu_3 \leq \dots \mu_n \rightarrow \infty,$$

if there is no risk of confusion. The difference $\mu_2 - \mu_1 = \mu_2$ is often referred to as *spectral gap*.

Clearly, the validity of the Kirchhoff condition implies that every vertex is incident with at least *one* e satisfying

$$\frac{\partial u_e}{\partial n}(\mathbf{v}) \geq 0$$

Definition 3.6. Given a metric graph \mathcal{G} and a non-negative continuously differentiable function $0 \leq u \in D(\Delta)$, a vertex $\mathbf{v} \in \mathbf{V}$ of degree $\deg \mathbf{v} \geq 2$ shall be called a *serious point* (for the function u) if $u(\mathbf{v}) \neq 0$ and there exist at least *two* edges $\mathbf{e}_1, \mathbf{e}_2 \sim \mathbf{v}$ such that

$$(3.8) \quad \frac{\partial u_{\mathbf{e}_i}}{\partial n}(\mathbf{v}) \geq 0, \quad i = 1, 2.$$

Observe that any local maximum of f is serious.

3.4. Examples of standard Laplacians.

Example 3.7. Let us present a few fundamental examples of a metric graphs: If all edges have the same length, then we call it *equilateral* (but beware the different convention in (10) below).

- (1) *Paths* are intervals identified with metric graphs.
- (2) *Loops* are constructed by identifying both endpoints of a path.
- (3) *Figure-8 graphs* are constructed from two loops $\mathcal{G}_1, \mathcal{G}_2$ (of possibly different lengths) upon identifying two vertices \mathbf{v}_1 in \mathcal{G}_1 and \mathbf{v}_2 in \mathcal{G}_2 .
- (4) *Flowers* consist of one central vertex (the *center*) and E loops (the *leaves*) attached to it.

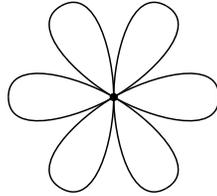


FIGURE 3. A flower on six edges (petals).

- (5) *Stars* consist of a central vertex \mathbf{v} (the *center*) and $E \geq 2$ edges radiating out from \mathbf{v} .
- (6) *Pumpkins* are built upon non-simple combinatorial graphs consisting of two vertices and e parallel edges, having both vertices as endpoints.

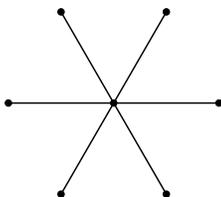


FIGURE 4. A star on 6 edges (rays).

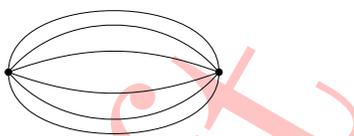


FIGURE 5. A pumpkin graph on six edges (slices).

- (7) *Pumpkin chains* consist of V vertices v_1, \dots, v_V and $E = \sum_{i=1}^{n-1} \sum_{j=1}^{m_i}$ edges, with m_i parallel edges between v_i, v_{i+1} . They are called η -*homogeneous* if $m_i \equiv \eta \in \mathbb{N}$, or *locally equilateral* if, for each $i = 1, \dots, n - 1$, the m_i parallel edges between v_i and v_{i+1} all have the same length (that is, the corresponding pumpkin subgraph is equilateral). In any case, we refer to v_1, v_V as the *antipodal points*.



FIGURE 6. A non-homogeneous pumpkin chain graph.

- (8) *Pumpkin stars* consist of a central vertex v (the *center*) and n pumpkins (each with m_1, \dots, m_n parallel edges) attached to it by either of their endpoints. They are called *homogeneous* if $m_i \equiv \eta \in \mathbb{N}$.
- (9) *Lasso (tadpole) graphs* are obtained from one path graph (the *handle*) \mathcal{G}_1 and one loop \mathcal{G}_2 upon identifying a vertex of \mathcal{G}_1 and an arbitrary point of \mathcal{G}_2 .

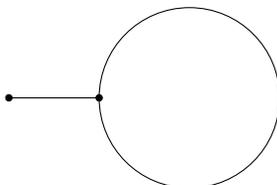


FIGURE 8. A lasso graph.

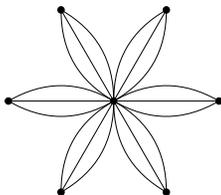
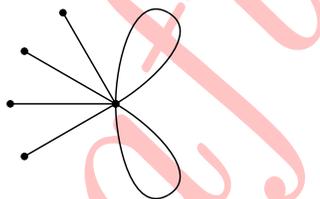


FIGURE 7. A homogeneous pumpkin star on 18 edges.

- (10) More generally, *stowers* are obtained gluing one flower graph and one star graph at their centers.⁴

FIGURE 9. A stower graph with $E_p = 2$ petals and $E_l = 4$ leaves.

- (11) *Complete metric graphs* are 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.

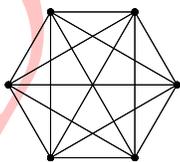


FIGURE 10. A complete graph on six vertices.

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. The following examples are taken from [119, 26, 160].

Lemma 3.8. *Let \mathcal{G} be a metric graph of total length $|\mathcal{G}|$. The following assertions hold.*

(a) *If \mathcal{G} is a path graph, then*

$$(3.9) \quad \mu_2 = \frac{\pi^2}{|\mathcal{G}|^2}.$$

⁴Exceptionally, we call stowers (and hence lasso graphs) *equilateral* if each of the flower's edges has *twice* the length of each of the star's edges.

(b) If \mathcal{G} is a loop, then

$$(3.10) \quad \mu_2 = \frac{4\pi^2}{|\mathcal{G}|^2}.$$

(c) If \mathcal{G} is a figure-8 graph, then

$$(3.11) \quad \mu_2 = \frac{4\pi^2}{|\mathcal{G}|^2}.$$

(d) If \mathcal{G} is an equilateral flower graph on $E \geq 2$ leaves, then

$$(3.12) \quad \mu_2 = \frac{\pi^2 E^2}{|\mathcal{G}|^2}.$$

(If $E = 1$, then \mathcal{G} is a loop.)

(e) If \mathcal{G} is an equilateral star graph on $E \geq 2$ edges, then

$$(3.13) \quad \mu_2 = \frac{\pi^2 E^2}{4|\mathcal{G}|^2}.$$

(f) If \mathcal{G} is an equilateral pumpkin graph on E edges, then

$$(3.14) \quad \mu_2 = \frac{\pi^2 E^2}{|\mathcal{G}|^2}.$$

(g) If \mathcal{G} is an η -homogeneous pumpkin chain, then

$$(3.15) \quad \mu_2 = \frac{\eta^2 \pi^2}{|\mathcal{G}|^2}.$$

(h) If \mathcal{G} is an η -homogeneous pumpkin star on $E = m\eta$ edges, $m \geq 2$, then

$$\mu_2 = \frac{\pi^2 E^2}{4|\mathcal{G}|^2}.$$

(i) If \mathcal{G} is a lasso graph with a handle of length ℓ_1 and a loop of length ℓ_2 , then k^2 is an eigenvalue of $\Delta_{\mathcal{G}}$ if and only if

$$(3.16) \quad \left(\cot k\ell_1 - 2 \tan \frac{k\ell_2}{2} \right) \sin \frac{k\ell_2}{2} = 0.$$

In particular,

$$\mu_2 = \frac{(\arcsin \frac{1}{\sqrt{3}})^2}{\ell^2}$$

if \mathcal{G} is equilateral (beware the above convention!), i.e., $\ell_2 = 2\ell_1$.

(j) If \mathcal{G} is an equilateral stower graph (beware the above convention!) on E_p petals and E_l leaves, with all leaves of equal length and all petals of (equal) double length, then

$$(3.17) \quad \mu_2 = \frac{\pi^2}{|\mathcal{G}|^2} \left(E_p + \frac{E_l}{2} \right)^2.$$

(k) If \mathcal{G} is an equilateral complete graph on V vertices, then

$$(3.18) \quad \mu_2 = \left(\arccos \frac{1}{1-V} \right)^2 \frac{V^2(V-1)^2}{4|\mathcal{G}|^2}.$$

Lemma 3.8.(k) has been used in [81] to prove an interesting result in differential geometry: given a compact manifold M of dimension $d \geq 3$, a Riemannian metric on M can be chosen such that the lowest positive eigenvalue of the corresponding Laplace–Beltrami operator has arbitrarily large multiplicity.

The proof of most of the items in Lemma 3.8 is based on a simple but crucial symmetry argument which we provide in Lemma 3.10 below. The main exceptions are given by Lemma 3.8.(c) and Lemma 3.8.(i): why (3.10) and (3.16) hold will be discussed in Example 6.5 below, whereas (3.16) can be proved as in Example 3.9 below.

Example 3.9. Lemma 3.15.(e) is based on the computation of a secular equation⁵ for a non-equilateral graph. Based on [41, Example 2.3], let us study again the 3-star graph of Example 3.1, assigning now a length $\ell_k > 0$ to each \mathbf{e}_k , $k = 1, 2, 3$.

Direct $\mathbf{e}_k \simeq [0, \ell_k]$ such that $0 \sim \mathbf{v}_k$, $\ell_k \sim \mathbf{v}_4$ (corresponding to the orientation in Figure 1-right). On each edge, in local coordinates, an eigenfunction ψ for some eigenvalue $\lambda > 0$ is just a solution of $-\psi'' = \lambda\psi$ and thus given by

$$\psi|_{\mathbf{e}_k}(x) = A_k \cos(\sqrt{\lambda}x) + B_k \sin(\sqrt{\lambda}x), \quad A_k, B_k \in \mathbb{R}, \quad k = 1, 2, 3.$$

The Kirchhoff condition reduces to $\psi'(\mathbf{v}_i) = 0$ for $i = 1, 2, 3$: thus $B_k = 0$, $k = 1, 2, 3$.

Continuity at \mathbf{v}_4 implies

$$(3.19) \quad A_1 \cos(\sqrt{\lambda}\ell_1) = A_2 \cos(\sqrt{\lambda}\ell_2) = A_3 \cos(\sqrt{\lambda}\ell_3).$$

The Kirchhoff condition at \mathbf{v}_4 implies

$$-\sqrt{\lambda}A_1 \sin(\sqrt{\lambda}\ell_1) - \sqrt{\lambda}A_2 \sin(\sqrt{\lambda}\ell_2) - \sqrt{\lambda}A_3 \sin(\sqrt{\lambda}\ell_3) = 0,$$

or

$$(3.20) \quad A_1 \sin(\sqrt{\lambda}\ell_1) + A_2 \sin(\sqrt{\lambda}\ell_2) + A_3 \sin(\sqrt{\lambda}\ell_3) = 0.$$

Taking into account (3.19) we reach at the secular equation

$$(3.21) \quad \tan(\sqrt{\lambda}\ell_1) + \tan(\sqrt{\lambda}\ell_2) + \tan(\sqrt{\lambda}\ell_3) = 0$$

that characterizes the (nonzero) eigenvalues of \mathcal{G} : we recover (3.13) if the star is equilateral.

In the following, we call a permutation O on the edge set \mathcal{E} of an equilateral metric graph \mathcal{G} an *automorphism* of \mathcal{G} if it respects adjacency, i.e., if Oe, Of share an endpoint whenever $e, f \in \mathcal{E}$ do. An automorphism is called *orientation-preserving* if, additionally, it respects *oriented* adjacency, i.e., if Oe, Of share an initial (resp., terminal) endpoint whenever $e, f \in \mathcal{E}$ do: in other words, we impose the condition that if \mathbf{v} is identified with 0 (resp., ℓ) on both e, f , then so is the common vertex of Oe, Of . If \mathcal{G} is equilateral, say $\ell_e \equiv \ell$, then any automorphism

⁵Note that secular equations are generally not unique!

O canonically induces an isomorphism from $L^2(\mathcal{G})$ to itself, which for simplicity we denote again by O , via

$$(Of)_e(x) = f_{Oe}(x), \quad \text{for a.e. } x \in (0, \ell).$$

Now, let us consider the orthogonal projector P_O onto the subspace of $L^2(\mathcal{G})$ -functions that are pointwise constant along the orbits:

$$L^2(\mathcal{G}) := L_s^2(\mathcal{G}) \oplus L_a^2(\mathcal{G}) := P_O L^2(\mathcal{G}) + (\text{Id} - P_O)L^2(\mathcal{G}).$$

Because O commutes with $\Delta_{\mathcal{G}}$, so does P_O : this implies that if the automorphism group generated by O acts transitively, the following spectral decomposition holds:

Lemma 3.10. *Let O be an automorphism of an equilateral metric graph \mathcal{G} such that given any two edges $e, f \in \mathbf{E}$ there is $n \in \mathbb{N}$ such that $f = O^n e$. Then the spectrum of the standard Laplacian on \mathcal{G} is the union of the spectra of $\Delta_{\mathcal{G}}|_{L_s^2(\mathcal{G})}$ and $\Delta_{\mathcal{G}}|_{L_a^2(\mathcal{G})}$ (including multiplicities).*

We can make good use of this decomposition: in particular, $L_s^2(\mathcal{G})$ is often isomorphic to $L^2(\tilde{\mathcal{G}})$ for a smaller graph that is easier to study, whereas the functions in the domain of $\Delta_{\mathcal{G}}|_{L_a^2(\mathcal{G})}$ can be shown, in many cases, to have vertices with Dirichlet conditions instead of standard vertex conditions: this has been used at least since [173] in the analysis of radially symmetric trees. A more detailed analysis [27, 23] on general symmetric graphs decomposes the space $L_a^2(\mathcal{G})$ into a sum over irreducible representations of the automorphism group. From this point of view, $L_s^2(\mathcal{G})$ is the part of the Hilbert space corresponding to the trivial representation.

Example 3.11. In the case of an equilateral stars \mathcal{S} on m edges, the Laplacian $\Delta_{\mathcal{S}}$ can be decomposed into a Laplacian on one interval with Neumann conditions at both endpoints; and Laplacians on $m - 1$ copies of the same interval with mixed Dirichlet/Neumann conditions. The same idea has been used in [172] to determine the spectrum of the Ornstein–Uhlenbeck operator on a star graph.

3.5. Dirichlet Laplacians. Because the eigenfunction associated with the lowest eigenfunction of the standard Laplacian is constant, all further eigenfunctions – and in particular the eigenfunction ψ associated with the second lowest eigenfunction – must be orthogonal to constants and, hence, change sign. By Proposition 3.18, eigenfunctions are continuous and, hence, must vanish at the interface between the support of their positive and negative parts. Such sets

$$\{x \in \mathcal{G} : \psi(x) \geq 0\} \quad \text{and} \quad \{x \in \mathcal{G} : \psi(x) \leq 0\}$$

define metric graphs in their own right, but ψ does not satisfy standard vertex conditions at all their vertices. This motivates to introduce a more general class of Dirichlet Laplacian. We let \mathbf{V}_D be a subset of \mathbf{V} – we will call it the *Dirichlet set* – and consider the same quadratic form as in (3.3), namely

$$(3.22) \quad a_{\mathcal{G}}^{\mathbf{V}_D}(u) := \int_{\mathcal{G}} |u'(x)|^2 dx = \sum_{e \in \mathbf{E}} \int_0^{\ell_e} |u'_e(x)|^2 dx,$$

but with the domain

$$(3.23) \quad H_0^1(\mathcal{G}; \mathbf{V}_D) := \{f \in H^1(\mathcal{G}) : f(\mathbf{v}) = 0 \text{ for all } \mathbf{v} \in \mathbf{V}_D\}.$$

We can then generalize Proposition 3.2 as follows.

Proposition 3.12. *Let $\mathbf{V}_D \subset \mathbf{V}$, then the self-adjoint operator $-\Delta_{\mathcal{G}}^{\mathbf{V}_D}$ associated with $a_{\mathcal{G}}^{\mathbf{V}_D}$ by means of*

$$D(-\Delta_{\mathcal{G}}^{\mathbf{V}_D}) := \{u \in H_0^1(\mathcal{G}; \mathbf{V}_D) : a_{\mathcal{G}}^{\mathbf{V}_D}(u, v) = (w, v)_{L^2(\mathcal{G})} \text{ for all } v \in H_0^1(\mathcal{G}; \mathbf{V}_D) \text{ and some } w \in L^2(\mathcal{G})\},$$

$$-\Delta_{\mathcal{G}}^{\mathbf{V}_D} u := w,$$

is explicitly given by

$$(3.24) \quad D(-\Delta_{\mathcal{G}}^{\mathbf{V}_D}) = \left\{ u \in \bigoplus H^2(\mathbf{e}) \text{ for all } \mathbf{e} \in \mathbf{E} : u \in C(\mathcal{G}), \begin{array}{l} u(\mathbf{v}) = 0 \text{ for all } \mathbf{v} \in \mathbf{V}_D \\ \partial u(\mathbf{v}) = 0 \text{ for all } \mathbf{v} \in \mathbf{V}_N \end{array} \right\},$$

$$-\Delta_{\mathcal{G}}^{\mathbf{V}_D} u = u''.$$

The operator $\Delta_{\mathcal{G}}^{\mathbf{V}_D}$ in (3.24) is called the *Laplacian with Dirichlet conditions in \mathbf{V}_D* or simply the *Dirichlet Laplacian*.

We obtain the following counterpart of Proposition 3.5.

Proposition 3.13. *If \mathbf{V}_D is not empty, then the spectrum of the Dirichlet Laplacian $\Delta_{\mathcal{G}}^{\mathbf{V}_D}$ is purely discrete and consists of infinitely many positive eigenvalues tending to $+\infty$. Its lowest eigenvalue is simple and strictly positive.*

The spectrum of the Dirichlet Laplacian with $\mathbf{V}_D \neq \emptyset$ will be denoted by

$$(3.25) \quad 0 < \lambda_1(\mathcal{G}; \mathbf{V}_D) < \lambda_2(\mathcal{G}; \mathbf{V}_D) \leq \lambda_3(\mathcal{G}; \mathbf{V}_D) \leq \dots \leq \lambda_n(\mathcal{G}; \mathbf{V}_D) \rightarrow \infty;$$

or by

$$(3.26) \quad 0 < \lambda_1^D < \lambda_2^D \leq \lambda_3^D \leq \dots \leq \lambda_n \rightarrow \infty.$$

if there is no risk of confusion concerning the Dirichlet set.

The following lemma compares the eigenvalues of $\Delta_{\mathcal{G}}$ with and without Dirichlet conditions. The proof is based on monotonicity and co-dimension of the domains (3.23), see [48, 146, 46].

Lemma 3.14. *For any $\mathbf{V}_D \subset \mathcal{G}$, $\mathbf{v} \in \mathcal{G}$ and $k \in \mathbb{N}$ we have*

$$(3.27) \quad \mu_k(\mathcal{G}) \leq \lambda_k(\mathcal{G}; \mathbf{V}_D) \leq \mu_{k+|\mathbf{V}_D|}(\mathcal{G}),$$

$$(3.28) \quad \lambda_k(\mathcal{G}; \mathbf{V}_D) \leq \lambda_k(\mathcal{G}; \mathbf{V}_D \cup \{\mathbf{v}\}) \leq \lambda_{k+1}(\mathcal{G}; \mathbf{V}_D).$$

Remarkably, upon imposing a Dirichlet condition at the center \mathbf{v}_c of equilateral stowers (and, in particular, of flowers or stars) we even have $\lambda_1(\mathcal{G}; \{\mathbf{v}_c\}) = \mu_2(\mathcal{G})$: metric graphs with this behavior are said to *obey the Dirichlet criterion* with respect to \mathbf{v} (in this case, $\mathbf{v} = \mathbf{v}_c$): this is a crucial property in the study of classes of graphs that are extremal with respect to μ_2 in [26].

Let us collect the values of λ_1 for a few fundamental examples: observe that many of the examples discussed in Lemma 3.8 become trivial upon imposing Dirichlet boundary conditions:

for instance, upon imposing a Dirichlet condition at its center vertex \mathbf{v}_c , the Laplacian on the flower graph (resp., on the star graph on $E \geq 2$ edges) becomes a direct sum of Laplacians on disjoint intervals with Dirichlet-only (resp., mixed Dirichlet/Neumann) boundary conditions.

Lemma 3.15. *Let \mathcal{G} be a metric graph of total length $|\mathcal{G}|$. The following assertions hold.*

(a) *If \mathcal{G} is a path graph with endpoints $\mathbf{v}_1, \mathbf{v}_2$, then*

$$(3.29) \quad \lambda_1(\mathcal{G}; \{\mathbf{v}_1\}) = \frac{\pi^2}{4|\mathcal{G}|^2} \quad \text{and} \quad \lambda_1(\mathcal{G}; \{\mathbf{v}_1, \mathbf{v}_2\}) = \frac{\pi^2}{|\mathcal{G}|^2}.$$

(b) *If \mathcal{G} is an equilateral star graph on $E \geq 2$ edges and $\mathbf{V}_D = \{\mathbf{v} \in \mathbf{V} : \deg(\mathbf{v}) = 1\}$, then*

$$(3.30) \quad \lambda_1(\mathcal{G}; \mathbf{V}_D) = \frac{\pi^2 E^2}{4|\mathcal{G}|^2}.$$

(c) *If \mathcal{G} is an η -homogeneous pumpkin chain with antipodal points $\mathbf{v}_1, \mathbf{v}_2$, then*

$$(3.31) \quad \lambda_1(\mathcal{G}; \{\mathbf{v}_1\}) = \frac{\eta^2 \pi^2}{4|\mathcal{G}|^2} \quad \text{and} \quad \lambda_1(\mathcal{G}; \{\mathbf{v}_1, \mathbf{v}_2\}) = \frac{\eta^2 \pi^2}{|\mathcal{G}|^2}.$$

(d) *If \mathcal{G} is a stower graph with center \mathbf{v}_c on E_p petals and E_l leaves, with all leaves of equal length and all petals of (equal) double length, then*

$$(3.32) \quad \lambda_1(\mathcal{G}; \{\mathbf{v}_c\}) = \frac{\pi^2}{|\mathcal{G}|^2} \left(E_p + \frac{E_l}{2} \right)^2.$$

(e) *If \mathcal{G} is a lasso graph with a handle of length ℓ_1 and a loop of length ℓ_2 , then k^2 is an eigenvalue of $\Delta_{\mathcal{G}}^{\mathbf{V}_D}$ if and only if $k > 0$ is a root of*

$$2 \sin(k\ell_1) (\cos(k\ell_2) - 1) + \cos(k\ell_1) \sin(k\ell_2) = 0.$$

3.6. Eigenvalue asymptotics. We know from the proof of Proposition 3.5 that the Laplacian with standard vertex conditions (and, possibly, Dirichlet conditions at a vertex set \mathbf{V}_D) has compact resolvent. Like in the case of a single interval, it is natural to wonder about the growth behavior of the eigenvalues. Because the embedding of $C(\mathcal{G}) \cap \bigoplus_{\mathbf{e} \in E} H^2(\mathbf{e})$ into $L^2(\mathbf{e})$ is not only compact, but even of trace class by Proposition 3.18, the resolvent $(\lambda - \Delta_{\mathcal{G}})^{-1}$ for each $\lambda < 0$ of trace class, hence its strictly positive eigenvalues must form a summable sequence. The following Weyl-type asymptotic delivers a finer description: in the equilateral case it has been known since [176], but this assumption was later removed in [200].

Proposition 3.16. *Let \mathcal{G} be a compact metric graph with total length $|\mathcal{G}|$ and let $\mathbf{V}_D \subset \mathbf{V}$ (possibly empty). Then*

$$\lambda_k(\Delta_{\mathcal{G}}^{\mathbf{V}_D}) = \frac{\pi^2 k^2}{|\mathcal{G}|^2} + \mathcal{O}(k) \quad \text{as } k \rightarrow \infty.$$

No explicit form for lower order terms can be obtained (with the exception of the single compact interval) since the eigenvalues form an almost periodic sequence being zeroes of a trigonometric polynomial [31, 150, 141].

Proof. For all $V_D \subset V$ the operator $-\Delta_{\mathcal{G}}^{V_D}$ can be sandwiched, in the sense of quadratic forms, between the operators associated with a^D, a^N : these are the forms that act as $a_{\mathcal{G}}$ on the domains

$$D(a^D) = \bigoplus_{e \in E} H_0^1(e), \quad D(a^N) = \bigoplus_{e \in E} H^1(e),$$

respectively. Their associated operators are the direct sums of the Laplacians with Dirichlet and Neumann conditions on each interval $e = (0, \ell_e)$, respectively, and we have already seen that the eigenvalues of both satisfy the Weyl asymptotics (2.9). \square

Because $\Delta_{\mathcal{G}}^{V_D}$ is a self-adjoint, negative semidefinite operators on $L^2(\mathcal{G})$, it generates a semigroup. Let us collect known information about it: we refer to [167, Chapter 6] for the proofs.

Proposition 3.17. *The quadratic form $a_{\mathcal{G}}$ in (3.22) is a Dirichlet form whenever defined on $D(a) = H_0^1(\mathcal{G}; V_D)$ for any (possibly empty) subset $V_D \subset V$. In particular, the strongly-continuous semigroups generated by this realization on $L^2(\mathcal{G})$ is positivity-preserving and L^∞ -contractive.*

If we denote by $\Delta_{\mathcal{G}}^{V_D}$ the Laplacian on \mathcal{G} with standard vertex conditions on $V \setminus V_D$ and Dirichlet conditions on V_D , and by $\Delta_{\mathcal{G}}$ the Laplacian on \mathcal{G} with standard vertex conditions on all vertices, then the domination inequalities

$$e^{t\Delta_{\mathcal{G}}^{V_{D_2}}} \leq e^{t\Delta_{\mathcal{G}}^{V_{D_1}}} \leq e^{t\Delta_{\mathcal{G}}}$$

hold, in the sense of Banach lattices, for all $\emptyset \neq V_{D_1} \subset V_{D_2} \subset V$.

Several embedding results are known for the relevant function spaces, with important consequences for the spectral properties of Laplacians on metric graphs, too. The following assertions have been proved in [72, Corollary 2.3], [167, Lemma 3.27], [171, Lemma 3.7] and [124, Lemma 3.2].

Proposition 3.18. *The following assertions hold.*

- (1) *The space $H^1(\mathcal{G})$ is compactly embedded into $C(\mathcal{G})$.*
- (2) *The space $W^{1,\infty}(\mathcal{G})$ is continuously embedded into $\text{Lip}(\mathcal{G})$.*
- (3) *The space $H^1(\mathcal{G})$ is continuously embedded into $C^{\frac{1}{2}}(\mathcal{G})$, and the $\frac{1}{2}$ -Hölder seminorm of any $f \in H^1(\mathcal{G})$ is no larger than $\|f'\|_{L^2(\mathcal{G})}$.*
- (4) *The embedding of $H^1(\mathcal{G})$ into $L^2(\mathcal{G})$ is of Hilbert-Schmidt class, while the embedding of $H^1(\mathcal{G}) \cap \bigoplus_{e \in E} H^2(0, \ell_e)$ into $L^2(\mathcal{G})$ is of trace class.*

Let us observe an immediate consequence of Proposition 3.18: the space $C(\mathcal{G}) \cap \bigoplus_{e \in E} H^2(0, \ell_e)$, and in particular the domain $\Delta_{\mathcal{G}}$, is continuously embedded into $\text{Lip}(\mathcal{G})$.

Corollary 3.19. *Let $V_D \subset V$ (possibly empty). Then all eigenfunctions of $\Delta_{\mathcal{G}}^{V_D}$ are Lipschitz continuous over \mathcal{G} .*

Furthermore, it follows from Proposition 3.18.(4) that the semigroup generated by $\Delta_{\mathcal{G}}^{V_D}$ is a trace class operator for all $t > 0$. The following short-time asymptotics of the trace has been known since [195, 175]: this is a first evidence of the fact that the spectrum allow us to

solve an inverse geometric problem, and in particular to reconstruct volume and some relevant combinatorial quantities associated with \mathcal{G} .

Theorem 3.20. *For a metric graph on V vertices and E edges there holds*

$$\mathrm{Tr}(e^{t\Delta_{\mathcal{G}}}) = \frac{|\mathcal{G}|}{\sqrt{4\pi t}} + \frac{V - E}{2} + o(t) \quad \text{as } t \rightarrow 0.$$

If \mathbf{V}_D is the set of all vertices of degree 1, then

$$\mathrm{Tr}(e^{t\Delta_{\mathcal{G}}^{\mathbf{V}_D}}) = \frac{|\mathcal{G}|}{\sqrt{4\pi t}} + \frac{V_r - E}{2} + o(t) \quad \text{as } t \rightarrow 0,$$

where V_r is the number of ramification vertices, i.e., of vertices of degree ≥ 3 .

3.7. First results in spectral geometry. This survey is devoted to the topic of spectral geometry, that is, how the metric and combinatorial feature of the underlying metric graph \mathcal{G} influence the spectrum (either the individual eigenvalues of their distribution as an ensemble) of the two Laplacian realizations on $L^2(\mathcal{G})$ we have just introduced. To give a flavor of this topic, let us first introduce two geometric quantities.

Definition 3.21. The *mean distance* $\mathrm{MeanDist}(\mathcal{G})$ and *diameter* $\mathrm{Diam}(\mathcal{G})$ are given by

$$\mathrm{MeanDist}(\mathcal{G}) := \frac{1}{|\mathcal{G}|^2} \int_{\mathcal{G}} \int_{\mathcal{G}} \mathrm{dist}(x, y) \, dx \, dy.$$

and

$$\mathrm{Diam}(\mathcal{G}) := \sup_{x, y \in \mathcal{G}} \mathrm{dist}(x, y),$$

respectively.

If $\mathbf{V}_D \neq \emptyset$, the *mean distance* $\mathrm{MeanDist}(\mathcal{G}; \mathbf{V}_D)$ and the *inradius* $\mathrm{Inr}(\mathcal{G}; \mathbf{V}_D)$ from \mathbf{V}_D are given by

$$\mathrm{MeanDist}(\mathcal{G}; \mathbf{V}_D) := \frac{1}{|\mathcal{G}|} \int_{\mathcal{G}} \mathrm{dist}(x, \mathbf{V}_D) \, dx,$$

and

$$\mathrm{Inr}(\mathcal{G}; \mathbf{V}_D) := \sup_{x \in \mathcal{G}} \inf_{v \in \mathbf{V}_D} \mathrm{dist}(x, v),$$

respectively.

We also introduce two further non-standard quantities: the *triameter* is

$$(3.33) \quad \mathrm{Triam}(\mathcal{G}) := \max_{x_1, x_2, x_3 \in \mathcal{G}} \min_{j \neq k} \mathrm{dist}(x_j, x_k);$$

while the *avoidance diameter* is

$$(3.34) \quad \mathrm{AvDiam}(\mathcal{G}) := \max_{\gamma \in \Gamma} \min_{t \in \mathbb{S}^1} \mathrm{dist}(\gamma(-t), \gamma(t)),$$

where \mathbb{S}^1 is the unit circle in \mathbb{C} and let Γ denote the class of injective continuous maps from \mathbb{S}^1 to \mathcal{G} .

In other words, the triameter measures the maximal pairwise separation among any *three* points on \mathcal{G} ; whereas the avoidance diameter measures how far apart two points can remain while exchanging places.

We can now provide two examples of spectral geometric results which can be derived from the variational properties of $\Delta_{\mathcal{G}}$ in an elementary way. The first one is [183, Theorem 4.4.3].

Corollary 3.22. *Let $\emptyset \neq \mathbf{V}_D \subset \mathbf{V}$. Then*

$$\lambda_1(\mathcal{G}; \mathbf{V}_D) \geq \frac{1}{|\mathcal{G}| \text{MeanDist}(\mathcal{G}; \mathbf{V}_D)} > \frac{1}{|\mathcal{G}| \text{Inr}(\mathcal{G}; \mathbf{V}_D)}.$$

Proof. We deduce from Proposition 3.18.(3) that

$$|f(x) - f(y)|^2 \leq \text{dist}(x, y) \|f'\|_{L^2(\mathcal{G})}^2$$

and in particular, letting y be the element of \mathbf{V}_D of minimal distance from x and integrating over x ,

$$(3.35) \quad \|f\|_{L^2(\mathcal{G})}^2 \leq \|f'\|_{L^2(\mathcal{G})}^2 \int_{\mathcal{G}} \text{dist}(x, \mathbf{V}_D) dx.$$

Now the assertion follows upon integrating (3.35) from $L^2 - L^\infty$ -Hölder inequality, with strict inequality because $\text{dist}(\cdot, \mathbf{V}_D)$ is not constant. \square

Furthermore, taking $\mathbf{V}_D = \{\mathbf{v}\}$ for some $\mathbf{v} \in \mathcal{G}$ such that

$$\text{MeanDist}(\mathcal{G}) = \frac{1}{|\mathcal{G}|} \int_{\mathcal{G}} \text{dist}(x, \mathbf{v}) dx$$

and combining (3.35) with Lemma 3.14, the following was deduced in [32].

Corollary 3.23. *There holds*

$$\mu_2(\mathcal{G}; \mathbf{V}_D) \geq \frac{1}{|\mathcal{G}| \text{MeanDist}(\mathcal{G})} > \frac{1}{|\mathcal{G}| \text{Diam}(\mathcal{G})}.$$

The bound in Corollary 3.22 will be improved in Section 5.3, whereas one further estimate by diameter sharpening Corollary 3.22 will be obtained in Section 5.3.2.

Remark 3.24. A particularly important class of non-standard vertex conditions are the so-called δ -type conditions. They are physically realizable and, curiously, can be used to approximate all other self-adjoint conditions [78]. They are interesting in the context of spectral optimization because they interpolate between standard and Dirichlet conditions at a vertex.

Letting $\mathbb{T} := \mathbb{R}/\pi\mathbb{Z}$ (in other words, \mathbb{T} is the interval $[-\frac{\pi}{2}, \frac{\pi}{2}]$ with its ends identified), we consider the operator $\Delta_{\mathcal{G}}^\gamma$ with parameters $\gamma : \mathbf{V} \rightarrow \mathbb{T}$ defined by

$$(3.36) \quad \left. \begin{aligned} D(\Delta_{\mathcal{G}}^\gamma) &= \left\{ u \in C(\mathcal{G}) \cap \bigoplus_{\mathbf{e}} H^2(0, \ell_{\mathbf{e}}) : \cos(\gamma_{\mathbf{v}}) \sum_{\mathbf{e} \sim \mathbf{v}} \frac{\partial u_{\mathbf{e}}}{\partial n}(\mathbf{v}) = \sin(\gamma_{\mathbf{v}}) u(\mathbf{v}) \right\}, \\ \Delta_{\mathcal{G}}^\gamma u &= u'' \end{aligned} \right\}$$

We remark that $u(\mathbf{v})$ is well-defined because the function u is continuous.

In particular, letting $\gamma_v = 0$ endows the vertex v with the standard vertex condition, while letting $\gamma_v = \frac{\pi}{2}$ turns the conditions to Dirichlet. The real number $\tan(\gamma_v)$ is sometimes called the strength of the δ potential at the vertex v . In this way, the Dirichlet condition corresponds to infinite strength. We wrote the conditions in the above way to allow treating the Dirichlet condition on an equal footing with others.

Remark 3.25. Just like the anti-periodic conditions are dual to the periodic conditions on an interval, it is also possible to consider a class of vertex conditions dual to the standard ones: they are usually referred to as *anti-Kirchhoff* or *anti-standard* conditions. Likewise, δ' -conditions are dual to δ -conditions. We refer to [38, 149, 192] for a discussion of these exotic conditions.

4. BASIC PROPERTIES OF THE SPECTRUM

Here we briefly list some fundamental properties of the spectrum of a compact graph.

4.1. Discreteness. The spectrum of a compact metric graph (i.e., a graph with finitely many edges of finite total length) with general self-adjoint vertex conditions is well-known to be discrete: it consists of isolated eigenvalues of finite multiplicity. The proof (see, for example, [49, Thm. 3.1.1]) proceeds using the standard technique: the resolvent is shown to be a compact operator in L^2 . Indeed, it is a bounded operator from L^2 to H^2 , which, in turn, is compactly embedded into L^2 .

4.2. Analyticity. Spectrum of the Laplacian on a metric graph has been shown in [48, 135] to be analytic with respect to the choice of the vertex conditions and edge lengths.

More precisely, taking the operator $\Delta_{\mathcal{G}}^{\gamma}$ as our setting, for every graph \mathcal{G} there is an analytic function $\Phi_{\mathcal{G}} : \mathbb{C}^V \times (\mathbb{C} \setminus \{0\})^E \times \mathbb{C} \rightarrow \mathbb{C}$ such that the eigenvalues λ are the roots of

$$(4.1) \quad \Phi_{\mathcal{G}}(\gamma, \{\ell_e\}, \lambda) = 0.$$

The multiplicity of the eigenvalue λ coincides with the algebraic multiplicity of the root.

We remark that equation 4.1 also describes the eigenvalues of non-self-adjoint operators (when γ are complex) on graphs with complex lengths. The latter are taken care of by an appropriate rescaling.

4.3. Secular manifold. An equation giving the eigenvalues of a particular graph is often called the *secular equation*, after [133]. In many cases, the secular equation is a trigonometric polynomial that depends on $\sqrt{\lambda}$ only in combination with edge lengths. In fact, this is true for any Laplacian $\Delta_{\mathcal{G}}^{\mathbb{V}_D}$, including $\mathbb{V}_D = \emptyset$, with one important caveat [37, 133, 130].

Proposition 4.1. *For every graph \mathcal{G} there is a multivariate polynomial $p \in \mathbb{C}[z_1, \dots, z_E]$ such that $\lambda = k^2 > 0$ is an eigenvalue of $\Delta_{\mathcal{G}}^{\mathbb{V}_D}$ if and only if*

$$(4.2) \quad p(e^{ik\ell_1}, \dots, e^{ik\ell_E}) = 0.$$

The multiplicity of the eigenvalue is equal to the algebraic multiplicity of the root.

There is a simple way to compute the polynomial p for any graph via the so-called bond scattering matrix, see [133] or [49, Sec. 2.1.2]. Equation (4.2) has only real roots (which makes it a Lee–Yang polynomial [11]), but the multiplicity of the root at zero does not match the multiplicity of 0 as the eigenvalue of $\Delta_{\mathcal{G}}^{\text{Vd}}$ [148]. We illustrate it in the following example.

Example 4.2. Consider a lasso graph with a Dirichlet condition at the vertex of degree 1. Following a standard procedure [41, Sec. 5.1] one can show its secular polynomial equation (4.2) to be

$$(4.3) \quad 2 \sin(k\ell_1)(\cos(k\ell_2) - 1) + \cos(k\ell_1) \sin(k\ell_2) = 0,$$

where ℓ_1 is the length of the handle and ℓ_2 is the length of the loop. Because of the Dirichlet condition, the operator is strictly positive. In other words, it has no eigenvalue zero despite $k = 0$ being a root of equation (4.3).

The particular form of equation (4.2) lead Barra and Gaspard [31] to view it as intersection times of the flow $k \mapsto (e^{ik\ell_1}, \dots, e^{ik\ell_E})$ on the torus $\mathbb{T}^E := \{|z_1| = \dots = |z_E| = 1\}$ with the *secular manifold* Σ defined⁶ by

$$(4.4) \quad \Sigma := \{(z_1, \dots, z_E) \in \mathbb{T}^E : p(z_1, \dots, z_E) = 0\}.$$

An illustrative example of the secular manifold is shown in Fig. 11 for the lasso graph from Example 4.2. Here the torus is parametrized as $\mathbb{T}^2 = (\mathbb{R}/2\pi\mathbb{Z})^2$ and the secular manifold is the set of solutions (κ_1, κ_2) of

$$(4.5) \quad 2 \sin(\kappa_1)(\cos(\kappa_2) - 1) + \cos(\kappa_1) \sin(\kappa_2) = 0.$$

For a generic choice of edge length ℓ_1, \dots, ℓ_E , the flow wraps around the torus covering it uniformly — this is known as the Weyl equidistribution [208]. Therefore, if one is interested in a spectral average (i.e., an average over many eigenvalues) of a quantity that can be read off Σ , one can instead integrate over Σ with an appropriate measure: the Barra–Gaspard measure [31, 53, 82, 9]. It is the cross-sectional measure of the sets on Σ , i.e., the measure of the projection of the given set onto the hyperplane normal to the vector (ℓ_1, \dots, ℓ_E) .

What interesting spectral quantities can be computed from a point on Σ ? Here is a partial list

- the distance to the next eigenvalue — the “nearest neighbor spacing” [31],
- the distribution of the eigenfunction L^2 norm between the graph’s edges [53, 82],
- the distance of a resonance from the real axis [44],
- the number of zeros of the eigenfunction [9] — via the nodal–magnetic connection [52],
- the distance to the corresponding eigenvalue of a perturbed graph [190] — even in the non-selfadjoint setting.

This idea can be also extended beyond the integration over Σ to yield, for example, the Weyl asymptotics of Proposition 3.16 or the the probability that a randomly chosen positive energy lies in the spectrum of an infinite periodic graph [22, 30, 29].

⁶It is apparent from the definition that Σ is not a manifold but an algebraic variety, but the term “secular manifold” is now standard.

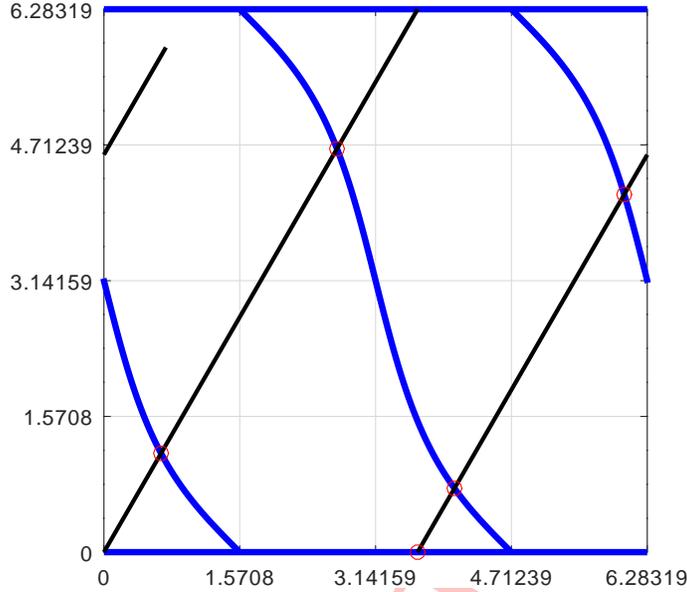


FIGURE 11. The secular manifold Σ (blue) corresponding to the lasso graph of Example 4.2 shown on the torus $\mathbb{T}^E = (\mathbb{R}/2\pi\mathbb{Z})^E$ and intersected by the flow $k \mapsto (k, k\sqrt{3})$ (which corresponds to edge lengths of the tadpole being $\ell_1 = 1$ and $\ell_2 = \sqrt{3}$). The intersection points are marked with circles and correspond numerically to $k = 0.6604, 2.6953, 3.6276, 4.0539, 6.0173$.

4.4. Setting edge lengths to zero. The case of zero lengths is notably absent from the statement of analyticity, equation (4.1). In the most general setting, convergence of the spectrum (and/or the resolvent) is a delicate issue [50, 66, 58], as in some cases the limiting graph has vertices with internal structure [79].

The most basic example showing that one must be careful is provided by the graph consisting of two disjoint intervals, one with Neumann and one with Dirichlet conditions. If the length of the Neumann interval tends to 0, the naive limiting graph is just the Dirichlet interval. But this “limiting operator” has no eigenvalue zero which is present for all non-zero values of the lengths. For other, more exotic, examples the reader is referred to [50, 43, 42].

However, in the case of the operator $\Delta_{\mathcal{G}}^\gamma$, all relevant spectral quantities (eigenvalues, eigenfunctions and the resolvent) do converge to what is intuitively the limiting graph [26, 66, 58], in the appropriate sense and under the following conditions (see [50, Lem 3.4]): the graph \mathcal{G} is connected, not all edges are shrunk to zero. We remark that in the limiting graph, the γ coefficient on a vertex v that is the result of a merger of vertices v_1, \dots, v_r is obtained from the condition

$$(4.6) \quad \tan(\gamma_v) = \sum_{j=1}^r \tan(\gamma_{v_j}).$$

Under the above conditions, it is tempting to compute the secular manifold of the limiting graph $\tilde{\mathcal{G}}$ by setting to zero the relevant variables in the secular manifold of the original graph \mathcal{G} . Unfortunately, this does not work as shown, again, by the tadpole graph: setting ℓ_2 to zero makes the secular trigonometric polynomial (4.3) identically zero.

To the best of our knowledge, it is not known whether the similar procedure works for the analytic function $\Phi_{\tilde{\mathcal{G}}}$, postulated in section 4.2.

4.5. Simplicity of the spectrum. Similar to the classical results for Laplace operator on domains and manifolds [205, 206], the eigenvalues of the graph operator $\Delta_{\mathcal{G}}^{\gamma}$ are generically simple and the eigenfunctions have full support (i.e., do not vanish entirely on any edge) — except for the eigenfunctions supported on a loop. The generic (in the Baire sense) simplicity of the eigenvalues was established in [98]. It was extended to include δ -type vertex conditions and to yield generic full support of eigenfunctions in [51]. The applicable notions of genericity were further strengthened [6] for graphs with standard conditions.

We state the theorem in the formulation of [51], since the result applies to graphs with standard, Dirichlet, or δ -conditions given by (3.36).

Theorem 4.3. *Let \mathcal{G} be a compact connected graph with some fixed choice of vertex parameters γ and with at least one vertex of degree other than 2 (i.e., \mathcal{G} is not a circle). Then the properties*

- (i) every eigenvalue of $\Delta_{\mathcal{G}}^{\gamma}$ is simple, and
- (ii) for each eigenfunction f of $\Delta_{\mathcal{G}}^{\gamma}$,
 - (a) either $f(v) \neq 0$ for each vertex v , or
 - (b) f is supported on only one loop of Γ

hold for the set of choices of edge lengths $(\ell_1, \dots, \ell_E) \in \mathbb{R}_+^E$ that is residual in \mathbb{R}_+^E (i.e., its complement is a meager set — a countable union of nowhere dense sets).

Naturally, if the graph \mathcal{G} has no loops, the case (iib) never occurs.

How bad can the eigenfunctions get in the non-generic case? If the edge lengths are rationally independent, there is a non-zero proportion of eigenfunctions of full support [8]. The same conclusion holds when the lengths are all proportional to a rational number [111]. Remarkably, for an arbitrary metric graph, we do not even know if there are infinitely many of eigenfunctions of full support: the following conjecture, put forward in [111], is still open.

Conjecture 1. *For any metric graph and any choice of a complete orthonormal sequence of eigenfunctions, there are infinitely many eigenfunctions with full support.*

The following partial solution can be found in [185].

Theorem 4.4. *Let \mathcal{G} be a metric tree, or else let $\mathbf{V}_D \neq \emptyset$. Then there exists a strictly increasing sequence of eigenvalues of multiplicity one and a sequence of corresponding eigenfunctions $(\psi_k)_{k \in \mathbb{N}}$ of $-\Delta_{\mathcal{G}}$ (resp., of $-\Delta_{\mathcal{G}}^{\mathbf{V}_D}$), so that each ψ_k does not vanish at the vertices of \mathcal{G} (apart from \mathbf{V}_D)*

Some further ideas were proposed in [140] and [6, Sec. 7.2].

5. GLOBAL METHODS

5.1. Symmetrization. Lemma 6.2 is sufficient to prove the following: this is the earliest result in spectral geometry of quantum graphs. We will recurrently recall it and use it as a field of application of new methods we wish to introduce.

Theorem 5.1. *Let \mathcal{G} be a metric graph of total length $|\mathcal{G}|$. Then the following assertions hold.*

(1) *The lowest positive eigenvalue of the Laplacian $\Delta_{\mathcal{G}}$ satisfies the estimate*

$$(5.1) \quad \mu_2(\mathcal{G}) \geq \frac{\pi^2}{|\mathcal{G}|^2} \quad \text{if } \mathbf{V}_D = \emptyset,$$

and

$$(5.2) \quad \lambda_1(\mathcal{G}; \mathbf{V}_D) \geq \frac{\pi^2}{4|\mathcal{G}|^2} \quad \text{if } \mathbf{V}_D \neq \emptyset.$$

In both cases there is equality if and only if \mathcal{G} is an interval, equipped with Neumann–Neumann conditions in (5.1), and mixed Dirichlet–Neumann conditions in (5.2).

(2) *If, additionally, \mathcal{G} is doubly edge connected, then*

$$(5.3) \quad \mu_2(\mathcal{G}) \geq \frac{4\pi^2}{|\mathcal{G}|^2} \quad \text{if } \mathbf{V}_D = \emptyset,$$

and

$$(5.4) \quad \lambda_1(\mathcal{G}; \mathbf{V}_D) \geq \frac{\pi^2}{|\mathcal{G}|^2} \quad \text{if } \mathbf{V}_D \neq \emptyset.$$

In both cases there is equality if and only if \mathcal{G} is a symmetric necklace with pure standard conditions if (5.3) holds, and in particular at both antipodal points; or with a Dirichlet condition at one antipodal point and standard conditions elsewhere.

Here, we call a metric graph with $\mathbf{V}_D = \emptyset$ *doubly edge connected* if no one cut in any interior point of any edge is sufficient to make \mathcal{G} disconnected (so, a flower graph is doubly edge connected, but a tree graph or a lasso graph are not); in the case of $\mathbf{V}_D \neq \emptyset$, this definition is slightly modified by stipulating that *all vertices in \mathbf{V}_D are identified* before counting (as above) the number of cuts that are necessary to make the graph disconnected.

The assertions in Theorem 5.1.(1) were originally discovered in [176] and rediscovered, generalized and sharpened several times, by different authors and with different proof techniques: we are going to focus on the proof delivered in [98, Theorem 1 and Lemma 3] for (5.1) and (5.2), respectively.

Based on the proof of Theorem 5.1.(1) delivered in [98], the estimates for the case of higher connectivity have been studied in [26, Theorem 2.1(2)] (inequality (5.3)) and in [45, Lemma 4.2] (inequality (5.4)), respectively. (A slightly sharper version of (5.3), also valid for homogeneous nonlinear operators, is proven in [45, Theorem 3.4].)

In view of its importance, we will present a fairly detailed proof of Theorem 5.1. We will begin by proving (5.2); (5.1) will be discussed at the end of this section, as an application of nodal geometry.

Proof. We begin by proving (5.2). We may, without loss of generality, assume \mathcal{G} to be connected after removal of all Dirichlet vertices.

Denote by ψ_1 an eigenfunction corresponding to $\lambda_1(\mathcal{G}; \mathbf{V}_D)$: in view of Proposition 3.17 and the Kreĭn–Rutman Theorem we deduce that ψ_1 is strictly positive a.e. – and in fact, even everywhere outside \mathbf{V}_D , see [139]. Let for notational simplicity $L := |\mathcal{G}|$ and construct a *symmetrised* (or *rearranged*) function ψ_1^* on $I = [0, L]$ as follows.

We first define the *upper level sets* of ψ_1 by

$$U_t := \{x \in \mathcal{G} : \psi_1(x) > t\}, \quad t \geq 0;$$

then $t \mapsto |U_t|$ (the total length of U_t) is a monotonically decreasing function from L at $t = 0$ to 0 at $t = M := \max_{x \in \mathcal{G}} \psi_1(x)$. We will also denote by

$$(5.5) \quad S_t := \{x \in \mathcal{G} : \psi_1(x) = t\}, \quad t \geq 0,$$

the corresponding “level surfaces”, $S_t = \partial U_t$ for $t \in (0, M)$, which in reality will generally be finite sets of points.

We define a function $\psi_1^* : [0, L] \rightarrow [0, M]$, the *decreasing rearrangement* of ψ_1 , by the rule

$$\psi_1^*(x) := t \quad \text{if and only if} \quad x = |U_t|, \quad x \in [0, L].$$

It is defined in such a way that its upper level sets have the same total length as the upper level sets of ψ_1 :

$$(5.6) \quad |U_t^*| = |\{y \in [0, L] : \psi_1^*(y) > t\}| = x = |U_t| = |\{y \in \mathcal{G} : \psi_1(y) > t\}|.$$

Thus ψ_1^* is monotonically decreasing in x (since $|U_t|$ is monotonically decreasing in t), with $\psi_1^*(0) = M$ and $\psi_1^*(L) = 0$, see Figure 12.

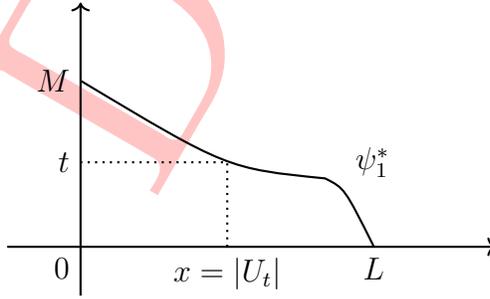


FIGURE 12. The rearranged function ψ_1^* on $[0, L]$.

One sees that $\psi_1^* \in H^1(0, L)$, while Cavalieri’s principle (using (5.6)) implies that $\|\psi_1^*\|_{L^2(0, L)} = \|\psi_1\|_{L^2(\mathcal{G})}$. Furthermore, the coarea formula implies that $\int_{\mathcal{G}} |\psi_1'|^2 dx \geq \int_0^L |(\psi_1^*)'|^2 dx$.

By the coarea formula,

$$\int_{\mathcal{G}} \varphi(x) |\psi_1'(x)| dx = \int_0^M \left(\sum_{x \in S_t} \varphi(x) \right) dt,$$

part of the assertion being that the integrand on the right-hand side is in fact integrable. Before we proceed, we also make two observations: first,

$$\sum_{x \in S_t} |\psi'_1(x)| \geq \left(\sum_{x \in S_t} \frac{1}{|\psi'_1(x)|} \right)^{-1}$$

almost everywhere (also noting that $\psi'_1(x)$ can vanish or be undefined only on a null set), since

$$(5.7) \quad \sum_{x \in S_t} \frac{1}{|\psi'_1(x)|} \sum_{y \in S_t} |\psi'_1(y)| \geq \sum_{x, y \in S_t} \frac{1}{|\psi'_1(y)|} \geq \sum_{x \in S_t} 1 = \#S_t,$$

where, for a.e. $t \in (0, M)$, $\#S_t \geq 1$. Secondly, if $y_t \in [0, L]$ is the unique point such that $\psi_1^*(y_t) = t$, i.e., $\{y_t\} = S_t^* = \partial U_t^*$, then the relation $|U_t| = |U_t^*|$ implies

$$\sum_{x \in S_t} \frac{1}{|\psi'_1(x)|} = \sum_{y \in S_t^*} \frac{1}{|(\psi_1^*)'(y)|} = \frac{1}{|(\psi_1^*)'(y_t)|}$$

for almost all $t \in [0, M]$. With these two observations, we can give the main calculation:

$$\begin{aligned} \int_{\mathcal{G}} |\psi'_1(x)|^2 dx &= \int_0^M \sum_{x \in S_t} |\psi'_1(x)| dt \\ &\geq \int_0^M \frac{1}{\sum_{x \in S_t} \frac{1}{|\psi'_1(x)|}} dt \\ &= \int_0^M \frac{1}{1/|(\psi_1^*)'(y_t)|} dt \\ &= \int_0^M |(\psi_1^*)'(y_t)| dt = \int_0^L |(\psi_1^*)'(y)|^2 dy, \end{aligned}$$

where the first line is the coarea formula, the second follows from the first observation, the third from the second observation, and the final line is another application of the coarea formula.

The proof of (5.2) now follows as with the theorem of Faber–Krahn in \mathbb{R}^d : since $\psi_1^*(L) = 0$,

$$\lambda_1(\mathcal{G}; \mathbf{V}_D) = \frac{\int_{\mathcal{G}} |\psi'_1|^2 dx}{\int_{\mathcal{G}} |\psi_1|^2 dx} \geq \frac{\int_0^L |(\psi_1^*)'|^2 dx}{\int_0^L |\psi_1^*|^2 dx} \geq \inf_{\substack{u \in H^1(0, L) \\ u(L) = 0}} \frac{\int_0^L |u'|^2 dx}{\int_0^L |u|^2 dx} = \lambda_1^{ND}(0, L) = \frac{\pi^2}{4|\mathcal{G}|^2}$$

by (2.4). This concludes the proof for general metric graphs \mathcal{G} . If \mathcal{G} is doubly connected, the proof of (5.4) is performed along the same chain of inequalities, and in particular (5.7), but using the improved estimate $\#S_t \geq 2$ for a.e. $t \in (0, M)$.

As announced, the proof of (5.1) and (5.3) is postponed to Section 5.3.2. \square

5.2. Test functions. When it comes to producing an *upper* counterpart of the *lower* bound in the previous section, there are two main paths we can follow. We can either apply surgical principles that modify in a controlled way the structure of the graph, eventually leading to a configuration that can be easily studied: this will be the guideline in Chapter 6. Else, we can use the variational characterization of eigenvalues: by the Min-max Theorem, the lowest positive eigenvalue μ_2 of the Laplacian with standard vertex conditions is the infimum of the Rayleigh quotient over the class of $H^1(\mathcal{G})$ -functions that are orthogonal to the constants; furthermore, this infimum is attained (and, hence, it is a minimum) if and only if the test function is an eigenfunction.

Accordingly, to find an upper bound on μ_2 it suffices to find a test function (not necessarily an eigenfunction!) and compute its Rayleigh quotient. For instance, such a test function could be a full sine wave supported on a longest edge in the graph, leading to the estimate

$$(5.8) \quad \mu_2(\mathcal{G}) \leq \frac{4\pi^2}{\ell_{\max}^2};$$

or else, considering a longest and a second-longest edges $\mathbf{e}_1, \mathbf{e}_2$ in \mathcal{G} , then considering the full sine wave supported on $\mathbf{e}_1, \mathbf{e}_2$ (more precisely: considering its positive part on \mathbf{e}_1 and its negative part on \mathbf{e}_2 , extending to the whole graph by 0, and adjusting the amplitude of the two waves to guarantee that the whole function is orthogonal to 1) leads to

$$f(x) := \begin{cases} \sin\left(\frac{\pi x}{\ell_1}\right) & \text{if } x \in \mathbf{e}_1, \\ -\frac{\ell_1}{\ell_2} \sin\left(\frac{\pi x}{\ell_2}\right) & \text{if } x \in \mathbf{e}_2, \end{cases}$$

and eventually at the estimate

$$(5.9) \quad \mu_2(\mathcal{G}) \leq \frac{4\pi^2}{(\ell_1 + \ell_2)^2}.$$

Alternatively, instead of searching *one* test function, we may well consider a whole family of $H^1(\mathcal{G})$ -functions whose Rayleigh quotient can be uniformly (and easily!) estimated, and then showing that it contains at least one admissible test function. A possible situation when one might want to do so is the following: Assume that \mathcal{G} is subdivided in k mutually disjoint, connected metric subgraphs $\mathcal{G}_1, \dots, \mathcal{G}_k$ in such a way that

$$\Lambda_{k,\infty}(\mathcal{P}) := \max_{1 \leq j \leq k} \lambda_1(\mathcal{G}_j, \partial\mathcal{G}_j)$$

is minimal among all possible such k -partitions \mathcal{P} of \mathcal{G} , where $\partial\mathcal{G}_i$ is the set $\overline{\mathcal{G}_i} \cap \bigcup_{j \neq i} \overline{\mathcal{G}_j}$. (That such a *spectral minimal partition* exists is not obvious, but has been proved in [118].) Now, upon taking the ground state ψ_j on each such \mathcal{G}_j , one may consider $\sum_{j=1}^k \psi_j$: while this function belongs to $H^1(\mathcal{G})$, it will not be an admissible test function as it is positive and, hence, certainly not orthogonal to the constants. However, one may look for a suitable linear combination

$$\psi_\alpha := \sum_{j=1}^k \alpha_j \psi_j \neq 0$$

such that $\int_{\mathcal{G}} \psi_{\alpha}(x) dx = 0$. The task of finding such a vector $\alpha \in \mathbb{R}^k$ can be easily accomplished, as it boils down to solving an algebraic system. In this way, one may use of known estimates on the *spectral minimal energy* $\Lambda_{k,\infty}(\mathcal{P})$ to derive upper estimates on μ_k : in this way, the estimate

$$(5.10) \quad \mu_k(\mathcal{G}) \leq \frac{\pi^2}{|\mathcal{G}|^2} \left(k - 1 + E - \left\lfloor \frac{N}{2} \right\rfloor \right)^2 \quad \text{for } k \text{ large}$$

has been obtained in [110]: here N is the number of vertices of degree 1 and E is, as usual, the number of edges. (We will encounter similar but more sophisticated estimates in Section 6.2.)

Here comes a “non-linear version” of this methods: it is taken from [47], as are its consequences.

Corollary 5.2. *Let $\psi: [0, 1] \rightarrow H^1(\mathcal{G}) \setminus \{0\}$ be such that $\psi_0 = -\psi_1$ and the mapping $t \mapsto \langle \psi_t, \mathbf{1} \rangle_{L^2(\mathcal{G})}$ is a continuous function $[0, 1] \rightarrow \mathbb{R}$. Then there exists t_0 such that*

$$(5.11) \quad \mu_2(\mathcal{G}) \leq \frac{\|\psi'_{t_0}\|_{L^2(\mathcal{G})}^2}{\|\psi_{t_0}\|_{L^2(\mathcal{G})}^2}.$$

Let us present a few applications of this basic method.

Proposition 5.3. *There holds*

$$(5.12) \quad \mu_2(\mathcal{G}) \leq \frac{24|\mathcal{G}|}{\text{Diam}(\mathcal{G})^3}.$$

Proof. Introduce the “tent” function

$$(5.13) \quad \tau_{y,d}(x) = \begin{cases} d - \text{dist}(x, y), & \text{if } \text{dist}(x, y) \leq d, \\ 0, & \text{otherwise,} \end{cases}$$

let $d = \text{Diam}(\mathcal{G})/2$, and take

$$(5.14) \quad \psi_t := \cos(\pi t)\tau_{x_1,d} + \sin(\pi t)\tau_{x_2,d},$$

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 5.2 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

$$(5.15) \quad \|\tau_{x_1,d}(x)\|_{L^2(\mathcal{G})}^2 \geq \int_0^d (d-x)^2 dx = \frac{d^3}{3},$$

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

$$\mu_2 \leq \frac{\cos^2(\pi t)L + \sin^2(\pi t)L}{\cos^2(\pi t)\frac{\text{Diam}(\mathcal{G})^3}{24} + \sin^2(\pi t)\frac{\text{Diam}(\mathcal{G})^3}{24}} \leq \frac{24L}{\text{Diam}(\mathcal{G})^3}.$$

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

Using the same technique, but a more sophisticated class of test functions, the following can be proved, where we use the notations from Definition 3.21.

Proposition 5.4. *There holds*

$$(5.16) \quad \mu_2(\mathcal{G}) \leq \frac{6|\mathcal{G}|}{(\text{AvDiam}(\mathcal{G}))^3}.$$

and

$$(5.17) \quad \mu_2(\mathcal{G}) \leq \frac{12|\mathcal{G}|}{(\text{Triam}(\mathcal{G}))^3}.$$

5.3. Graph decomposition. In Section 5.1 we have reviewed some isoperimetric inequalities obtained by symmetrization methods: however theoretically and historically important, their proofs are based on “spreading around” the mass distribution of the ground state all over the metric graph, without respecting its fine structure.

Let $(\mathcal{G}_i)_{1 \leq i \leq N}$ be a family of mutually disjoint metric subgraphs of \mathcal{G} such that $\mathcal{G} = \bigsqcup_{i=1}^N \mathcal{G}_i$: accordingly,

$$\|f'\|_{L^2(\mathcal{G})}^2 = \sum_{i=1}^N \|f'\|_{L^2(\mathcal{G}_i)}^2 \quad \text{and} \quad \|f\|_{L^2(\mathcal{G})}^2 = \sum_{i=1}^N \|f\|_{L^2(\mathcal{G}_i)}^2.$$

Because the restriction to each \mathcal{G}_i of any eigenfunction φ on \mathcal{G} is again a valid test function for the Rayleigh quotient on \mathcal{G}_i , we apply the Poincaré inequality to each \mathcal{G}_i and deduce that

$$(5.18) \quad \|\varphi'\|_{L^2(\mathcal{G})}^2 \geq \min_{1 \leq i \leq N} \lambda_1(\mathcal{G}_i; \partial\mathcal{G}_i) \|\varphi\|_{L^2(\mathcal{G})}^2,$$

if φ can be guaranteed to vanish on a suitable subset $\partial\mathcal{G}_i$ of each \mathcal{G}_i : for instance because each \mathcal{G}_i contains at least one Dirichlet vertex, or else because \mathcal{G}_i are designed on purpose in such a way that the eigenfunctions vanish at all kissing points $\mathcal{G}_i \cap \mathcal{G}_j$.

A refinement of the lower estimates in Section 5.1 can, thus, be obtained if \mathcal{G} is conveniently decomposed into metric subgraphs \mathcal{G}_i that allow for enhanced eigenvalue bounds: either because of their geometry (say, because we choose \mathcal{G}_i to be fairly homogeneous with respect to some relevant quantity) or because of the spectral properties of the Laplacian restricted to such subgraphs (e.g., because the subgraphs are designed to mirror some properties of the eigenfunctions on \mathcal{G}). In this section we are going to discuss three approaches to this general method.

5.3.1. Voronoi cells. The first method we present here is based on the notion of *Voronoi decomposition* that has been developed for combinatorial graphs in [154] and suitably adapted to metric graphs in [183].

The following refinement of Corollary 3.22 is [183, Theorem 4.5.11].

Theorem 5.5. *Let \mathcal{G} be a compact metric graph with total length $|\mathcal{G}|$ and inradius $\text{Inr}(\mathcal{G}; \mathbf{V}_D)$ with respect to some $\emptyset \neq \mathbf{V}_D \subset \mathbf{V}$. Then*

$$\lambda_1(\mathcal{G}; \mathbf{V}_D) \geq \frac{1}{\sup_{\mathbf{v} \in \mathbf{V}_D} |B(\mathbf{v}, \text{Inr}(\mathcal{G}; \mathbf{V}_D)) \cap \mathcal{G}|}.$$

In the proof, we are going to decompose \mathcal{G} into a family $(\mathcal{G}_i)_{1 \leq i \leq N} \equiv (\mathcal{U}_v)_{v \in \mathbf{V}_D}$ of Voronoi cells: let us introduce this notion.

Definition 5.6. Let $\emptyset \neq \mathbf{V}_D \subset \mathbf{V}$. A family $(\mathcal{U}_v)_{v \in \mathbf{V}_D}$ of metric subgraphs of \mathcal{G} is called a *Voronoi decomposition* with respect to \mathbf{V}_D if the following conditions are satisfied:

- Let $\mathbf{v} \in \mathbf{V}_D$. Then $\mathbf{v} \in \mathcal{U}_v$ and for any further $x \in \mathcal{U}_v$ there exists a geodesic $\gamma \subset \mathcal{G}$ whose endpoints are x, \mathbf{v} and whose trace lies in \mathcal{U}_v .
- Let $\mathbf{v}, \mathbf{w} \in \mathbf{V}_D$ and $x \in \mathcal{U}_v$. If $\mathbf{v} \neq \mathbf{w}$, then $\text{dist}_{\mathcal{G}}(\mathbf{v}, x) \leq \text{dist}_{\mathcal{G}}(\mathbf{w}, x)$.
- Let $\mathbf{v}, \mathbf{w} \in \mathbf{V}_D$. If $\mathbf{v} \neq \mathbf{w}$, then $\mathcal{U}_v \cap \mathcal{U}_w$ has empty interior.

Roughly speaking, such a family $(\mathcal{U}_v)_{v \in \mathbf{V}_D}$ decomposes \mathcal{G} into a mutually disjoint metric subgraphs in such a way that each element of \mathcal{U}_v is closer to $\mathbf{v} \in \mathbf{V}_D$ than to any further $\mathbf{w} \in \mathbf{V}_D$. It is not at all obvious that a Voronoi decomposition of any given \mathcal{G} always exists: indeed, proving that such decomposition is based on a delicate application of the Zorn's Lemma [183, Theorem 4.5.6].

Example 5.7. Unlike in the case of domains, a Voronoi decomposition is generally not unique. Let \mathcal{G} be a metric star consisting of three equilateral edges $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ with centrum \mathbf{v}_0 (the center of the star) and leaves $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$. If $\mathbf{V}_D = \{\mathbf{v}_1, \mathbf{v}_2\}$, then there are precisely two Voronoi decompositions of \mathcal{G} : either $\mathcal{U}_{\mathbf{v}_1}$ consists of $\mathbf{e}_1, \mathbf{e}_3$ and $\mathcal{U}_{\mathbf{v}_2}$ consists of \mathbf{e}_2 , or $\mathcal{U}_{\mathbf{v}_1}$ consists of \mathbf{e}_1 and $\mathcal{U}_{\mathbf{v}_2}$ consists of $\mathbf{e}_2, \mathbf{e}_3$.

Proof. Decomposing \mathcal{G} into Voronoi cells $(\mathcal{U}_v)_{v \in \mathbf{V}_D}$ also allows for a decomposition of the numerator and the denominator of the Rayleigh quotient:

$$\|f'\|_{L^2(\mathcal{G})}^2 = \sum_{\mathbf{v} \in \mathbf{V}} \|f'\|_{L^2(\mathcal{U}_v)}^2 \quad \text{and} \quad \|f\|_{L^2(\mathcal{G})}^2 = \sum_{\mathbf{v} \in \mathbf{V}} \|f\|_{L^2(\mathcal{U}_v)}^2,$$

where the Dirichlet boundary of each \mathcal{U}_v is the singleton $\{\mathbf{v}\}$. We can now observe that for each such cell

$$\|f'\|_{L^2(\mathcal{U}_v)}^2 \geq \frac{1}{|\mathcal{U}_v| \text{Inr}(\mathcal{U}_v; \{\mathbf{v}\})} \|f\|_{L^2(\mathcal{U}_v)}^2 \geq \frac{1}{B(\mathbf{v}; \text{Inr}(\mathcal{G}; \mathbf{V}_D)) \text{Inr}(\mathcal{U}_v; \{\mathbf{v}\})} \|f\|_{L^2(\mathcal{U}_v)}^2,$$

where the second inequality follows by general properties of Voronoi decompositions (and, indeed, holds uniformly with respect to *any* Voronoi decomposition!). The claim then follows summing over all cells. \square

5.3.2. *Nodal domains.* To prove (5.1) using this approach, we apply (5.2) to each *nodal domain* of the second eigenfunctions. This idea is very effective, so we will elaborate on it.

Definition 5.8. Let $\varphi \in C(\mathcal{G})$. We call

- (a) the closed set $N(\varphi) := \{x \in \mathcal{G} : \varphi(x) = 0\}$ the *nodal set* of φ ;
 (b) $\Omega \subset \mathcal{G}$ a *nodal domain* of φ if it is the closure of a connected component of $\mathcal{G} \setminus N(\varphi)$.

Example 5.9. If $\mathcal{G} = I = [0, L]$ is just a bounded interval, and $\psi_k \sim \lambda_k$ is a k th eigenfunction of $-\frac{d^2}{dx^2} + q$ on I ($q \in L^\infty(I)$), then by Sturm–Liouville theory, ψ_k has exactly $k - 1$ zeros in the interior of I , and thus exactly k nodal domains $\Omega_1, \dots, \Omega_k$.

As a more explicit example, if $q = 0$ and $k = 2$, then $\psi_2(x) = A \cos(\frac{\pi x}{L})$ is an eigenfunction for $\lambda_2 = \frac{\pi^2}{|\mathcal{G}|^2}$; $N(\psi_2) = \{\frac{L}{2}\}$ (independently of $A \neq 0$), and so $\Omega_1 = [0, \frac{L}{2}]$, $\Omega_2 = [\frac{L}{2}, L]$.

Remark 5.10. If $k \geq 2$, then $\psi_k \sim \mu_k(\mathcal{G})$ changes sign on \mathcal{G} (since it is orthogonal in $L^2(\mathcal{G})$ to the function ψ_1 , which is positive everywhere). In particular, if $k = 2$, then there exist nodal domains Ω^+ and Ω^- where ψ_k is positive and negative, respectively.

The following is [117, Lemma 2.3].

Lemma 5.11. *Suppose ψ_k is an eigenfunction for $\lambda_k(\mathcal{G})$ on \mathcal{G} and $\Omega \subset \mathcal{G}$ is any nodal domain of ψ_k . Denote by $\lambda_1(\Omega; \partial\Omega)$ the first eigenvalue of the Laplacian on Ω with Dirichlet conditions on $\partial\Omega$ and standard conditions at all other vertices, i.e.,*

$$\lambda_1(\Omega) = \inf_{\substack{0 \neq u \in H^1(\Omega) \\ u(x)=0 \forall x \in \partial\Omega}} \frac{\int_{\Omega} |u'|^2 dx}{\int_{\Omega} |u|^2 dx}.$$

Then $\lambda_k(\mathcal{G}) = \lambda_1(\Omega; \partial\Omega)$ and $\psi_k|_{\Omega}$ is an eigenfunction for $\lambda_1(\Omega; \partial\Omega)$.

Proof. By assumption ψ_k satisfies the eigenvalue equation $-\psi_k = \mu_k \psi_k$ strongly (indeed pointwise) in \mathcal{G} , and hence in Ω . But it also satisfies all vertex conditions in Ω by construction. Thus it is equal to *some* eigenfunction on Ω ; in particular, $\mu_k = \lambda_j(\Omega)$ for some $k \geq 1$.

Now since ψ_k does not change sign in Ω , and $\lambda_1(\Omega)$ is the only eigenvalue on Ω with a non-sign-changing eigenfunction, we must have $j = 1$. \square

We can finally complete the proof of Theorem 5.1.

Proof of (5.1). Fix an eigenfunction $\psi_1^{\mathcal{G}} \sim \lambda_1(\mathcal{G})$, then ψ_1 has (at least) two nodal domains Ω^+ , Ω^- ; at least one of them, say Ω^+ , has total length $\leq |\mathcal{G}|/2$. Since $\partial\Omega^+ \neq \emptyset$, i.e., Ω^+ has at least one Dirichlet vertex, by Lemma 5.11 and (5.3), there holds

$$\lambda_1(\mathcal{G}) = \lambda_1(\Omega^+) \geq \frac{\pi^2}{4|\Omega^+|^2} \geq \frac{\pi^2}{|\mathcal{G}|^2}.$$

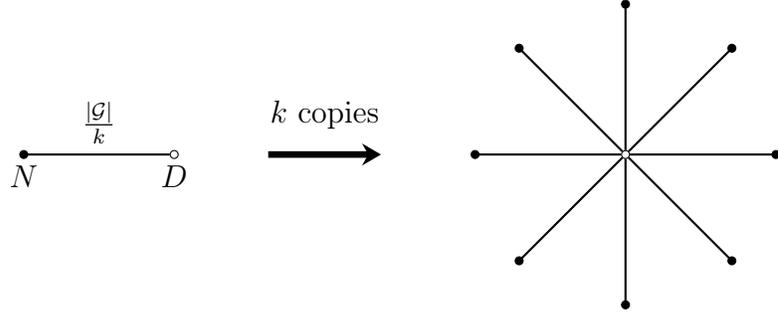
We can prove (5.3) likewise. \square

The symmetrization method allows for a generalization of the inequality to the higher eigenvalues, as proved in [98, Theorem 1].

Theorem 5.12. *If $V_D = \emptyset$, then the k -th-lowest eigenvalue satisfies*

$$(5.19) \quad \lambda_k(\mathcal{G}) \geq \frac{\pi^2(k+1)^2}{4|\mathcal{G}|^2} \quad \text{for all } k \geq 1.$$

Equality is attained in (5.19) if and only if \mathcal{G} is an equilateral k -star.



Proof. If ψ_k has k nodal domains, then at least one has length $\leq L/k$; apply Theorem 5.1 (in the version for $V_D \neq \emptyset$). Otherwise, there exists a linear combination of ψ_1, \dots, ψ_k which does have k nodal domains. Apply the symmetrization technique to one of these. \square

If \mathcal{G} is not a tree, a lower bound on λ_1 in terms of diameter only is impossible, as shown in [119, Example 5.1]; see Proposition 6.7 for the case of trees. However, the following lower bound holds [183, Theorem 4.4.6].

Proposition 5.13. *If $V_D = \emptyset$, then*

$$(5.20) \quad \mu_k \geq \frac{\nu_k}{|\mathcal{G}| \text{Diam}(\mathcal{G})} \quad \text{for all } k \geq 2,$$

where ν_k is the number of nodal domains of an eigenfunction associated with μ_k .

Proof. Let ψ_k be an eigenfunction associated with μ_k : then by Lemma 5.11 the restriction of ψ_k to each of its nodal domains Ω_i , $i = 1, \dots, \nu_k$ is the ground state of the Laplacian with Dirichlet conditions at the boundary of $\partial\Omega_i$ and we can apply Corollary 3.22 to each of the nodal domains. We conclude that

$$\lambda_k(\mathcal{G}) \geq \frac{1}{|\Omega_j| \text{Inr}(\Omega; \partial\Omega_j)} \geq \frac{\nu_k}{|\mathcal{G}| \text{Diam}(\mathcal{G})},$$

where the last inequality follows from the pidgeonhole principle and the obvious estimate $\text{Inr}(\tilde{\mathcal{G}}; V_D) \leq \text{Diam}(\tilde{\mathcal{G}})$, which holds for all graphs $\tilde{\mathcal{G}}$. \square

Because any eigenfunction associated with μ_2 has certainly two nodal domains, one deduces in particular the estimate

$$(5.21) \quad \mu_2 \geq \frac{2}{|\mathcal{G}| \text{Diam}(\mathcal{G})}.$$

5.3.3. *Double covers.* The starting point of a further approach to decompositions is (5.18). If φ does not necessarily disappear at the boundary of each $\partial\mathcal{G}_i$, then we have to resort to the Poincaré-Wirtinger inequality to find

$$\|\varphi'\|_{L^2(\mathcal{G}_i)}^2 \geq \mu_2(\mathcal{G}_i) \int_{\mathcal{G}_i} \left(\varphi(x) - \int_{\mathcal{G}_i} \varphi \right)^2 dx :$$

now, by the Jensen inequality and summing over i , we deduce

$$(5.22) \quad \|\varphi'\|_{L^2(\mathcal{G})}^2 \geq \min_{1 \leq i \leq N} \mu_2(\mathcal{G}_i) \left(\|\varphi\|_{L^2(\mathcal{G})}^2 - \sum_{i=1}^N \frac{1}{|\mathcal{G}_i|} \left(\int_{\mathcal{G}_i} \varphi(x) dx \right)^2 \right).$$

Alas, the restriction of φ to \mathcal{G}_i need not have zero mean, hence it is generally not a valid test function for the Rayleigh quotient on \mathcal{G}_i . A way to circumvent this problem, based on the notion of cover of \mathcal{G} , has been proposed in [14] and later generalized in [170]. Unlike in the previously considered decompositions of \mathcal{G} , we remove the condition that the cells are mutually disjoint; on the contrary, we assume that almost each point of \mathcal{G} belongs to precisely m different cells.

Definition 5.14. Let $m \in \mathbb{N}$. An m -fold cover of a metric graph \mathcal{G} is a finite family $(\mathcal{U}_i)_{1 \leq i \leq N}$ of connected metric subgraphs of \mathcal{G} such that for almost every $x \in \mathcal{G}$ there exist m distinct indices $1 \leq i_1 < \dots < i_m \leq N$ such that $x \in \mathcal{U}_{i_1} \cap \dots \cap \mathcal{U}_{i_m}$ and $x \notin \mathcal{U}_i$ for $i \notin \{i_1, \dots, i_m\}$.

The associated vicinity graph Γ is a simple weighted graph with vertex set $\{1, \dots, N\}$ and edge weights $\mu_{ij} := |\mathcal{U}_i \cap \mathcal{U}_j|$ for vertices $i \neq j$ and $\mu_{ii} = 0$.

We denote by $\alpha_i(\mathcal{L}_\Gamma)$ the i -th-lowest eigenvalue of the normalized Laplacian \mathcal{L}_Γ , defined e.g. as in [80, Chapter 1]:

$$\mathcal{L}_\Gamma := \mathcal{I} \mathcal{M} \mathcal{I} :$$

here \mathcal{M} is the diagonal matrix that contains the weights of Γ and \mathcal{I} is the signed incidence matrix of an arbitrary orientation of Γ . The following was obtained in [14, Theorem 1.2] for $m = 2$ and in [170, Theorem 2.1] for general m .

Theorem 5.15. Let \mathcal{G} be a metric graph. Given an m -fold cover $(\mathcal{U}_i)_{1 \leq i \leq N}$ of \mathcal{G} with associated vicinity graph Γ , we have

$$(5.23) \quad \mu_i(\mathcal{G}) \geq \frac{m-1}{m} \alpha_i(\mathcal{L}_\Gamma) \min_{1 \leq j \leq N} \mu_2(\mathcal{U}_j), \quad i = 1, \dots, N.$$

Proof. We consider the linear bounded operator $\Phi : L^2(\mathcal{G}) \rightarrow \mathbb{R}^N$ given by

$$(\Phi f)_i := \frac{1}{\sqrt{|\mathcal{U}_i|}} \int_{\mathcal{U}_i} f dx, \quad i = 1, \dots, N.$$

Using the Min-max Theorem and because $(\mathcal{U}_i)_{1 \leq i \leq N}$ is an m -fold cover of \mathcal{G} , one can show that

$$\mu_i(\mathcal{G}) \geq \frac{1}{m} \alpha_i(m \text{Id}_{\mathbb{R}^N} - \Phi \Phi^*) \min_{1 \leq j \leq k} \mu_2(\mathcal{U}_j), \quad i = 1, \dots, N$$

where Φ^* is the adjoint of Φ and $\alpha_i(m \text{Id}_{\mathbb{R}^N} - \Phi \Phi^*)$ denotes the i -th-lowest eigenvalue of the operator $m \text{Id}_{\mathbb{R}^N} - \Phi \Phi^*$. The entries of $\Phi \Phi^*$ with respect to Cartesian coordinates on \mathbb{R}^N are

$$(\Phi \Phi^*)_{ij} = \frac{|\mathcal{U}_i \cap \mathcal{U}_j|}{\sqrt{|\mathcal{U}_i|} |\mathcal{U}_j|}$$

and, thus, $(mI - \Phi\Phi^*)_{ii} = m - 1$ and

$$(mI - \Phi\Phi^*)_{ij} = -\frac{|\mathcal{U}_i \cap \mathcal{U}_j|}{\sqrt{|\mathcal{U}_i||\mathcal{U}_j|}} = -(m-1)\frac{\mu_{ij}}{\sqrt{d_i^\mu d_j^\mu}}$$

for $i \neq j$, because $(\mathcal{U}_i)_{1 \leq i \leq N}$ is an m -fold cover. Therefore,

$$m \text{Id}_{\mathbb{R}^N} - \Phi\Phi^* = (m-1)D^{-\frac{1}{2}}\mathcal{I}\mathcal{M}\mathcal{I}D^{-\frac{1}{2}},$$

where D denotes the diagonal matrix of weighted vertex degrees. Because

$$\mu_i(\mathcal{G}) \geq \frac{1}{m}\alpha_i(m \text{Id}_{\mathbb{R}^N} - \Phi\Phi^*) \min_{1 \leq j \leq N} \mu_2(\mathcal{U}_j)$$

the claim follows, once we observe that the normalized Laplacian \mathcal{L}_Γ and its symmetric version $\tilde{\mathcal{L}}_\Gamma := D^{-\frac{1}{2}}\mathcal{I}\mathcal{M}\mathcal{I}D^{-\frac{1}{2}}$ have same eigenvalues. \square

The simplest application of Theorem 5.15 is obtained upon considering the so-called *star double cover* $(\mathcal{S}_v)_{v \in \mathbf{V}}$ of \mathcal{G} : each \mathcal{S}_v consists of the vertex $v \in \mathbf{V}$ and of all incident edges, i.e., $\mathcal{S}_v = \mathbf{E}_v$. We can thus apply Theorem 5.15 for $m = 2$ and obtain the following, cf. [14, Theorem 3.4].

Corollary 5.16. *Let \mathcal{G} be a metric graph. We have*

$$(5.24) \quad \mu_i(\mathcal{G}) \geq \frac{\pi^2}{8\ell_{\max}^2}\alpha_i(\mathcal{L}_\mathcal{G}), \quad i = 1, \dots, V,$$

where $\alpha_i(\mathcal{L}_\mathcal{G})$ is the i -th-lowest eigenvalue of the normalized Laplacian $\mathcal{L}_\mathcal{G}$ of the weighted combinatorial graph \mathbf{G} underlying \mathcal{G} , with edge weights $\mu_e := \ell_e$.

Proof. Applying Theorem 5.15 with $\mathcal{U}_v := \mathcal{S}_v$ we deduce

$$\mu_i(\mathcal{G}) \geq \frac{1}{2}\alpha_i(\mathcal{L}_\mathcal{G}) \min_{v \in \mathbf{V}} \mu_2(\mathcal{S}_v), \quad i = 1, \dots, V,$$

The right-hand side can be further estimated using

$$\mu_2(\mathcal{S}_v) \geq \frac{\pi^2}{4\ell_{\max}^2} \quad \text{for all } v \in \mathbf{V},$$

which follows combining Corollary 6.12.1 below with (3.13). \square

6. LOCAL METHODS

Not only can eigenvalues be described by means of the Courant–Fischer Minmax Principle: a fundamental consequence of the description of the Laplacians with standard vertex conditions (with or without Dirichlet vertices) in terms of quadratic forms is that *surgical operations on the metric graph have a functional analytical counterpart as operations on the form domain.*

In this section we wish to explore *surgery methods*. Surgery is primarily a tool to modify metric graphs in order to produce new graphs whose spectrum (as a whole, or perhaps in terms of individual eigenvalues) is behaving in a consistently monotone way. Ideally, the spectral theory of the target graph will be easier to perform.

6.1. Elementary surgery methods. We wish to explore the related principle that loosening connections, or “cutting through the graph” lowers the eigenvalues. This is a prototypical *surgery principle*: examining how making a local topological, geometric or metric change to a graph (“surgery”) affects its Laplacian spectrum. Some such principles were implicit in the works of Nicaise [176] and Friedlander [98], but only started being studied systematically in the 2010s with [48, 146]. The standard reference is now probably [46].

6.1.1. *Rank-one perturbations.*

Definition 6.1. We say $\tilde{\mathcal{G}}$ is formed from \mathcal{G} by *cutting through the vertex* $\mathbf{v} \in \mathbf{V}(\mathcal{G})$ if \mathbf{v} is replaced by $p \geq 2$ vertices $\mathbf{v}_1, \dots, \mathbf{v}_p \in \mathbf{V}(\tilde{\mathcal{G}})$ such that all other incidence and adjacency relations are preserved. In this case the *rank* of the cut is defined to be $p - 1$.

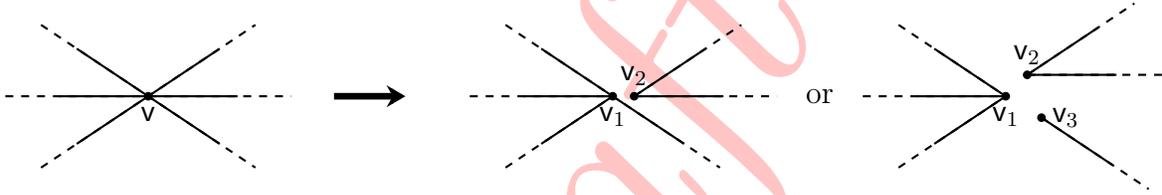


FIGURE 13. Two examples of cutting through a vertex of degree 6. The first (center) has rank 1; the second (right) has rank 2, and is also a rank 1 cut of the first.

The inverse process is called *gluing* vertices.

This notion is reflected at the level of function spaces.

Lemma 6.2. *Let \mathcal{G} be a metric graph and let $\tilde{\mathcal{G}}$ be the metric graph obtained gluing p distinct vertices $\mathbf{v}_1, \dots, \mathbf{v}_p$ of \mathcal{G} to form \mathbf{v}_0 . Then up to a canonical identification $C(\mathcal{G})$ is a subspace of $C(\tilde{\mathcal{G}})$ of codimension $p - 1$. Accordingly, the same is true of $H^1(\mathcal{G})$ and $H^1(\tilde{\mathcal{G}})$; and of $H_0^1(\tilde{\mathcal{G}})$ and $H_0^1(\mathcal{G})$, as long as standard conditions are imposed at all of $\mathbf{v}_0, \dots, \mathbf{v}_p$.*

More precisely, we can define a natural isomorphism $\Phi : L^2(\mathcal{G}) \rightarrow L^2(\tilde{\mathcal{G}})$ via the identification

$$L^2(\mathcal{G}) \simeq \bigoplus_{e \in \mathcal{E}} L^2(0, \ell_e) \simeq L^2(\tilde{\mathcal{G}}),$$

where \mathcal{E} is the common set of edges of the two graphs. Moreover, if $f \in C(\mathcal{G})$ (in particular if $f \in H^1(\mathcal{G})$) satisfies $f(\mathbf{v}_1) = \dots = f(\mathbf{v}_m)$, then also $\Phi(f) \in C(\tilde{\mathcal{G}})$ (correspondingly, $\Phi(f) \in H^1(\tilde{\mathcal{G}})$).

Also note that by inserting dummy vertices as necessary we can thus cut/glue any p points in the graph.

Now a rank $r \geq 2$ cut (or gluing) can easily be defined by concatenating r rank-1 cuts (see also [109, Section 2.2]), so it makes sense to analyze rank-1 operations as the base case. Here, Lemma 6.2 translates into the following interlacing inequality for the eigenvalues of the standard

Laplacian, although Dirichlet (or other self-adjoint) vertex conditions may be imposed at any vertices not affected by the gluing. The following can be traced back to [46, Corollary 3.4] and also [49, Theorems 3.1.8 and 3.1.10] as well as [144, 192].

Theorem 6.3. *If the graph $\tilde{\mathcal{G}}$ is obtained from \mathcal{G} by gluing two vertices, then their eigenvalues satisfy the interlacing inequalities*

$$(6.1) \quad \lambda_k(\mathcal{G}) \leq \lambda_k(\tilde{\mathcal{G}}) \leq \lambda_{k+1}(\mathcal{G}) \leq \lambda_{k+1}(\tilde{\mathcal{G}}), \quad k \geq 1.$$

If a given value Λ has multiplicities m and \tilde{m} in the spectra of \mathcal{G} and $\tilde{\mathcal{G}}$, respectively, then $|m - \tilde{m}| \leq 1$ and, with the identification just described, the intersection of the respective Λ -eigenspaces has dimension $\min(m, \tilde{m})$.

The following immediate consequence was observed in [46, Corollary 3.6].

Corollary 6.4. *Suppose $\mathbf{v}_1, \dots, \mathbf{v}_m \in \mathbf{V}(\mathcal{G})$ and for some $k \geq 1$ there exist eigenfunctions ψ_1, \dots, ψ_k corresponding to $\lambda_1(\mathcal{G}), \dots, \lambda_k(\mathcal{G})$, respectively, such that*

$$\psi_1(\mathbf{v}_1) = \dots = \psi_1(\mathbf{v}_m), \quad \dots, \quad \psi_k(\mathbf{v}_1) = \dots = \psi_k(\mathbf{v}_m).$$

Let $\tilde{\mathcal{G}}$ be the graph formed from \mathcal{G} by gluing $\mathbf{v}_1, \dots, \mathbf{v}_m$. Then

$$\lambda_1(\tilde{\mathcal{G}}) = \lambda_1(\mathcal{G}), \quad \dots, \quad \lambda_k(\tilde{\mathcal{G}}) = \lambda_k(\mathcal{G}).$$

Moreover, ψ_1, \dots, ψ_k are eigenfunctions on $\tilde{\mathcal{G}}$ associated with $\lambda_1(\tilde{\mathcal{G}}), \dots, \lambda_k(\tilde{\mathcal{G}})$, respectively.

Example 6.5. A surprising consequence of Corollary 6.4 is that all figure-8 graphs of same total length are “semi-co-spectral”: by this we mean that *the half of their eigenvalues agree*: more precisely, $\frac{4k^2\pi^2}{|\mathcal{G}|^2}$ is an eigenvalue of all of them for each $k = 1, 2, \dots$

Indeed, let \mathcal{G} be a loop. Then $\Delta_{\mathcal{G}}$ is nothing but the second derivative with periodic boundary conditions on the interval $[0, |\mathcal{G}|]$, whose eigenfunctions are given by (2.6). Each eigenfunction associated with λ_k attains each of its values $2k$ times: in particular, by the translation symmetry of $\psi_k := \cos(\sqrt{\lambda_k} \cdot)$ we can regard any two points of \mathcal{G} as vertices where ψ_k attains the same value: gluing them will not change λ_k . In this way, we can form any figure-8 graph $\tilde{\mathcal{G}}$.

As noted at the beginning of the section, the basic principle goes back decades; the inequality in its sharp form (with characterization of equality) is from [46, Theorem 3.4]. Since the result is driven by the form domains, instead of the Laplacian one could consider a more general self-adjoint uniformly elliptic second-order operator (in particular allowing a potential) and the conclusion would be the same.

Remark 6.6. What happens if other conditions than standard are imposed at the vertices being glued can be far more involved, depending on the conditions in question; in particular, one may elect to impose different conditions in $\tilde{\mathcal{G}}$ than in \mathcal{G} . The issue was quite thoroughly investigated in [192, Section 4], where all self-adjoint conditions of radially symmetric type (that is, where the vertex conditions are independent of permutations of the edges at a vertex); this includes δ - and δ' -type, as well as anti-Kirchhoff, see Remark 3.25. Whether $\lambda_k(\mathcal{G}) \leq \lambda_k(\tilde{\mathcal{G}})$

or $\lambda_k(\mathcal{G}) \geq \lambda_k(\tilde{\mathcal{G}})$ depends on the conditions imposed; in particular, negative δ - or δ' -potentials may lead to an inversion of the inequality.

To illustrate the effectivity of Theorem 6.3, let us present an alternative proof of Theorem 5.1: it first appeared in [176] and historically it arguably is the first proof of spectral geometric flavour in metric graph theory.

Second proof of Theorem 5.1. This is based on *Nicaise' doubling trick*, as introduced in the proof of [176, Théorème 3.1]. Let us first begin with the case $V_D = \emptyset$.

We begin by replacing each edge in \mathcal{G} by two parallel edges, thus introducing the graph \mathcal{G}_2 of double length, each of whose vertices have even degree: by a well-known graph theoretical result that goes back to Euler, the underlying combinatorial graph contains at least one Eulerian cycle. We cut through arbitrarily many vertices in V_N , until \mathcal{G} is turned into such a Eulerian cycle C , which we may identify with a graph \mathcal{G}' with all vertices of degree 2, see Figure 14.

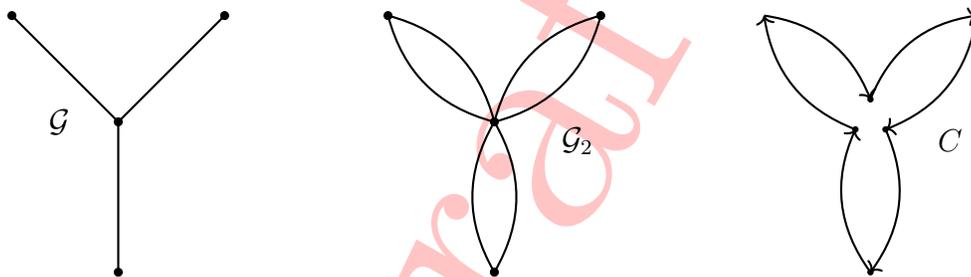


FIGURE 14. The original graph \mathcal{G} (left); the “doubled graph” \mathcal{G}_2 (center); an Eulerian cycle C (right), which forms a closed cycle in \mathcal{G}_2 , traversing every edge exactly once.

In this way, we have transformed the assignment of minimizing the Rayleigh quotient over $H^1(\mathcal{G})$ to the assignment of minimizing it over the space of test functions $H^1(\mathcal{G}')$: with the above construction, and in view of Corollary 6.4, $\lambda_1(\mathcal{G}) \geq \lambda_1(\mathcal{G}')$, whereas by (2.5) we find that

$$\lambda_1(\mathcal{G}') = \frac{4\pi^2}{|\mathcal{G}'|^2} = \frac{4\pi^2}{4|\mathcal{G}|^2}.$$

This yields (5.1). Also (5.2) can be proved likewise: the main difference is that the (combinatorial) Eulerian cycle contains one point on which Dirichlet conditions are imposed. Therefore, we have to invoke (2.2) instead of (2.5), thus obtaining

$$\lambda_1(\mathcal{G}') = \frac{\pi^2}{|\mathcal{G}'|^2} = \frac{\pi^2}{4|\mathcal{G}|^2}.$$

This concludes the proof. □

It was observed in [146] that if \mathcal{G} already contains an Eulerian cycle, then the “doubling trick” is not necessary and the improved estimate

$$\lambda_1(\mathcal{G}) \geq \lambda_1(\text{cycle } C \text{ of length } |\mathcal{G}|) = \frac{4\pi^2}{|\mathcal{G}|^2}$$

holds. This is a special case of Theorem 5.1.(2), since each Eulerian graph is doubly edge connected. Intuitively, graphs which are more connected, i.e., have more non-overlapping paths between any pairs of points, necessarily have larger λ_1 and thus faster convergence of diffusion processes to equilibrium. Higher graph connectivity and its effect on the eigenvalues is also explored in [45]. This closely parallels results for discrete graph Laplacians which have been known for many decades [95], where the discrete counterpart of λ_1 is even called the *algebraic connectivity* of the graph.

Proposition 6.7. *Let \mathcal{G} be a tree with $V_D = \{v \in V : \deg(v) = 1\}$, i.e., with Dirichlet conditions imposed at the leaves and standard conditions elsewhere. Then*

$$(6.2) \quad \lambda_1(\mathcal{G}; V_D) \geq \frac{\pi^2}{\text{Diam}(\mathcal{G})^2},$$

where $\text{Diam } \mathcal{G}$ is the diameter of the graph.

If \mathcal{G} has one Neumann leaf and all other leaves Dirichlet, the bound is

$$(6.3) \quad \lambda_1(\mathcal{G}; V_D) \geq \frac{\pi^2}{4 \text{Diam}(\mathcal{G})^2},$$

Proof. We repeatedly apply Proposition 6.23 at vertices of degree three or more, choosing the graph with the minimal $\lambda_1(\mathcal{G}_{E_D})$ at every step. We stop when there are no vertices of degree larger than 2 and we absorb all vertices of degree two into the edges. The graph is thus reduced to a collection of disjoint intervals with Dirichlet conditions, and the first eigenvalue comes from the longest of them. The longest interval possible is the path giving the diameter of the graph.

If the tree has one Neumann leaf, we double the tree and reflect its eigenfunction across this leaf to obtain a tree with all leaves Dirichlet and the diameter less than or equal to $2 \text{Diam } \mathcal{G}$. \square

We will now consider operations that expand the graph in some way, either by scaling up a part of it or by attaching a new subgraph to it.

Definition 6.8. Let v_0 be a vertex of \mathcal{G} whose set of incident edges is $\{e_1, \dots, e_k\}$ and let \mathcal{H} be another metric graph. Form a new graph $\tilde{\mathcal{G}}$ by removing v_0 from \mathcal{G} and, for each $i = 1, \dots, k$, attaching edge e_i to some vertex $w = w(i)$ of \mathcal{H} instead. Let w_1, \dots, w_m , $m \leq k$ be the list of vertices of \mathcal{H} to which an edge has been so attached. If v_0 is equipped with the δ -potential of strength $\gamma(v_0) \in (-\infty, \infty)$, then δ -potentials should be placed at the vertices w_1, \dots, w_m in such a way that they sum to $\gamma(v_0)$. We then say that $\tilde{\mathcal{G}}$ is formed by *inserting \mathcal{H} into \mathcal{G} at v_0* .

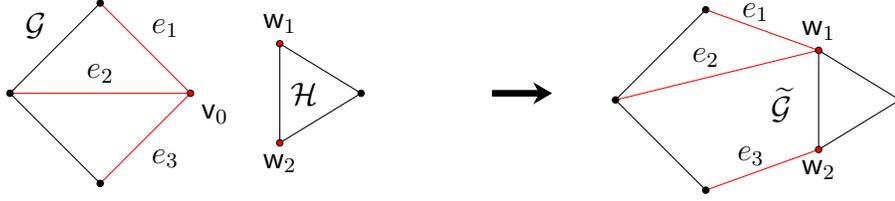


FIGURE 15. Inserting \mathcal{H} into \mathcal{G} at v_0 , we obtain the graph $\tilde{\mathcal{G}}$ on the right.

Whenever $w_1 = \dots = w_m$ we have the following special case.

Definition 6.9. Assume that \mathcal{G} and \mathcal{H} are given, with one distinguished vertex in each graph, say $v_1 \in \mathcal{G}$ and $w_1 \in \mathcal{H}$. If $\tilde{\mathcal{G}}$ is formed by gluing together v_1 and w_1 , we speak of attaching the pendant graph \mathcal{H} to \mathcal{G} .

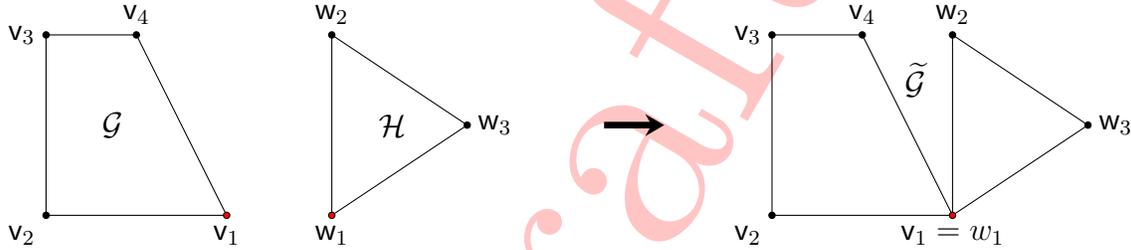


FIGURE 16. By gluing together v_1, w_1 we can attach the graph \mathcal{H} to \mathcal{G} , thus obtaining the graph $\tilde{\mathcal{G}}$ on the right.

Theorem 6.10. *The following operations decrease the given eigenvalues.*

- (1) Suppose $\tilde{\mathcal{G}}$ is formed from \mathcal{G} by attaching a pendant metric graph \mathcal{H} at a vertex $v_0 \in V(\mathcal{G})$. If, for some r and k ,

$$(6.4) \quad \lambda_r(\mathcal{H}) \leq \lambda_k(\mathcal{G}),$$

then

$$(6.5) \quad \lambda_{k+r-1}(\tilde{\mathcal{G}}) \leq \lambda_k(\mathcal{G}).$$

The inequality in (6.5) is strict if the eigenvalue $\lambda_k(\mathcal{G})$ has an eigenfunction which does not vanish at v_0 , $\lambda_k(\mathcal{G}) > \lambda_{k-1}(\mathcal{G})$ and $\lambda_k(\mathcal{G}) > \lambda_r(\mathcal{H})$.

- (2) Suppose $\tilde{\mathcal{G}}$ is formed by inserting a graph \mathcal{H} at a vertex v_0 of \mathcal{G} . Assume that only standard conditions were imposed at the vertices of \mathcal{H} prior to insertion. Then, for all k such that $\lambda_k(\mathcal{G}) \geq 0$,

$$(6.6) \quad \lambda_k(\tilde{\mathcal{G}}) \leq \lambda_k(\mathcal{G}).$$

The inequality in (6.6) is strict if $\lambda_k(\mathcal{G}) > \max(0, \lambda_{k-1}(\mathcal{G}))$ and the eigenvalue $\lambda_k(\mathcal{G})$ has an eigenfunction which does not vanish at v_0 .

Remark 6.11. An important special case of Theorem 6.10 is when the conditions are standard at all vertices of \mathcal{H} . In this case

$$(6.7) \quad 0 = \lambda_1(\mathcal{H}) \leq \lambda_1(\mathcal{G}) \leq \lambda_k(\mathcal{G})$$

and Theorem 6.10.(1) with $r = 1$ shows that attaching the pendant lowers *all* eigenvalues of \mathcal{G} :

$$(6.8) \quad \lambda_k(\tilde{\mathcal{G}}) \leq \lambda_k(\mathcal{G}) \quad \text{for all } k \geq 1.$$

The inequality (6.8) was noted in [144, Theorem 2] (for $V_D = \emptyset$ and $k = 1$) and [191, Proposition 3.1] (for $V_D = \emptyset$ and general k).

Several useful inequalities now follow.

Corollary 6.12. (1) *Let $\tilde{\mathcal{G}}$ be obtained from \mathcal{G} by lengthening the edge e , i.e., replacing e by an edge e' of length $\ell_{e'} > \ell_e$. Then*

$$(6.9) \quad \lambda_k(\tilde{\mathcal{G}}) \leq \lambda_k(\mathcal{G}) \quad \text{for all } k \geq 1.$$

The inequality is strict if $\lambda_k(\mathcal{G}) > \max(0, \lambda_{k-1}(\mathcal{G}))$ and there is an eigenfunction corresponding to $\lambda_k(\mathcal{G})$ which does not vanish identically on e .

(2) *Suppose there exist $\mathbf{v}, \mathbf{w} \in V(\mathcal{G})$ and a choice of $n \geq 1$ first eigenfunctions ψ_1, \dots, ψ_n such that*

$$(6.10) \quad \psi_k(\mathbf{v}) = \psi_k(\mathbf{w})$$

for all $k = 1, \dots, n$. If $\lambda_k(\mathcal{G}) \geq 0$, then the graph $\tilde{\mathcal{G}}$ formed by inserting an edge of arbitrary length between \mathbf{v}, \mathbf{w} satisfies

$$\lambda_k(\tilde{\mathcal{G}}) \leq \lambda_k(\mathcal{G}), \quad k = 1, \dots, n.$$

(3) *Suppose $\tilde{\mathcal{G}}$ is formed by adding an edge of length ℓ connecting existing vertices \mathbf{v}, \mathbf{w} of \mathcal{G} . Then $(\pi/\ell)^2 \leq \lambda_{k_0}(\mathcal{G})$ implies $\lambda_k(\tilde{\mathcal{G}}) \leq \lambda_k(\mathcal{G})$ for all $k \geq k_0$.*

(4) *Let $V_D = \emptyset$. Suppose there exist an eigenfunction ψ associated with $\lambda_1(\mathcal{G})$ and an edge e of \mathcal{G} such that $\psi|_e \equiv 0$. Then the graph $\tilde{\mathcal{G}}$ formed by shrinking e to a point (i.e., removing e and gluing its incident vertices together) satisfies $\lambda_1(\tilde{\mathcal{G}}) = \lambda_1(\mathcal{G})$, and $\psi|_{\mathcal{G} \setminus e}$ is an eigenfunction associated with $\lambda_1(\tilde{\mathcal{G}})$ (up to the canonical identification described in Lemma 6.2).*

Obtaining upper estimates tends to be easier. We have already seen in Section 5.2 how to derive first elementary bounds by finding the energy of a test function. Alternatively, how can we make λ_1 as large as possible using surgery methods, i.e., comparing a given graph \mathcal{G} with a new graph \mathcal{G}' whose lowest eigenvalue is both larger and explicitly known? Example 3.7.(2) shows that there cannot be a complementary upper bound to (5.1). But the principle that gluing vertices increases the eigenvalues has been exploited in [119, Theorem 4.2] and later in [26, Corollary 2.9] (without and with the correcting term N , respectively) to obtain the following bound in terms of the mean edge length.

Theorem 6.13. *If \mathcal{G} has $E \geq 2$ edges, no vertices of degree 2, and $N \geq 0$ vertices of degree 1, then*

$$(6.11) \quad \mu_2(\mathcal{G}) \leq \frac{\pi^2}{|\mathcal{G}|^2} \left(E - \frac{N}{2} \right)^2$$

unless \mathcal{G} is a path graph, a loop, or a lasso graph. Equality – among others cases – if \mathcal{G} is an equilateral pumpkin or flower graph, or else any figure-8-graph.

Besides Theorem 6.3, for the proof we need two further surgery principles.

Definition 6.14. We say that a closed subset $\mathcal{G}' \subset \mathcal{G}$ of a given graph \mathcal{G} is a *pendant subgraph* of \mathcal{G} if it is attached to the rest of \mathcal{G} at a single point (without loss of generality, a vertex), that is, the set

$$\overline{\mathcal{G}' \cap \mathcal{G} \setminus \mathcal{G}'}$$

is a singleton.

Lemma 6.15. *Suppose $\tilde{\mathcal{G}}$ is formed from \mathcal{G} by deleting a pendant subgraph $\mathcal{G}' \subset \mathcal{G}$ (equivalently, \mathcal{G} is formed from $\tilde{\mathcal{G}}$ by gluing a new graph \mathcal{G}' to $\tilde{\mathcal{G}}$ at a single vertex). Then*

$$\mu_k(\tilde{\mathcal{G}}) \geq \mu_k(\mathcal{G})$$

for all $k \geq 1$.

Proof. Given \mathcal{G} and its subgraph \mathcal{G}' attached to $\tilde{\mathcal{G}} = \mathcal{G} \setminus \mathcal{G}'$ at the vertex \mathbf{v} , form a new, disconnected graph

$$\mathcal{G}' \sqcup \tilde{\mathcal{G}}$$

via a suitable cut through \mathbf{v} . This is a cut of rank 1, thus, by Theorem 6.3,

$$\mu_k(\mathcal{G}' \sqcup \tilde{\mathcal{G}}) \geq \mu_{k-1}(\mathcal{G})$$

for all $k \geq 2$. Now the set of eigenvalues of $\mathcal{G}' \sqcup \tilde{\mathcal{G}}$ is just the union of the set of eigenvalues of \mathcal{G}' and the set of eigenvalues of $\tilde{\mathcal{G}}$ (where eigenvalues are always repeated according to their multiplicities). Since $\mu_1(\mathcal{G}) = \mu_1(\tilde{\mathcal{G}}) = 0$ has multiplicity 2, it follows that $\lambda_1(\tilde{\mathcal{G}})$ can, at best, correspond to $\mu_3(\mathcal{G}' \sqcup \tilde{\mathcal{G}})$, $\mu_3(\tilde{\mathcal{G}})$ at best to $\mu_4(\mathcal{G}' \sqcup \tilde{\mathcal{G}})$, and so on. Thus, in general,

$$\mu_k(\tilde{\mathcal{G}}) \geq \mu_{k+1}(\mathcal{G}' \sqcup \tilde{\mathcal{G}}) \geq \mu_k(\mathcal{G}) \quad \text{for all } k \geq 1. \quad \square$$

Finally, we need to discuss how μ_2 changes upon redistributing length to make pendant edges and/or pendant loops equilateral. The following can be deduced from [26, Corollary 7.2].

Lemma 6.16. *Given \mathcal{G} consisting of $E \geq 3$ edges, n of which are pendant edges (of length $\ell_{p,1}, \dots, \ell_{p,n}$) attached to some vertex \mathbf{v}_0 , and m of which are loops (of length $\ell_{l,1}, \dots, \ell_{l,m}$) attached to the same vertex \mathbf{v}_0 . Construct $\tilde{\mathcal{G}}$ from \mathcal{G} replacing the n pendant edges by the same number of pendant edges, each of equal length*

$$\ell_p := \frac{1}{n} \sum_{j=1}^n \ell_{p,j};$$

and replacing the m loops by the same number of loops, each of equal length

$$\ell_l := \frac{1}{m} \sum_{k=1}^m \ell_{l,k}.$$

Then

$$(6.12) \quad \mu_2(\mathcal{G}) \leq \mu_2(\tilde{\mathcal{G}}).$$

Provided $\mu_2(\tilde{\mathcal{G}}) = \frac{\pi^2}{4\ell_p^2}$ (resp., $\mu_2(\tilde{\mathcal{G}}) = \frac{\pi^2}{\ell_p^2}$), equality holds in (6.12) if and only if $\ell_{p,j} \equiv \ell_p$ (resp., $\ell_{l,k} \equiv \ell_l$).

Proof of Theorem 6.13. Glue together all vertices of \mathcal{G} that have degree larger than 2. This forms a stower (a flower, if $n = 0$) \mathcal{S} with the same number of edges and the same total length as \mathcal{G} . We conclude that

$$\mu_2(\mathcal{G}) \leq \mu_2(\mathcal{S})$$

by Lemma 6.16. The claim now follows from Lemma 3.8. \square

Remark 6.17. An important motivation for the development of spectral geometry in metric graph theory has been the pioneering investigation in [95] for the discrete Laplacian $\mathcal{L}_{\mathcal{G}}$ on simple combinatorial graphs \mathcal{G} . In particular, Fiedler proved that the lowest strictly positive eigenvalue of $\mathcal{L}_{\mathcal{G}}$ is minimal for path graphs and maximal for (and only for) complete graphs. Therefore, Theorem 5.1.(1) is seen to be a direct counterpart of Fiedler's *lower* bound. On the other hand, the interpretation of the upper bound in Equation 6.11 is less immediate, even dropping the correction term N (or simply assuming $N = 0$). Indeed, this illustrates in a nice way a heuristic but robust role: the role played by vertices in the spectral theory of combinatorial graphs is usually played by edges in the spectral theory of metric graphs. In particular, "complete metric graphs" are those metric graphs for which any two edges are "adjacent", i.e., share an endpoint: these are precisely the pumpkin stars, cf. Example 3.7 (and in particular pumpkin and flowers).

Remark 6.18. It was mistakenly stated in [119, Theorem 4.2] that equilateral pumpkin and flower graphs are the only classes of metric graphs maximising the estimate in (6.11). This is wrong, as it was pointed out in [26] based on Example 6.5. It turns out that the situation is even more complicated: so-called *inflated stars* form a class of isospectral graphs with respect to the normalized Laplacian matrix, see [64, 155]. This isospectrality result can be immediately extended to metric graphs in view of the transference principle in Theorem 8.1 below, see [169, Remark 6.3], showing in particular that equilateral flower graphs have many isospectral metric graphs.

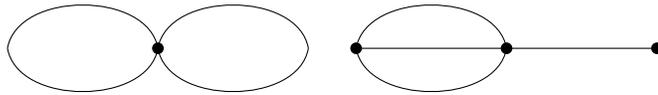


FIGURE 17. An equilateral flower on two edges and a further isospectral metric graph.

Indeed, it turns out that inflated stars are precisely the combinatorial graphs underlying the pumpkin stars introduced in Remark 6.17.

Just like the lower estimate can be improved in the class of doubly connected metric graphs, the upper estimate can be improved in the class of simply connected metric graphs, i.e., of metric tree graphs. The following upper bound is [191, Theorem 3.2].

Theorem 6.19. *Let \mathcal{G} be a metric tree. Then*

$$(6.13) \quad \mu_k(\mathcal{G}) \leq \frac{k^2 \pi^2 E^2}{4|\mathcal{G}|^2} \quad \text{for all } k \in \mathbb{N},$$

with equality being attained if and only if

- $k = 2$ and \mathcal{G} is an equilateral star graph, or
- $k \geq 3$ and \mathcal{G} is a path graph.

Proof. Let us see how (6.13) can be deduced from surgery principles. Pick one edge of maximal length and an edge of the next maximal length within \mathcal{G} , say $\mathbf{e}_1, \mathbf{e}_2$. Upon iteratively deleting pendant edges, we can transform \mathcal{G} into the (unique) path $\mathcal{P} \subset \mathcal{G}$ that contains $\mathbf{e}_1, \mathbf{e}_2$, which can be regarded as an interval of length $|\mathcal{P}|$ with Neumann boundary conditions. Then it follows from Lemma 6.15 that

$$\mu_k(\mathcal{G}) \leq \mu_k(\mathcal{P}) = \frac{\pi^2 k^2}{|\mathcal{P}|^2} \leq \frac{\pi^2 k^2 E^2}{|\mathbf{e}_1|^2 + |\mathbf{e}_2|^2} \leq \frac{\pi^2 k^2 E^2}{4|\mathcal{G}|^2}. \quad \square$$

The following refinement for $k = 2$ has been observed in [26, Theorem 2.2]: its proof is based on the bound

$$E_l \text{Diam}(\mathcal{G}) \geq 2|\mathcal{G}|,$$

which is sharp and rigid: it becomes an equality precisely for equilateral stars.

Proposition 6.20. *Let \mathcal{G} be a metric tree with $E_l \geq 2$ leaves. Then*

$$\mu_2(\mathcal{G}) \leq \frac{\pi^2 E_l^2}{4|\mathcal{G}|^2},$$

with equality being attained if and only if \mathcal{G} is a star graph.

Metric trees are in many respects interpolating between intervals and higher dimensional domains. For instance, we mention the following bound [191, Theorem 4.1], which is reminiscent of Friedlander's inequality (2.11).

Proposition 6.21. *Let \mathcal{G} be a metric tree. Then*

$$\mu_k(\mathcal{G}) \leq \lambda_k(\mathcal{G}; \mathbf{V}_D = \mathbf{V}) \quad \text{for all } k \in \mathbb{N}.$$

Equality holds for at least one k if and only if all edge lengths are rationally dependent.

The perhaps more widely known result from [191], namely [191, Theorem 3.4], states that on a metric tree it is possible to find an upper bound on μ_k purely in terms of the diameter; in fact, this is a direct consequence of Lemma 6.15. This may be combined with the intertwining

principle for cutting through vertices, Theorem 6.3, to obtain the following general result, which also appeared as [90, Theorem 5.2] (in a slightly more general context, namely among graphs of finite total length and finite number of cycles but with a possibly infinite number of edges). In the following, we call

$$\beta := E - V + 1$$

the *first Betti number* of a (metric) graph with E edges and V vertices: by an easy combinatorial argument, β is the number of independent cycles in the graph; in particular, metric trees are characterized as those metric graphs with vanishing Betti number.

Theorem 6.22. *Let \mathcal{G} have Betti number $\beta \in \mathbb{N}_0$. Then*

$$(6.14) \quad \mu_k(\mathcal{G}) \leq (k + \beta - 1)^2 \frac{\pi^2}{\text{Diam}(\mathcal{G})^2} \quad \text{for all } k \in \mathbb{N}.$$

Proof. Since \mathcal{G} has Betti number β , it is possible to cut it β times to produce a tree \mathcal{T} , which obviously satisfies $\text{Diam } \mathcal{T} \geq \text{Diam}(\mathcal{G})$. By Theorem 6.3, we have $\mu_k(\mathcal{G}) \leq \mu_{k+\beta}(\mathcal{T})$. Now, by iteratively deleting pendant edges we may prune \mathcal{T} until we are left with a path graph of length $\text{Diam } \mathcal{T}$, whose eigenvalues are those of the second derivative with Neumann boundary conditions. We conclude that

$$\mu_k(\mathcal{G}) \leq \mu_{k+\beta}(\mathcal{T}) \leq \frac{\pi^2(k + \beta - 1)^2}{\text{Diam}(\mathcal{T})^2} \leq \frac{\pi^2(k + \beta - 1)^2}{\text{Diam}(\mathcal{G})^2}. \quad \square$$

6.2. Further interlacing techniques. The following interlacing estimate, which is comparable to Theorem 6.3, is [24, Lemma 4.2].

Proposition 6.23. *Let \mathcal{G} be a metric graph with a vertex \mathbf{v} of degree d with standard conditions, whose removal separates the graph into d disjoint subgraphs. Denote by $\mathbf{E}_{\mathbf{v}}$ the set of edges incident in \mathbf{v} and let $r < d$ be a nonnegative integer. For a subset $\mathbf{E}_{\mathbf{D}}$ of $\mathbf{E}_{\mathbf{v}}$, with $|\mathbf{E}_{\mathbf{D}}| = r$, define $\mathcal{G}_{\mathbf{E}_{\mathbf{D}}}$ to be the modification of the graph \mathcal{G} obtained by imposing the Dirichlet condition at \mathbf{v} for edges from $\mathbf{E}_{\mathbf{D}}$ and leaving the edges from $\mathbf{E}_{\mathbf{v}} \setminus \mathbf{E}_{\mathbf{D}}$ connected at \mathbf{v} with the standard condition. Then*

$$(6.15) \quad \mu_n(\mathcal{G}) \leq \min_{|\mathbf{E}_{\mathbf{D}}|=r} \lambda_n(\mathcal{G}_{\mathbf{E}_{\mathbf{D}}}; \{\mathbf{v}\}) \leq \mu_{n+1}(\mathcal{G}) \leq \max_{|\mathbf{E}_{\mathbf{D}}|=r} \lambda_n(\mathcal{G}_{\mathbf{E}_{\mathbf{D}}}; \{\mathbf{v}\}) \leq \mu_{n+2}(\mathcal{G}).$$

The following is [45, Theorem 4.7].

Theorem 6.24. *Let \mathcal{G} have Betti number β . Then*

$$(6.16) \quad \mu_{k+1}(\mathcal{G}) \geq \left(k - \frac{N + \beta}{2}\right)^2 \frac{\pi^2}{|\mathcal{G}|^2} \quad \text{for all } k \geq \max\{2, N + \beta\} \quad \text{if } \mathbf{V}_{\mathbf{D}} = \emptyset$$

and

$$(6.17) \quad \lambda_k(\mathcal{G}; \mathbf{V}_{\mathbf{D}}) \geq \left(k - \frac{N + \beta}{2}\right)^2 \frac{\pi^2}{|\mathcal{G}|^2} \quad \text{for all } k \geq N + \beta \quad \text{if } \mathbf{V}_{\mathbf{D}} \neq \emptyset,$$

where N is the number of vertices of degree 1 on which a standard (i.e., Neumann) condition is imposed.

Proof. If \mathcal{G} is not a tree, we find an edge whose removal would not disconnect the graph. Let \mathbf{v} be a vertex to which this edge is incident; since \mathcal{G} is not a cycle, without loss of generality we can assume its degree is 3 or larger (otherwise this vertex can be absorbed into the edge). We disconnect the edge from this vertex, reducing β by one and creating an extra vertex of degree 1 where we impose the Neumann condition. We keep standard conditions at \mathbf{v} . Then the new graph is not a cycle, as a new vertex of degree 1 was created. We may therefore repeat the process inductively until we obtain a tree \mathcal{T} with $N' = N + \beta$ Neumann vertices.

Since the eigenvalues are reduced at every step, $\lambda_k(\mathcal{G}) \geq \lambda_k(\mathcal{T})$. It is therefore enough to verify the inequality for trees.

Given a tree \mathcal{T} , by Theorem 4.4 we can choose the k -th eigenvalue to be simple and the associated eigenfunction to be nonzero on vertices [51], hence to have exactly k nodal domains [187, 198]. Each nodal domain is a subtree \mathcal{T}_j and $\lambda_k(\mathcal{T})$ is the first eigenvalue of the subtree.

There are at most $|N|$ subtrees with some Neumann conditions on their leaves. Since these are nodal subtrees ($k > 1$), there are also some leaves with Dirichlet conditions and we can use (5.2) in the form $L_j \sqrt{\lambda} \geq \pi/2$. The same conclusion is true if $k = 1$ and \mathcal{T} has at least one Dirichlet vertex.

If $k \geq |N|$, we also have at least $k - |N|$ subtrees with *only* Dirichlet conditions at the leaves, for which we can use the bound of Proposition 6.7 but with the diameter substituted by the total length of the subtree, i.e., $L_j \sqrt{\lambda} \geq \text{Diam}(\mathcal{T}_j) \sqrt{\lambda} \geq \pi$. We therefore have

$$L \sqrt{\lambda_k(\mathcal{T})} = \sum_{j=1}^k L_j \sqrt{\lambda_1(\mathcal{T}_j)} \geq N \frac{\pi}{2} + (k - N)\pi = \left(k - \frac{N}{2}\right) \pi. \quad \square$$

An upper bound that is similar in spirit was obtained in [45, Theorem 4.9].

Theorem 6.25. *Let \mathcal{G} be a connected quantum graph with Dirichlet or Neumann conditions at the vertices of degree 1 and standard condition elsewhere. If \mathcal{G} is not a cycle, then*

$$(6.18) \quad \lambda_k(\mathcal{G}) \leq \left(k - 2 + \beta + D + \frac{N+\beta}{2}\right)^2 \frac{\pi^2}{|\mathcal{G}|^2} \quad \text{for all } k \in \mathbb{N},$$

where $D := |\mathbf{V}_D|$ and N is number of vertices of degree 1 that do not belong to \mathbf{V}_D .

Proof. If \mathcal{G} is not a tree (i.e., if $\beta > 0$) and not a cycle, we repeat the process described at the beginning of the proof of Theorem 6.24, disconnecting β edges at vertices and creating a tree \mathcal{T} with β additional Neumann vertices of degree 1. At every step, the eigenvalue goes down, but by Theorem 6.3 not further than the next eigenvalue, therefore we have $\lambda_k(\mathcal{G}) \leq \lambda_{k+\beta}(\mathcal{T})$ and the bound for general graphs follows from the bound for trees, $\beta = 0$.

We will prove the result assuming \mathcal{G} is a tree by induction on the number of edges. The inequality turns into equality for a single edge with either Dirichlet, Neumann or mixed conditions.

Choose an arbitrary vertex \mathbf{v} of degree three or more and apply Proposition 6.23 (the third inequality) with $r = 1$. Let \mathcal{G}' be the graph realizing this inequality; it is a disjoint union of two trees – denote them by \mathcal{T}_1 and \mathcal{T}_2 . Without loss of generality, $\lambda_k(\mathcal{G}')$ is an eigenvalue of \mathcal{T}_1 ;

denote its position in the spectrum of \mathcal{T}_1 by $j \leq k$. We therefore have

$$\lambda_k(\mathcal{G}') = \lambda_j(\mathcal{T}_1) \quad \text{and} \quad \lambda_k(\mathcal{G}') \leq \lambda_{k-j+1}(\mathcal{T}_2).$$

Denoting by L_1 and L_2 the total lengths of the two trees, we have $L = L_1 + L_2$. Denoting by D_1 and D_2 the number of Dirichlet vertices, we also have $D = D_1 + D_2 - 1$, since one Dirichlet vertex was added in the process of application of Proposition 6.23 with $r = 1$. We now use the inductive hypothesis for the two trees \mathcal{T}_1 and \mathcal{T}_2 to get

$$\begin{aligned} L\sqrt{\lambda_k(\mathcal{G})} &\leq L_1\sqrt{\lambda_j(\mathcal{T}_1)} + L_2\sqrt{\lambda_{k-j+1}(\mathcal{T}_2)} \\ &\leq \pi\left(j - 2 + D_1 + \frac{N_1}{2}\right) + \pi\left(k - j + 1 - 2 + D_2 + \frac{N_2}{2}\right) \\ &= \pi\left(k - 3 + D + 1 + \frac{N}{2}\right). \end{aligned}$$

This completes the proof. \square

Remark 6.26. (a) The first expression in (6.16) gives a better bound than (5.19) for all $k \geq |N| + \beta$. Theorem 6.24 is asymptotically sharp in the sense that both the eigenvalue and its bound have the same asymptotic form $\frac{k^2\pi^2}{|\mathcal{G}|^2} + o(1)$ as $k \rightarrow \infty$. It was proved in [151] that Theorem 6.25 is asymptotically sharp, too: there exists a sequence of metric graphs for which the error in (6.18) vanishes asymptotically.

Further asymptotically sharp bounds were obtained in [176, Théorème 2.4]: namely

$$(6.19) \quad \frac{(k-1-|\mathcal{G}|)^2\pi^2}{|\mathcal{G}|^2} \leq \lambda_k(\mathcal{G}) \leq \frac{(k-1+|\mathcal{G}|)^2\pi^2}{|\mathcal{G}|^2}$$

if \mathcal{G} is equilateral. For some (equilateral!) \mathcal{G} , (6.19) is tighter than (6.18).

(b) Applying Theorem 5.1 for each of the k nodal subtrees in the proof of Theorem 6.24, we can recover again Theorem 5.12.

6.3. Pumpkin chains, Sturm–Liouville problems, and diameter. In this and the next section we will look at advanced techniques for obtaining eigenvalue bounds (for simplicity in the special case of μ_2) by comparing a given graph with special classes of more structured graphs. It turns out that the *pumpkin chains* introduced in Example 3.7 will play an important role for both upper and lower bounds.

Lemma 6.27. *Let \mathcal{G} be compact and connected. Then there exist two locally equilateral pumpkin chains $\mathcal{P}_1, \mathcal{P}_2$ such that*

$$\mu_2(\mathcal{P}_1) \leq \mu_2(\mathcal{G}) \leq \mu_2(\mathcal{P}_2),$$

where \mathcal{P}_1 has the same or lesser total length as \mathcal{G} , and the total length of its bridges is no longer than the bridges within \mathcal{G} ; while \mathcal{P}_2 can be taken to have the same diameter as \mathcal{G} and the same number or fewer vertices.

The lower bound, proved in [46, Lemmas 5.1 and 5.3], requires a *local symmetrization* technique in addition to sharp forms of gluing and removing superfluous pendants.

The upper bound/construction is proved in [119, Section 5.2], by fixing any two diametral points in \mathcal{G} , and successively considering all non-backtracking paths in the graph between

them, shortening the paths, gluing them together at selected points, and deleting the rest of the graph to obtain the desired comparison graph \mathcal{P}_2 . It combines the gluing principle, Theorem 6.3 in its simplest form (gluing vertices cannot decrease the eigenvalues), together with the principles that shortening edges and deleting pendant graphs cannot decrease the eigenvalues (Corollary 6.12.(1) and Theorem 6.10.(1), respectively). It is also explained in full in [59, Section 2].

Locally equilateral pumpkin chains have the advantage that, up to the right choice of basis, their eigenfunctions (associated with the standard Laplacian, although a Dirichlet condition may be assumed at either of the antipodal vertices) decompose naturally into *longitudinal* (depending only on the distance to the antipodal vertices) and *transversal* ones (supported only on a single pumpkin, and in particular vanishing on all vertices), see [46, Lemma 5.4]. In particular, we have the following.

Lemma 6.28. *Let \mathcal{P} be a locally equilateral pumpkin chain which is not just a pumpkin graph. Then $\mu_2(\mathcal{P})$ is simple and its eigenfunction is longitudinal, that is, in the notation of Example 3.7.(7) it depends only on $\text{dist}(\cdot, \mathbf{v}_1)$.*

As noted, the result continues to hold if one or two antipodal vertices are equipped with a Dirichlet condition instead; see [46, Lemma 5.5].

This means that, if \mathcal{P} is a locally equilateral pumpkin chain, then $\mu_2(\mathcal{P})$ is equal to the spectral gap of a suitable weighted Sturm–Liouville problem on an interval of length $\text{dist}(\mathbf{v}_1, \mathbf{v}_\mathbf{v}) = \text{Diam } \mathcal{P}$, and there is a natural correspondence between their respective eigenfunctions, as explained in [119, Section 5.2]:

Lemma 6.29. *Letting $D = \text{Diam } \mathcal{P}$, we have that $\mu_2(\mathcal{P})$ is equal to the spectral gap (smallest nontrivial eigenvalue) of the problem*

$$\begin{aligned} -(\omega u)' &= \lambda \omega u && \text{in } (0, D), \\ u'(0) &= u'(D) = 0, \end{aligned}$$

where, in the notation of Example 3.7(7), $\omega \in L^\infty(0, D)$ is a positive step function defined by $\omega(x) = m_i$, the number of parallel edges between \mathbf{v}_i and \mathbf{v}_{i+1} , if $\text{dist}(\mathbf{v}_i, \mathbf{v}_1) < x < \text{dist}(\mathbf{v}_{i+1}, \mathbf{v}_1)$.

Both this principle of mapping onto a Sturm–Liouville problem, and the upper bound method in Lemma 6.27 were originally developed to study upper bounds for μ_2 in terms of diameter which, in particular, do *not* involve the total length (unlike, e.g., Proposition 5.3); in particular, it was shown in [119, Section 5.2] that no upper bound purely in terms of diameter is possible:

Example 6.30. There exists a sequence \mathcal{G}_n of graphs of fixed diameter, such that $\mu_2(\mathcal{G}_n) \rightarrow \infty$.

The graphs are taken to be pumpkin chains of increasing complexity but constant diameter $D > 0$, whose associated Sturm–Liouville weights ω_n are assumed to be sufficiently close in $L^\infty(0, D)$ to the exponential (smooth) weights $\tilde{\omega}_n(x) = e^{nx}$. An explicit calculation shows that the spectral gap for $\tilde{\omega}_n$ behaves like $\frac{n^2}{4}$. These weights correspond to “cusp-like” pumpkin chains, where the number of parallel edges within each pumpkin grows exponentially as one traverses the chain.

On the other hand, if one fixes the number of vertices (and thus the degree of complexity of the graph, in some sense) one can obtain a sharp upper bound.

Theorem 6.31. *Let \mathcal{G} have V vertices and diameter $\text{Diam } \mathcal{G} > 0$. Then*

$$(6.20) \quad \mu_2(\mathcal{G}) \leq \frac{\pi^2(V+2)^2}{4(\text{Diam } \mathcal{G})^2}.$$

The estimate is sharp in the sense that there exists a sequence of pumpkin chains \mathcal{G}_n with fixed diameter and number of vertices, realizing equality in (6.20) in the asymptotic limit.

This was proved in [59, Theorem 1.1], sharpening an earlier estimate [119, Theorem 6.1]. In either case, as noted Lemma 6.27 allows one to reduce to considering only locally equilateral pumpkin chains. One then uses a test function argument to control the spectral gap of the latter, based on sinusoidal functions of $\text{dist}(\cdot, v_1)$. In [59] this test function argument is analyzed carefully and brought into its sharpest form.

A similar test function argument applied to pumpkin chains does, however, also allow one to obtain an upper bound which also involves the total length, see [119, Theorem 7.1]:

Theorem 6.32. *We have*

$$\mu_2(\mathcal{G}) \leq \frac{\pi^2}{(\text{Diam } \mathcal{G})^2} \cdot \frac{4|\mathcal{G}| - 3 \text{Diam } \mathcal{G}}{\text{Diam } \mathcal{G}}.$$

This is broadly similar to Proposition 5.3 but has quite a different form (and was obtained several years earlier). Unlike Theorem 6.31, to the best of our knowledge neither this bound nor the bound in Proposition 5.3 has been optimized, that is, they are unlikely to be sharp.

We finish this section by recalling a few other complementary bounds and non-bounds involving diameter from [119]. If one looks for corresponding *lower* bounds in terms of just $\text{Diam } \mathcal{G}$, or even $\text{Diam } \mathcal{G}$ and $|\mathcal{V}|$, then none are possible, as a simple example ([119, Example 5.1]) shows:

Example 6.33. Form \mathcal{G}_n by taking an interval of length $\frac{1}{3}$ and, to each of its two endpoints, join a flower graphs on n edges of length $\frac{1}{3}$ each (\mathcal{G}_n is thus a “flower dumbbell”). Then \mathcal{G}_n has exactly two vertices, and $\text{Diam } \mathcal{G}_n = 1$. However, a simple test function argument shows that $\mu_2(\mathcal{G}_n) \rightarrow 0$; take the function to be $+1$ on one flower, -1 on the other and sinusoidal (or linear) on the handle of the dumbbell.

Since our graphs may have multiple parallel edges, and indeed this property is critical in many of the constructions above, fixing the number of edges the graph may have is a much stronger restriction than fixing its number of vertices; it was observed in [119, Remark 6.3] that both upper and lower bounds on μ_2 are possible if one fixes the diameter and the number of edges.

Proposition 6.34. *Let \mathcal{G} have E edges and diameter $\text{Diam } \mathcal{G}$, then*

$$\frac{\pi^2}{E^2(\text{Diam } \mathcal{G})^2} \leq \mu_2(\mathcal{G}) \leq \frac{4\pi^2 E^2}{(\text{Diam } \mathcal{G})^2}.$$

Neither bound is likely to be optimal; improving them is an open problem. The upper bound follows from a trivial test function argument, completely analogous to (5.8): since at least one edge must have length at least $\frac{\text{Diam } \mathcal{G}}{E}$, one may place a full sine wave on that edge. The lower bound follows from the basic lower bound, Theorem 5.1.(1), plus the trivial estimate $|\mathcal{G}| \leq E \text{Diam } \mathcal{G}$.

6.4. Cutting along eigenfunctions. In this section we are presenting a refinement of the notion of *cutting through a vertex* introduced in Definition 6.1. The following idea goes back to [40, Sec 3.1] and [46], but it has first been fully exploited in [47], where it is crucially used to prove Proposition 6.37 below. In the following it will be fundamental to allow for δ -conditions at the vertices of \mathcal{G} , as introduced in Section 8.9, i.e., continuity across each vertex along with

$$\sum_{e \sim \mathbf{v}} \frac{\partial u_e}{\partial n}(\mathbf{v}) = \gamma(\mathbf{v})u(\mathbf{v})$$

for some vector $(\gamma(\mathbf{v}))_{\mathbf{v} \in \mathcal{V}}$ of strengths of δ -potentials: remarkably, they will appear in the proof of Proposition 6.37, even though the assertion only deals with the Laplacian with standard vertex conditions. We regard the following as a *hybrid* surgical operation, in that it modifies a metric graph and the associated Laplacian at the same time.

Definition 6.35 (Cutting through vertices along a function). Assume we are given a function $\psi \in H^1(\mathcal{G})$ satisfying a δ -condition with strength $\gamma(\mathbf{v})$ at \mathbf{v} . The following surgery transformation will be called *cutting through the vertex \mathbf{v} along the function ψ* :

- (1) cutting the metric graph \mathcal{G} through a vertex \mathbf{v} , thus producing $p \geq 2$ new (“descendant”) vertices $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_p$ and
- (2) endowing the new vertex \mathbf{v}_i with the *strength*

$$(6.21) \quad \gamma(\mathbf{v}_i) = -\frac{1}{\psi(\mathbf{v})} \sum_{e \sim \mathbf{v}_i} \frac{\partial \psi_e}{\partial n}(\mathbf{v}), \quad i = 1, \dots, p,$$

where the summation is over the edges that are attached to the relevant descendant of \mathbf{v} . By convention, when $\psi(\mathbf{v}) = 0$, we impose Dirichlet conditions at all vertices $\mathbf{v}_1, \dots, \mathbf{v}_p$.

A few observations are in order. On one hand, since $\gamma(\mathbf{v}) = \sum_{i=1}^p \gamma(\mathbf{v}_i)$, the analogue of Theorem 6.3 still holds. Namely, denoting by \mathcal{G}^{cut} the graph obtained by cutting,

$$(6.22) \quad \lambda_k(\mathcal{G}^{\text{cut}}) \leq \lambda_k(\mathcal{G}) \leq \lambda_{k+(p-1)}(\mathcal{G}^{\text{cut}}), \quad k \geq 1,$$

see, for example, [48, Thm. 5.3].

On the other hand if ψ was an eigenfunction before cutting, it is also an eigenfunction of the cut graph \mathcal{G}^{cut} , *with the same eigenvalue*. Importantly, the label of the eigenvalue in the spectrum may have changed, but (6.22) gives some control on the change in the label. This can be used, as in [40], to give a bound on the number of zeros of the eigenfunction ψ . Conversely, as in Proposition 6.37 below, using the knowledge of the number of zeros, one can identify the label of the new eigenvalue.

We will illustrate the power of this idea by proving an estimate on the girth of \mathcal{G} : this is defined as follows.

Definition 6.36. The *girth* of a connected metric graph \mathcal{G} is

$$\text{Girth}(\mathcal{G}) := \min\{|\mathbf{c}| : \mathbf{c} \subset \mathcal{G} \text{ is a cycle in } \tilde{\mathcal{G}}\},$$

where $\tilde{\mathcal{G}}$ is obtained from \mathcal{G} by gluing together all Dirichlet vertices of \mathcal{G} , if any are present. The girth is defined to be zero if $\tilde{\mathcal{G}}$ is a tree.

Proposition 6.37. *If $\mathbf{V}_D \neq \emptyset$, then*

$$(6.23) \quad \lambda_1(\mathcal{G}; \mathbf{V}_D) \leq \frac{\pi^2}{\text{Girth}(\mathcal{G})^2}.$$

Equality is attained if and only if \mathcal{G} is an equilateral star graph with $n \geq 2$ edges of length $\text{Girth}(\mathcal{G})/2$ with Dirichlet conditions at all degree 1 vertices.

Proof. 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 1 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 by Remark 6.11; a Dirichlet condition imposed at a vertex of degree d separates the vertex into d copies.

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

$$(6.24) \quad \psi''(x) = -\lambda_1(\mathcal{G}; \mathbf{V}_D)\psi(x) < 0.$$

For the purpose of this proof all internal (to an edge) local maxima are to be considered vertices. We may and do assume, without loss of generality, that there are no further vertices of degree two. Now, the set of serious points (in the sense of Definition 3.6) of ψ is a nonempty 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 $\frac{\partial \psi_{\mathbf{e}_{\pm 1}}}{\partial n}(\mathbf{v}_0) \geq 0$.

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 (6.24) 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 $\frac{\partial \psi_{\mathbf{e}_2}}{\partial n}(\mathbf{v}_1) \geq 0$. 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 18 and 19.

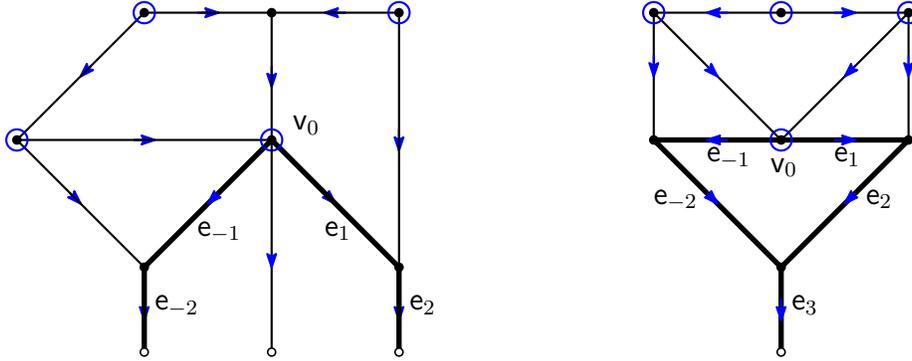


FIGURE 18. Examples of metric graphs with Dirichlet vertices (marked as small empty disks) and with a schematic depiction of the first eigenfunction as a gradient flow (blue arrows). The serious points are now the vertices with at least two outward-pointing arrows; they are circled in blue. The paths that are constructed in the course of the proof of Proposition 6.37 are shown as thicker edges.

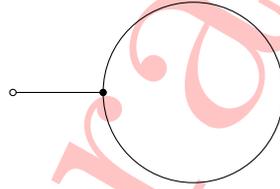


FIGURE 19. A lasso graph with one Dirichlet vertex.

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 . 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

$$\sum_{\substack{e \sim \mathbf{v}_i \\ e \in \tilde{\mathcal{G}}}} \frac{\partial u_e}{\partial n}(\mathbf{v}_i) + \gamma_{\mathbf{v}_i} u(\mathbf{v}_i) = 0,$$

where

$$(6.25) \quad \gamma_{\mathbf{v}_i} := \frac{1}{\psi(\mathbf{v}_i)} \sum_{\substack{e \sim \mathbf{v}_i \\ e \in \mathcal{G} \setminus \tilde{\mathcal{G}}}} \frac{\partial \psi_e}{\partial n}(\mathbf{v}_i) = -\frac{1}{\psi(\mathbf{v}_i)} \sum_{\substack{e \sim \mathbf{v}_i \\ e \in \tilde{\mathcal{G}}}} \frac{\partial \psi_e}{\partial n}(\mathbf{v}_i),$$

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 $\tilde{\mathcal{G}}$: we will eventually compare $\tilde{\mathcal{G}}$ with an interval or a tadpole (lasso) without δ -potentials, yielding the inequality.

Now, $\lambda_1(\mathcal{G})$ is still an eigenvalue, and, since ψ is non-negative, $\lambda_1(\mathcal{G}) = \lambda_1(\tilde{\mathcal{G}})$ by (6.22).

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 $\frac{\partial \psi_{\mathbf{e}}}{\partial n}(\mathbf{v}_i) \geq 0$; hence all derivatives in the first sum in (6.25) 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 [49, Thm 3.1.8], replacing all $\gamma_{\mathbf{v}_i}$ with 0 can only increase the eigenvalues. Therefore, $\lambda_1(\mathcal{G})$ 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 (5.11).

Finally, we discuss the case of equality. Sufficiency is clear. To prove necessity, we first observe that $\psi|_{\tilde{\mathcal{G}}}$ is a simple eigenfunction that 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 handle 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 6.3). The same reasoning yields $\frac{\partial \psi_{\mathbf{e}_{\pm 1}}}{\partial n}(\mathbf{v}_0) = 0$.

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

$$(6.26) \quad \sum_{\mathbf{e} \sim \mathbf{v}_0, \mathbf{e} \neq \mathbf{e}_{\pm 1}} \frac{\partial \psi_{\mathbf{e}}}{\partial n}(\mathbf{v}_0) = 0,$$

and therefore there is another edge $\tilde{\mathbf{e}}_1$ with $\frac{\partial \psi_{\tilde{\mathbf{e}}_1}}{\partial n}(\mathbf{v}_0) \geq 0$. 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 $\frac{\partial \psi_{\tilde{\mathbf{e}}_1}}{\partial n}(\mathbf{v}_0) = 0$. Proceeding by induction (and applying (6.26) 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, $\frac{\partial \psi_{\mathbf{e}}}{\partial n}(\mathbf{v}_0) = 0$ for every incident edge \mathbf{e} , therefore – since the eigenvalue is π^2/s^2 – the edge length must be $s/2$. \square

A simple symmetry argument now yields the following estimate for graphs without Dirichlet conditions: it has been obtained in [47], too.

Corollary 6.38. *Suppose the connected metric graph \mathcal{G} is obtained from two copies of another connected graph, $\hat{\mathcal{G}}$, by pairwise gluing of finitely many pairs of the duplicated vertices. Then*

$$(6.27) \quad \mu_2(\mathcal{G}) \leq \frac{4\pi^2}{\text{Girth}(\mathcal{G})^2}.$$

Equality is attained if \mathcal{G} is an equilateral pumpkin graph.

The following counterpart of Proposition 6.23 is [90, Lemma 4.18].

Proposition 6.39. *Let \mathcal{G} be a locally finite, connected metric graph, and $\mathbf{V}_D \subset \{\mathbf{v} \in \mathbf{V} : \deg(\mathbf{v}) = 1\}$. Suppose that \mathcal{G}_1 and \mathcal{G}_2 are two mutually disjoint, complementary metric subgraphs of \mathcal{G} such that $\overline{\mathcal{G}_1} \cap \overline{\mathcal{G}_2}$ consists of finitely many vertices of \mathcal{G} . Let $\psi \geq 0$, $\psi \not\equiv 0$, be*

an eigenfunction corresponding to $\lambda_1(\mathcal{G}; \mathbf{V}_D)$. If, for each vertex $\mathbf{v} \in \mathcal{G}_1 \cap \mathcal{G}_2$ and each edge \mathbf{e} connecting \mathbf{v} with a vertex \mathbf{w} in \mathcal{G}_2 , the derivative of ψ at \mathbf{v} pointing into \mathbf{e} is non-positive, then

$$(6.28) \quad \lambda_1(\mathcal{G}, \mathbf{V}_D) \geq \lambda_1(\mathcal{G}_1, \mathbf{V}_{D_1})$$

holds, where $\mathbf{V}_{D_1} := \mathcal{G}_1 \cap \mathbf{V}_D$. The inequality is strict if and only if at least one of the above-mentioned derivatives is strictly negative.



FIGURE 20. A partition of a graph \mathcal{G} into two subgraphs \mathcal{G}_1 and \mathcal{G}_2 . To apply Lemma 6.39 the derivatives of the eigenfunction ψ at the vertices \mathbf{v}_1 and \mathbf{v}_2 pointing into the respective edges \mathbf{e}_1 , \mathbf{e}_2 and \mathbf{e}_3 have to be nonpositive.

Proof. Let E_1 denote the edge set of \mathcal{G}_1 and let ψ_1 denote the restriction of ψ to \mathcal{G}_1 . For a given vertex $\mathbf{v} \in \mathcal{G}_1 \cap \mathcal{G}_2$ let $E_{2,\mathbf{v}}$ denote the set of edges in \mathcal{G}_2 that are incident to \mathbf{v} , and suppose that for each such edge $\mathbf{e} \simeq [0, \ell_{\mathbf{e}}]$ the vertex \mathbf{v} is identified with 0. Then, $\psi'_{\mathbf{e}}(0) \leq 0$ for all $\mathbf{e} \in E_{2,\mathbf{v}}$ by assumption. One sees immediately that

$$(6.29) \quad \begin{aligned} \|\psi'_1\|_{L^2(\mathcal{G}_1)}^2 &= \sum_{\mathbf{e} \in E_1} \int_0^{\ell_{\mathbf{e}}} |\psi'_{\mathbf{e}}(x)|^2 dx = \sum_{\mathbf{e} \in E_1} \psi_{\mathbf{e}} \psi'_{\mathbf{e}} \Big|_0^{\ell_{\mathbf{e}}} - \sum_{\mathbf{e} \in E_1} \int_0^{\ell_{\mathbf{e}}} \psi_{\mathbf{e}}(x) \psi''_{\mathbf{e}}(x) dx \\ &= \sum_{\mathbf{v} \in \mathcal{G}_1 \cap \mathcal{G}_2} \psi(\mathbf{v}) \sum_{\mathbf{e} \in E_{2,\mathbf{v}}} \psi'_{\mathbf{e}}(0) + \lambda_1(\mathcal{G}, \mathbf{V}_D) \|\psi_1\|_{L^2(\mathcal{G}_1)}^2 \\ &\leq \lambda_1(\mathcal{G}, \mathbf{V}_D) \|\psi\|_{L^2(\mathcal{G}_1)}^2, \end{aligned}$$

This implies (6.28); moreover, (6.29) – and hence (6.28) – is strict if $\psi'_{\mathbf{e}}(0) < 0$ for some $\mathbf{v} \in \mathcal{G}_1 \cap \mathcal{G}_2$ and some $\mathbf{e} \in E_{2,\mathbf{v}}$. The converse implication holds because $\psi_1 = \psi|_{\mathcal{G}_1}$ can be proven to be a ground state of $\mathcal{H}_{\mathbf{V}_{D_1}}$ if $\psi'_{\mathbf{e}}(\mathbf{v}) = 0$ at all cutpoints \mathbf{v} of $\mathcal{G}_1, \mathcal{G}_2$ and all $\mathbf{e} \in E_{2,\mathbf{v}}$. \square

Proposition 6.39 can be used to prove the following lower estimate, which improves Theorem 5.1 on a special class of trees. It bears a certain similarity to the celebrated *Makai inequality* for bounded, simply connected, planar domains.

Theorem 6.40. *Let \mathcal{G} be a metric tree and assume that there is a vertex $\mathbf{v}_c \in \mathcal{G}$ which has same distance from all the (further) vertices of degree 1. Then the lowest eigenvalue $\lambda_1(\mathcal{G}, \mathbf{V}_D)$ admits the lower bound*

$$(6.30) \quad \lambda_1(\mathcal{G}, \mathbf{V}_D) \geq \frac{\pi^2}{4 \text{Inr}(\mathcal{G}; \mathbf{V}_D)^2},$$

where $V_D := \{v \in V \setminus v_c : \deg(v) = 1\}$.

Observe that under the assumptions of Theorem 6.40, Dirichlet conditions are imposed on all but at most one vertices of degree 1.

Proof. Let \mathcal{G} be a metric tree. We first consider the special case that $\deg(v_c) = 1$. If $|V_D| = 1$, then \mathcal{G} is isometrically isomorphic to an interval with mixed Dirichlet/Neumann conditions in the degree 1 vertices and therefore $\lambda_1(\mathcal{G}; V_D) = \frac{\pi^2}{4 \text{Inr}(\mathcal{G}; V_D)^2}$. Next assume that $|V_D| \geq 2$. Let ψ denote a nonnegative eigenfunction corresponding to $\lambda_1(\mathcal{G}; V_D)$. Using induction and the Kirchhoff condition, it can be shown that there exists a path \mathcal{P} in \mathcal{G} connecting the center point v_c and a vertex $v \in V_D$ such that ψ is decreasing along \mathcal{P} . Since $|V_D| \geq 2$, and hence \mathcal{G} is not an interval, \mathcal{P} passes at least one vertex other than v, v_c . Let w denote the unique vertex in $V \setminus V_D$ that is adjacent to v , let \mathcal{G}' denote the graph obtained after removing the edge vw from \mathcal{G} and let $V_{D'} := V_D \setminus \{v\}$. Since ψ is decreasing on the edge vw , we may apply Proposition 6.39 to obtain $\lambda_1(\mathcal{G}; V_D) \geq \lambda_1(\mathcal{G}', V_{D'})$; however, by construction of v_c , $\text{Inr}(\mathcal{G}; V_D) = \text{dist}(v_c, w)$ for all $w \in \mathcal{G}$, whence $\text{Inr}(\mathcal{G}; V_D) = \text{Inr}(\mathcal{G}'; V_{D'})$. Repeating this argument inductively, after a finite number of steps we are reduced to $|V_D| = 1$, which proves the estimate (6.30) for all metric trees with $\deg(v_c) = 1$.

Let us now assume that $\deg(v_c) > 1$. Again let ψ denote a nonnegative eigenfunction corresponding to $\lambda_1(\mathcal{G}; V_D)$. Since ψ satisfies Kirchhoff conditions in v_c , there exists an edge e incident to v_c such that ψ has nonpositive derivative on e at v_c . Now, cutting through the center vertex $d - 1$ times yields d disjoint trees; for each of these, v_c continues to be the center vertex (and in particular each has the same inradius). From these trees, let \mathcal{G}_2 denote the tree containing the edge e and let \mathcal{G}_1 denote its complement in \mathcal{G} , the (restored) union of the other $d - 1$ trees. In \mathcal{G}_1 the center vertex v_c has degree $d - 1$. Setting $V_{D1} := V_D \cap \mathcal{G}_1$ and applying Lemma 6.39 we obtain $\lambda_1(\mathcal{G}; V_D) \geq \lambda_1(\mathcal{G}_1, V_{D1})$. Because the claim is already known to hold whenever $\deg(v_c) = 1$, an induction argument now yields (6.30) for all metric trees. \square

7. M-FUNCTIONS

Titchmarsh-Weyl M-function is proven to be an important tool in the studies of one-dimensional Schrödinger equation [207]. It is usually defined via

$$M(\lambda) = \frac{u'(0)}{u(0)}, \quad \text{Im } \lambda \neq 0,$$

where u is any square integrable solution to the stationary Schrödinger equation

$$-u''(x) + q(x)u(x) = \lambda u(x), \quad x \in [0, \infty).$$

One may think about the point $x = 0$ as the unique boundary point allowing to collect information about solutions of the Schrödinger equation on the half-line. Therefore M-function is an effective tool to solve inverse problems, in particular it can be used to determine the spectral measure.

Introducing M-function for metric graphs one usually picks up few existing vertices, which can be seen as points on \mathcal{G} through which investigation of the metric graph can be carried out.

The corresponding M-function is then a matrix-valued Nevanlinna-Herglotz function (see discussion below) and contains all information on the metric graph \mathcal{G} , which can be obtained by observing solution of the stationary Schrödinger equation on \mathcal{G} at the contact set. It can be seen as energy dependent Dirichlet-to-Neumann map. It has deep connections to the Wigner's reaction R-matrix proposed to model atomic collisions [209].

The goal of this section is to provide a comprehensive introduction into the theory of graph's M-function and illustrate how these functions can be used in graph's surgery and solving inverse problems. The interested readers may consult [142, Chapters 17 and 18].

7.1. Definition of the M-function.

Definition 7.1. A *contact set* $\partial\mathcal{G}$ is any finite subset of vertices in \mathcal{G} . All other vertices in \mathcal{G} are called *internal vertices* and will be denoted by $\partial\mathcal{G}^c$.

The contact set can be chosen arbitrarily, it usually contains all degree 1 vertices and is smaller than the total set of vertices in order to avoid overdetermined problems. For example in the case of single interval, to solve the inverse problem it is enough to have only one of the end points in the contact set. On the other hand, every inner point on an edge can be seen as a degree two vertex and may therefore be a member of the contact set, if necessary.

Definition 7.2. For any $\lambda, \text{Im } \lambda \neq 0$, consider the set of solutions to the equation

$$(7.1) \quad -\psi''(x) = \lambda\psi(x),$$

satisfying:

- standard vertex conditions at all internal vertices $\partial\mathcal{G}^c$,
- (only) continuity conditions at the contact vertices $\partial\mathcal{G}$.

Every such solution is uniquely determined by its values on $\partial\mathcal{G}$. Then the M-function associated with the graph \mathcal{G} and the contact set $\partial\mathcal{G}$ is the $|\partial\mathcal{G}| \times |\partial\mathcal{G}|$ map defined by

$$(7.2) \quad \mathbf{M}(\lambda) : \psi|_{\partial\mathcal{G}} \mapsto \partial\psi|_{\partial\mathcal{G}}.$$

where $\psi|_{\partial\mathcal{G}}$ and $\partial\psi|_{\partial\mathcal{G}}$ are the vectors of function values and sums of normal derivatives values, respectively, taken at the contact points:

$$(7.3) \quad \psi|_{\partial\mathcal{G}} = (\psi(v_j))_{v_j \in \partial\mathcal{G}}, \quad \partial\psi|_{\partial\mathcal{G}} = (\partial\psi(v_j))_{v_j \in \partial\mathcal{G}}.$$

The functions are assumed to be continuous at the contact vertices, therefore the values $\psi(v_j)$ are well-defined. The sum of normal derivatives has already been used in (3.5)

$$\partial u(\mathbf{v}) \equiv \sum_{\mathbf{e} \sim \mathbf{v}} \frac{\partial u_{\mathbf{e}}}{\partial n}(\mathbf{v}).$$

We state without proving few properties of the M-functions:

- Every M-function associated with the graph \mathcal{G} and contact set $\partial\mathcal{G}$ is a *Herglotz-Nevanlinna matrix valued function*, i.e., it is
 - analytic outside the real axis $\lambda \notin \mathbb{R}$;

– with positive imaginary part in the upper half-plane

$$\operatorname{Im} \lambda > 0 \Rightarrow \operatorname{Im} \mathbf{M}(\lambda) := \frac{1}{2i} \left(\mathbf{M}(\lambda) - (\mathbf{M}(\lambda))^* \right) \geq 0;$$

– symmetric with respect to the real axis

$$(\mathbf{M}(\lambda))^* = \mathbf{M}(\bar{\lambda}).$$

- $\mathbf{M}(\lambda)$ originally defined for $\operatorname{Im} \lambda \neq 0$ can be extended to a meromorphic operator-valued function on \mathbb{C} . Each of the singularities is an eigenvalue of the Dirichlet Laplacian on \mathcal{G} – the Laplace operator determined by Dirichlet conditions at the contact vertices $\partial\mathcal{G}$ and standard conditions at the internal vertices $\partial\mathcal{G}^C$.
- Similarly $-\mathbf{M}^{-1}(\lambda)$ is also a matrix-valued Herglotz-Nevalinna function. Each singularity of $-\mathbf{M}^{-1}(\lambda)$ is an eigenvalue of the standard Laplacian on \mathcal{G} – the Laplace operator determined by standard conditions at both contact and internal vertices of \mathcal{G} .

Note that not all eigenvalues of the Dirichlet Laplacian lead to singularities of the M-function. Metric graphs have localised eigenfunctions and their support can be disjoint from the contact set $\partial\mathcal{G}$. Similarly not all eigenvalues of the standard Laplacian lead to singularities of the inverse M-function.

Introducing M-function it is not necessary to require that standard conditions are assumed at all internal vertices $\partial\mathcal{G}^C$ – one may use any Hermitian vertex conditions there.

7.2. Elementary examples. The goal of this subsection is to describe how to obtain M-functions for elementary graphs assuming standard vertex conditions.

Single interval with two contact points. Assume that $\mathcal{G}_1 = [0, \ell]$ is the graph formed by one edge, its end-points forming two vertices $v_1 = \{0\}$ and $v_2 = \{\ell\}$. We assume in addition that the contact set contains both vertices $\partial\mathcal{G} = \{v_1, v_2\}$.

To calculate the M-function we determine first all solutions to the differential equation

$$\begin{aligned} -\psi''(x) &= \underbrace{\lambda}_{=k^2} \psi \\ \Rightarrow \psi(x) &= a_1 e^{ikx} + a_2 e^{-ik(x-\ell)}, \quad a_1, a_2 \in \mathbb{C}. \end{aligned}$$

This solution can be expressed using its values at the end-points as

$$\psi(x) = \frac{i}{2 \sin k\ell} \left((e^{-ik\ell} \psi(0) - \psi(\ell)) e^{ikx} + (-\psi(0) + e^{-ik\ell} \psi(\ell)) e^{-ik(x-\ell)} \right).$$

The normal derivatives at the end-points are:

$$\begin{aligned} \partial\psi(v_1) &= \psi'(0) = -k \cot k\ell \psi(0) + \frac{k}{\sin k\ell} \psi(\ell), \\ \partial\psi(v_2) &= -\psi'(\ell) = \frac{k}{\sin k\ell} \psi(0) - k \cot k\ell \psi(\ell). \end{aligned}$$

Taking into account that

$$\psi(v_1) = \psi(0), \quad \psi(v_2) = \psi(\ell),$$

we get the M-function

$$(7.4) \quad \mathbf{M}_{\mathcal{G}_1}(\lambda) = \begin{pmatrix} -k \cot k\ell & \frac{k}{\sin k\ell} \\ \frac{k}{\sin k\ell} & -k \cot k\ell \end{pmatrix}.$$

It is easy to see that the function has singularities at the zeroes of $\sin k\ell$ – the spectrum of the Dirichlet operator on the interval of length ℓ .

Single interval with one contact point. Consider the same graph \mathcal{G}_1 , but choose the contact set consisting of just one vertex, say $\partial\mathcal{G} = \{v_1\}$ ($\partial\mathcal{G}^C = v_2$).

To determine the M-function we need to look at the solution of the same differential equation satisfying standard, i.e., Neumann, condition at $x = \ell$. Such solution is unique up to a multiplicative constant:

$$\psi(x) = \cos k(x - \ell).$$

The formula determining the M-function coincides with the classical formula used by Weyl:

$$\mathbf{M}_{\mathcal{G}_1}(\lambda) = \frac{\psi'(0)}{\psi(0)} = \frac{-k \sin k(0 - \ell)}{\cos k(0 - \ell)} = k \tan k\ell.$$

This formula differs from the formula in the first example since we have a different contact set and the M-function is a scalar-valued function.

The singularities coincide with the spectrum of the Laplacian on the interval $[0, \ell]$ with Dirichlet condition at $x = 0$ and Neumann condition at $x = \ell$.

Lasso graph with one contact point. Consider the lasso graph \mathcal{G}_2 formed by the loop of length ℓ and handle of length s . Assume that the contact set is formed by the single degree 1 vertex. Writing general solutions of the differential equations on the edges and taking into account standard vertex conditions at the central vertex one easily calculates the M-function

$$M_{\mathcal{G}_2}(\lambda) = k \frac{\cos \frac{k\ell}{2} \sin ks + 2 \sin \frac{k\ell}{2} \cos ks}{\cos \frac{k\ell}{2} \cos ks - 2 \sin \frac{k\ell}{2} \sin ks}.$$

Independently of the value of s , the Laplacian on \mathcal{G}_2 has eigenvalues $(\frac{2\pi}{\ell})^2$ corresponding to the eigenfunctions supported by the loop and identically equal to zero on the handle. These eigenfunctions are not seen from the contact vertex and therefore do not cause any singularities in the M-function.

7.3. Explicit formulas for the M-function. We have seen that singularities of the M-function and its inverse are always connected with the eigenvalues of the following two Laplacians on \mathcal{G} :

- the Dirichlet Laplacian $-\Delta^D(\mathcal{G})$ determined by Dirichlet conditions on $\partial\mathcal{G}$ and standard conditions at the inner vertices $\partial\mathcal{G}^C$;
- the standard Laplacian $-\Delta^{\text{st}}(\mathcal{G})$ determined by standard conditions at all vertices.

Let us denote by λ_n^D, ψ_n^D and $\lambda_n^{\text{st}}, \psi_n^{\text{st}}$, $n = 1, 2, \dots$, the eigenvalues and the normalised (in the $L_2(\mathcal{G})$) eigenfunctions of the Dirichlet and standard Laplacians, respectively. Then the following two explicit formulas for the M-functions hold [142, 147, 138]:

$$(7.5) \quad \mathbf{M}_{\mathcal{G}}(\lambda) = - \left(\sum_{n=1}^{\infty} \frac{\langle \psi_n^{\text{st}} |_{\partial\mathcal{G}}, \cdot \rangle_{\ell_2(\partial\mathcal{G})} \psi_n^{\text{st}} |_{\partial\mathcal{G}}}{\lambda_n^{\text{st}} - \lambda} \right)^{-1},$$

and

$$(7.6) \quad \mathbf{M}_{\mathcal{G}}(\lambda) - \mathbf{M}_{\mathcal{G}}(\lambda') = \sum_{n=1}^{\infty} \frac{\lambda - \lambda'}{(\lambda_n^D - \lambda)(\lambda_n^D - \lambda')} \langle \partial\psi_n^D |_{\partial\mathcal{G}}, \cdot \rangle_{\ell_2(\partial\mathcal{G})} \partial\psi_n^D |_{\partial\mathcal{G}}.$$

Here $\psi_n |_{\partial\mathcal{G}}$ and $\partial\psi_n |_{\partial\mathcal{G}}$ as in the definition of the M-function denote the vectors formed by the values of the eigenfunctions and by the sums of normal derivatives of the eigenfunctions at the contact vertices, respectively.

The first formula can be written as

$$-(\mathbf{M}_{\mathcal{G}}(\lambda))^{-1} = \sum_{n=1}^{\infty} \frac{\langle \psi_n^{\text{st}} |_{\partial\mathcal{G}}, \cdot \rangle_{\ell_2(\partial\mathcal{G})} \psi_n^{\text{st}} |_{\partial\mathcal{G}}}{\lambda_n^{\text{st}} - \lambda}.$$

It determines the M-function uniquely. It is clear that the singularities of $-\mathbf{M}_{\mathcal{G}}^{-1}(\lambda)$ coincide with those eigenvalues of $-\Delta_{\mathcal{G}}^{\text{st}}$ for which the traces of the eigenfunctions $\psi_n^{\text{st}} |_{\partial\mathcal{G}}$ are not identically zero. These singularities are often called *generalised zeroes* of $\mathbf{M}_{\mathcal{G}}(\lambda)$. They are not zeroes of the M-function as it might happen that no vector \vec{b} exists such that $\mathbf{M}_{\mathcal{G}}(\lambda_n^{\text{st}}) \vec{b} = 0$.

The second formula does not determine the M-function uniquely – to recover $\mathbf{M}_{\mathcal{G}}(\lambda)$ it is necessary to know $\mathbf{M}_{\mathcal{G}}(\lambda')$ – the value of $\mathbf{M}_{\mathcal{G}}$ at any non-singular reference point λ' . Nevertheless the singularities of the M-function are uniquely determined – they coincide with those eigenvalues of $-\Delta_{\mathcal{G}}^D$ for which the normal derivatives of the eigenfunctions $\partial\psi_n^{\text{st}} |_{\partial\mathcal{G}}$ are not identically zero.

These formulas not only explain in details the relation between the eigenvalues of the two Laplacians on \mathcal{G} (the operators $-\Delta_{\mathcal{G}}^D$ and $-\Delta_{\mathcal{G}}^{\text{st}}$) and the singularities and generalised zeroes of $\mathbf{M}_{\mathcal{G}}(\lambda)$, but provide a clear interpretation for Wigner's formulas. In [209] it was suggested to look at scalar functions of the form:

$$R(E) = \sum_{\mu} \frac{\gamma_{\mu}^2}{E_{\mu} - E}.$$

Resemblance with formula (7.5) is striking. The main difference is that our formula not only extends Wigner's class to matrix-valued functions, but provides clear interpretation of the weights γ_{μ}^2 as traces of the eigenfunctions.

Moreover, formula (7.6) can be re-written as

$$(7.7) \quad \mathbf{M}_{\mathcal{G}}(\lambda) = \mathbf{M}_{\mathcal{G}}(\lambda') + \sum_{n=1}^{\infty} \left(\frac{\langle \partial\psi_n^D |_{\partial\mathcal{G}}, \cdot \rangle_{\ell_2(\partial\mathcal{G})} \partial\psi_n^D |_{\partial\mathcal{G}}}{\lambda_n^D - \lambda} - \frac{\langle \partial\psi_n^D |_{\partial\mathcal{G}}, \cdot \rangle_{\ell_2(\partial\mathcal{G})} \partial\psi_n^D |_{\partial\mathcal{G}}}{\lambda_n^D - \lambda'} \right),$$

which reminds of Wigner's formula

$$R(z) = \alpha z + \beta + \sum_{\mu} \left(\frac{\gamma_{\mu}^2}{Z_{\mu} - z} - \frac{\gamma_{\mu}^2}{Z_{\mu}} \right).$$

The two formulas coincide in the scalar case if one puts $\lambda' = 0$ and assumes that the linear terms is absent $\alpha = 0$.

It is worth to mention that formulas (7.5) and (7.6) are not specific for Laplacians on metric graphs. Similar formulas can be obtained considering two self-adjoint extensions of a symmetric operator with equal finite (or even infinite) deficiency indices using for example the language of boundary triples [35]. To get analogs of formula (7.6) with the linear term present it is enough to consider extensions which are self-adjoint operator relations (instead of self-adjoint operators) or fractional transformations of the M-functions.

7.4. M-function and spectral estimates. Let us discuss how M-functions can be used to obtain spectral estimates and analyse behaviour of the spectrum and of the spectral gap in particular under surgery transformations.

7.4.1. M-function and spectra of Dirichlet and standard Laplacians. Formulas (7.5) and (7.6) suggest to divide spectra of the operators $-\Delta_{\mathcal{G}}^{\text{D}}$ and $-\Delta_{\mathcal{G}}^{\text{st}}$ (only discrete eigenvalues are present) into visible and invisible eigenvalues. Invisible eigenvalues are common eigenvalues for these two operators with the eigenfunctions satisfying both Dirichlet and standard conditions at the contact points. These eigenvalues give no contribution into formulas (7.5) and (7.6). These eigenvalues do not change when two graphs are glued together and are relatively easy to take care of. Therefore in what follows we shall often assume that all eigenvalues are visible, i.e., the corresponding eigenfunctions satisfy just one set of vertex conditions on the contact set and therefore determine singularities and generalised zeroes of the M-function.

Let us introduce the *signed eigenvalue counting function*

$$(7.8) \quad N_{\mathcal{G}}(\lambda) := \#\left\{\lambda_n^{\text{st}} : \lambda_n^{\text{st}} \leq \lambda\right\} - \#\left\{\lambda_n^{\text{D}} : \lambda_n^{\text{D}} \leq \lambda\right\}.$$

This function is right continuous by definition. The function is identically equal to zero for $\lambda < 0$ and is positive for $\lambda \geq 0$, since $\lambda = 0$ is an eigenvalue of the standard Laplacian and inequality $\lambda_n^{\text{D}} \geq \lambda_n^{\text{st}}$ follows from Rayleigh quotient and the fact that the domain of the quadratic form for $-\Delta_{\mathcal{G}}^{\text{st}}$ is strictly larger than the domain of the quadratic form for $-\Delta_{\mathcal{G}}^{\text{D}}$.

The eigenvalue counting function satisfies the upper estimate

$$N_{\mathcal{G}}(\lambda) \leq |\partial\mathcal{G}|,$$

since $-\Delta_{\mathcal{G}}^{\text{D}}$ and $-\Delta_{\mathcal{G}}^{\text{st}}$ are two self-adjoint extensions of the symmetric operator obtained by restricting these two operators to their common domain – the set of functions from $H^2(\mathcal{G})$ satisfying both Dirichlet and standard conditions on $\partial\mathcal{G}$ and just standard conditions at all inner vertices. This symmetric operator has equal deficiency indices $|\partial\mathcal{G}|$, hence the number of eigenvalues on each interval may differ by at most $|\partial\mathcal{G}|$.

Precise value of the eigenvalue counting function is determined by the number n^+ of positive eigenvalues in the matrix $\mathbf{M}_{\mathcal{G}}(\lambda)$:

$$(7.9) \quad N_{\mathcal{G}}(\lambda) = n^+(\mathbf{M}_{\mathcal{G}}(\lambda)) := \#\left\{\mu_m : \mathbf{M}_{\mathcal{G}}(\lambda)\mathbf{f}_m = \mu_m\mathbf{f}_m, \mu_m \geq 0\right\}, \quad \lambda \neq \lambda_n^{\text{D}}.$$

To prove this formula one may look at the energy curves $\mu_m(\lambda)$, $m = 1, 2, \dots, |\partial\mathcal{G}|$ for the M-matrix. These eigenvalues are nothing else than Steklov eigenvalues for the problem associated with \mathcal{G} and its contact set $\partial\mathcal{G}$. These curves have singularities only at the eigenvalues of $L_{\mathcal{G}}^{\text{D}}$ as can be seen from formula (7.6). The number of curves tending to $+\infty$ when approaching certain λ_0 from the left is equal to the multiplicity of λ_0 as an eigenvalue of $L_{\mathcal{G}}^{\text{D}}$. These curves come back from $-\infty$ to the right of the singularities. All other energy curves are continuous at these points.

Between the singularities all curves are continuous monotonically increasing functions of $\lambda \in \mathbb{R}$. Note that we do not claim that the curves are given by analytic functions, also it is often the case. The analyticity of $\mu_j(\lambda)$ may be broken when two curves intersect each other, i.e., when $\mathbf{M}_{\mathcal{G}}(\lambda)$ has multiple eigenvalues. The eigenvalues of the standard Laplacian are precisely those values of λ for which one of the energy curves crosses the line $\mu = 0$. For negative values of λ the M-function is strictly negative as can be seen from formula (7.5) taking into account that all λ_n^{st} are non-negative. Therefore if no Dirichlet eigenvalues λ_n^{D} are involved then the number of times the energy curves cross the zero line to the left of λ coincides with the number of positive eigenvalues of $\mathbf{M}_{\mathcal{G}}(\lambda)$. For every simple Dirichlet eigenvalue one energy curve disappears to $+\infty$ and $\mathbf{M}_{\mathcal{G}}$ gains an extra negative eigenvalue. Similarly Dirichlet eigenvalues of higher multiplicity lower the number of positive Steklov eigenvalues accordingly.

Formula (7.9) can be used to determine the number of the eigenvalues of the standard Laplacian to the left of λ

$$(7.10) \quad \#\left\{\lambda_n^{\text{st}} : \lambda_n^{\text{st}} \leq \lambda\right\} = \#\left\{\lambda_n^{\text{D}} : \lambda_n^{\text{D}} \leq \lambda\right\} + \#\left\{\mu_m : \mathbf{M}_{\mathcal{G}}(\lambda)\mathbf{f}_m = \mu_m\mathbf{f}_m, \mu_m \geq 0\right\}.$$

This formula is proven under the assumption that no invisible eigenvalues occur, but existence of such eigenvalues does not destroy the formula as they contribute equally to the left and right hand sides.

7.4.2. Gluing graphs and the spectral gap. Let us discuss behaviour of the spectral gap when two graphs $\mathcal{G}_1 = (\mathbf{E}_1, \mathbf{V}_1)$ and $\mathcal{G}_2 = (\mathbf{E}_2, \mathbf{V}_2)$ are glued together. Without loss of generality we may assume that the corresponding contact sets $\partial\mathcal{G}_1$ and $\partial\mathcal{G}_2$ have equal sizes $|\partial\mathcal{G}_1| = |\partial\mathcal{G}_2|$. The new glued graph $\mathcal{G} = (\mathbf{E}, \mathbf{V})$ is obtained by taking the union of the edge sets $\mathbf{E} = \mathbf{E}_1 \cup \mathbf{E}_2$, identifying vertices from the two contact sets $\partial\mathcal{G}_1 = \partial\mathcal{G}_2$ and keeping all internal vertices coming from the original graphs: $\mathbf{V} = \mathbf{V}_1 \cup \mathbf{V}_2$. The standard Laplacian on \mathcal{G} is obtained by imposing standard vertex conditions at the contact vertices $\partial\mathcal{G} = \partial\mathcal{G}_1 \equiv \partial\mathcal{G}_2$.

Let \mathbf{M}_1 and \mathbf{M}_2 be the two M-functions associated with the contact sets $\partial\mathcal{G}_1$ and $\partial\mathcal{G}_2$ respectively. Then the M-function for \mathcal{G} with the contact set $\partial\mathcal{G}$ is equal to the sum of M-functions

$$(7.11) \quad \mathbf{M}(\lambda) = \mathbf{M}_1(\lambda) + \mathbf{M}_2(\lambda).$$

This formula holds since we assume standard conditions at the vertices where \mathcal{G}_1 and \mathcal{G}_2 are joined together.

The lowest standard and Dirichlet eigenvalues on metric graphs are always visible from the corresponding M-functions. The eigenfunctions corresponding to the lowest eigenvalues of the standard and Dirichlet Laplacians on every (connected) \mathcal{G} can be chosen strictly positive [139], i.e., positive except at those vertices, where Dirichlet conditions are assumed. As a result the traces at $\partial\mathcal{G}$ of the ground state eigenfunctions for $-\Delta_{\mathcal{G}}^{\text{st}}$ are all non-zero, as well as the sums of normal derivatives for the ground state of $-\Delta_{\mathcal{G}}^{\text{D}}$. In particular the points λ_1^{D} are always singular points for $\mathbf{M}_{\mathcal{G}}(\lambda)$. The point $\lambda_1 = 0$ is the lowest eigenvalue of $-\Delta_{\mathcal{G}}$ and a solution of the secular equation

$$\det \mathbf{M}(\lambda) = 0,$$

since $\mathbf{M}(0)\mathbf{1} = 0$ and $\lambda = 0$ is a regular point since all Dirichlet eigenvalues λ_n^{D} are strictly positive.

What can be said about the new M-function in terms of the M-functions for the parts glued together?

- Every singularity of each of $\mathbf{M}_j(\lambda)$, $j = 1, 2$, is also a singularity of $\mathbf{M}(\lambda)$ since every Dirichlet eigenfunction on \mathcal{G} is also a Dirichlet eigenfunction on at least of one of \mathcal{G}_j .
- The eigenvalues of $-\Delta_{\mathcal{G}}$ lying below the ground states of the Dirichlet Laplacians $-\Delta_{\mathcal{G}_j}^{\text{D}}$, $j = 1, 2$, are always visible in $\mathbf{M}_{\mathcal{G}}(\lambda)$. This follows from the fact every such $\lambda_n^{\text{st}}(\mathcal{G})$ is a regular point for $\mathbf{M}_{\mathcal{G}}(\lambda)$ and any eigenfunction with zero trace on $\partial\mathcal{G}$ leads to a Dirichlet eigenfunction on one of \mathcal{G}_j .
- Provided the ground states of the Dirichlet Laplacians on \mathcal{G}_j are different, $\lambda_1^{\text{D}}(\mathcal{G}_1) \neq \lambda_1^{\text{D}}(\mathcal{G}_2)$, the spectral gap for $-\Delta_{\mathcal{G}}$ cannot exceed $\lambda_M := \max\{\lambda_1^{\text{D}}(\mathcal{G}_1), \lambda_1^{\text{D}}(\mathcal{G}_2)\}$. This follows from the elementary estimates:

$$\begin{aligned} 0 \leq N_{\mathcal{G}}(\mu) &= \#\{\lambda_n^{\text{st}} : \lambda_n^{\text{st}} \leq \lambda_M\} - \underbrace{\#\{\lambda_n^{\text{D}} : \lambda_n^{\text{D}} \leq \lambda_M\}}_{\geq 2} \\ &\Rightarrow \#\{\lambda_n^{\text{st}} : \lambda_n^{\text{st}} \leq \lambda_M\} \geq 2. \end{aligned}$$

- The spectral gap for $-\Delta_{\mathcal{G}}$ is less than $\lambda_m := \min\{\lambda_1^{\text{D}}(\mathcal{G}_1), \lambda_1^{\text{D}}(\mathcal{G}_2)\}$ if and only if $\mathbf{M}_{\mathcal{G}}$ has at least two positive eigenvalues immediately to the left of μ . For sufficiently small $\epsilon > 0$ we have

$$n^+(\mathbf{M}_{\mathcal{G}}(\lambda_m - \epsilon)) = N_{\mathcal{G}}(\lambda_m - \epsilon) = \underbrace{\#\{\lambda_n^{\text{st}} : \lambda_n^{\text{st}} \leq \lambda_m - \epsilon\}}_{\geq 2} - \underbrace{\#\{\lambda_n^{\text{D}} : \lambda_n^{\text{D}} \leq \lambda_m - \epsilon\}}_{= 0} \geq 2.$$

When two graphs are glued together, then the new graph has larger total length and therefore it is natural to expect that the spectral gap is going to decrease. Already gluing two intervals of different lengths $\ell_1 < \ell_2$ into a circle graph of length $\ell_1 + \ell_2$, one observes that the spectral gap

increases from $\left(\frac{\pi}{\ell_2}\right)^2$ to $\left(\frac{2\pi}{\ell_1+\ell_2}\right)^2 < \left(\frac{\pi}{\ell_2}\right)^2$ [144]. In general situation behaviour of the spectral gap depends on the number n^+ of positive eigenvalues of the M-function at the spectral gap of one of \mathcal{G}_j . Note that it is not enough to know the number of positive Steklov eigenvalues for the original two graphs. We finish this section by providing complete characterization when does the spectral gap increases gluing arbitrary metric graphs.

Theorem 7.3. *The spectral gap for the standard Laplacian does not decrease when two graphs \mathcal{G}_1 and \mathcal{G}_2 are glued together into \mathcal{G}*

$$(7.12) \quad \lambda_2(\mathcal{G}) \geq \min_j \{\lambda_2(\mathcal{G}_j)\},$$

if and only if the M-function for \mathcal{G} has the following number of positive eigenvalues:

$$(1) \min_j \{\lambda_2(\mathcal{G}_j)\} \leq \min_j \{\lambda_1^D(\mathcal{G}_j)\} \text{ and}$$

$$\lim_{\epsilon \searrow 0} n^+ \left(\mathbf{M}_{\mathcal{G}}(\min_j \{\lambda_2(\mathcal{G}_j)\} - \epsilon) \right) = 1;$$

$$(2) \min_j \{\lambda_1^D(\mathcal{G}_j)\} < \min_j \{\lambda_2(\mathcal{G}_j)\} < \max_j \{\lambda_1^D(\mathcal{G}_j)\} \text{ and}$$

$$\lim_{\epsilon \searrow 0} n^+ \left(\mathbf{M}_{\mathcal{G}}(\min_j \{\lambda_2(\mathcal{G}_j)\} - \epsilon) \right) = 0;$$

$$(3) \lambda_1^D(\mathcal{G}_1) = \lambda_1^D(\mathcal{G}_2) = \min_j \{\lambda_2(\mathcal{G}_j)\} \text{ and}$$

$$\lim_{\epsilon \searrow 0} n^+ \left(\mathbf{M}_{\mathcal{G}}(\min_j \{\lambda_2(\mathcal{G}_j)\} - \epsilon) \right) = 1.$$

It is surprising that the result is determined by the number of positive eigenvalues of $\mathbf{M}_{\mathcal{G}}$ and is independent of the properties of the eigenvectors. This property can be traced back to [36], where the number of negative eigenvalues for the Laplacian with general vertex conditions was calculated.

We do not have enough space to discuss solution of the inverse problems starting with M-functions. This approach is well-developed in Chapters 14-15 and 19-23 of [142]. Only in the case of trees (graphs without cycles) the M-function associated with all degree 1 vertices determines the metric graph, potential on the edges and vertex conditions (under mild additional assumptions) [18, 19] and [142, Chapter 20]. To solve the inverse problem for graphs with cycles one may use *magnetic boundary control* – spectral data depending on the magnetic fluxes through the cycles. This approach has been developed in [136, 143, 137] and [142, Chapters 22 and 23].

7.5. M-function and isospectrality. M-functions can be successfully used to explain isospectrality of some pairs of metric graphs. Some of these graphs are known from the spectral theory of discrete Laplacians, but new families can be constructed, leading in particular to new families of discrete graphs. We present here the main ideas, interested readers may consult our recent paper [145].

Definition 7.4. Two metric graphs \mathcal{G}_1 and \mathcal{G}_2 with contact sets $\partial\mathcal{G}_1$ and $\partial\mathcal{G}_2$, respectively, are called *Steklov-equivalent* if and only if the corresponding M-functions coincide: $\mathbf{M}_{\mathcal{G}_1}(\lambda) = \mathbf{M}_{\mathcal{G}_2}(\lambda)$.

It is clear that two Steklov-equivalent graphs are isospectral, the opposite implication does not always hold.

We start with two elementary observations:

- Let \mathcal{G}_1 and \mathcal{G}_2 be two Steklov-equivalent graphs, then gluing them to the same metric graph \mathcal{K} yields a new pair of isospectral graphs.
- Let the metric graph \mathcal{G} contain two Steklov-equivalent subgraphs \mathcal{G}_1 and \mathcal{G}_2 , then exchanging the subgraphs we obtain a graph \mathcal{G}' isospectral to the original graph \mathcal{G} .

The following two methods used procedure, which we call *swapping Steklov subspaces*

Theorem 7.5. Let \mathcal{K} be a metric graph with a degenerate Steklov eigenvalue $\mu(\lambda)$ with the eigensubspace $V(\lambda)$, $\dim V(\lambda) > 1$. Let \mathcal{Q}_i , $i = 1, 2$, be two isospectral metric graphs such that

$$\begin{aligned} \mathbf{M}_{\mathcal{Q}_1}(\lambda)|_{V(\lambda)} &\stackrel{\text{unitarily}}{\sim} \mathbf{M}_{\mathcal{Q}_2}(\lambda)|_{V(\lambda)}, \\ \mathbf{M}_{\mathcal{Q}_1}(\lambda)|_{V(\lambda)^\perp} &= \mathbf{M}_{\mathcal{Q}_2}(\lambda)|_{V(\lambda)^\perp}. \end{aligned}$$

Then the graphs obtained by gluing together \mathcal{K} and \mathcal{Q}_i , $i = 1, 2$, are isospectral.

The theorem can be proven by just noting that the corresponding eigenfunctions can be chosen equal on the *common* graph \mathcal{K} . An example of isospectral graphs constructed using this approach is presented in Fig. 21.

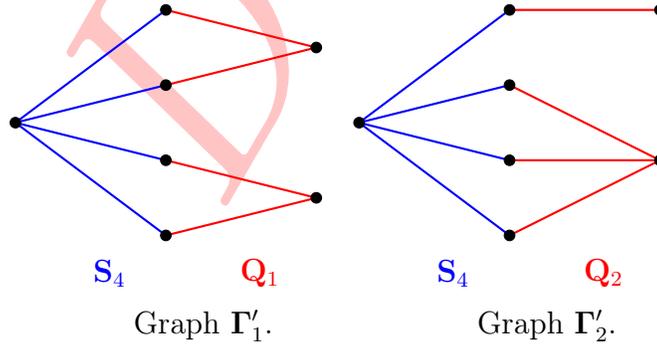


FIGURE 21. Two isospectral graphs extending \mathbf{S}_4 .

This example can be simplified as follows.

One may slightly modify the proposed method as.

Theorem 7.6. Let $(\mathcal{K}_1, \mathcal{K}_2)$ and $(\mathcal{Q}_1, \mathcal{Q}_2)$ be two pairs of graphs with the same number of contact points and each pair having unitarily equivalent M-functions, that is

$$(7.13) \quad \mathbf{M}_{\mathcal{K}_1}(\lambda) \stackrel{\text{unitarily}}{\sim} \mathbf{M}_{\mathcal{K}_2}(\lambda), \quad \mathbf{M}_{\mathcal{Q}_1}(\lambda) \stackrel{\text{unitarily}}{\sim} \mathbf{M}_{\mathcal{Q}_2}(\lambda).$$

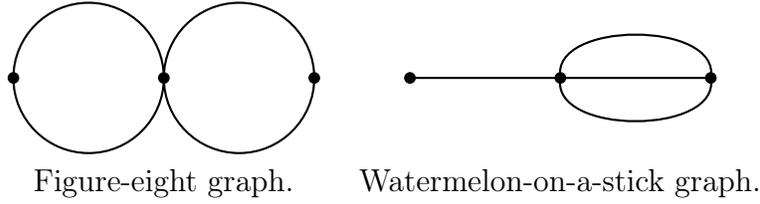


FIGURE 22. The simplest pair of isospectral metric graphs.

Let us denote by $\mu_s^{\mathcal{K}_1}(\lambda) = \mu_s^{\mathcal{K}_2}(\lambda)$ and $\mu_s^{\mathcal{Q}_1}(\lambda) = \mu_s^{\mathcal{Q}_2}(\lambda)$ the Steklov eigenvalues. Assume that for each i and s the eigenspaces for $\mathbf{M}_{\mathcal{K}_i}(\lambda)$ and $\mathbf{M}_{\mathcal{Q}_i}(\lambda)$ can be chosen equal,

$$V_s^{\mathcal{K}_i}(\lambda) = V_s^{\mathcal{Q}_i}(\lambda), \quad s = 1, 2, \dots, S, \quad i = 1, 2.$$

If in addition the graphs $\mathcal{K}_1 \cup \mathcal{Q}_1$ and $\mathcal{K}_2 \cup \mathcal{Q}_2$ (as disjoint unions) are isospectral, then the graphs \mathcal{G}_1 and \mathcal{G}_2 obtained by gluing together \mathcal{K}_i and \mathcal{Q}_i for the respective values of $i = 1, 2$ are also isospectral.

Combining the two observations and two methods formulated above one may construct broad families of isospectral graphs. These families extend existing approaches to construct isospectral graphs such as

- Seidel switching formulated and analysed in [199, 61, 64];
- Butler–Grout construction from [64, 155, 169].

It seems that proposed approach is an alternative to Sunada construction and its different modifications [204, 61, 105, 27, 181, 23].

8. GENERALIZATIONS, APPLICATIONS AND FURTHER TOPICS

8.1. Geometry of eigenfunctions: nodal domains and hot spots. Much less is known about the Laplacian eigenfunctions than the eigenvalues. In analogy with the Euclidean case, two problems of interest are:

- (1) Count the number of *nodal domains* of a k -th eigenfunction ψ_k , that is, the connected components of

$$\{x \in \mathcal{G} : \psi_k(x) \neq 0\};$$

- (2) Study the *hot and cold spots*, that is, the number and location of local and global maxima and minima of the eigenfunction, in particular in the case $k = 2$.

Problem (1) has been extensively studied on metric graphs, usually under the assumption that every eigenvalue is simple and no eigenfunction vanishes on any (non-dummy) vertex, assumptions which are known to be generic (that is, given a fixed graph topology, different from a loop, the set of all edge lengths for which these assertions hold is of the second Baire category in \mathbb{R}_+^V). It has been known for many years that under these assumptions the k -th eigenfunction of the standard Laplacian has between $k - \beta$ and k nodal domains [40], and in recent years attention has been devoted to studying the distribution of the so-called *nodal deficit*, the difference between the number of nodal domains of ψ_k and k , see [8, 9]. What can

happen in the non-generic case where eigenfunctions may vanish at the vertices was studied in [111]. One may also consider *Neumann domains*, which are, roughly speaking, the connected components of $\{x \in \mathcal{G} : \psi'_k(x) \neq 0\}$ [7, 10].

Problem (2) is inspired in part by the *hot spots conjecture* of Rauch for the Neumann Laplacian on domains, see [63, 116, 123, 203], which asks when the maximum and minimum values of any second Neumann Laplacian eigenfunction on a domain $\Omega \subset \mathbb{R}^d$ are located on $\partial\Omega$. On graphs \mathcal{G} , natural questions are how many maxima and minima the eigenfunction can have, and, more nebulously, how these can be distributed throughout \mathcal{G} . Relatively little is known, see [121, 122]. In particular, it is an open problem to show that, generically (in the same sense as above), the second eigenfunction has exactly one global maximum and one global minimum.

8.2. Spectral correspondence with difference operators. We have already seen a way of computing the spectrum of $\Delta_{\mathcal{G}}$ in terms of the zeros of a polynomial in Section 4.3. There is another, older way of associating the eigenvalues of $\Delta_{\mathcal{G}}$ with the characteristic polynomial of a finite-dimensional operator that can be interpreted as a discrete Laplace-type matrix on the combinatorial graph underlying \mathcal{G} . The following is the main result in [37]. To formulate it, we will need to introduce the normalized Laplacian $\mathcal{L}_{\text{norm}}^{\mathcal{G}}$ of the combinatorial graph underlying \mathcal{G} : it is given by

$$\mathcal{L}_{\text{norm}}^{\mathcal{G}} f(\mathbf{v}) := \frac{1}{\deg^{[\ell]}(\mathbf{v})} \sum_{\mathbf{w} \sim \mathbf{v}} \frac{f(\mathbf{v}) - f(\mathbf{w})}{\ell_e}$$

where $\deg^{[\ell]}$ is the metric degree defined by

$$\deg^{[\ell]}(\mathbf{v}) := \sum_{e \in E_{\mathbf{v}}} \ell_e$$

Observe that if \mathcal{G} is equilateral, then $\mathcal{L}_{\text{norm}}^{\mathcal{G}} = \text{Id}_{\mathbf{V}} - \mathcal{D}^{-1} \mathcal{A}_{\mathcal{G}}$, where $\mathcal{D}_{\mathcal{G}}$ is the diagonal matrix whose entries are the vertex degrees and $\mathcal{A}_{\mathcal{G}}$.

Theorem 8.1. *Let \mathcal{G} be an equilateral metric graph, with underlying combinatorial graph \mathcal{G} . Let us denote by κ the number of its connected components and by κ_b the number of its connected components that are additionally bipartite.*

If u is an eigenvector of $-\Delta_{\mathcal{G}}$ with associated eigenvalue $\lambda > 0$, then the corresponding vector $u|_{\mathbf{V}} \in \mathbb{C}^{\mathbf{V}}$ of vertex evaluations is a (right) eigenvector of the normalized Laplacian $\mathcal{L}_{\text{norm}}^{\mathcal{G}}$: more precisely,

$$(8.1) \quad \mathcal{L}_{\mathcal{G}} u|_{\mathbf{V}} = (1 - \cos \sqrt{\lambda}) u|_{\mathbf{V}}.$$

Conversely, if $1 - \cos \sqrt{\lambda} > 0$ is an eigenvalue of $\mathcal{L}_{\mathcal{G}}$ of multiplicity $\text{mult}(\cos \sqrt{\lambda})$ and $u|_{\mathbf{V}}$ is an associated eigenvector, then λ is an eigenvalue of $-\Delta_{\mathcal{G}}$ and $u|_{\mathbf{V}}$ is the vector of node values

of some eigenvector associated with the eigenvalue λ . The multiplicities are

$$\text{mult}(\lambda) = \begin{cases} \kappa & \text{if } \lambda = 0, \\ \text{mult}(1 - \cos \sqrt{\lambda}) & \text{if } \sin \sqrt{\lambda} \neq 0, \\ |E| - |V| + 2\kappa & \text{if } \cos \sqrt{\lambda} = 1, \lambda > 0, \\ |E| - |V| + 2\kappa_b & \text{if } \cos \sqrt{\lambda} = -1, \lambda > 0. \end{cases}$$

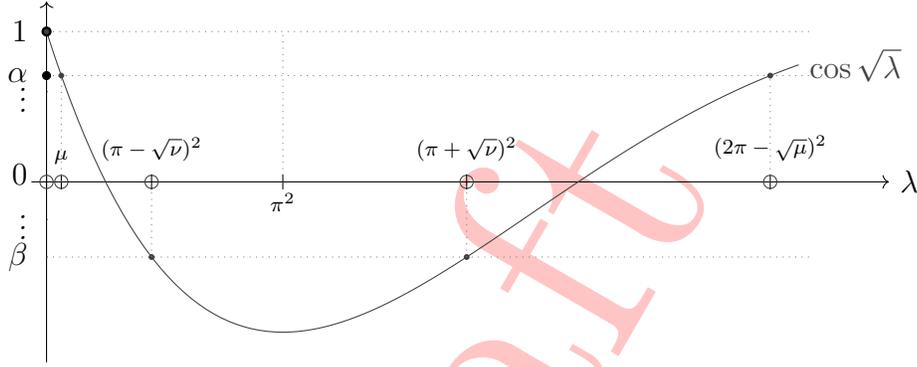


FIGURE 23. On the abscissa, the eigenvalues of $-\Delta_{\mathcal{G}}$ are plotted in correspondence with the associated eigenvalues of \mathcal{T} on the ordinate axis.

In other words,

$$\mu_2(\mathcal{G}) = \arccos(1 - \mu_2(\mathbf{G}))^2$$

if $\mu_2(\mathbf{G}) \in [0, 2)$, where $\mu_2(\mathcal{G})$ denotes the lowest positive eigenvalue of $\mathcal{L}_{\text{norm}}^{\mathcal{G}}$.

Similar results have been recovered in [175] (whenever standard conditions are replaced by Dirichlet conditions in some nodes), [38] (where anti-Kirchhoff conditions are considered), in [75, 180, 153] (for infinite metric graphs), and [74, Section 3 and Section 4] (for Schrödinger operators with nonzero potential).

In the case of non-equilateral graphs, it is easy to see that the relation (8.1) cannot generally hold. However, the following *inequality* has been obtained in [125] and later extended to all k in [184, Corollary 2.2].

Proposition 8.2. *Let \mathcal{G} be connected and such that the underlying combinatorial graph is simple, i.e., it contains no loops and no parallel edges. Then*

$$\mu_k(\Delta_{\mathcal{G}}) \leq \frac{\pi^2}{2} \mu_k(\mathcal{L}_{\mathcal{G}}) \quad \text{for all } k = 1, \dots, |V|.$$

A smart application of these spectral correspondence principles has allowed for estimates on $\mu_2(\mathcal{G})$ based on the lowest positive eigenvalue of the discrete Laplacian on an appropriate graph: a prototypical case is presented in [14], where good use is made of spectral upper estimates on

the underlying combinatorial graph \mathbf{G} . These estimates have been further developed in [184], where the bounds

$$\mu_k(\mathcal{G}) \leq C \frac{d_{\max}^{[\ell]}(g+k)}{\ell_{\min}^2 |\mathcal{G}|} \quad \text{and} \quad \mu_k(\mathcal{G}) \leq C \frac{d_{\max}(\beta+k-1)(g+k)}{|\mathcal{G}|^2}$$

(respectively for small and large k), in terms of the genus g of \mathbf{G} and the (metric) degree $\deg^{[\ell]}$ have been deduced using sophisticated techniques including the kissing caps invented in [202]. The techniques presented in Section 5.3.3 have been tweaked in [170] to also derive the lower bound

$$\mu_k(\mathcal{G}) \geq 2\pi^2 \alpha_k(\mathbf{G}_d) \min_{1 \leq j \leq N} \frac{1}{|\mathcal{C}_j|^2}, \quad k = 1, \dots, N,$$

whenever \mathcal{G} is planar or, more generally, it admits a cycle double cover $(\mathcal{C}_i)_{1 \leq i \leq N}$: this lower bound entails the eigenvalues α_k , $k = 1, \dots, N$ of the normalized Laplacian of \mathbf{G}_d , a weighted version of the dual graph induced by these cycles.

8.3. Infinite metric graphs. Infinite metric graphs have been studied since [158]. A very rich theory of infinite metric graphs has been developed since the 1990s [5, 75, 76, 77, 70, 71]. Modern results about spectrum, extension and potential theory, and heat kernels have been obtained ever since in [201, 178, 156, 62, 69, 166, 104, 73, 188, 153, 128, 93, 115, 177, 125, 33]. In this context, the role of *graph ends* was implicitly touched upon in [173, 72, 174] and has been fully appreciated in [124]: ends can be understood as “points at infinity” of infinite metric graphs and they are connected in a subtle way to the deficiency indices and, in particular, to the self-adjointness of the Laplacian, see also [126] and the recent survey [127]. If a graph end has a suitably small neighborhood of finite volume, then additional conditions (say, of Dirichlet or Neumann type) have to be imposed there, leading to new Laplacian realizations. The issue of the discreteness of the spectrum of these realizations has been discussed in [125, 90]: it turns out that the spectrum can be discrete even though the graph has infinite volume. The possibility of a Weyl-type eigenvalue asymptotics for certain fractal-like infinite metric graphs has been studied in [120]. Indeed, self-similar infinite metric graphs can often be interpreted as fractals, see e.g., [13]. Also, there is a very broad literature about the application of Floquet theory to metric graphs including [179, 34]. More recently, a notion of convergence for sequences of sparse combinatorial graphs that goes back to [39] has been adapted in [16] to the case of metric graphs to prove sophisticated results about the band structure of the spectrum of infinite metric trees: this has made possible to demonstrate quantum ergodicity (i.e., eigenfunctions with eigenvalues lying in a certain band are spatially delocalized) in [15, 17].

8.4. Heat kernels. Because the Laplacian with standard vertex conditions is a self-adjoint, positive semi-definite operator, by the Spectral Theorem it generates a strongly continuous semigroup of contractions. Indeed, this semigroup consists of integral operators whose kernel $p^{\mathcal{G}} = p_t^{\mathcal{G}}(x, y)$ is usually referred to as *heat kernel*. It turns out that the heat kernel encodes much information about the metric graph. In particular, the *heat trace* $\text{Tr}^{\mathcal{G}}(t) := \int_{\mathcal{G}} p_t^{\mathcal{G}}(x, x) dx$ – especially its short-time asymptotics – allows one to read off the total length of the metric graph and its first Betti number: this was first proved by Roth [194, 195] (a simple corollary

of Roth's trace formula was presented as Theorem 3.20) and comparable results have been re-discovered several times, and generalized to more general vertex conditions: we refer to [132, 148, 129, 56, 55].

Using Roth's formula for the heat kernel, it can be proved that the point evaluations of any sequence $(\psi_n)_{n \in \mathbb{N}}$ of eigenfunctions of $-\Delta_{\mathcal{G}}$ at any point of the graph is Cesàro square summable: the following *local Weyl law* was proved in [60, Theorem 4.1].

Theorem 8.3. *For any $x \in \mathcal{G}$ there holds*

$$\lim_{N \rightarrow \infty} \sum_{j=1}^N \psi_j(x)^2 = \frac{2}{\deg(x)|\mathcal{G}|},$$

where $\deg(x)$ is the degree of x if $x \in \mathbf{V}$, or 2 else.

Another proof based on an ergodic theorem for functions supported on the secular manifold has been obtained in [28]. A generalization of Theorem 8.3 for Schrödinger operators with δ -conditions has been obtained in [54]: by its means, it could be proved in [54, Theorem 1] that the sequence of discrepancies of the eigenvalues of a Schrödinger operator from those of the free Laplacian on the same \mathcal{G} is Cesàro summable. A special case of this assertion was proved in [190].

8.5. Torsional geometry. If Dirichlet conditions are imposed on a nonempty vertex set \mathbf{V}_D in \mathcal{G} , then $\int_0^\infty \int_{\mathcal{G}} \int_{\mathcal{G}} p_t^{\mathcal{G}}(x, y) dx dy$ – or equivalently the $L^1(\mathcal{G} \times \mathcal{G})$ -norm of the Green function of $\Delta^{\mathcal{G}}$ – is called *torsional rigidity* $T(\mathcal{G}; \mathbf{V}_D)$ of \mathcal{G} : it is an old notion that was introduced by Pólya for planar domains, and in [65, 83] on metric graphs. It turns out that this quantity can be used to estimate $\lambda_1(\mathcal{G}; \mathbf{V}_D)$ both from above and from below. Indeed, the *Pólya–Szegő Inequality*

$$\lambda_1(\mathcal{G}; \mathbf{V}_D) T(\mathcal{G}; \mathbf{V}_D) < |\mathcal{G}|$$

and the *Kohler–Jobin Inequality*

$$\left(\frac{\pi}{\sqrt[3]{24}} \right)^2 \leq \lambda_1(\mathcal{G}; \mathbf{V}_D) T(\mathcal{G}; \mathbf{V}_D)^{\frac{2}{3}}$$

have been proved in [171] (with the latter bound improved by a factor $2^{\frac{2}{3}}$ if the graph is doubly edge connected); a similar result in the more general context of metric measure spaces was obtained in [164]. An interesting feature of these estimates is that the torsional rigidity $T(\mathcal{G})$ can be easily computed by solving an algebraic system in $|\mathbf{V} \setminus \mathbf{V}_0|$ (the number of non-Dirichlet vertices) unknowns and equations that involves a weighted version of the discrete Laplacian.

Another lower estimate on $\lambda_1(\mathcal{G}; \mathbf{V}_D)$ in terms of the maximum of a so-called *torsion functions* has been originally observed by Donsker–Varadhan [86, 87] and later re-discovered in [20] and then again in [101]: the abstract version in [168] can be applied to metric graphs, too, as long as Dirichlet conditions are imposed on at least one vertex.

8.6. Spectral Minimal Partitions. Imagine one wants to subdivide a metric graph \mathcal{G} into k parts. An arguably natural choice is to look for the nodal domains of a k -th eigenfunction ψ_k , i.e., for the connected components of the set $\{x \in \mathcal{G} : \psi_k(x) \neq 0\}$. Indeed, it was shown in [102] (under certain technical assumptions, later removed in [111]) that ψ_k has at most k nodal domains, and this bound is sharp as it is attained by trees [4, 187, 186] (this has been used already in the proof of Theorem 6.24); indeed, it is rigid, as it is only attained by trees [21].

So, a different approach is needed if one looks for a spectral way of partitioning \mathcal{G} . One possible way of doing so is based on the theory of *spectral minimal partitions* [108, 57]: roughly speaking, one partitions \mathcal{G} in k connected subgraphs (*clusters*), imposes Dirichlet conditions at the cutpoints, takes the maximum among all the ground state energies on such clusters, and then infimizes among all possible way of subdividing \mathcal{G} into k clusters. It was proved in [118] that such infimum $\mathcal{L}_k(\mathcal{G})$ is attained – i.e., there exists a spectral minimal k -partition – for all \mathcal{G} and all k . Remarkably, such spectral minimal energies satisfy a Weyl-type asymptotic [111]: in particular, it is known

$$\lim_{k \rightarrow \infty} \frac{\mathcal{L}_k(\mathcal{G})}{k^2} = \frac{\pi^2}{|\mathcal{G}|^2} \quad \text{for all } \mathcal{G},$$

which can be regarded as a metric graph counterpart of Caffarelli and Lin’s – hitherto open – *hexagonal conjecture* for planar domains [67].

8.7. Symmetrization and NLS equations. A slightly adapted version of the symmetrization method discussed in Section 5.1 has also been used to study nonlinear problems, in particular Nonlinear Schrödinger (NLS) equations, mostly on unbounded graphs. In a series of landmark papers [1, 2, 3], the authors studied minimizers (so-called *ground states*), graphs \mathcal{G} with at least one edge of infinite length (half lines), of the NLS energy

$$E_{\mathcal{G}}(u) = \frac{1}{2} \int_{\mathcal{G}} |u'|^2 dx - \frac{1}{p} \int_{\mathcal{G}} |u|^p dx$$

on $H^1(\mathcal{G})$ under a mass constraint (i.e. fixed L^2 -norm) in the subcritical regime $2 \leq p < 6$, that is, in which the embedding $H^1(\mathcal{G}) \hookrightarrow L^p(\mathcal{G})$ is continuous. Critical points of this functional are solutions of the equation

$$u'' + |u|^{p-2}u = \lambda u$$

edgewise in \mathcal{G} , with standard conditions at any vertices. We note that ground states exist and are explicitly known on both $\mathcal{G} = \mathbb{R}$ and $\mathcal{G} = \mathbb{R}_+$, being given by a properly scaled soliton (sech function), and that $\min E_{\mathbb{R}_+} < \min E_{\mathbb{R}}$.

The authors showed that $\inf E_{\mathcal{G}}$ is always between $\min E_{\mathbb{R}_+}$ and $\min E_{\mathbb{R}}$, but that existence or non-existence of minimizers depends subtly on the topology of the graph. In particular, if \mathcal{G} satisfies what is known as the *(H)-condition* (essentially, that upon deletion of an arbitrary point of \mathcal{G} , the resulting graph does not have any bounded connected components; equivalently, for any $x \in \mathcal{G}$ there are at least two distinct *paths to infinity* emanating from x), then the infimal energy $E_{\mathcal{G}}$ can attain is equal to $E_{\mathbb{R}}$, but the infimum is attained if and only if \mathcal{G} can

be obtained from \mathbb{R} by gluing a finite number of points to create a pumpkin chain of locally equilateral 2-pumpkins with two copies of \mathbb{R}_+ attached to one of its antipodal points.

The key point is that the (H)-condition guarantees that the level surfaces S_t (see (5.5)) of any positive function $\psi \in H^1(\mathcal{G})$ will have size $\#S_t \geq 2$ for almost all $t \in (0, \|\psi\|_\infty)$, allowing one to symmetrize ψ onto a positive function in $H^1(\mathbb{R})$ which is symmetrically decreasing about $0 \in \mathbb{R}$, decreasing its gradient; one can then analyze when equality is possible. Without the (H)-condition, in general one only knows that $\#S_t \geq 1$ and can thus only symmetrize onto monotonically decreasing functions on \mathbb{R}_+ ; in this case there do exist graphs admitting ground states.

A large literature has emerged studying such NLS equations in various regimes (including the critical and supercritical cases, $p = 6$ and $p > 6$), and variants (for example, quintic rather than cubic nonlinearities, or with a potential, or other vertex conditions), both for ground states and other positive solutions and sign-changing solutions. It would go well beyond the scope of this article to give a proper survey of the literature on NLS on metric graphs, a topic which warrants its own survey – instead, we refer to the recent papers [84, 88] –, but we mention that there are some other parallels between techniques used, for example, some surgery-type principles, such as the idea of gluing vertices, and studying when this does or does not change the infimal value of the functional (already present [2, Theorem 2.5]), are also used here, having been developed independently of the analysis of the spectral geometry of the Laplacian.

8.8. p -Laplacians. Another nonlinear problem related to the Laplacian, which is arguably a more direct variant, is the p -Laplacian, which corresponds to the equation

$$(8.2) \quad -(|u|^{p-2}u')' = \lambda|u|^{p-2}u$$

edgewise in the compact metric graph \mathcal{G} , plus a suitable adaptation of standard conditions, for $1 < p < \infty$, the cases $p = 1$ and $p = \infty$ being singular.

For $1 < p < \infty$, the corresponding weak formulation is given in $W^{1,p}(\mathcal{G}) = \{u \in L^p(\mathcal{G}) : u' \in L^p(\mathcal{G})\}$, and in place of the spectral gap one studies the smallest *positive* critical point of the functional

$$E_p(u) := \int_{\mathcal{G}} |u'|^p dx$$

subject to the constraint that $\|u\|_{L^p(\mathcal{G})} = 1$. This was done in [45], where an isoperimetric-type inequality is proved using a p -variant of the symmetrization method from Section 5.1.

Alternatively, one may impose Dirichlet conditions on one or more vertices and then study the infimum of E_p among all $W_0^{1,p}$ -functions of L^p -norm 1, the corresponding eigenfunction is a ground state. This was done in [85], where the authors also studied the limits $p \rightarrow 1$ and $p \rightarrow \infty$, showing that, just as for Euclidean domains, there is convergence of the eigenvalue and eigenfunction to their counterparts for the 1- and the ∞ -Laplacians, which the authors describe.

In the former case, the correct setting is the space of functions of bounded variation, and the eigenvalue corresponds to a so-called *Cheeger cut* of the graph. A theory of BV functions on

graphs was developed, and links to the Cheeger problem were studied, in [161, 162], see also [163].

There are still many open problems for the p -Laplacian on compact graphs, including to show that the sequence of variational critical points of E_p , obtainable by the usual Ljusternik–Schnirelman method, actually represent all solutions of the p -Laplace equation (8.2) in $W^{1,p}(\mathcal{G})$, something which is known on intervals [89] but unknown on Euclidean domains. One could also consider (p, q) -variants, where one fixes a suitable L^q -norm of the function, rather than the L^p -norm. Developing surgery principles for these eigenvalues also remains to be done. A version of Weyl’s law for the Ljusternik–Schnirelman variational eigenvalues of (8.2), and an analysis of the number of nodal domains of the corresponding eigenvalues, is given in [111].

8.9. Other self-adjoint realizations of the Laplacian. Just like in the case of individual intervals, discussed in Remark 2.2, we can consider infinitely many further self-adjoint realizations of the Laplacian on a metric graph. In particular, the transmission condition parametrization

$$(8.3) \quad \begin{pmatrix} u(0) \\ u(L) \end{pmatrix} \in Y, \quad \begin{pmatrix} -u'(0) \\ u'(L) \end{pmatrix} + R \begin{pmatrix} u(0) \\ u(L) \end{pmatrix} \in Y^\perp$$

for any subspace Y of $\mathbb{C}^{2|E|}$ and any self-adjoint operator R on Y , has been popularized in [134]. Standard vertex conditions can be represented in this formalism by imposing that Y is an appropriate space associated with the so-called *signed incidence matrix* of any orientation of the metric graph \mathcal{G} , see [38, Example 2.4] for details.

Various other parametrizations have been considered, among others, in [130, 106, 131, 100] (see [49, Thm. 1.4.4] for a side-by-side comparison of most of them). More recently, several classes of non-standard vertex conditions inducing (possibly non-self-adjoint) Laplacian realization that do or dot preserve relevant quantum mechanical symmetries have been studied in [114, 94, 113, 29].

While the Laplacian with standard conditions (and possibly Dirichlet conditions on a nonempty subset of V) has nonnegative eigenvalues only, general self-adjoint realizations may certainly have negative eigenvalues for suitable coefficient matrices R : this is true already in the case of δ -conditions as introduced in Remark 3.24. A formula for the number of negative eigenvalues has been derived in [36].

For a recent survey of the spectral theory of Laplacians and Schrödinger operators on metric graphs with δ and δ' conditions, including spectral geometric considerations, see [193].

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