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ABSTRACT

A "quantum graph" is a Laplacian differential operator on a metric graph, that is a combinatorial graph where edges are identified with intervals of certain lengths. Introduced by L. Pauling in the 1930s, this concept has found various applications in chemistry, physics and biology. Finite quantum graphs (i.e., the metric graph has finitely many vertices and edges) are rather widely studied. On the other hand, less is known about quantum graphs on infinite metric graphs and in particular, a large part of the existing literature relies on an additional geometrical assumption, the existence of a uniform positive lower bound on the edge lengths. However, this is known to exclude certain interesting phenomena and spectral properties.

The present thesis is concerned with several aspects of the spectral theory of infinite quantum graphs. Particular focus lies on infinite graphs without additional geometrical assumptions and the specific phenomena arising in this situation.

The first part of the thesis is devoted to spectral estimates for the Kirchhoff Laplacian. We introduce a notion of an isoperimetric constant for infinite metric graphs and obtain a Cheeger-type estimate. This leads in particular to purely combinatorial criteria for the Kirchhoff Laplacian to have uniformly positive or discrete spectrum.

The second part contains a study of the isoperimetric constant for tessellating metric graphs. Motivated by similar concepts in the setting of combinatorial graphs, this is carried out in terms of a curvature-like quantity.

In the third part we investigate radially symmetric antitrees, a special class of infinite graphs with a high degree of symmetry. We perform a detailed spectral analysis and provide examples of antitrees for which the Kirchhoff Laplacian has absolutely continuous spectrum equal to the positive halfline.

The goal of the fourth part is to develop basic extension theory for the minimal Kirchhoff Laplacian. The geometric standard assumption implies self-adjointness and hence there has been little prior work on this subject. In our approach, we study the connection between self-adjoint extensions and the notion of graph ends, an ideal boundary for infinite graphs introduced independently by Freudenthal and Halin. We obtain a sharp lower estimate on the deficiency indices and a geometric characterization of uniqueness of a Markovian extension.

The fifth part can be seen as a complement to the previous. We introduce the Gaffney Laplacian on an infinite metric graph, prove results regarding its closedness and provide an explicit formula for the deficiency indices of the minimal Gaffney Laplacian in terms of graph ends.

ZUSAMMENFASSUNG

Der Begriff „Quantengraph” bezeichnet einen Laplace-Differentialoperator auf einem metrischen Graphen (ein kombinatorischer Graph, dessen Kanten als Intervalle unterschiedlicher Länge aufgefasst werden). Dieses Konzept wurde von L. Pauling in den 1930er-Jahren eingeführt und fand zahlreiche Anwendungen in der Chemie, Physik und Biologie. Endliche Quantengraphen (d.h., der metrische Graph besitzt endlich viele Knoten und Kanten) wurden in den letzten Jahren intensiv studiert. Über die Eigenschaften von Quantengraphen auf unendlichen Graphen ist weniger bekannt und ein großer Teil der existierenden Literatur behandelt diese nur unter einer zusätzlichen geometrischen Annahme, der Existenz einer strikt positiven unteren Schranke für die Kantenlängen. Gleichzeitig ist jedoch bekannt, dass dies gewisse interessante Phänomene und spektrale Eigenschaften bereits ausschließt.

Die vorliegende Arbeit befasst sich mit verschiedenen Aspekten der Spektraltheorie von unendlichen Quantengraphen. Besonderer Fokus liegt dabei auf unendlichen Graphen ohne zusätzliche geometrische Bedingungen und den besonderen Phänomenen, die in diesem Fall auftreten können.

Der erste Teil der Arbeit widmet sich Spektralabschätzungen für den Kirchhoff Laplace-Operator. Wir definieren eine isoperimetische Konstante für unendliche Quantengraphen und beweisen eine Cheeger-Abschätzung. Dies ergibt insbesondere rein kombinatorische Bedingungen unter denen der Kirchhoff Laplace-Operator strikt positives oder rein diskretes Spektrum besitzt.

Im zweite Teil studieren wir die isoperimetrische Konstante für den Spezialfall von planaren metrische Graphen näher. Motiviert durch ähnliche Konzepte für kombinatorische Graphen benützen dafür wir eine Krümmungsgröße.

Im dritten Teil untersuchen wir radialsymmetrische Antibäume, eine spezielle Klasse von unendlichen Graphen mit besonderen Symmetrieeigenschaften. Wir analysieren grundlegende spektrale Eigenschaften und konstruieren Beispiele von Antibäumen, für die das absolutstetige Spektrum des Kirchhoff Laplace-Operators gleich der positiven Halbachse ist.

Das Ziel des vierten Teils ist die Entwicklung grundlegender Erweiterungstheorie für den minimalen Kirchhoff Laplace-Operator. Unter der oben erwähnten geometrischen Annahme ist dieser Operator selbst-adjungiert und daher gibt es zu diesem Thema bisher nur wenige Resultate. Wir studieren den Zusammenhang zwischen selbst-adjungierten Erweiterungen und Graphenden, einem klassischen Randbegriff für unendliche Graphen, der unabhängig von Freudenthal und Halin eingeführt wurde. Dabei erhalten wir eine scharfe untere Abschätzung für die Defektindizes und eine geometrische Charakterisierung der Existenz einer eindeutigen markowschen Erweiterung.

Der fünfte und letzte Teil stellt ein Komplement zum vorigen dar. Wir definieren den Gaffney Laplace-Operator im Kontext von unendlichen metrischen Graphen, beweisen Resultate im Zusammenhang mit seiner Abgeschlossenheit und finden unter der Verwendung von Graphenden eine explizite Formel für die Defektindizes des minimalen Gaffney Laplace-Operators.

INTRODUCTION

In the last few decades, the study of quantum graphs has developed into an important and active mathematical field. A quantum graph is a Schrödinger operator on a metric graph (i.e. a discrete graph where edges are identified with intervals of certain lengths), acting on edgewise smooth functions satisfying certain coupling conditions at the vertices. The most studied quantum graph is the Kirchhoff Laplacian, which corresponds to a Laplacian without potential or weights and provides the analog of the Laplace–Beltrami operator in this setting.

The notion of quantum graphs was introduced by Pauling in the 1930s in order to model free electrons in organic molecules [76]. After being rediscovered in the 1980s (see e.g. [44, 51, 77]), the concept was used in various other branches of physics, mathematical biology and material sciences, where many applications are based on a one-dimensional graph approximation of a thin wire-like material. Having a different motivation in mind, Kottos and Smilansky provoked further interest in the subject in [67, 68], where they proposed quantum graphs as interesting but still comparably accessible models to study complex phenomena in quantum chaos. For an overview and further references on quantum graphs in applications and quantum chaos we refer to [18, 21, 42, 52, 78].

From a more theoretical point of view, an interesting aspect of quantum graphs is their close relationship to (weighted) discrete Laplacians (for details on discrete Laplacians see e.g. [14, 34, 83]). Whereas in some situations discrete Laplacians are easier to study, since they are based on difference expressions rather than differential equations, the situation is in fact opposite from the perspective of stochastic properties. The framework of Dirichlet forms [49] links both operator classes to certain stochastic processes: in this sense quantum graphs relate to Brownian motions on metric graphs and moreover, the Dirichlet form of a quantum graph is typically strongly local, e.g. [53]. This allows to use a large number of general results, see for instance [82]. On the other hand, weighted discrete Laplacian lead to continuous-time random walks and pure jump forms [14, 48, 58, 87], which are typically much harder to analyze. Nevertheless, it turns out that certain stochastic aspects of quantum graphs and discrete Laplacians are related. In this context, metric graphs are also referred to as "cable graphs" and sometimes allow to transfer results from the continuous to the discrete setting and back [15, 17, 40, 48, 55, 70, 71].

Moreover, it turns out that these two operator classes are connected in terms of basic spectral properties. In fact, there is a close link between the eigenvalues of the Kirchhoff Laplacian on an equilateral (i.e., all edges have the same length) metric graph and the normalized (also known as physical) discrete Laplacian: they can be computed from each other in terms of a simple formula [85]. These relations were generalized considerably in [27, 31, 78] and in particular it was shown in [69] that these two operators are in a certain sense locally unitarily equivalent. In the non-equilateral case, connections between quantum graphs and a specific class of weighted discrete Laplacians were established in [43]. For eigenvalue estimates involving another type of weighted discrete Laplacians see also [4].

In the last two decades the study of graphs has also become an important topic in tropical and algebraic geometry. Discrete and metrics graph appear for instance as degenerations of algebraic curves and allow certain parallels to compact Riemann surfaces in terms of divisor theory, see e.g. [2, 3, 6, 7, 8, 9, 11, 33, 80, 89]. In this context, discrete Laplacians are used in the definition of the divisor of a rational function on a graph [9, page 768], which can be seen as a generalization of the Laplace–Deligne formula [9, Remark 1.4]. Quantum graphs were related to the Arakelov–Green function in [10] and the notion of divisorial gonality in [5].

Due to these motivations, in the last years a tremendous amount of works was dedicated to finite quantum graphs (i.e., the metric graph has finitely many vertices and edges). In this setting, the Kirchhoff Laplacian is always self-adjoint with purely discrete spectrum and its spectral theory has been developed in many different directions. For an overview and further references we refer to [18, 21, 42, 52, 78]; for more recent articles see e.g. spectral gap estimates [5, 19, 20, 41, 60, 79], new results in quantum chaos [23, 24, 56, 84] and other topics [1, 4, 13, 22].

In contrast to this, less is known about the properties of quantum graph operators on infinite graphs (i.e., the metric graph has countably many vertices and edges). The major part of the existing literature treats infinite metric graphs only under rather restrictive geometric assumptions. The best understood models are radially symmetric metric trees: due to strong symmetry assumptions, the corresponding Kirchhoff Laplacian reduces to an infinite sum of one-dimensional Sturm–Liouville operators [28, 72, 81], which allows a rather detailed treatment of this example (see, e.g. [25, 28, 36, 39, 45, 72, 73, 81]).

Apart from this rather explicit model, the most common geometric assumption is the existence of a strictly positive lower bound on the lengths of the edges (compare e.g. [21, Assumption 1.4.12] and [78, Assumption 2.1.1]). This permits for instance to study periodic quantum graphs: their spectra are known to have band-gap structure [21, Chapter 4]. More recent articles investigate universal properties of the relative density of the bands [12], explicit constructions of Bethe–Sommerfeld graphs (i.e. the number of gaps in the spectrum is finite) [47] and examples of periodic quantum graphs with empty absolutely continuous spectrum [46].

However, in general the existence of a uniform lower bound on the edge lengths is a rather restrictive condition and already excludes several interesting models and effects. For instance, it already implies that the Kirchhoff Laplacian is self-adjoint [21, Theorem 1.4.19] and has non-empty essential spectrum [43, Corollary 4.1]. As another consequence, the metric graph is complete with its standard metric and hence the results from [82] directly apply. Metric graphs violating this assumption are sometimes called fractal metric graphs [78, Section 1.6.7] and appear for example as models in mathematical biology [57, 78]. The literature explicitly dedicated to this case is rather scarce and we refer to [29, 30, 43].

The present thesis is devoted to several topics in the spectral analysis of infinite quantum graphs. Particular focus lies on infinite metric graphs without any additional geometric assumptions and the specific spectral phenomena arising in this situation. The thesis consists of five research articles which were written during the course of my doctoral studies. They have been included under their original title as the following chapters:

1. Spectral estimates for infinite quantum graphs [63],
2. Strong Isoperimetric Inequality for Tessellating Quantum Graphs [75],
3. Quantum graphs on radially symmetric antitrees [64],
4. Self-adjoint and Markovian extensions of infinite quantum graphs [66],
5. A note on the Gaffney Laplacian on metric graphs [65].

We finish this introduction with an overview of the manuscripts and a description of the main results. Detailed information on their publication status is contained as well. The articles [63, 64, 65] were written in joint work with my advisor Aleksey Kostenko, and [66] in additional collaboration with Delio Mugnolo.

1. **Spectral estimates for infinite quantum graphs**,
   (joint with A. Kostenko)
   Calc. Var. Partial Differential Equations **58***, no. 1, Art. 15 (2019).*

   The first article [63] is concerned with spectral estimates for the Kirchhoff Laplacian on an infinite metric graph, which play a crucial role in the study of the corresponding heat semigroup. We introduce a notion of an isoperimetric constant and obtain a Cheeger-type inequality (Theorem 3.4). Whereas due to certain geometric parallels [16, 32, 74] this result is expected, the main discovery is that in contrast to manifolds and finite metric graphs [32, 74] the isoperimetric constant of an infinite metric graph has a combinatorial structure.

   This in particular leads to combinatorial criteria for the Kirchhoff Laplacian to have strictly positive or purely discrete spectrum (Corollary 4.5). For instance, if the isoperimetric constant of the underlying combinatorial graph is strictly positive, then the spectrum is strictly positive if and only if edge lengths are uniformly bounded above; the spectrum is purely discrete if and only if edge lengths go to zero upon removing compact subgraphs. This class of graphs includes several important examples such as regular tessellations of hyperbolic space and Cayley graphs of non-amenable countable finitely generated groups. In case of Cayley graphs we also mention that by Lemma 8.12, the group is amenable if and only if for every choice of edge lengths (with edge lengths bounded above) the Kirchhoff Laplacian has strictly positive spectrum. This can in some sense be interpreted as a metric graph analog of the classical criteria by Kesten involving the discrete normalized Laplacian, which is the generator of the simple random walk on the Cayley graph [61, 62].

2. **Strong Isoperimetric Inequality for Tessellating Quantum Graphs**,
   Proceedings of the 2017 Bielefeld Conference in the Theory of Networks, Oper. Theory: Adv. Appl., Birkhäuser, to appear
   (accepted on 24. December 2018).

   The results of [63] make it natural to search for lower estimates for the isoperimetric constant. For discrete Laplacians on tessellating graphs such estimates are available in terms of discrete curvature notions [54, 59, 86]. In the second article [75], we provide similar results for metric tessellating graphs. We modify the edge curvature introduced in [86] and define a notion of a characteristic value for edges of tessellating metric graphs (Section

2.2). In terms of this notion, we obtain a lower estimate on the isoperimetric constant (Theorem 3.3).

3. **Quantum graphs on radially symmetric antitrees**,
(joint with A. Kostenko)
J. Spectral Theory, to appear (accepted on 24. May 2019).

The third article [64] is devoted to radially symmetric antitrees, a special class of infinite metric graphs with particular symmetry properties. Historically, (discrete) antitrees appear first as (counter-) examples in context with the question of stochastic completeness for continuous-time random walks [88]. Our goal in this article is to provide a class of graphs which can be fully analyzed, but at the same time features very different properties in comparison with the frequently considered class of symmetric trees.

Based on a decomposition of the Kirchhoff Laplacian into one-dimensional Sturm–Liouville operators (Theorem 3.2), we are able to perform a detailed spectral analysis by employing spectral theory of Krein strings. For instance, we prove that the Kirchhoff Laplacian is self-adjoint if and only if the total volume of the antitree is infinite (Theorem 4.1). This characterization is in some sense surprising: the condition of infinite total volume is a much weaker assumption than the Gaffney-type self-adjointness criteria (for general graphs) discussed in [66], which require completeness of the graph for suitable metrics. This can be interpreted as a hint that metric completion (a radially symmetric antitree is metrically complete exactly when it has infinite diameter) might not be the right notion of a graph boundary for the self-adjointness problem. In the finite volume case, we prove that deficiency indices are equal to 1 and describe all self-adjoint extensions (Theorem 4.1 (ii)). Moreover, we compute the isoperimetric constant in terms of sphere numbers and edge lengths (Section 7) and construct non-periodic antitrees with a large amount of absolutely continuous spectrum (Section 9). In this context we also refer to [37], where the decomposition result, Theorem 3.2, was employed to construct antitrees for which the Kirchhoff Laplacian has zero Lebesgue measure spectrum and nontrivial singular continuous spectrum.

During the submission process of [64], we also learned about the recent article [26], where the authors prove a decomposition result (similar to Theorem 3.2) for an abstract class of metric graphs satisfying certain symmetry assumptions. Radially symmetric antitrees are particular examples of this graph class, but we stress that our focus is on the spectral analysis, wheras the main aim of [26] is to provide a decomposition result in a rather general situation. In fact, it appears that the methods of [64] can easily be generalized to the setting of [26], leading to a detailed spectral description of the Kirchhoff Laplacian on this abstract graph class.

4. **Self-adjoint and Markovian extensions of infinite quantum graphs**,
(joint with A. Kostenko and D. Mugnolo), *submitted*.

The objective of the fourth article [66] is to study the self-adjointness problem for the Kirchhoff Laplacian. There has been little prior work on this subject and most of the known results rely on the common assumption of a positive uniform lower bound on edge lengths (which implies self-adjointness). Recently, a few results based on completeness properties with respect to suitable metrics have appeared (cf. [43, §4]). Motivated by the results on radially symmetric antitrees [64], we pursue a different approach and employ the notion of graph ends, a classical graph boundary introduced independently by Freudenthal and Halin. Modifying this concept slightly, we introduce the notion of *graph ends of finite volume* (Definition 3.7) and investigate their connection to self-adjoint extensions of the Kirchhoff Laplacian.

Our first main result is a lower estimate on the deficiency indices in terms of the number of finite volume graph ends (Theorem 4.1). This estimate is sharp and we also provide a criterion for the equality to hold. In particular equality holds for radially symmetric antitrees, which explains the criteria from [64] (see Example 4.11 and Section 7). Our second main result is a geometric characterization of the uniqueness of Markovian extensions: this holds true if and only if all graph ends have infinite volume (Corollary 5.5; see also [38] for detailed information on the importance and relationship of self-adjoint and Markovian uniqueness). In particular, for graphs with only one graph end (e.g. tessellating graphs, antitrees, Cayley graphs of amenable groups which are not virtually infinite cyclic) this condition reduces to the simple assumption that the graph has infinite total volume (Remark 3.8). Moreover, in case of only finitely many ends of finite volume, we provide an explicit description of the so-called finite energy extensions, a special class of self-adjoint extensions containing all Markovian extensions (Theorem 6.11). In particular, the Markovian extensions form a rather small one-parameter family for the above examples of graphs having just one end (Section 7 contains an example of an antitree such that the corresponding Kirchhoff Laplacian has infinite deficiency indices).

5. **A note on the Gaffney Laplacian on metric graphs**,
(joint with A. Kostenko), *in preparation.*

The fifth article [65] is a complement to [66] and investigates the Gaffney Laplacian on a metric graph (see Section 3), which is the analog of the Laplacian on Riemannian manifolds studied by Gaffney in [50]. Namely, the Gaffney Laplacian is the restriction of the maximal Kirchhoff Laplacian to functions having finite energy (Dirichlet integral). The main goal is to provide a new, transparent perspective on the main results of [66]: first of all, the self-adjointness of the Gaffney Laplacian is equivalent to the uniqueness of Markovian extensions of the Kirchhoff Laplacian (Lemma 3.4) and its deficiency indices coincide exactly with the number of graph ends of finite volume (Theorem 3.8). Moreover, the finite energy extensions studied in [66] are exactly the self-adjoint restrictions of the Gaffney Laplacian (Lemma 3.5). However, the main disadvantage of the Gaffney Laplacian is that it is not necessarily closed and we address this question in Theorem 3.9 (see also Proposition 4.1 and Remark 4.2). In case of finite total volume, closedness of the Gaffney Laplacian is equivalent to the number of graph ends being finite (Corollary 3.10). All these results are demonstrated by examples in the final section.

If the Gaffney Laplacian is not closed, the next natural question is the description of its closure. In the one-dimensional setting, the Gaffney operator coincides with the maximal one and based on a certain kind of dimension reduction [28, 72, 81], we show that for radially symmetric trees (in fact, for the general class of radially symmetric metric graphs of [26]) this effect prevails in the sense that the closure of the Gaffney Laplacian coincides with the maximal Kirchhoff Laplacian (Lemma 4.6 and Remark 4.7).

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SPECTRAL ESTIMATES FOR INFINITE QUANTUM GRAPHS

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Abstract. We investigate the bottom of the spectra of infinite quantum graphs, i.e., Laplace operators on metric graphs having infinitely many edges and vertices. We introduce a new definition of the isoperimetric constant for quantum graphs and then prove the Cheeger-type estimate. Our definition of the isoperimetric constant is purely combinatorial and thus it establishes connections with the combinatorial isoperimetric constant, one of the central objects in spectral graph theory and in the theory of simple random walks on graphs. The latter enables us to prove a number of criteria for quantum graphs to be uniformly positive or to have purely discrete spectrum. We demonstrate our findings by considering trees, antitrees and Cayley graphs of finitely generated groups.

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1. Introduction

The main focus of our paper is on the study of spectra of quantum graphs. The notion of "quantum graph" refers to a graph $\mathcal{G}$ considered as a one-dimensional simplicial complex and equipped with a differential operator. The spectral and

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scattering properties of Schrödinger operators on such structures attracted a considerable interest during the last two decades, as they provide, in particular, relevant models of nanostructured systems (we only mention recent collected works and monographs with a comprehensive bibliography: [9], [10], [25], [58]).

Let $\mathcal{G}$ be a locally finite connected metric graph, that is, a locally finite connected combinatorial graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$, where each edge $e \in \mathcal{E}$ is identified with a copy of the interval $[0, |e|]$ and $|\cdot|$ denotes the edge length. We shall always assume throughout the paper that *each edge has finite length*, that is, $|\cdot|\colon \mathcal{E} \to (0,\infty)$. In the Hilbert space $L^2(\mathcal{G}) = \bigoplus_{e\in\mathcal{E}} L^2(e)$, we can define the Hamiltonian $\mathbf{H}$ which acts in this space as the (negative) second derivative $-\frac{d^2}{dx_e^2}$ on every edge $e \in \mathcal{E}$. To give $\mathbf{H}$ the meaning of a quantum mechanical energy operator, it must be self-adjoint and hence one needs to impose appropriate boundary conditions at the vertices. Kirchhoff (also known as Kirchhoff–Neumann) conditions (2.6) are the most standard ones (cf. [10]) and the corresponding operator denoted by $\mathbf{H}$ is usually called a Kirchhoff (Kirchhoff–Neumann) Laplacian (we refer to Sections 2.2–2.4 for a precise definition of the operator $\mathbf{H}$). If the graph $\mathcal{G}$ is finite ($\mathcal{G}$ has finitely many vertices and edges), then the spectrum of $\mathbf{H}$ is purely discrete (see, e.g., [10]). During the last few years, a lot of effort has been put in estimating the first nonzero eigenvalue of the operator $\mathbf{H}$ (notice that 0 is always a simple eigenvalue if $\mathcal{G}_d$ is connected) and also in understanding its dependence on various characteristics of the corresponding metric graph including the number of *essential* vertices of the graph (vertices of degree 2 are called *inessential*); the number or the total length of the graph's edges; the edge connectivity of the underlying (combinatorial) graph, etc. For further information we refer to a brief selection of recent articles [3], [4], [8], [41], [42], [45], [59].

If the graph $\mathcal{G}$ is infinite (there are infinitely many vertices and edges), then the corresponding pre-minimal operator $\mathbf{H}_0$ defined by (2.7) is not automatically essentially self-adjoint. One of the standard conditions to ensure the essential self-adjointness of $\mathbf{H}_0$ is the existence of a positive lower bound on the edges lengths, $\ell_*(\mathcal{G}) = \inf_{e\in\mathcal{E}} |e| > 0$ (see [10]). Only recently several self-adjointness conditions without this rather restrictive assumption have been established in [26], [44] (see Section 2.3 for further details). Of course, the next natural question is the structure of the spectrum of the operator $\mathbf{H}$. Clearly, the spectrum of an infinite quantum graph is not necessarily discrete and hence one is interested in the location of the bottom of the spectrum, $\lambda_0(\mathbf{H})$, as well as of the bottom of the essential spectrum, $\lambda_0^{\mathrm{ess}}(\mathbf{H})$, of $\mathbf{H}$. Since the graph is infinite, many quantities of interest for finite quantum graphs (e.g., the number of vertices, edges, or its total length) are no longer suitable for these purposes and the corresponding bounds usually lead to trivial estimates. However, it is widely known that quantum graphs in a certain sense interpolate between Laplacians on Riemannian manifolds and difference Laplacians on combinatorial graphs and hence quantum graphs can be investigated by modifying techniques that have been developed for operators on manifolds and graphs and we explore these analogies in the present paper. Notice that this insight has already proved to be very fruitful and it has led to many important results in spectral theory of operators on metric graphs (see, e.g., [10]). Although quantum graphs are essentially operators on one dimensional manifolds, our point of view is that the corresponding results and estimates should be of combinatorial nature.

Our central result is a Cheeger-type estimate for quantum graphs, which establishes lower bounds for $\lambda_0(\mathbf{H})$ and $\lambda_0^{\mathrm{ess}}(\mathbf{H})$ in terms of the isoperimetric constant $\alpha(\mathcal{G})$ of the metric graph $\mathcal{G}$ (Theorem 3.4). Although the Cheeger-type bound for (finite) quantum graphs was proved 30 years ago by S. Nicaise (see [51, Theorem 3.2]), we give a new purely combinatorial definition of the isoperimetric constant (see Definition 3.2) and as a result this establishes a connection with isoperimetric constants for combinatorial graphs (see Lemma 4.2 and also (4.10)–(4.11)). To a certain extent this connection is expected (cf. Theorem 2.11 and also [6, 15, 11, 58]). Moreover, it was observed recently in [26, 44] by using the ideas from [43] that spectral properties of the operator $\mathbf{H}$ are closely connected with the corresponding properties of the discrete Laplacian defined in $\ell^2(\mathcal{V}; m)$ by the expression

$$(\tau_{\mathcal{G}} f)(v) := \frac{1}{m(v)} \sum_{u \sim v} \frac{f(v) - f(u)}{|e_{u,v}|}, \quad v \in \mathcal{V}, \tag{1.1}$$

where the weight function $m\colon \mathcal{V} \to \mathbb{R}_{>0}$ is given by

$$m\colon v \mapsto \sum_{u \sim v} |e_{u,v}|. \tag{1.2}$$

Using this connection, several criteria for $\lambda_0(\mathbf{H})$ and $\lambda_0^{\mathrm{ess}}(\mathbf{H})$ to be positive have been established in [26], however, in terms of isoperimetric constants and volume growth of the combinatorial graphs, which were introduced, respectively, in [5] and [28], [34] (in this paper we obtain these results as simple corollaries of our estimate (3.8)).

Despite the combinatorial nature of (3.3) and (3.4), it is known that computation of the combinatorial isoperimetric constant is an NP-hard problem [49] (see also [35, 37] for further details). Motivated by [5] and [21], we introduce a quantity, which sometimes is interpreted as a curvature of a graph, leading to estimates for the isoperimetric constants $\alpha(\mathcal{G})$ and $\alpha_{\mathrm{ess}}(\mathcal{G})$. It also turns out to be very useful in many situations of interest as we show by the examples of trees and antitrees. Another way to estimate isoperimetric constants is provided by the volume growth. Namely, we can apply the exponential volume growth estimates for regular Dirichlet forms from [63] (see also [34], [52]) to prove upper bounds (Brooks-type estimates [7]) for quantum graphs (see Theorem 7.1). However, this can be done under the additional assumption that the metric graph is complete with respect to the natural path metric (notice that in this case $\mathbf{H}_0$ is essentially self-adjoint and $\mathbf{H}$ coincides with its closure, see Corollary 2.3).

The quantities $\lambda_0(\mathbf{H})$ and $\lambda_0^{\mathrm{ess}}(\mathbf{H})$ are of fundamental importance for several reasons. From the spectral theory point of view, the positivity of $\lambda_0(\mathbf{H})$ or $\lambda_0^{\mathrm{ess}}(\mathbf{H})$ corresponds to bounded invertibility or Fredholmness of the operator $\mathbf{H}$. Moreover, $\lambda_0^{\mathrm{ess}}(\mathbf{H}) = +\infty$ holds precisely when the spectrum of $\mathbf{H}$ is purely discrete, which is further equivalent to the compactness of the embedding $H_0^1(\mathcal{G})$ into $L^2(\mathcal{G})$ (the definition of the form domain $H_0^1(\mathcal{G})$ is given in Section 2.4). It is difficult to overestimate the importance of $\lambda_0(\mathbf{H})$ and $\lambda_0^{\mathrm{ess}}(\mathbf{H})$ in applications. For example, in the theory of parabolic equations $\lambda_0(\mathbf{H})$ gives the speed of convergence of the system towards equilibrium. On the other hand, Cheeger-type inequalities have a venerable history. Starting from the seminal work of J. Cheeger [16], where a connection between the isoperimetric constant of a compact manifold and a first nontrivial eigenvalue of the Laplace–Beltrami operator was found, this topic became an active area of research in both manifolds and graphs settings. One of the most fruitful applications of Cheeger's inequality in graph theory (this inequality was first proved independently in [20, 22] and [1, 2]) is in the study of networks connectivity, namely, in constructing expanders (see [17, 19, 35, 47]). Notice also that the positivity of the isoperimetric constant (also known as a *strong isoperimetric inequality*) is of fundamental importance in the study of random walks on graphs (we refer to [65] for further details).

Let us now finish the introduction by describing the content of the article. First of all, we review necessary notions and facts on infinite quantum graphs in Section 2, where we introduce the pre-minimal operator $\mathbf{H}_0$ (Section 2.2), discuss its essential self-adjointness (Section 2.3) and the corresponding quadratic form $\mathfrak{t}_{\mathcal{G}}$ (Section 2.4), and also touch upon its connection with the difference Laplacian (1.1) (Section 2.5).

Section 3 contains our first main result, Theorem 3.4, which provides the Cheeger-type estimate for quantum graphs. Its proof follows closely the line of arguments as in the manifold case with the only exception, Lemma 3.7, which enables us to replace the isoperimetric constant (3.12) having the form similar to that of in [51] (see also [41, 57]) by the quantity (3.3) having a combinatorial structure. The latter also reveals connections with the combinatorial isoperimetric constant α_{comb} from [2, 20], which measures connectedness of the underlying combinatorial graph, and with the discrete isoperimetric constant α_d introduced recently in [5] for the difference Laplacian (1.1). Bearing in mind the importance of both α_{comb} and α_d in applications as well as the fact that these quantities are widely studied, we discuss these connections in Sections 4.

Similar to manifolds and combinatorial Laplacians, one can estimate $\lambda_0(\mathbf{H})$ and $\lambda_0^{\mathrm{ess}}(\mathbf{H})$ by using the isoperimetric constant not only from below but also from above (Lemma 5.1). However, the price we have to pay is the existence of a positive lower bound on the edges lengths, $\inf_{e\in\mathcal{E}}|e| > 0$. Combining these estimates with the results from Section 4, we conclude that in this case the positivity of $\lambda_0(\mathbf{H})$ (resp., $\lambda_0^{\mathrm{ess}}(\mathbf{H})$) is equivalent to the validity of a strong isoperimetric inequality, i.e., $\alpha_{\mathrm{comb}} > 0$ (resp., $\alpha_{\mathrm{comb}}^{\mathrm{ess}} > 0$).

In Section 6, we introduce a quantity which may be interpreted as a curvature of a metric graph. Firstly, using this quantity we are able to obtain estimates on the isoperimetric constant. Secondly, we discuss its connection with the curvatures introduced for combinatorial Laplacians in [21] and for unbounded difference Laplacians in [5]. The latter, in particular, enables us to obtain simple discreteness criteria for $\sigma(\mathbf{H})$ (see Lemma 6.5 and Corollary 6.6), which to a certain extent can be seen as the analogs of the discreteness criteria from [23] and [31].

The estimates in terms of the volume growth are given in Section 7. In Section 8, we consider several illustrative examples. The case of trees is treated in Section 8.1. We show that for trees without inessential vertices and loose ends (vertices having degree 1), $\lambda_0(\mathbf{H}) > 0$ if and only if $\sup_e|e| < \infty$. Moreover, the spectrum of $\mathbf{H}$ is purely discrete if and only if the number $\#\{e\in\mathcal{E}\colon |e| > \varepsilon\}$ is finite for every $\varepsilon > 0$. Notice that under the additional symmetry assumption that a given metric tree is regular similar results, however, for the so-called Neumann Laplacian were observed by M. Solomyak [62]. The case of antitrees is considered in Section 8.2. We provide some general estimates and also focus on two particular examples of exponentially and polynomially growing antitrees. In particular, it turns out that for a polynomially growing antitree, our results provide rather good estimates for $\lambda_0(\mathbf{H})$ and $\lambda_0^{\mathrm{ess}}(\mathbf{H})$ (see Example 8.9). In the last subsection, we consider the case of Cayley graphs of finitely generated groups. Similar to combinatorial Laplacians, the amenability/non-amenability of the underlying group plays a crucial role.

Finally, in Appendix A we provide a slight improvement to the Cheeger estimates from [5] by noting that one can replace intrinsic path metrics in the definition of isoperimetric constants simply by edge weight functions having *an intrinsic* property.

2. Quantum graphs

2.1. **Combinatorial and metric graphs.** In what follows, $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ will be an unoriented graph with countably infinite sets of vertices $\mathcal{V}$ and edges $\mathcal{E}$. For two vertices u, $v \in \mathcal{V}$ we shall write $u \sim v$ if there is an edge $e_{u,v} \in \mathcal{E}$ connecting u with v. For every $v \in \mathcal{V}$, we denote the set of edges incident to the vertex v by $\mathcal{E}_v$ and

$$\deg_{\mathcal{G}}(v) := \#\{e|\, e \in \mathcal{E}_v\} \tag{2.1}$$

is called *the degree* (or *combinatorial degree*) of a vertex $v \in \mathcal{V}$. When there is no risk of confusion which graph is involved, we shall write deg instead of $\deg_{\mathcal{G}}$. By $\#(S)$ we denote the cardinality of a given set S. *A path* $\mathcal{P}$ of length $n \in \mathbb{Z}_{>0} \cup \{\infty\}$ is a sequence of vertices $\{v_0, v_1, \dots, v_n\}$ such that $v_{k-1} \sim v_k$ for all $k \in \{1, \dots, n\}$. If $v_0 = v_n$, then $\mathcal{P}$ is called a *cycle*.

We shall always make the following assumption.

Hypothesis 2.1. *The infinite graph $\mathcal{G}_d$ is* locally finite *(*$\deg(v) < \infty$ *for every $v \in \mathcal{V}$),* connected *(for any two vertices $u, v \in \mathcal{V}$ there is a path connecting u and v), and* simple *(there are no loops or multiple edges).*

Next we assign each edge $e \in \mathcal{E}$ a finite length $|e| \in (0, \infty)$. In this case $\mathcal{G} := (\mathcal{V}, \mathcal{E}, |\cdot|) = (\mathcal{G}_d, |\cdot|)$ is called *a metric graph.* The latter enables us to equip $\mathcal{G}$ with a topology and metric. Namely, by assigning each edge a direction and calling one of its vertices the initial vertex e_0 and the other one the terminal vertex e_i, every edge $e \in \mathcal{E}$ can be identified with a copy of the interval $\mathcal{I}_e = [0, |e|]$; moreover, the ends of the edges that correspond to the same vertex v are identified as well. Thus, $\mathcal{G}$ can be equipped with *the natural path metric* ϱ_0 (the distance between two points $x, y \in \mathcal{G}$ is defined as the length of the "shortest" path connecting x and y). Moreover, a metric graph $\mathcal{G}$ can be considered as a topological space (one-dimensional simplicial complex). For further details we refer to, e.g., [10, Chapter 1.3].

Also throughout this paper we shall assume the following conditions.

Hypothesis 2.2. *There is a finite upper bound for lengths of graph edges:*

$$\ell^*(\mathcal{G}) := \sup_{e \in \mathcal{E}} |e| < \infty. \tag{2.2}$$

In fact, Hypothesis 2.2 is not a restriction for our purposes (see Lemma 2.8 and also Remark 2.9(i)).

Hypothesis 2.3. *All edges in $\mathcal{G}$ are essential, that is,* $\deg(v) \neq 2$ *for all $v \in \mathcal{V}$.*

This assumption is not a restriction at all since vertices of degree 2 are irrelevant for the spectral properties of the Kirchhoff Laplacian and hence can be removed (see, e.g., [41]).

2.2. **Kirchhoff's Laplacian.** Let $\mathcal{G}$ be a metric graph satisfying Hypothesis 2.1–2.3. Upon identifying every $e \in \mathcal{E}$ with a copy of the interval $\mathcal{I}_e$ and considering $\mathcal{G}$ as the union of all edges glued together at certain endpoints, let us introduce the Hilbert space $L^2(\mathcal{G})$ of functions $f\colon \mathcal{G} \to \mathbb{C}$ such that

$$L^2(\mathcal{G}) = \bigoplus_{e\in\mathcal{E}} L^2(e) = \Big\{ f = \{f_e\}_{e\in\mathcal{E}} \big| \, f_e \in L^2(e), \ \sum_{e\in\mathcal{E}} \|f_e\|^2_{L^2(e)} < \infty \Big\}.$$

The subspace of compactly supported $L^2(\mathcal{G})$ functions will be denoted by

$$L^2_c(\mathcal{G}) = \big\{ f \in L^2(\mathcal{G}) | \ f \neq 0 \text{ only on finitely many edges } e \in \mathcal{E} \big\}.$$

Next let us equip $\mathcal{G}$ with the Laplace operator. For every $e \in \mathcal{E}$ consider the maximal operator $\mathrm{H}_{e,\max}$ acting on functions $f \in H^2(e)$ as a negative second derivative. Here and below $H^n(e)$ for $n \in \mathbb{Z}_{\geq 0}$ denotes the usual Sobolev space. In particular, $H^0(e) = L^2(e)$ and

$$H^1(e) = \{ f \in AC(e)\colon f' \in L^2(e)\}, \quad H^2(e) = \{ f \in H^1(e)\colon f' \in H^1(e)\}.$$

Now consider the maximal operator on $\mathcal{G}$ defined by

$$\mathbf{H}_{\max} = \bigoplus_{e\in\mathcal{E}} \mathrm{H}_{e,\max}, \qquad \mathrm{H}_{e,\max} = -\frac{\mathrm{d}^2}{\mathrm{d}x_e^2}, \quad \mathrm{dom}(\mathrm{H}_{e,\max}) = H^2(e). \tag{2.3}$$

For every $f_e \in H^2(e)$ the following quantities

$$f_e(e_o) := \lim_{x\to e_o} f_e(x), \qquad\qquad f_e(e_i) := \lim_{x\to e_i} f_e(x), \tag{2.4}$$

and

$$f_e'(e_o) := \lim_{x\to e_o} \frac{f_e(x) - f_e(e_o)}{|x - e_o|}, \qquad f_e'(e_i) := \lim_{x\to e_i} \frac{f_e(x) - f_e(e_i)}{|x - e_i|}, \tag{2.5}$$

are well defined. The Kirchhoff (or Kirchhoff–Neumann) boundary conditions at every vertex $v \in \mathcal{V}$ are then given by

$$\begin{cases} f \text{ is continuous at } v, \\ \sum_{e\in\mathcal{E}_v} f_e'(v) = 0. \end{cases} \tag{2.6}$$

Imposing these boundary conditions on the maximal domain $\mathrm{dom}(\mathbf{H}_{\max})$ and then restricting to compactly supported functions we get the pre-minimal operator

$$\begin{aligned} &\mathbf{H}_0 = \mathbf{H}_{\max} \restriction \mathrm{dom}(\mathbf{H}_0), \\ &\quad \mathrm{dom}(\mathbf{H}_0) = \{ f \in \mathrm{dom}(\mathbf{H}_{\max}) \cap L^2_c(\mathcal{G}) | \, f \text{ satisfies (2.6)}, \ v \in \mathcal{V}\}. \end{aligned} \tag{2.7}$$

Integrating by parts one obtains that $\mathbf{H}_0$ is symmetric. We call its closure *the minimal Kirchhoff Laplacian*. Notice that the values of f at the vertices (2.4) and one-sided derivatives (2.5) do not depend on the choice of orientation on $\mathcal{G}$. Moreover, the second derivative is also independent of orientation on $\mathcal{G}$ and hence so is the operator $\mathbf{H}_0$.

Remark 2.1. *If* $\deg(v) = 1$*, then Kirchhoff's condition* (2.6) *at* v *is simply the Neumann condition*

$$f_e'(v) = 0. \tag{2.8}$$

Let us mention that one can replace it by the Dirichlet condition

$$f_e(v) = 0 \tag{2.9}$$

and we shall consider the operator $\mathbf{H}_0$ with mixed boundary conditions (either Neumann or Dirichlet) at the vertices $v \in \mathcal{V}$ of the graph $\mathcal{G}$ such that $\deg(v) = 1$*.*

In the rest of our paper, we shall denote by $\mathcal{V}_D$ (respectively, by $\mathcal{V}_N$) the set of vertices $v \in \mathcal{V}$ such that $\deg(v) = 1$ and the Dirichlet condition (2.9) (respectively, the Neumann condition (2.8)) is imposed at v. The sets of corresponding edges will be denoted by $\mathcal{E}_D$ and $\mathcal{E}_N$, respectively.

2.3. **Self-adjointness.** In the rest of our paper we shall always assume that the graph $\mathcal{G}_d$ is infinite, that is, both sets $\mathcal{V}$ and $\mathcal{E}$ are infinite (since $\mathcal{G}_d$ is assumed to be locally finite). In this case the operator $\mathbf{H}_0$ is not necessarily essentially self-adjoint (that is, its closure may have nonzero deficiency indices) and finding self-adjointness criteria is a challenging open problem. The next results were proved recently in [26]. Define the weight function $m\colon \mathcal{V} \to \mathbb{R}_{>0}$ by

$$m\colon v \mapsto \sum_{e\in\mathcal{E}_v} |e|, \tag{2.10}$$

and then let $p_m\colon \mathcal{E} \to \mathbb{R}_{>0}$ be given by

$$p_m\colon e_{u,v} \mapsto m(u) + m(v). \tag{2.11}$$

The path metric ϱ_m on $\mathcal{V}$ generated by p_m is defined by

$$\varrho_m(u, v) := \inf_{\mathcal{P}=\{v_0,\dots,v_n\}\colon\, v_0=u\ \ v_n=v} \sum_k p_m(e_{v_{k-1},v_k}), \tag{2.12}$$

where the infimum is taken over all paths connecting u and v.

Theorem 2.2 ([26])**.** *If $(\mathcal{V}, \varrho_m)$ is complete as a metric space, then $\mathbf{H}_0$ is essentially self-adjoint. In particular, $\mathbf{H}_0$ is essentially self-adjoint if*

$$\inf_{v\in\mathcal{V}} m(v) > 0. \tag{2.13}$$

Replacing p_m in (2.12) by the edge length $|\cdot|$, we end up with the natural path metric ϱ_0 on $\mathcal{V}$. Clearly, $(\mathcal{V}, \varrho_m)$ is complete if so is $(\mathcal{V}, \varrho_0)$ and hence we arrive at the following Gaffney-type theorem for quantum graphs.

Corollary 2.3 ([26])**.** *If $\mathcal{G}$ equipped with a natural path metric is complete as a metric space, then $\mathbf{H}_0$ is essentially self-adjoint.*

The next well known result (see [10, Theorem 1.4.19]) also immediately follows from Theorem 2.2.

Corollary 2.4. *If*

$$\ell_*(\mathcal{G}) := \inf_{e\in\mathcal{E}} |e| > 0, \tag{2.14}$$

then $\mathbf{H}_0$ is essentially self-adjoint.

2.4. **Quadratic forms.** In this section we present the variational definition of the Kirchhoff Laplacian. Consider the quadratic form

$$\mathfrak{t}^0_{\mathcal{G}}[f] := (\mathbf{H}_0 f, f)_{L^2(\mathcal{G})}, \qquad f \in \operatorname{dom}(\mathfrak{t}^0_{\mathcal{G}}) := \operatorname{dom}(\mathbf{H}_0). \tag{2.15}$$

For every $f \in \operatorname{dom}(\mathbf{H}_0)$, an integration by parts gives

$$\mathfrak{t}^0_{\mathcal{G}}[f] = \int_{\mathcal{G}} |f'(x)|^2\, dx = \|f'\|^2_{L^2(\mathcal{G})}. \tag{2.16}$$

Clearly, the form $\mathfrak{t}^0_{\mathcal{G}}$ is nonnegative. Moreover, it is closable since $\mathbf{H}_0$ is symmetric. Let us denote its closure by $\mathfrak{t}_{\mathcal{G}}$ and the corresponding domain by $H^1_0(\mathcal{G}) := \mathrm{dom}(\mathfrak{t}_{\mathcal{G}})$. By the first representation theorem, there is a unique nonnegative self-adjoint operator corresponding to the form $\mathfrak{t}_{\mathcal{G}}$.

Definition 2.5. The self-adjoint nonnegative operator $\mathbf{H}$ associated with the form $\mathfrak{t}_{\mathcal{G}}$ in $L^2(\mathcal{G})$ will be called *the Kirchhoff Laplacian.*

If the pre-minimal operator $\mathbf{H}_0$ is essentially self-adjoint, then $\mathbf{H}$ coincides with its closure. In the case when $\mathbf{H}_0$ is a symmetric operator with nontrivial deficiency indices, the operator $\mathbf{H}$ is the Friedrichs extension of $\mathbf{H}_0$.

Remark 2.6. *Of course, one may consider the maximally defined form*

$$\mathfrak{t}^{(N)}_{\mathcal{G}}[f] := \int_{\mathcal{G}} |f'(x)|^2\, dx, \qquad f \in \mathrm{dom}(\mathfrak{t}^{(N)}_{\mathcal{G}}), \tag{2.17}$$

where

$$\mathrm{dom}(\mathfrak{t}^{(N)}_{\mathcal{G}}) := \{f \in L^2(\mathcal{G})|\ f \in H^1_{\mathrm{loc}}(\mathcal{G}),\ f' \in L^2(\mathcal{G})\} =: H^1(\mathcal{G}), \tag{2.18}$$

and then associate a self-adjoint positive operator, let us denote it by $\mathbf{H}^N$*, with this form in* $L^2(\mathcal{G})$*. Clearly, the forms* $\mathfrak{t}_{\mathcal{G}}$ *and* $\mathfrak{t}^{(N)}_{\mathcal{G}}$ *coincide if and only if* $\mathbf{H}$ *is the unique positive self-adjoint extension of* $\mathbf{H}_0$ *(this in particular holds if* $\mathbf{H}_0$ *is essentially self-adjoint). We are not aware of a description of the self-adjoint operator* $\mathbf{H}^N$ *associated with the form* $\mathfrak{t}^{(N)}_{\mathcal{G}}$ *if the pre-minimal operator has nontrivial deficiency indices (however, see the recent work* [13, 38]*). Moreover, to the best of our knowledge, the description of deficiency indices of* $\mathbf{H}_0$ *and its self-adjoint extensions is a widely open problem.*

If at some vertices $v \in \mathcal{V}$ with $\deg(v) = 1$ the Neumann condition (2.8) is replaced by the Dirichlet condition (2.9), then the corresponding form domain will be denoted by $\widetilde{H}^1_0(\mathcal{G})$. Notice that

$$\widetilde{H}^1_0(\mathcal{G}) = \{f \in H^1_0(\mathcal{G})|\ f_e(v) = 0,\ v \in \mathcal{V}_D\}. \tag{2.19}$$

By abusing the notation, we shall denote the corresponding self-adjoint operator by $\mathbf{H}$. The bottom of the spectrum of $\mathbf{H}$ can be found by using the Rayleigh quotient

$$\lambda_0(\mathbf{H}) := \inf \sigma(\mathbf{H}) = \inf_{\substack{f \in \widetilde{H}^1_0(\mathcal{G}) \\ f \neq 0}} \frac{(\mathbf{H}f, f)_{L^2(\mathcal{G})}}{\|f\|^2_{L^2(\mathcal{G})}} = \inf_{\substack{f \in \widetilde{H}^1_0(\mathcal{G}) \\ f \neq 0}} \frac{\|f'\|^2_{L^2(\mathcal{G})}}{\|f\|^2_{L^2(\mathcal{G})}}. \tag{2.20}$$

Moreover, the bottom of the essential spectrum is given by

$$\lambda^{\mathrm{ess}}_0(\mathbf{H}) := \inf \sigma_{\mathrm{ess}}(\mathbf{H}) = \sup_{\widetilde{\mathcal{G}} \subset \mathcal{G}} \inf_{\substack{f \in \widetilde{H}^1_0(\mathcal{G} \setminus \widetilde{\mathcal{G}}) \\ f \neq 0}} \frac{\|f'\|^2_{L^2(\mathcal{G} \setminus \widetilde{\mathcal{G}})}}{\|f\|^2_{L^2(\mathcal{G} \setminus \widetilde{\mathcal{G}})}}, \tag{2.21}$$

where the sup is taken over all finite subgraphs $\widetilde{\mathcal{G}}$ of $\mathcal{G}$. Here for any $\widetilde{\mathcal{G}} \subset \mathcal{G}$ we define $\widetilde{H}^1_0(\mathcal{G} \setminus \widetilde{\mathcal{G}})$ as the set of $H^1_0(\mathcal{G} \setminus \widetilde{\mathcal{G}})$ functions satisfying the following boundary conditions: for vertices in $\mathcal{G} \setminus \widetilde{\mathcal{G}}$ having one or more edges in $\widetilde{\mathcal{G}}$, we change the boundary conditions from Kirchhoff–Neumann to Dirichlet; for all other vertices in $\mathcal{G} \setminus \widetilde{\mathcal{G}}$, we leave them the same. This equality is known as a Persson-type theorem (or Glazman's decomposition principle in the Russian literature, see [33]) and its proof in the case of quantum graphs is analogous to the case of Schrödinger operators (see, e.g., [18, Theorem 3.12]).

Remark 2.7. *Let us mention that the following equivalence holds true*

$$\lambda_0(\mathbf{H}) = 0 \qquad \Longleftrightarrow \qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) = 0. \tag{2.22}$$

The implication " $\Leftarrow$ " is obvious. However, $\lambda_0(\mathbf{H}) = 0$ *and* $\lambda_0^{\mathrm{ess}}(\mathbf{H}) \neq 0$ *holds only if* 0 *is an isolated eigenvalue. On the other hand,* (2.16) *implies that* 0 *is an eigenvalue of* $\mathbf{H}$ *only if* $\mathbb{1} \in L^2(\mathcal{G})$*. The latter happens exactly when*

$$\mathrm{mes}(\mathcal{G}) := \sum_{e\in\mathcal{E}} |e| < \infty.$$

and hence the equivalence (2.22) *holds true whenever* $\mathrm{mes}(\mathcal{G}) = \infty$*,*

On the other hand, it turns out that $\mathbb{1} \notin H_0^1(\mathcal{G})$ *if* $\mathrm{mes}(\mathcal{G}) < \infty$ *and hence* 0 *is never an eigenvalue of* $\mathbf{H}$ *(see Corollary 3.5(iv)). In particular, the latter implies that* $\mathfrak{t}_{\mathcal{G}} \neq \mathfrak{t}_{\mathcal{G}}^{(N)}$ *if the metric graph* $\mathcal{G}$ *has finite total volume,* $\mathrm{mes}(\mathcal{G}) < \infty$*. The analysis of this case is postponed to a separate publication.*

If $\mathcal{G}_1$, $\mathcal{G}_2$ are finite subgraphs with $\mathcal{G}_1 \subseteq \mathcal{G}_2 \subset \mathcal{G}$, then $\widetilde{H}_0^1(\mathcal{G}\setminus\mathcal{G}_2) \subseteq \widetilde{H}_0^1(\mathcal{G}\setminus\mathcal{G}_1)$ in the sense that every function in $\widetilde{H}_0^1(\mathcal{G}\setminus\mathcal{G}_2)$ can be extended to be in $\widetilde{H}_0^1(\mathcal{G}\setminus\mathcal{G}_1)$ by setting it zero on remaining edges. Thus,

$$\inf_{\substack{f\in\widetilde{H}_0^1(\mathcal{G}\setminus\mathcal{G}_2)\\ f\neq 0}} \frac{\|f'\|^2_{L^2(\mathcal{G}\setminus\mathcal{G}_2)}}{\|f\|^2_{L^2(\mathcal{G}\setminus\mathcal{G}_2)}} \geq \inf_{\substack{f\in\widetilde{H}_0^1(\mathcal{G}\setminus\mathcal{G}_1)\\ f\neq 0}} \frac{\|f'\|^2_{L^2(\mathcal{G}\setminus\mathcal{G}_1)}}{\|f\|^2_{L^2(\mathcal{G}\setminus\mathcal{G}_1)}}.$$

Let $\mathcal{K}_{\mathcal{G}}$ be the set of all finite, connected subgraphs of $\mathcal{G}$ ordered by the inclusion relation "$\subseteq$" and hence $\mathcal{K}_{\mathcal{G}}$ is a net. Moreover,

$$\lambda_0^{\mathrm{ess}}(\mathbf{H}) = \sup_{\widetilde{\mathcal{G}}\in K_{\mathcal{G}}} \inf_{\substack{f\in\widetilde{H}_0^1(\mathcal{G}\setminus\widetilde{\mathcal{G}})\\ f\neq 0}} \frac{\|f'\|^2_{L^2(\mathcal{G}\setminus\widetilde{\mathcal{G}})}}{\|f\|^2_{L^2(\mathcal{G}\setminus\widetilde{\mathcal{G}})}} = \lim_{\widetilde{\mathcal{G}}\in K_{\mathcal{G}}} \inf_{\substack{f\in\widetilde{H}_0^1(\mathcal{G}\setminus\widetilde{\mathcal{G}})\\ f\neq 0}} \frac{\|f'\|^2_{L^2(\mathcal{G}\setminus\widetilde{\mathcal{G}})}}{\|f\|^2_{L^2(\mathcal{G}\setminus\widetilde{\mathcal{G}})}}, \tag{2.23}$$

where the limit is understood in the sense of nets and in this case we will say that $\widetilde{\mathcal{G}}$ tends to $\mathcal{G}$.

The next result provides an estimate, which easily follows from (2.20)–(2.21).

Lemma 2.8. *Set*

$$\ell^*_{\mathrm{ess}}(\mathcal{G}) := \inf_{\widetilde{\mathcal{E}}} \sup_{e\in\mathcal{E}\setminus\widetilde{\mathcal{E}}} |e|, \tag{2.24}$$

where the infimum is taken over all finite subsets $\widetilde{\mathcal{E}}$ *of* $\mathcal{E}$*. Then*

$$\lambda_0(\mathbf{H}) \leq \frac{\pi^2}{\ell^*(\mathcal{G})^2}, \qquad\qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) \leq \frac{\pi^2}{\ell^*_{\mathrm{ess}}(\mathcal{G})^2}. \tag{2.25}$$

Proof. By construction, the set $\widetilde{H}_c^1(\mathcal{G}) := \widetilde{H}_0^1(\mathcal{G}) \cap L_c^2(\mathcal{G})$ is a core for $\mathfrak{t}_{\mathcal{G}}$. Moreover, every $f \in \widetilde{H}_0^1(\mathcal{G})$ admits a unique decomposition $f = f_{\mathrm{lin}} + f_0$, where $f_{\mathrm{lin}} \in \widetilde{H}_0^1(\mathcal{G})$ is piecewise linear on $\mathcal{G}$ (that is, it is linear on every edge $e \in \mathcal{E}$) and $f_0 \in \widetilde{H}_0^1(\mathcal{G})$ takes zero values at the vertices $\mathcal{V}$. It is straightforward to check that

$$\mathfrak{t}_{\mathcal{G}}[f] = \int_{\mathcal{G}} |f'(x)|^2 dx = \int_{\mathcal{G}} |f'_{\mathrm{lin}}(x)|^2 dx + \int_{\mathcal{G}} |f'_0(x)|^2 dx = \mathfrak{t}_{\mathcal{G}}[f_{\mathrm{lin}}] + \mathfrak{t}_{\mathcal{G}}[f_0]. \tag{2.26}$$

Now the estimates (2.25) and (2.24) easily follow from the decomposition (2.26). Indeed, for every $f = f_0 \in \widetilde{H}_0^1(\mathcal{G})$

$$\mathfrak{t}_{\mathcal{G}}[f_0] = \sum_{e\in\mathcal{E}} \|f'_{0,e}\|^2_{L^2(e)}, \tag{2.27}$$

where $f_{0,e} := f_0 \restriction e \in H_0^1(e)$. Noting that

$$\inf_{f \in H_0^1([0,l])} \frac{\|f'\|_{L^2}^2}{\|f\|_{L^2}^2} = \left(\frac{\pi}{l}\right)^2,$$

and then taking into account (2.20) and (2.21), we arrive at (2.25). $\square$

Remark 2.9. *A few remarks are in order:*

(i) *The estimate* (2.25) *shows that the condition* (2.2) *is not a restriction since in the case* $\ell^*(\mathcal{G}) = \infty$ *one immediately gets* $\lambda_0(\mathbf{H}) = \lambda_0^{\mathrm{ess}}(\mathbf{H}) = 0$. *Moreover, in this case* $\sigma(\mathbf{H})$ *coincides with the positive semi-axis* $\mathbb{R}_{\geq 0}$ *(see* [61, Theorem 5.2]*).*

(ii) *The second inequality in* (2.25) *implies that* (2.24) *is necessary for the spectrum of* $\mathbf{H}$ *to be purely discrete. Notice that* $\ell^*_{\mathrm{ess}}(\mathcal{G}) = 0$ *means that the number* $\#\{e \in \mathcal{E} \,|\, |e| > \varepsilon\}$ *is finite for every* $\varepsilon > 0$.

(iii) *The estimates* (2.25) *can be slightly improved by noting that we can use other test functions on the edges* $e \in \mathcal{E}_N$ *to improve the bound* $(\pi/|e|)^2$ *by* $(\pi/2|e|)^2$. *For example, we get the following estimate*

$$\lambda_0(\mathbf{H}) \leq \min\left\{ \inf_{e \in \mathcal{E} \setminus \mathcal{E}_N} \left(\frac{\pi}{|e|}\right)^2, \inf_{e \in \mathcal{E}_N} \left(\frac{\pi}{2|e|}\right)^2 \right\}. \tag{2.28}$$

2.5. **Connection with the difference Laplacian.** In this section we restrict for simplicity to the case of Neumann boundary conditions at the loose ends, that is, $f_e'(v) = 0$ for all $v \in \mathcal{V}$ with $\deg(v) = 1$. Let the weight function $m\colon \mathcal{V} \to \mathbb{R}_{>0}$ be given by (2.10). Consider the difference Laplacian defined in $\ell^2(\mathcal{V}; m)$ by the expression

$$(\tau_{\mathcal{G}} f)(v) := \frac{1}{m(v)} \sum_{u \sim v} \frac{f(v) - f(u)}{|e_{u,v}|}, \quad v \in \mathcal{V}. \tag{2.29}$$

Namely, $\tau_{\mathcal{G}}$ generates in $\ell^2(\mathcal{V}; m)$ the pre-minimal operator

$$\mathbf{h}_0\colon \quad \begin{array}{ccc} \mathrm{dom}(\mathbf{h}_0) & \to & \ell^2(\mathcal{V}; m) \\ f & \mapsto & \tau_{\mathcal{G}} f \end{array}, \qquad \mathrm{dom}(\mathbf{h}_0) := C_c(\mathcal{V}), \tag{2.30}$$

where $C_c(\mathcal{V})$ is the space of finitely supported functions on $\mathcal{V}$. The operator $\mathbf{h}_0$ is a nonnegative symmetric operator. Denote its Friedrichs extension by $\mathbf{h}$.

It was observed in [26] that the operators $\mathbf{H}$ and $\mathbf{h}$ are closely connected (for instance, by [26, Corollary 4.1(i)], $\mathbf{H}_0$ and $\mathbf{h}_0$ are essentially self-adjoint only simultaneously). In fact, it is not difficult to notice a connection between $\mathbf{H}$ and $\mathbf{h}$ by considering their quadratic forms (see [26, Remark 3.7]). Namely, let $\mathcal{L} = \ker(\mathbf{H}_{\max})$ be the kernel of $\mathbf{H}_{\max}$, which consists of piecewise linear functions on $\mathcal{G}$. Every $f \in \mathcal{L}$ can be identified with its values $\{f(e_i), f(e_o)\}_{e \in \mathcal{E}}$ on $\mathcal{V}$ and, moreover,

$$\|f\|^2_{L^2(\mathcal{G})} = \sum_{e \in \mathcal{E}} |e| \frac{|f(e_i)|^2 + \mathrm{Re}(f(e_i) f(e_o)^*) + |f(e_o)|^2}{3}. \tag{2.31}$$

Now restrict ourselves to the subspace $\mathcal{L}_{cont} = \mathcal{L} \cap C_c(\mathcal{G})$. Clearly,

$$\sum_{e \in \mathcal{E}} |e| (|f(e_i)|^2 + |f(e_o)|^2) = \sum_{v \in \mathcal{V}} |f(v)|^2 \sum_{e \in \mathcal{E}_v} |e| = \|f\|^2_{\ell^2(\mathcal{V}; m)}$$

defines an equivalent norm on $\mathcal{L}_{cont}$ since the Cauchy–Schwarz inequality immediately implies

$$\frac{1}{6}\|f\|^2_{\ell^2(\mathcal{V};m)} \le \|f\|^2_{L^2(\mathcal{G})} \le \frac{1}{2}\|f\|^2_{\ell^2(\mathcal{V};m)}. \tag{2.32}$$

On the other hand, for every $f \in \mathcal{L}_{cont}$ we get

$$\begin{aligned}\mathfrak{t}_{\mathcal{G}}[f] = (\mathbf{H}f, f)_{L^2(\mathcal{G})} &= \sum_{e\in\mathcal{E}} \int_e |f'(x_e)|^2 dx_e = \sum_{e\in\mathcal{E}} \frac{|f(e_o) - f(e_i)|^2}{|e|} \\ &= \frac{1}{2}\sum_{u,v\in\mathcal{V}} \frac{|f(v) - f(u)|^2}{|e_{u,v}|} = (\mathbf{h}f, f)_{\ell^2(\mathcal{V};m)} =: \mathfrak{t}_{\mathbf{h}}[f].\end{aligned} \tag{2.33}$$

Hence we end up with the following estimate.

Lemma 2.10.

$$\lambda_0(\mathbf{H}) \le 6\lambda_0(\mathbf{h}), \qquad\qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) \le 6\lambda_0^{\mathrm{ess}}(\mathbf{h}). \tag{2.34}$$

Proof. Clearly, the Rayleigh quotient (2.20) together with (2.32) and (2.33) imply

$$\begin{aligned}\lambda_0(\mathbf{H}) = \inf_{f\in H^1_0(\mathcal{G})} \frac{\mathfrak{t}_{\mathcal{G}}[f]}{\|f\|^2_{L^2(\mathcal{G})}} &\le \inf_{f\in\mathcal{L}_{cont}} \frac{\mathfrak{t}_{\mathcal{G}}[f]}{\|f\|^2_{L^2(\mathcal{G})}} \\ &\le \inf_{f\in C_c(\mathcal{V})} \frac{\mathfrak{t}_{\mathbf{h}}[f]}{\frac{1}{6}\|f\|^2_{\ell^2(\mathcal{V};m)}} = 6\lambda_0(\mathbf{h}).\end{aligned}$$

□

If $\mathcal{G}$ is *equilateral* (that is, $|e| = 1$ for all $e \in \mathcal{E}$), then $m(v) = \deg(v)$ for all $v \in \mathcal{V}$ and hence $\tau_{\mathcal{G}}$ coincides with the *combinatorial Laplacian*

$$(\tau_{\mathrm{comb}} f)(v) := \frac{1}{\deg_{\mathcal{G}}(v)} \sum_{u\sim v} f(v) - f(u), \quad v \in \mathcal{V}. \tag{2.35}$$

In this particular case spectral relations between $\mathbf{H}$ and $\mathbf{h}$ have already been observed by many authors (see [6], [15, Theorem 1], [24] and [11, Theorem 3.18]).

Theorem 2.11. *If $|e| = 1$ for all $e \in \mathcal{E}$, then*

$$\lambda_0(\mathbf{h}) = 1 - \cos\big(\sqrt{\lambda_0(\mathbf{H})}\big), \qquad \lambda_0^{\mathrm{ess}}(\mathbf{h}) = 1 - \cos\big(\sqrt{\lambda_0^{\mathrm{ess}}(\mathbf{H})}\big). \tag{2.36}$$

Remark 2.12. *Actually, far more than* (2.36) *is known in the case of equilateral quantum graphs. In fact, there is a sort of unitary equivalence between equilateral quantum graphs and the corresponding combinatorial Laplacians (see* [53, 54] *and also* [46]*).*

Hence for equilateral graphs we obtain

$$\lambda_0(\mathbf{h}) \le \frac{1}{2}\lambda_0(\mathbf{H}), \qquad\qquad \lambda_0^{\mathrm{ess}}(\mathbf{h}) \le \frac{1}{2}\lambda_0^{\mathrm{ess}}(\mathbf{H}).$$

The latter together with (2.34) imply that for equilateral graphs the following equivalence holds true

$$\lambda_0(\mathbf{H}) > 0 \quad \big(\lambda_0^{\mathrm{ess}}(\mathbf{H}) > 0\big) \qquad \Longleftrightarrow \qquad \lambda_0(\mathbf{h}) > 0 \quad \big(\lambda_0^{\mathrm{ess}}(\mathbf{h}) > 0\big). \tag{2.37}$$

In fact, it was proved recently in [26, Corollary 4.1] that the equivalence (2.37) holds true if the metric graph $\mathcal{G}$ satisfies Hypothesis 2.2. Unfortunately, there is no such simple connection like (2.36) if $\mathcal{G}$ is not equilateral.

Remark 2.13. *Spectral gap estimates for combinatorial Laplacians is an established topic with a vast literature because of their numerous applications (see* [1, 2, 17, 19, 20, 27, 35, 65] *and references therein). Recently there was a considerable interest in the study of spectral bounds for discrete (unbounded) Laplacians on weighted graphs (see* [5, 40]*). On the one hand,* (2.36) *and* (2.37) *indicate that there must be analogous estimates for quantum graphs, however, we should stress that* (2.36) *holds only for equilateral graphs. On the other hand, these connections also indicate that spectral estimates for quantum graphs should have a combinatorial nature.*

Remark 2.14. *Since* $\frac{4}{\pi^2}x \le 1-\cos(\sqrt{x})$ *for all* $x\in[0,\pi^2/4]$, (2.36) *implies the following estimate for equilateral quantum graphs*

$$\lambda_0(\mathbf{H}) \le \frac{\pi^2}{4}\lambda_0(\mathbf{h}), \qquad\qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) \le \frac{\pi^2}{4}\lambda_0^{\mathrm{ess}}(\mathbf{h}),$$

which improves (2.34)*. Moreover, the constant* $\pi^2/4$ *is sharp in the equilateral case. However, it remains unclear to us how sharp is the estimate* (2.34)*.*

3. The Cheeger-type bound

For every $\widetilde{\mathcal{G}}\in\mathcal{K}_{\mathcal{G}}$ we define *the boundary of* $\widetilde{\mathcal{G}}$ *with respect to the graph* $\mathcal{G}$ as the set of all vertices $v\in\widetilde{\mathcal{V}}\setminus\mathcal{V}_N$ such that either $\deg_{\widetilde{\mathcal{G}}}(v)=1$ or $\deg_{\widetilde{\mathcal{G}}}(v)<\deg_{\mathcal{G}}(v)$, that is,

$$\partial_{\mathcal{G}}\widetilde{\mathcal{G}} := \bigl\{v\in\tilde{\mathcal{V}} \mid v\in\mathcal{V}_D \text{ or } \deg_{\widetilde{\mathcal{G}}}(v)<\deg_{\mathcal{G}}(v)\bigr\}. \tag{3.1}$$

For a given finite subgraph $\widetilde{\mathcal{G}}\subset\mathcal{G}$ we then set

$$\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}}) := \sum_{v\in\partial_{\mathcal{G}}\widetilde{\mathcal{G}}}\deg_{\widetilde{\mathcal{G}}}(v). \tag{3.2}$$

Remark 3.1. *Let us stress that our definition of a boundary is different from the combinatorial one. In particular, we define the boundary as the set of vertices whereas the combinatorial definition counts the number of edges connecting* $\widetilde{\mathcal{V}}$ *with its complement* $\mathcal{V}\setminus\widetilde{\mathcal{V}}$.

Definition 3.2. (i) *The isoperimetric (or Cheeger) constant* of a metric graph $\mathcal{G}$ is defined by

$$\alpha(\mathcal{G}) := \inf_{\widetilde{\mathcal{G}}\in\mathcal{K}_{\mathcal{G}}}\frac{\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}})}{\mathrm{mes}(\widetilde{\mathcal{G}})}\in[0,\infty), \tag{3.3}$$

where $\mathrm{mes}(\widetilde{\mathcal{G}})$ denotes the Lebesgue measure of $\widetilde{\mathcal{G}}$, $\mathrm{mes}(\widetilde{\mathcal{G}}) := \sum_{e\in\widetilde{\mathcal{E}}}|e|$.

(ii) *The isoperimetric constant at infinity* is defined by

$$\alpha_{\mathrm{ess}}(\mathcal{G}) := \sup_{\widetilde{\mathcal{G}}\in\mathcal{K}_{\mathcal{G}}}\alpha(\mathcal{G}\setminus\widetilde{\mathcal{G}})\in[0,\infty]. \tag{3.4}$$

Recall that for any $\widetilde{\mathcal{G}}\in\mathcal{K}_{\mathcal{G}}$ we consider $\mathcal{G}\setminus\widetilde{\mathcal{G}}$ with the following boundary conditions: for vertices in $\mathcal{G}\setminus\widetilde{\mathcal{G}}$ having one or more edges in $\widetilde{\mathcal{G}}$, we change the boundary conditions from Kirchhoff–Neumann to Dirichlet; for all other vertices in $\mathcal{G}\setminus\widetilde{\mathcal{G}}$, we leave them the same. These boundary conditions imply that for a subgraph $\mathcal{Y}\in\mathcal{K}_{\mathcal{G}\setminus\widetilde{\mathcal{G}}}$,

$$\partial_{\mathcal{G}\setminus\widetilde{\mathcal{G}}}\mathcal{Y} = \partial_{\mathcal{G}}\mathcal{Y}, \tag{3.5}$$

where the left-hand side is the boundary of $\mathcal{Y}$ with respect to $\mathcal{G} \setminus \widetilde{\mathcal{G}}$ (with the new Dirichlet conditions) and the right-hand side is the boundary with respect to the original graph $\mathcal{G}$. Hence,

$$\alpha(\mathcal{G} \setminus \widetilde{\mathcal{G}}) = \inf_{\mathcal{Y} \in \mathcal{K}_{\mathcal{G} \setminus \widetilde{\mathcal{G}}}} \frac{\deg(\partial_{\mathcal{G} \setminus \widetilde{\mathcal{G}}} \mathcal{Y})}{\mathrm{mes}(\mathcal{Y})} = \inf_{\mathcal{Y} \in \mathcal{K}_{\mathcal{G} \setminus \widetilde{\mathcal{G}}}} \frac{\deg(\partial_{\mathcal{G}} \mathcal{Y})}{\mathrm{mes}(\mathcal{Y})}$$

and $\alpha(\mathcal{G} \setminus \mathcal{G}_1) \le \alpha(\mathcal{G} \setminus \mathcal{G}_2)$ whenever $\mathcal{G}_1 \subseteq \mathcal{G}_2$. Thus,

$$\alpha_{\mathrm{ess}}(\mathcal{G}) = \sup_{\widetilde{\mathcal{G}} \in \mathcal{K}_{\mathcal{G}}} \alpha(\mathcal{G} \setminus \widetilde{\mathcal{G}}) = \lim_{\widetilde{\mathcal{G}} \in \mathcal{K}_{\mathcal{G}}} \alpha(\mathcal{G} \setminus \widetilde{\mathcal{G}}). \tag{3.6}$$

Remark 3.3. *Choosing $\widetilde{\mathcal{G}}$ as an edge $e \in \mathcal{E}$ or a star $\mathcal{E}_v$ with some $v \in \mathcal{V}$, one gets the following simple bounds on the isoperimetric constant*

$$\alpha(\mathcal{G}) \le \frac{2}{\ell^*(\mathcal{G})}, \qquad \alpha(\mathcal{G}) \le \inf_{v \in \mathcal{V}} \frac{\deg_{\mathcal{G}}(v)}{m(v)}. \tag{3.7}$$

The next result is the analog of the famous Cheeger estimate for Laplacians on manifolds [16].

Theorem 3.4.

$$\lambda_0(\mathbf{H}) \ge \frac{1}{4}\alpha(\mathcal{G})^2, \qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) \ge \frac{1}{4}\alpha_{\mathrm{ess}}(\mathcal{G})^2. \tag{3.8}$$

As an immediate corollary we get the following result.

Corollary 3.5. (i) $\mathbf{H}$ *is uniformly positive whenever* $\alpha(\mathcal{G}) > 0$.
 (ii) $\lambda_0^{\mathrm{ess}}(\mathbf{H}) > 0$ *if* $\alpha_{\mathrm{ess}}(\mathcal{G}) > 0$.
 (iii) *The spectrum of* $\mathbf{H}$ *is purely discrete if* $\alpha_{\mathrm{ess}}(\mathcal{G}) = \infty$.
 (iv) *If the metric graph $\mathcal{G}$ has finite total volume,* $\mathrm{mes}(\mathcal{G}) < \infty$*, then* $\mathbf{H}$ *is a uniformly positive operator with purely discrete spectrum.*

Proof. Clearly, we only need to prove (iv). Since $\mathrm{mes}(\mathcal{G}) < \infty$ and taking (3.3) into account, we immediately obtain

$$\alpha(\mathcal{G}) \ge \frac{1}{\mathrm{mes}(\mathcal{G})}, \tag{3.9}$$

which together with (3.8) implies the inequality $\lambda_0(\mathbf{H}) > 0$. Next, using (3.4) together with the estimate (3.9) and the net property of $\mathcal{K}_{\mathcal{G}}$, one gets $\alpha_{\mathrm{ess}}(\mathcal{G}) = \infty$, which finishes the proof. ☐

Before proving the estimates (3.8) we need several preliminary lemmas. In what follows, for every $U \subseteq \mathcal{G}$, we shall denote by ∂U the boundary of a set U in the sense of the natural metric topology on $\mathcal{G}$ (see Section 2.1). For every measurable function $h \colon \mathcal{G} \to \mathbb{R}$ and every $t \in \mathbb{R}$ let us define the set

$$\Omega_h(t) := \{x \in \mathcal{G} |\ h(x) > t\}. \tag{3.10}$$

The next statement is known as the *co-area formula* and we give its proof for the sake of completeness.

Lemma 3.6. *If $h \colon \mathcal{G} \to \mathbb{R}$ is continuous on $\mathcal{G}$ and continuously differentiable on every edge $e \in \mathcal{E}$, then*

$$\int_{\mathcal{G}} |h'(x)|\, dx = \int_{\mathbb{R}} \#(\partial\Omega_h(t))\, dt. \tag{3.11}$$

Proof. Assume first that $\operatorname{supp}(h) \subset e$ for some $e \in \mathcal{E}$. We can identify e with the open interval $(0,|e|)$ and hence

$$M_e := \{x \in e |\ h'(x) \neq 0\}$$

can be written as $M_e = \bigcup_n I_n$ for (at most countably many) disjoint open intervals $I_n \subseteq (0,|e|)$. Since h is strictly monotone on each of these intervals,

$$\begin{aligned}\int_{\mathcal{G}} |h'(x)|\, dx &= \int_e |h'(x)|\, dx = \int_{M_e} |h'(x)|\, dx \\ &= \sum_n \int_{I_n} |h'(x)|\, dx = \sum_n \operatorname{mes}(h(I_n)) = \sum_n \int_{\mathbb{R}} \mathbb{1}_{h(I_n)}(s)\, ds.\end{aligned}$$

Here $\operatorname{mes}(X)$ denotes the Lebesgue measure of $X \subseteq \mathbb{R}$. Moreover, by continuity of h, it is straightforward to check that $\mathbb{1}_{h(I_n)}(t) = \#(\partial\Omega_h(t) \cap I_n)$ for all $t \in \mathbb{R}$. Hence we end up with

$$\sum_n \int_{\mathbb{R}} \mathbb{1}_{h(I_n)}(t)\, dt = \sum_n \int_{\mathbb{R}} \#(\partial\Omega_h(t) \cap I_n)\, dt = \int_{\mathbb{R}} \#(\partial\Omega_h(t) \cap M_e)\, dt.$$

Now assume that $t \in \mathbb{R}$ is such that $\partial\Omega_h(t) \cap M_e^c \neq \varnothing$, where

$$M_e^c := e \setminus M_e = \{x \in e |\ h'(x) = 0\}$$

is the set of critical points of h. By Sard's Theorem [60], $h(M_e^c)$ has Lebesgue measure zero and hence

$$\int_{\mathbb{R}} \#(\partial\Omega_h(t) \cap M_e)\, dt = \int_{\mathbb{R}} \#(\partial\Omega_h(t) \cap e)\, dt.$$

Assume now that $h\colon \mathcal{G} \to \mathbb{R}$ is an arbitrary function satisfying the assumptions. Then we get

$$\begin{aligned}\int_{\mathcal{G}} |h'(x)|\, dx &= \sum_{e\in\mathcal{E}} \int_e |h'(x)|\, dx \\ &= \sum_{e\in\mathcal{E}} \int_{\mathbb{R}} \#(\partial\Omega_h(t) \cap e)\, dt = \int_{\mathbb{R}} \#(\partial\Omega_h(t) \cap (\mathcal{G}\backslash\mathcal{V}))\, dt.\end{aligned}$$

If $\partial\Omega_h(t) \cap \mathcal{V} \neq \varnothing$, then $t \in h(\mathcal{V})$. Since $\mathcal{V}$ is countable, we arrive at (3.11). $\square$

Next it will turn out useful to rewrite the Cheeger constant (3.3) in the following way. Let

$$\widetilde{\alpha}(\mathcal{G}) := \inf_{U\in\mathcal{U}_{\mathcal{G}}} \frac{\#(\partial U)}{\operatorname{mes}(U)}, \tag{3.12}$$

where $\mathcal{U}_{\mathcal{G}} = \cup_{\widetilde{\mathcal{G}}\in\mathcal{K}_{\mathcal{G}}} \mathcal{U}_{\widetilde{\mathcal{G}}}$ and

$$\mathcal{U}_{\widetilde{\mathcal{G}}} = \{U \subseteq \widetilde{\mathcal{G}} |\ U \text{ is open, } U \cap \mathcal{V}_D = \varnothing \text{ and } \partial U \cap \mathcal{V} = \varnothing\}. \tag{3.13}$$

Lemma 3.7. *Let* $\alpha(\mathcal{G})$ *be defined by* (3.3). *Then*

$$\alpha(\mathcal{G}) = \widetilde{\alpha}(\mathcal{G}). \tag{3.14}$$

Proof. (i) It easily follows from the definition of $\widetilde{\alpha}(\mathcal{G})$ that

$$\widetilde{\alpha}(\mathcal{G}) \leq \alpha(\mathcal{G}).$$

Indeed, assume first that $\widetilde{\mathcal{G}} \in \mathcal{K}_{\mathcal{G}}$ and identify $\widetilde{\mathcal{G}}$ with a closed subset of the graph. For a sufficiently small $\varepsilon > 0$, we cut out a ball $B_\varepsilon(v)$ of radius ε at each point in $v \in \partial_{\mathcal{G}}\widetilde{\mathcal{G}}$ and obtain the set

$$U := \widetilde{\mathcal{G}} \setminus \bigcup_{v \in \partial_{\mathcal{G}}\widetilde{G}} B_\varepsilon(v).$$

We have $U \in \mathcal{U}_{\mathcal{G}}$ and, moreover, ∂U has precisely $\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}})$ points. In total,

$$\frac{\#(\partial U)}{\mathrm{mes}(U)} = \frac{\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}})}{\mathrm{mes}(\widetilde{\mathcal{G}}) - \varepsilon \deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}})}.$$

Letting ε tend to zero, we obtain the desired inequality.

(ii) To prove the other inequality, let $U \in \mathcal{U}_{\mathcal{G}}$ and $\widetilde{\mathcal{G}} = (\widetilde{\mathcal{V}}, \widetilde{\mathcal{E}})$ be the finite subgraph consisting of all edges $e \in \mathcal{E}$ with $e \cap U \neq \varnothing$ and all vertices incident to such an edge. Clearly, $\mathrm{mes}(U) \le \mathrm{mes}(\widetilde{\mathcal{G}})$. Also, by (3.2),

$$\begin{aligned}\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}}) = \sum_{v \in \partial\widetilde{\mathcal{G}}} \deg_{\widetilde{\mathcal{G}}}(v) =& \#\{e \in \widetilde{\mathcal{E}} |\ e \text{ connects } \partial_{\mathcal{G}}\widetilde{\mathcal{G}} \text{ and } \widetilde{\mathcal{G}} \setminus \partial_{\mathcal{G}}\widetilde{\mathcal{G}}\} \\ &+ 2\#\{e \in \widetilde{\mathcal{E}} |\ \text{ both vertices are in } \partial_{\mathcal{G}}\widetilde{\mathcal{G}}\}.\end{aligned}$$

Since U is open, every point of $\partial_{\mathcal{G}}\widetilde{\mathcal{G}}$ is not in U. Therefore, every edge in the subgraph $\widetilde{\mathcal{G}}$ connected to a vertex in $\partial_{\mathcal{G}}\widetilde{\mathcal{G}}$ must contain at least one boundary point of U. If both vertices of the edge are in $\partial_{\mathcal{G}}\widetilde{\mathcal{G}}$, it must even contain at least two boundary points of U. Also, since $\mathcal{V} \cap \partial U = \varnothing$, the boundary points lie in the strict interior of each edge and therefore cannot coincide for different edges. Thus, $\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}}) \le \#(\partial U)$.

Finally, notice that $\widetilde{\mathcal{G}}$ might be disconnected. If it is the case, then write $\widetilde{\mathcal{G}} = \dot\cup_n \widetilde{\mathcal{G}}_n$ as a disjoint, finite union of connected subgraphs $\widetilde{\mathcal{G}}_n \in \mathcal{K}_{\mathcal{G}}$. Then

$$\frac{\#(\partial U)}{\mathrm{mes}(U)} \ge \frac{\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}})}{\mathrm{mes}(\widetilde{\mathcal{G}})} = \frac{\sum_n \deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}}_n)}{\sum_n \mathrm{mes}(\widetilde{\mathcal{G}}_n)} \ge \min_n \frac{\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}}_n)}{\mathrm{mes}(\widetilde{\mathcal{G}}_n)},$$

which implies that $\widetilde{\alpha}(\mathcal{G}) \ge \alpha(\mathcal{G})$. □

Now we are in position to prove the Cheeger-type estimates (3.8).

Proof of Theorem 3.4. Let us show that the following inequality

$$\alpha(\mathcal{G})\, \|f\|_{L^2(\mathcal{G})} \le 2\|f'\|_{L^2(\mathcal{G})} \tag{3.15}$$

holds true for all $f \in \mathrm{dom}(\mathfrak{t}^0_{\mathcal{G}}) = \mathrm{dom}(\mathbf{H}_0)$. Without loss of generality we can restrict ourselves to real-valued functions. So, suppose $f \in \mathrm{dom}(\mathbf{H}_0)$ is real-valued. Observe that (see, e.g., [32, Lemma I.4.1])

$$\|f\|^2_{L^2(\mathcal{G})} = \int_{\mathcal{G}} f(x)^2\, dx = \int_0^\infty \mathrm{mes}(\Omega_{f^2}(t))\, dt.$$

Next we want to use Lemma 3.7 with $h = f^2$. If $t > 0$ is such that $\partial\Omega_{f^2}(t) \cap \mathcal{V} \neq \varnothing$, then $t \in f^2(\mathcal{V})$ by continuity of f^2. Since $\mathcal{V}$ and hence $f^2(\mathcal{V})$ are countable, we get that $\Omega_{f^2}(t) \in \mathcal{U}_{\mathcal{G}}$ for almost every $t > 0$. Thus, in view of Lemma 3.7

$$\alpha(\mathcal{G})\|f\|^2_{L^2} \le \int_0^\infty \#(\partial\Omega_{f^2}(t))\, dt. \tag{3.16}$$

On the other hand, applying Lemma 3.6 to $h = f^2$ and then the Cauchy–Schwarz inequality, we get

$$\int_0^\infty \#(\partial\Omega_{f^2}(t))dt = 2\int_{\mathcal{G}} |f(x)f'(x)|dx \le 2\|f\|_{L^2(\mathcal{G})}\|f'\|_{L^2(\mathcal{G})}. \tag{3.17}$$

Combining the last two inequalities, we arrive at (3.15), which together with the Rayleigh quotient (2.20) proves the first inequality in (3.8).

The proof of the second inequality in (3.8) follows the same line of reasoning since by (2.21)

$$\lambda_0^{\mathrm{ess}}(\mathbf{H}) \ge \inf_{\substack{f\in\widetilde{H}_0^1(\mathcal{G}\setminus\widetilde{\mathcal{G}})\\ f\neq 0}} \frac{\|f'\|^2_{L^2(\mathcal{G}\setminus\widetilde{\mathcal{G}})}}{\|f\|^2_{L^2(\mathcal{G}\setminus\widetilde{\mathcal{G}})}},$$

for every finite subgraph $\widetilde{\mathcal{G}}$ of $\mathcal{G}$. Notice that the boundary conditions on $\mathcal{G}\setminus\widetilde{\mathcal{G}}$ are defined after (3.4). □

Remark 3.8. *The Cheeger estimate for finite quantum graphs was first proved in* [51] *(see also* [57, §6] *and* [40]*). Our result extends* [51, Theorem 3.2] *to the case of infinite graphs and also provides a bound on the essential spectrum of* $\mathbf{H}$. *However, our definition of the isoperimetric constant* (3.8) *is purely combinatorial since the infimum is taken over finite connected subgraphs of* $\mathcal{G}$*, although the definition in* [51] *(see also* [41, 57]*) is similar to* (3.12).

Let us mention that one can obtain a similar statement for the operator $\mathbf{H}^N$ *that is related to the maximally defined quadratic form (see Remark 2.6). However, one needs to take the infimum in the definition of the isoperimetric constant over all subgraphs of finite volume.*

Taking into account the equivalence (2.22), let us finish this section with the next observation.

Lemma 3.9. *The following equivalence holds true*

$$\alpha(\mathcal{G}) = 0 \qquad \Longleftrightarrow \qquad \alpha_{\mathrm{ess}}(\mathcal{G}) = 0. \tag{3.18}$$

Proof. Clearly, we only need to prove the implication $\alpha(\mathcal{G}) = 0 \Rightarrow \alpha_{\mathrm{ess}}(\mathcal{G}) = 0$. Assume the converse, that is, there is an infinite graph $\mathcal{G}$ satisfying Hypotheses 2.1–2.3 such that $\alpha(\mathcal{G}) = 0$ and $\alpha_{\mathrm{ess}}(\mathcal{G}) > 0$. Then by (3.3), there is a sequence $\{\mathcal{G}_n\} \subset \mathcal{K}_{\mathcal{G}}$ such that

$$\alpha(\mathcal{G}) = \lim_{n\to\infty} \frac{\deg(\partial_{\mathcal{G}}\mathcal{G}_n)}{\mathrm{mes}(\mathcal{G}_n)} = 0.$$

On the other hand, (3.4) implies that there is $\widetilde{\mathcal{G}} \in \mathcal{K}_{\mathcal{G}}$ such that $\alpha(\mathcal{G}\setminus\widetilde{\mathcal{G}}) = \alpha_0 > 0$. In particular, taking into account (3.5), the latter is equivalent to the fact that

$$\frac{\deg(\partial_{\mathcal{G}\setminus\widetilde{\mathcal{G}}}\mathcal{Y})}{\mathrm{mes}(\mathcal{Y})} = \frac{\deg(\partial_{\mathcal{G}}\mathcal{Y})}{\mathrm{mes}(\mathcal{Y})} \ge \alpha_0 > 0$$

for every finite subgraph $\mathcal{Y} \subset \mathcal{G}\setminus\widetilde{\mathcal{G}}$.

Next observe that

$$\lim_{n\to\infty} \frac{\deg(\partial_{\mathcal{G}}(\mathcal{G}_n\setminus\widetilde{\mathcal{G}}))}{\mathrm{mes}(\mathcal{G}_n\setminus\widetilde{\mathcal{G}})} = 0,$$

which leads to a contradiction. Indeed, by construction, $\lim_{n\to\infty} \mathrm{mes}(\mathcal{G}_n) = \infty$ and hence $\mathrm{mes}(\mathcal{G}_n \setminus \widetilde{\mathcal{G}}) = \mathrm{mes}(\mathcal{G}_n)(1 + o(1))$ as $n \to \infty$. It remains to note that

$$\deg(\partial_{\mathcal{G}}\mathcal{G}_n) - \deg(\widetilde{\mathcal{G}}) \le \deg(\partial_{\mathcal{G}}(\mathcal{G}_n \setminus \widetilde{\mathcal{G}})) \le \deg(\partial_{\mathcal{G}}\mathcal{G}_n) + \deg(\widetilde{\mathcal{G}}). \qquad \square$$

4. Connections with discrete isoperimetric constants

For every vertex set $X \subseteq \mathcal{V}$, we define its boundary and interior edges by

$$\mathcal{E}_b(X) = \{e \in \mathcal{E} |\ e \text{ connects } X \text{ and } \mathcal{V}\backslash X\},$$
$$\mathcal{E}_i(X) = \{e \in \mathcal{E} |\ \text{all vertices incident to } e \text{ are in } X\}.$$

Also, for a vertex set $X \subseteq \mathcal{V}$ we set

$$m(X) := \sum_{v\in X} m(v),$$

where $m\colon \mathcal{V} \to (0, \infty)$ is defined by (2.10) (in fact, $m(v) = \mathrm{mes}(\mathcal{E}_v)$ for every $v \in \mathcal{V}$). *The (discrete) isoperimetric constant* $\alpha_d(Y)$ of $Y \subseteq \mathcal{V}$ is defined by

$$\alpha_d(Y) := \inf_{\substack{X\subseteq Y\\ X \text{ is finite}}} \frac{\#(\mathcal{E}_b(X))}{m(X)} \in [0, \infty). \tag{4.1}$$

The discrete isoperimetric constant of the graph $\mathcal{G}$ is then given by

$$\alpha_d(\mathcal{V}) := \inf_{\substack{X\subseteq \mathcal{V}\\ X \text{ is finite}}} \frac{\#(\mathcal{E}_b(X))}{m(X)} \in [0, \infty). \tag{4.2}$$

Moreover, we need the *discrete isoperimetric constant at infinity*

$$\alpha_d^{\mathrm{ess}}(\mathcal{V}) := \sup_{\substack{X\subseteq \mathcal{V}\\ X \text{ is finite}}} \alpha_d(\mathcal{V} \setminus X) \in [0, \infty]. \tag{4.3}$$

Remark 4.1. *Our definition of the isoperimetric constants follows the one provided in Appendix A (see Remark A.4). This definition is slightly different from the one given in* [5]*, which uses the notion of an intrinsic metric on $\mathcal{V}$ (cf.* [29]*). In particular, the natural path metric ϱ_0 (cf. Section 2.3) is intrinsic in the sense of* [5, 29] *and in certain cases (if, for example, $\mathcal{G}_d$ is a tree) the corresponding definitions from* [5] *coincide with* (4.2) *and* (4.3)*. Notice that the following Cheeger-type estimates for the discrete Laplacian* (2.29)–(2.30) *(see* [5, Theorems 3.1 and 3.3] *and Theorem A.1) hold true*

$$\lambda_0(\mathbf{h}) \ge \frac{1}{2}\alpha_d(\mathcal{V})^2, \qquad \lambda_0^{\mathrm{ess}}(\mathbf{h}) \ge \frac{1}{2}\alpha_d^{\mathrm{ess}}(\mathcal{V})^2. \tag{4.4}$$

The next result provides a connection between isoperimetric constants.

Lemma 4.2. *The isoperimetric constants* (3.3) *and* (4.2) *can be related by*

$$\frac{1}{2}\alpha(\mathcal{G}) \le \alpha_d(\mathcal{V}), \qquad \frac{2}{\alpha(\mathcal{G})} \le \frac{1}{\alpha_d(\mathcal{V})} + \ell^*(\mathcal{G}). \tag{4.5}$$

In particular, the isoperimetric constants at infinity (3.4) *and* (4.3) *satisfy*

$$\frac{1}{2}\alpha_{\mathrm{ess}}(\mathcal{G}) \le \alpha_d^{\mathrm{ess}}(\mathcal{V}), \qquad \frac{2}{\alpha_{\mathrm{ess}}(\mathcal{G})} \le \frac{1}{\alpha_d^{\mathrm{ess}}(\mathcal{V})} + \ell^*_{\mathrm{ess}}(\mathcal{G}). \tag{4.6}$$

Proof. (i) First, let $X \subset \mathcal{V}$ be finite. Let also $\widetilde{\mathcal{G}} = (\widetilde{\mathcal{V}}, \widetilde{\mathcal{E}})$ be the finite subgraph of $\mathcal{G}$ consisting of all edges with at least one vertex in the set X. Observe that

$$\widetilde{\mathcal{E}} = \bigcup_{v \in X} \mathcal{E}_v = \mathcal{E}_i(X) \cup \mathcal{E}_b(X).$$

Then

$$m(X) = \sum_{v \in X} m(v) = 2 \sum_{e \in \mathcal{E}_i(X)} |e| + \sum_{e \in \mathcal{E}_b(X)} |e| \leq 2 \sum_{e \in \widetilde{\mathcal{E}}} |e| = 2 \operatorname{mes}(\widetilde{\mathcal{G}}).$$

Note that for every $v \in X$, the whole star $\mathcal{E}_v$ attached to it is in $\widetilde{\mathcal{G}}$. Therefore, every vertex from $\partial_{\mathcal{G}} \widetilde{\mathcal{G}}$ is not in X. Now consider an edge e in the subgraph $\widetilde{\mathcal{G}}$ which is connected to a vertex $v \in \partial_{\mathcal{G}} \widetilde{\mathcal{G}}$. Then its other endpoint must be in X (because of the definition of $\widetilde{\mathcal{G}}$). Hence

$$\begin{aligned}
\deg(\partial_{\mathcal{G}} \widetilde{\mathcal{G}}) = \sum_{v \in \partial \widetilde{\mathcal{G}}} \deg_{\widetilde{\mathcal{G}}}(v) &= \sum_{v \in \partial \widetilde{\mathcal{G}}} \#\{e |\ e \text{ connects } v \text{ and } X\} \\
&\leq \#\{e \in \widetilde{\mathcal{E}} |\ e \text{ connects } X \text{ and } \mathcal{V} \backslash X\} = \#(\mathcal{E}_b(X)).
\end{aligned}$$

Splitting $\widetilde{\mathcal{G}}$ in finitely many connected components as in the proof of Lemma 3.7, we arrive at the first inequality in (4.5).

To prove the second inequality, assume $\widetilde{\mathcal{G}} \in \mathcal{K}_{\mathcal{G}}$. Write $\widetilde{\mathcal{E}} = \widetilde{\mathcal{E}}_0 \cup \widetilde{\mathcal{E}}_1 \cup \widetilde{\mathcal{E}}_2$, where $\widetilde{\mathcal{E}}_0$, $\widetilde{\mathcal{E}}_1$, $\widetilde{\mathcal{E}}_2$ are the sets of edges in the subgraph with, respectively, none, one, and two vertices in $\partial_{\mathcal{G}} \widetilde{\mathcal{G}}$. Clearly,

$$\deg(\partial_{\mathcal{G}} \widetilde{\mathcal{G}}) = \#(\widetilde{\mathcal{E}}_1) + 2\#(\widetilde{\mathcal{E}}_2). \tag{4.7}$$

Now define the finite vertex set $X := \widetilde{\mathcal{V}} \backslash \partial_{\mathcal{G}} \widetilde{\mathcal{G}}$. We have

$$\mathcal{E}_i(X) = \widetilde{\mathcal{E}}_0, \qquad\qquad \mathcal{E}_b(X) = \widetilde{\mathcal{E}}_1.$$

Thus,

$$\begin{aligned}
2 \frac{\operatorname{mes}(\widetilde{\mathcal{G}})}{\deg(\partial_{\mathcal{G}} \widetilde{\mathcal{G}})} &= 2 \frac{\sum_{e \in \widetilde{\mathcal{E}}_0} |e| + \sum_{e \in \widetilde{\mathcal{E}}_1} |e| + \sum_{e \in \widetilde{\mathcal{E}}_2} |e|}{\#(\widetilde{\mathcal{E}}_1) + 2\#(\widetilde{\mathcal{E}}_2)} \\
&= \frac{2 \sum_{e \in \mathcal{E}_i(X)} |e| + \sum_{e \in \mathcal{E}_b(X)} |e|}{\#(\mathcal{E}_b(X)) + 2\#(\widetilde{\mathcal{E}}_2)} + \frac{\sum_{e \in \mathcal{E}_b(X)} |e| + 2 \sum_{e \in \widetilde{\mathcal{E}}_2} |e|}{\#(\mathcal{E}_b(X)) + 2\#(\widetilde{\mathcal{E}}_2)} \\
&= \frac{m(X)}{\#(\mathcal{E}_b(X)) + 2\#(\widetilde{\mathcal{E}}_2)} + \frac{\sum_{e \in \mathcal{E}_b(X)} |e| + 2 \sum_{e \in \widetilde{\mathcal{E}}_2} |e|}{\#(\mathcal{E}_b(X)) + 2\#(\widetilde{\mathcal{E}}_2)} \\
&\leq \frac{m(X)}{\#(\mathcal{E}_b(X))} + \frac{\sum_{e \in \mathcal{E}_b(X)} |e| + 2 \sum_{e \in \widetilde{\mathcal{E}}_2} |e|}{\#(\mathcal{E}_b(X)) + 2\#(\widetilde{\mathcal{E}}_2)} \leq \frac{m(X)}{\#(\mathcal{E}_b(X))} + \sup_{e \in \mathcal{E}} |e|.
\end{aligned}$$

(ii) To prove (4.6), let first $X \subseteq \mathcal{V}$ be a finite and connected (in the sense that for two vertices in X, there always exists a path connecting them and only passing through vertices in X) set of vertices. Then the subgraph $\widetilde{\mathcal{G}}_X \subseteq \mathcal{G}$ consisting of all edges with both vertices in X is finite and connected. Now note that for a finite vertex set $Y \subseteq \mathcal{V} \setminus X$, the subgraph $\widetilde{\mathcal{G}}_Y$ defined above is contained in $\mathcal{G} \setminus \widetilde{\mathcal{G}}_X$. Hence taking into account (3.5) and using the same line of reasoning as in (i), we get $\alpha(\mathcal{G} \setminus \widetilde{\mathcal{G}}_X) \leq 2\alpha_d(\mathcal{V} \setminus X)$. Finally, choose an increasing sequence $\{X_n\} \subseteq \mathcal{V}$ of finite and connected vertex sets such that every finite vertex set $X \subseteq \mathcal{V}$ is eventually contained in X_n. Then the corresponding sequence $\{\widetilde{\mathcal{G}}_n\} \subseteq \mathcal{K}_{\mathcal{G}}$ of subgraphs is increasing and every finite, connected subgraph $\widetilde{\mathcal{G}} \in \mathcal{K}_{\mathcal{G}}$ is eventually contained in $\widetilde{\mathcal{G}}_n$. In view of (3.6), we obtain the first inequality in (4.6) by taking limits.

To prove the second, for a subgraph $\mathcal{G}_0 \in \mathcal{K}_{\mathcal{G}}$, choose X to be the set of vertices in $\mathcal{G}_0$. Let $\widetilde{\mathcal{G}} \in \mathcal{K}_{\mathcal{G}\setminus\mathcal{G}_0}$. If a vertex v is both in $\widetilde{\mathcal{V}}$ and in X, then it has at least one incident edge which lies in the cut out graph $\mathcal{G}_0$ and therefore $v \in \partial_{\mathcal{G}}\widetilde{\mathcal{G}}$. Thus, the vertex set $Y = \widetilde{\mathcal{V}}\backslash\partial_{\mathcal{G}}\widetilde{\mathcal{G}}$ satisfies $Y \cap X = \varnothing$. Refining the previous estimate,

$$2\frac{\operatorname{mes}(\widetilde{\mathcal{G}})}{\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}})} \le \frac{m(Y)}{\#(\mathcal{E}_b(Y))} + \frac{\sum_{e\in\mathcal{E}_b(Y)}|e| + 2\sum_{e\in\widetilde{\mathcal{E}}_2}|e|}{\#(\mathcal{E}_b(Y)) + 2\#(\widetilde{\mathcal{E}}_2)} \le \frac{m(Y)}{\#(\mathcal{E}_b(Y))} + \ell^*(\mathcal{G}\setminus\mathcal{G}_0).$$

and hence

$$\frac{2}{\alpha(\mathcal{G}\setminus\mathcal{G}_0)} \le \frac{1}{\alpha_d(\mathcal{V}\setminus X)} + \ell^*(\mathcal{G}\setminus\mathcal{G}_0).$$

Choosing an increasing sequence $\{\mathcal{G}_n\} \subseteq \mathcal{K}_{\mathcal{G}}$ such that every $\mathcal{G}_0 \in \mathcal{K}_{\mathcal{G}}$ is eventually contained in $\mathcal{G}_n$ and applying the same limit argument as before, we arrive at the second inequality in (4.6). $\square$

Remark 4.3. *It can be seen by examples that the estimates* (4.5) *and* (4.6) *are sharp. Indeed, on the equilateral Bethe lattice (see Example 8.3), one gets equalities in the second inequalities* (4.5) *and* (4.6) *(cf.* (8.3)*).*

Combining (4.5) with Corollary 3.5, we obtain Theorem 4.18 from [26].

Corollary 4.4 ([26])**.** (i) *$\lambda_0(\mathbf{H}) > 0$ if $\alpha_d(\mathcal{V}) > 0$.*
(ii) *$\lambda_0^{\mathrm{ess}}(\mathbf{H}) > 0$ if $\alpha_d^{\mathrm{ess}}(\mathcal{V}) > 0$.*
(iii) *The spectrum of $\mathbf{H}$ is purely discrete if the number $\#\{e \in \mathcal{E} \colon |e| > \varepsilon\}$ is finite for every $\varepsilon > 0$ and $\alpha_d^{\mathrm{ess}}(\mathcal{V}) = \infty$.*

Proof. We only need to mention that $\ell^*_{\mathrm{ess}}(\mathcal{G}) = 0$ if and only if the number $\#\{e \in \mathcal{E} \colon |e| > \varepsilon\}$ is finite for every $\varepsilon > 0$. Moreover, in this case it follows from (4.6) that $\alpha^{\mathrm{ess}}(\mathcal{G}) = \alpha_d^{\mathrm{ess}}(\mathcal{V})$. $\square$

Finally, let us mention that in the case of equilateral graphs the discrete isoperimetric constants coincide with the combinatorial isoperimetric constants introduced in [22]:

$$\alpha_{\mathrm{comb}}(\mathcal{V}) = \inf_{X\in\mathcal{V}} \frac{\#(\partial X)}{\deg(X)}, \qquad \alpha_{\mathrm{comb}}^{\mathrm{ess}}(\mathcal{V}) = \sup_{\substack{X\subseteq\mathcal{V}\\ X \text{ is finite}}} \alpha_{\mathrm{comb}}(\mathcal{V}\setminus X) \tag{4.8}$$

Comparing (4.8) with (4.2) and (4.3) and noting that

$$\ell_*(\mathcal{G})\deg_{\mathcal{G}}(v) \le m(v) \le \ell^*(\mathcal{G})\deg_{\mathcal{G}}(v)$$

for all $v \in \mathcal{V}$, one easily derives the estimates

$$\frac{\alpha_{\mathrm{comb}}(\mathcal{V})}{\ell^*(\mathcal{G})} \le \alpha_d(\mathcal{V}) \le \frac{\alpha_{\mathrm{comb}}(\mathcal{V})}{\ell_*(\mathcal{G})}, \qquad \frac{\alpha_{\mathrm{comb}}^{\mathrm{ess}}(\mathcal{V})}{\ell^*_{\mathrm{ess}}(\mathcal{G})} \le \alpha_d^{\mathrm{ess}}(\mathcal{V}) \le \frac{\alpha_{\mathrm{comb}}^{\mathrm{ess}}(\mathcal{V})}{\ell_*^{\mathrm{ess}}(\mathcal{G})}.$$

Here

$$\ell_*^{\mathrm{ess}}(\mathcal{G}) := \sup_{\widetilde{\mathcal{E}}} \inf_{e\in\mathcal{E}\setminus\widetilde{\mathcal{E}}} |e|, \tag{4.9}$$

and the supremum is taken over all finite subsets $\widetilde{\mathcal{E}}$ of $\mathcal{E}$. Moreover, taking into account Lemma 4.2, we get the following connection between our isoperimetric constants and the combinatorial ones:

$$\frac{2\,\alpha_{\mathrm{comb}}(\mathcal{V})}{\ell^*(\mathcal{G})(1+\alpha_{\mathrm{comb}}(\mathcal{V}))} \le \alpha(\mathcal{G}) \le \frac{2\,\alpha_{\mathrm{comb}}(\mathcal{V})}{\ell_*(\mathcal{G})} \tag{4.10}$$

and

$$\frac{2\,\alpha^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{V})}{\ell^*_{\mathrm{ess}}(\mathcal{G})(1+\alpha^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{V}))} \le \alpha^{\mathrm{ess}}(\mathcal{G}) \le \frac{2\,\alpha^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{V})}{\ell^{\mathrm{ess}}_*(\mathcal{G})}. \tag{4.11}$$

Since $\alpha_{\mathrm{comb}}(\mathcal{V}) \in [0,1)$, we end up with the following result.

Corollary 4.5. *Let $\mathcal{G}$ be a metric graph such that $\ell^*(\mathcal{G}) < \infty$. Then:*

(i) $\lambda_0(\mathbf{H}) > 0$ *if* $\alpha_{\mathrm{comb}}(\mathcal{V}) > 0$.
(ii) $\lambda_0^{\mathrm{ess}}(\mathbf{H}) > 0$ *whenever* $\alpha^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{V}) > 0$.
(iii) *The spectrum of* $\mathbf{H}$ *is purely discrete if* $\ell^*_{\mathrm{ess}}(\mathcal{G}) = 0$ *and* $\alpha^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{V}) > 0$.

5. Upper bounds via the isoperimetric constant

It is possible to use the isoperimetric constants to estimate $\lambda_0(\mathbf{H})$ and $\lambda_0^{\mathrm{ess}}(\mathbf{H})$ from above, however, for this we need to impose additional restrictions on the metric graph.

Lemma 5.1. *Suppose that $\ell_*(\mathcal{G}) = \inf_{e\in\mathcal{E}} |e| > 0$. Then*

$$\lambda_0(\mathbf{H}) \le \frac{\pi^2}{2\,\ell_*(\mathcal{G})}\alpha(\mathcal{G}), \qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) \le \frac{\pi^2}{2\,\ell^{\mathrm{ess}}_*(\mathcal{G})}\alpha_{\mathrm{ess}}(\mathcal{G}). \tag{5.1}$$

Proof. To estimate $\lambda_0(\mathbf{H})$, choose any $\phi \in H^1([0,1])$ with $\phi(0) = 0$, $\phi(1) = 1$ and $\|\phi\|_{L^2(0,1)} = 1$ and set

$$\widetilde{\phi}(x) := \mathbb{1}_{[0,1/2]}(x)\phi(2x) + \mathbb{1}_{(1/2,1]}(x)\phi(2-2x), \qquad x \in [0,1].$$

Assume a subgraph $\mathcal{G}_0 \in \mathcal{K}_{\mathcal{G}}$ and a finite, connected subgraph $\widetilde{\mathcal{G}} = (\widetilde{\mathcal{V}}, \widetilde{\mathcal{E}})$ of $\mathcal{G}\setminus\mathcal{G}_0$. Then define $g \in \widetilde{H}^1_c(\mathcal{G}\setminus\mathcal{G}_0)$ by setting

$$g(x_e) := \begin{cases} 0, & e \in \mathcal{E}_{\mathcal{G}\setminus\mathcal{G}_0},\ e \notin \widetilde{\mathcal{E}} \\ 1, & e \in \widetilde{\mathcal{E}}_0 \\ \phi(\frac{|x_e-u|}{|e|}), & e = e_{u,\tilde{u}} \in \widetilde{\mathcal{E}}_1, u \in \partial\widetilde{\mathcal{G}} \\ \widetilde{\phi}(\frac{|x_e-e_o|}{|e|}), & e \in \widetilde{\mathcal{E}}_2 \end{cases},$$

where $\widetilde{\mathcal{E}}_0$, $\widetilde{\mathcal{E}}_1$, $\widetilde{\mathcal{E}}_2$ are defined as in the previous subsection and $|x_e - y|$ denotes the distance between $x_e \in e$ and some $y \in e$. If $\mathcal{G}_0 \neq \varnothing$ and $v \in \mathcal{G}\setminus\mathcal{G}_0$ is a vertex with at least one incident edge in $\mathcal{G}_0$, then either v is not in $\widetilde{\mathcal{V}}$ or v is a boundary vertex of $\widetilde{\mathcal{G}}$. In both cases, g vanishes at v. Therefore, $g \in \widetilde{H}^1(\mathcal{G}\setminus\mathcal{G}_0)$. Next we get

$$\|g\|^2_{L^2(\mathcal{G}\setminus\mathcal{G}_0)} = \sum_{e\in\widetilde{\mathcal{E}}_0} |e| + \sum_{e\in\widetilde{\mathcal{E}}_1} |e|\|\phi\|^2_{L^2(0,1)} + \sum_{e\in\widetilde{\mathcal{E}}_2} 2\frac{|e|}{2}\|\phi\|^2_{L^2(0,1)} = \mathrm{mes}(\widetilde{\mathcal{G}}),$$

and, in view of (4.7),

$$\begin{aligned}\|g'\|^2_{L^2(\mathcal{G}\setminus\mathcal{G}_0)} &= \sum_{e\in\widetilde{\mathcal{E}}_1} \frac{1}{|e|}\|\phi'\|^2_{L^2(0,1)} + \sum_{e\in\widetilde{\mathcal{E}}_2} \frac{4}{|e|}\|\phi'\|^2_{L^2(0,1)} \\ &\le \frac{\|\phi'\|^2_{L^2(0,1)}}{\ell_*(\mathcal{G}\setminus\mathcal{G}_0)}(\#(\widetilde{\mathcal{E}}_1) + 4\#(\widetilde{\mathcal{E}}_2)) \le \frac{2\|\phi'\|^2_{L^2(0,1)}}{\ell_*(\mathcal{G}\setminus\mathcal{G}_0)}\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}}).\end{aligned}$$

Choosing $\phi(x) = \sqrt{2}\sin(\frac{\pi}{2}x)$, we obtain the estimate

$$\frac{\|g'\|^2_{L^2(\mathcal{G}\setminus\mathcal{G}_0)}}{\|g\|^2_{L^2(\mathcal{G}\setminus\mathcal{G}_0)}} \le \frac{\pi^2}{2\,\ell_*(\mathcal{G}\setminus\mathcal{G}_0)}\frac{\deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}})}{\mathrm{mes}(\widetilde{\mathcal{G}})}.$$

Choosing $\mathcal{G}_0 = \varnothing$, (2.20) and (3.8) imply the first inequality in (5.1). Now assume $\mathcal{G}_0 \neq \varnothing$. Then

$$\inf_{\substack{f\in\widetilde{H}^1(\mathcal{G}\setminus\mathcal{G}_0)\\ f\neq 0}} \frac{\|f'\|^2_{L^2(\mathcal{G}\setminus\mathcal{G}_0)}}{\|f\|^2_{L^2(\mathcal{G}\setminus\mathcal{G}_0)}} \le \frac{\pi^2}{2\,\ell_*(\mathcal{G}\setminus\mathcal{G}_0)}\alpha(\mathcal{G}\setminus\mathcal{G}_0).$$

Finally, using (2.23) and (3.6) we end up with

$$\lambda_0^{\mathrm{ess}}(\mathbf{H}) \le \lim_{\mathcal{G}_0\in\mathcal{K}_{\mathcal{G}}} \frac{\pi^2}{2\,\ell_*(\mathcal{G}\setminus\mathcal{G}_0)}\alpha(\mathcal{G}\setminus\mathcal{G}_0) = \frac{\pi^2}{2\,\ell_*^{\mathrm{ess}}(\mathcal{G})}\alpha_{\mathrm{ess}}(\mathcal{G}). \qquad \square$$

Combining Lemma 5.1 with the Cheeger-type bounds (3.8) and the estimates (4.10)–(4.11) and taking into account Lemma 3.9, we immediately get the following result.

Corollary 5.2. *If $\ell_*(\mathcal{G}) > 0$ and $\ell^*(\mathcal{G}) < \infty$, then the following are equivalent:*

(i) $\lambda_0(\mathbf{H}) > 0$,
(ii) $\lambda_0^{\mathrm{ess}}(\mathbf{H}) > 0$,
(iii) $\alpha_{\mathrm{comb}}(\mathcal{G}) > 0$,
(iv) $\alpha_{\mathrm{comb}}^{\mathrm{ess}}(\mathcal{G}) > 0$.

Remark 5.3. *A few remarks are in order:*

(i) *If $\ell_*(\mathcal{G}) = 0$, then the estimate in* (5.1) *becomes trivial.*
(ii) *Notice that* (5.1) *is better than* (2.25) *only if the isoperimetric constant satisfies*

$$\alpha(\mathcal{G}) < \frac{2\,\ell_*(\mathcal{G})}{\ell^*(\mathcal{G})^2}.$$

(iii) *In* [12], *Buser noticed that the isoperimetric constant can be used for obtaining upper estimates on the spectral gap for Laplacians on compact Riemannian manifolds. Hence estimates of the type* (5.1) *are often called Buser-type estimates. Let us mention that for combinatorial Laplacians a Buser-type estimate was first proved in* [2] *(see also* [17, 19]*). For finite quantum graphs, a Buser-type bound can be found in* [41, Proposition 0.3], *which is, however, different from our estimate* (5.1).

6. Bounds by curvature

Despite the combinatorial nature of isoperimetric constants (3.3) and (3.4), it is known that computation of the combinatorial isoperimetric constant (4.8) is an NP-hard problem (see [35, 37, 49] for further details). Our next aim is to introduce a quantity, which provides estimates for $\alpha(\mathcal{G})$ and $\alpha_{\mathrm{ess}}(\mathcal{G})$ and also turns out to be very useful in many situations (see Section 8).

Suppose now that our graph is oriented, that is, every edge is assigned a direction. For every $v \in \mathcal{V}$, let $\mathcal{E}_v^+$ and $\mathcal{E}_v^-$ be the sets of outgoing and incoming edges, respectively. Next define the function $\mathrm{K}\colon \mathcal{V} \to \mathbb{R}\cup\{-\infty\}$ by

$$\mathrm{K}\colon v \mapsto \frac{\#(\mathcal{E}_v^+) - \#(\mathcal{E}_v^-)}{\#(\mathcal{E}_v^+)} \inf_{e\in\mathcal{E}_v^+}\frac{1}{|e|}. \tag{6.1}$$

Note that K can take both positive and negative values, and $\mathrm{K}(v) = -\infty$ whenever $\#(\mathcal{E}_v^+) = \emptyset$.

Lemma 6.1. *Assume $\mathcal{G}$ is an oriented graph such that the function* K *is positive. Then the isoperimetric constant* (3.3) *satisfies*

$$\alpha(\mathcal{G}) \geq \mathrm{K}(\mathcal{G}) := \inf_{v\in\mathcal{V}} \mathrm{K}(v) \geq 0. \tag{6.2}$$

Proof. Let $\widetilde{\mathcal{G}} \in \mathcal{K}_{\mathcal{G}}$ be a finite and connected subgraph. For every $v \in \widetilde{\mathcal{V}}$, denote by $\mathcal{E}_v^+(\widetilde{\mathcal{G}})$ and $\mathcal{E}_v^-(\widetilde{\mathcal{G}})$ the sets of outgoing and incoming edges in $\widetilde{\mathcal{G}}$. Since $\mathrm{K}(v) > 0$ is positive, we get

$$\sup_{e\in\mathcal{E}_v^+} |e| \leq \frac{1}{\mathrm{K}(v)}\Big(1 - \frac{\#(\mathcal{E}_v^-)}{\#(\mathcal{E}_v^+)}\Big),$$

for all $v \in \mathcal{V}$. Therefore,

$$\begin{aligned}\mathrm{mes}(\widetilde{\mathcal{G}}) = \sum_{e\in\widetilde{\mathcal{E}}} |e| = \sum_{v\in\widetilde{\mathcal{V}}} \sum_{e\in\mathcal{E}_v^+(\widetilde{\mathcal{G}})} |e| &\leq \frac{1}{\mathrm{K}(\mathcal{G})} \sum_{v\in\widetilde{\mathcal{V}}} \sum_{e\in\mathcal{E}_v^+(\widetilde{\mathcal{G}})} 1 - \frac{\#(\mathcal{E}_v^-)}{\#(\mathcal{E}_v^+)} \\ &= \frac{1}{\mathrm{K}(\mathcal{G})} \sum_{v\in\widetilde{\mathcal{V}}} \#(\mathcal{E}_v^+(\widetilde{\mathcal{G}}))\Big(1 - \frac{\#(\mathcal{E}_v^-)}{\#(\mathcal{E}_v^+)}\Big).\end{aligned}$$

First observe that

$$\sum_{v\in\widetilde{\mathcal{V}}} \#(\mathcal{E}_v^+(\widetilde{\mathcal{G}})) = \sum_{v\in\widetilde{\mathcal{V}}} \#(\mathcal{E}_v^-(\widetilde{\mathcal{G}})) = \#(\widetilde{\mathcal{E}}).$$

Moreover, for any non-boundary point $v \in \widetilde{\mathcal{V}} \setminus \partial_{\mathcal{G}}\widetilde{\mathcal{G}}$, the whole star $\mathcal{E}_v$ is contained in $\widetilde{\mathcal{G}}$ and hence $\mathcal{E}_v^\pm(\widetilde{\mathcal{G}}) = \mathcal{E}_v^\pm$. Therefore, we get

$$\begin{aligned}\sum_{v\in\widetilde{\mathcal{V}}} \#(\mathcal{E}_v^+(\widetilde{\mathcal{G}}))\Big(1 - \frac{\#(\mathcal{E}_v^-)}{\#(\mathcal{E}_v^+)}\Big) &= \sum_{v\in\widetilde{\mathcal{V}}} \#(\mathcal{E}_v^+(\widetilde{\mathcal{G}})) - \sum_{v\in\widetilde{\mathcal{V}}} \#(\mathcal{E}_v^+(\widetilde{\mathcal{G}}))\frac{\#(\mathcal{E}_v^-)}{\#(\mathcal{E}_v^+)} \\ &= \sum_{v\in\widetilde{\mathcal{V}}} \#(\mathcal{E}_v^-(\widetilde{\mathcal{G}})) - \sum_{v\in\widetilde{\mathcal{V}}} \#(\mathcal{E}_v^+(\widetilde{\mathcal{G}}))\frac{\#(\mathcal{E}_v^-)}{\#(\mathcal{E}_v^+)} \\ &= \sum_{v\in\partial_{\mathcal{G}}\widetilde{\mathcal{G}}} \#(\mathcal{E}_v^-(\widetilde{\mathcal{G}})) - \#(\mathcal{E}_v^+(\widetilde{\mathcal{G}}))\frac{\#(\mathcal{E}_v^-)}{\#(\mathcal{E}_v^+)} \\ &\leq \sum_{v\in\partial_{\mathcal{G}}\widetilde{\mathcal{G}}} \deg_{\widetilde{\mathcal{G}}}(v) = \deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}}).\end{aligned}$$

Combining this with the previous estimates, we end up with the following bound

$$\mathrm{mes}(\widetilde{\mathcal{G}}) \leq \frac{1}{\mathrm{K}(\mathcal{G})} \deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}}),$$

which proves the claim. □

Remark 6.2. *The function* K *is sometimes interpreted as* curvature*. Several notions of curvature have been introduced for discrete and combinatorial Laplacians. Perhaps, the closest one to* (6.1) *have been introduced in* [39]*. Namely, since the natural path metric ϱ_0 is intrinsic, define the function $\mathrm{K}_d\colon \mathcal{V} \to \mathbb{R}$ by*

$$\mathrm{K}_d\colon v \mapsto \frac{\#(\mathcal{E}_v^+) - \#(\mathcal{E}_v^-)}{m(v)}. \tag{6.3}$$

Moreover, $m(v) = \deg(v)$ for all $v \in \mathcal{V}$ if the corresponding metric graph is equilateral (i.e., $|e| \equiv 1$), and hence (6.3) *coincides with the definition suggested for combinatorial Laplacians in* [21]. *Notice that for equilateral graphs* (6.1) *reads*

$$\mathrm{K}(v) = \mathrm{K}_{\mathrm{comb}}(v) := 1 - \frac{\#(\mathcal{E}_v^-)}{\#(\mathcal{E}_v^+)}, \quad v \in \mathcal{V}, \tag{6.4}$$

and hence in this case

$$\frac{2}{\mathrm{K}(v)} = \frac{2}{\mathrm{K}_{\mathrm{comb}}(v)} = 1 + \frac{1}{\mathrm{K}_d(v)}, \quad v \in \mathcal{V}. \tag{6.5}$$

It seems there is no nice connection between K *and* K_d *in the general case.*

Remark 6.3. *Let us also mention that Lemma 6.1 can be seen as the analog of* [5, Theorem 6.2]*, where the following bound for the discrete isoperimetric constant was established:*

$$\alpha_d(\mathcal{V}) \geq \mathrm{K}_d(\mathcal{V}) := \inf_{v \in \mathcal{V}} \mathrm{K}_d(v), \tag{6.6}$$

if K_d is nonnegative on $\mathcal{V}$. *Combining* (6.6) *with the second inequality in* (4.5)*, we end up with the following bound*

$$\frac{2}{\alpha(\mathcal{G})} \leq \frac{1}{\mathrm{K}_d(\mathcal{V})} + \ell^*(\mathcal{G}). \tag{6.7}$$

In what follows we shall call the function $\mathrm{K}_{\mathrm{comb}} \colon \mathcal{V} \to \mathbb{Q} \cup \{-\infty\}$ defined by (6.4) as the *combinatorial curvature* (in [21, p. 32], $\mathrm{K_d}$ is called a *curvature of the combinatorial distance spheres*). Note that the curvature can take both positive and negative values, and $\mathrm{K}_{\mathrm{comb}}(v) = -\infty$ whenever $\#(\mathcal{E}_v^+) = \emptyset$. The next simple estimate turns out to be very useful in applications.

Lemma 6.4. *Assume* K_{comb} *is positive on* $\mathcal{V}$ *and*

$$\mathrm{K}_{\mathrm{comb}}(\mathcal{V}) := \inf_{v \in \mathcal{V}} \mathrm{K}_{\mathrm{comb}}(v).$$

Then the isoperimetric constant (3.3) *satisfies*

$$\alpha(\mathcal{G}) \geq \frac{\mathrm{K}_{\mathrm{comb}}(\mathcal{V})}{\ell^*(\mathcal{G})}. \tag{6.8}$$

Proof. Noting that $\mathrm{K}_{\mathrm{comb}}$ is positive and comparing (6.4) with (6.1), we get

$$\frac{\mathrm{K}_{\mathrm{comb}}(v)}{\ell^*(\mathcal{G})} \leq \mathrm{K}(v) \tag{6.9}$$

for all $v \in \mathcal{V}$. Hence the claim follows from Lemma 6.1. □

With a little extra effort and using an argument similar to that in the proof of (4.5) one can show the following bounds.

Lemma 6.5. *Assume* $\mathcal{G}$ *is an oriented graph such that the function* K *(and hence* $\mathrm{K}_{\mathrm{comb}}$*) is positive on* $\mathcal{V}$ *and set*

$$\mathrm{K}^{\mathrm{ess}}(\mathcal{G}) := \liminf_{v \in \mathcal{V}} \mathrm{K}(v), \qquad \mathrm{K}^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{V}) := \liminf_{v \in \mathcal{V}} \mathrm{K}_{\mathrm{comb}}(v). \tag{6.10}$$

Then the isoperimetric constant at infinity (3.4) *satisfies*

$$\alpha_{\mathrm{ess}}(\mathcal{G}) \geq \mathrm{K}^{\mathrm{ess}}(\mathcal{G}), \tag{6.11}$$

and

$$\frac{\mathrm{K}^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{V})}{\ell^*_{\mathrm{ess}}(\mathcal{G})} \leq \alpha_{\mathrm{ess}}(\mathcal{G}) \leq \frac{2}{\ell^*_{\mathrm{ess}}(\mathcal{G})}, \tag{6.12}$$

Combining Lemma 6.5 with the Cheeger-type estimate, we immediately get the following result.

Corollary 6.6. *If $\mathcal{G}$ is an oriented graph such that the function* $\mathrm{K}_{\mathrm{comb}}$ *is nonnegative on $\mathcal{V}$, then*

$$\lambda_0(\mathbf{H}) \ge \frac{\mathrm{K}_{\mathrm{comb}}(\mathcal{V})^2}{4\,\ell^*(\mathcal{G})^2}, \qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) \ge \frac{\mathrm{K}^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{V})^2}{4\,\ell^*_{\mathrm{ess}}(\mathcal{G})^2}. \tag{6.13}$$

In particular, if $\mathrm{K}^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{V}) > 0$, then the spectrum of $\mathbf{H}$ is purely discrete precisely when $\ell^*_{\mathrm{ess}}(\mathcal{G}) = 0$.

Remark 6.7. *Let us mention that in the case when $\mathrm{K}^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{V}) = 0$ the condition $\ell^*_{\mathrm{ess}}(\mathcal{G}) = 0$ is no longer sufficient for the discreteness. For further details we refer to Section 8.2 and, more specifically, to the example of polynomially growing antitrees (see Example 8.7).*

7. Growth volume estimates

Here we plan to exploit the results from [63] to get upper bounds on the spectra of quantum graphs in terms of the exponential volume growth rates, the so-called Brooks-type estimates (cf. [7], [34], [63] for further details and references). Following [63], we introduce the following notation. For every $x \in \mathcal{G}$ and $r > 0$, let

$$B_r(x) := \{y \in \mathcal{G} |\ \varrho_0(x, y) < r\}. \tag{7.1}$$

Here ϱ_0 is the natural path metric on $\mathcal{G}$. Let also

$$\mathrm{vol}_x(r) := \mathrm{mes}(B_r(x)), \tag{7.2}$$

and

$$\mathrm{vol}_*(r) := \inf_{x\in\mathcal{G}} \frac{\mathrm{mes}(B_r(x))}{\mathrm{mes}(B_1(x))}. \tag{7.3}$$

Next we define the following numbers

$$\mu_x(\mathcal{G}) := \liminf_{r\to\infty} \frac{\log(\mathrm{vol}_x(r))}{r}, \qquad \mu_*(\mathcal{G}) := \liminf_{r\to\infty} \frac{\log(\mathrm{vol}_*(r))}{r}. \tag{7.4}$$

Notice that $\mu_x(\mathcal{G})$ does not depend on $x \in \mathcal{G}$ if $\mathcal{G} = \cup_{r>0} B_r(x)$ for some (and hence for all) $x \in \mathcal{G}$. If both conditions are satisfied, then we shall write $\mu(\mathcal{G})$ instead of $\mu_x(\mathcal{G})$.

Theorem 7.1. *Suppose $(\mathcal{V}, \varrho_0)$ is complete as a metric space. Then*

$$\lambda_0(\mathbf{H}) \le \lambda_0^{\mathrm{ess}}(\mathbf{H}) \le \frac{1}{4}\mu_*(\mathcal{G})^2 \le \frac{1}{4}\mu(\mathcal{G})^2. \tag{7.5}$$

Proof. The first and the last inequalities in (7.5) are obvious and hence it remains to show that

$$\lambda_0^{\mathrm{ess}}(\mathbf{H}) \le \frac{1}{4}\mu_*(\mathcal{G})^2.$$

Notice that by Corollary 2.3, the pre-minimal operator $\mathbf{H}_0$ is essentially self-adjoint and hence $\mathbf{H}$ is its closure. Let us consider the corresponding quadratic form $\mathfrak{t}_{\mathcal{G}}$ defined as the closure in $L^2(\mathcal{G})$ of the form $\mathfrak{t}^0_{\mathcal{G}}$ (see (2.15) and (2.16)). It is not difficult to check that the form $\mathfrak{t}_{\mathcal{G}}$ is a strongly local regular Dirichlet form (see [30] for definitions). On the other hand, using the Hopf–Rinow type theorem for graphs (see [36]), with a little work one can show that every ball $B_r(x)$ is relatively compact if $(\mathcal{V}, \varrho_0)$ is complete. Therefore, by [63, Theorem 5] and [52, Theorem 1], [34, Theorem 1.1], we get

$$\lambda_0(\mathbf{H}) \le \frac{1}{4}\mu_*(\mathcal{G})^2, \qquad\qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) \le \frac{1}{4}\mu(\mathcal{G})^2.$$

Noting that $\mathrm{mes}(B_1(x)) \ge 1$ for all $x \in \mathcal{G}$ and taking into account [34, Remark (e) on p.885], we arrive at the desired estimate. $\square$

The next result is straightforward from Theorem 7.1.

Corollary 7.2. *Let $(\mathcal{V}, \varrho_0)$ be complete as a metric space. Then:*

(i) $\lambda_0(\mathbf{H}) = \lambda_0^{\mathrm{ess}}(\mathbf{H}) = 0$ *if* $\mu(\mathcal{G}) = 0$.
(ii) *The spectrum of* $\mathbf{H}$ *is not discrete if* $\mu_*(\mathcal{G}) < \infty$.

Remark 7.3. *Clearly, to compute or estimate $\mu_*(\mathcal{G})$ is a much more involved problem comparing to that of $\mu(\mathcal{G})$. However, it might happen that $\mu_*(\mathcal{G}) < \mu(\mathcal{G})$ and hence $\mu_*(\mathcal{G})$ provides a better bound (see Example 8.4).*

Remark 7.4. *Let us mention that these results have several further consequences for the heat semigroup $\mathrm{e}^{-t\mathbf{H}}$ generated by the operator $\mathbf{H}$. For example, $\mu_*(\mathcal{G}) = 0$ implies the exponential instability of the corresponding heat semigroup on $L^p(\mathcal{G})$ for all $p \in [1, \infty]$ (see* [63, Corollary 2]*).*

We finish this section with comparing the estimates (7.5) with the ones obtained in [26] in terms of the volume growth of the corresponding discrete graph. Following [34] (see also [26, §4.3]), define the constant

$$\mu_d(\mathcal{G}) := \liminf_{r\to\infty} \frac{\log m(B_r(v))}{r} \tag{7.6}$$

for a fixed $v \in \mathcal{V}$. Here

$$m(B_r(v)) = \sum_{u\in B_r(v)} m(u), \qquad v \in \mathcal{V}.$$

Notice that $\mu_d(\mathcal{G})$ does not depend on the choice of $v \in \mathcal{V}$ if $\mathcal{G} = \cup_{r>0} B_r(x)$.

Lemma 7.5. *If $\ell^*(\mathcal{G}) < \infty$ and $(\mathcal{V}, \varrho_0)$ is complete as a metric space, then*

$$\mu(\mathcal{G}) = \mu_d(\mathcal{G}). \tag{7.7}$$

Proof. First observe that

$$m(B_r(v)) = 2\sum_{\{u,\tilde u\}\subset B_r(v)} |e_{u,\tilde u}| + \sum_{\substack{\{u,\tilde u\}\not\subset B_r(v)\\ \{u,\tilde u\}\cap B_r(v)\neq\varnothing}} |e_{u,\tilde u}| \ge \mathrm{mes}(B_r(v)) = \mathrm{vol}_v(r).$$

for all $v \in \mathcal{V}$ and $r > 0$, which immediately implies $\mu(\mathcal{G}) \le \mu_d(\mathcal{G})$. Similarly, we also get

$$m(B_r(v)) \le 2\mathrm{mes}(B_{r+\ell^*}(v)) \tag{7.8}$$

for all $v \in \mathcal{V}$ and $r > 0$ and hence

$$\mu_d(\mathcal{G}) \le \liminf_{r\to\infty} \frac{\log(2\mathrm{vol}_v(r+\ell^*))}{r} = \mu(\mathcal{G}),$$

which finishes the proof of (7.7). $\square$

Remark 7.6. *A few remarks are in order.*

(i) *On the one hand, it does not look too surprising that the exponential growth rates for two Dirichlet forms* $\mathfrak{t}_{\mathcal{G}}$ *and* $\mathfrak{t}_{\mathbf{h}}$ *coincide. In particular this reflects the equivalence* (2.37) *in the case of sub-exponential growth rates. However, comparing* (7.7) *with the fact that there is no equality between* $\lambda_0(\mathbf{H})$ *and* $\lambda_0(\mathbf{h})$ *(see Section 2.5), one can conclude that in the case of an exponential growth of volume balls,* (7.5) *might not lead to qualified estimates (and examples of trees and antitrees in the next section confirm this observation).*

(ii) *Combining* (7.7) *with Corollary 7.2 we obtain Theorem 4.19 from* [26].

8. Examples

In this section we are going to apply our results to certain classes of graphs (trees, antitrees, and Cayley graphs of finitely generated groups). Let us also recall that we always assume Hypotheses 2.1–2.3 to be satisfied.

8.1. **Trees.** Let us first recall some basic notions. A connected graph without cycles is called *a tree*. We shall denote trees (both combinatorial and metric) by $\mathcal{T}$. Notice that for any two vertices u, v on a tree $\mathcal{T} = (\mathcal{V}, \mathcal{E})$ there is exactly one path $\mathcal{P}$ connecting u and v. A tree $\mathcal{T} = (\mathcal{V}, \mathcal{E})$ with a distinguished vertex $o \in \mathcal{V}$ is called *a rooted tree* and o is called *the root* of $\mathcal{T}$. In a rooted tree the vertices can be ordered according to (combinatorial) spheres. Namely, let $d(\cdot) := d(o, \cdot)$ be the combinatorial distance to the root o and S_n be the n-th (combinatorial) sphere, i.e., the set of vertices $v \in \mathcal{V}$ with $d(v) = n$. A vertex in the $(n+1)$-th sphere, which is connected to v in the n-th sphere, is called *a forward neighbor* of v. In what follows, we define an orientation on a rooted tree according to combinatorial spheres, that is, for every edge e its initial vertex belongs to the smaller combinatorial sphere.

We begin with the following simple estimate for rooted trees. According to the choice of orientation, we get $\mathrm{K}_{\mathrm{comb}}(o) = \deg(o)$ and

$$\mathrm{K}_{\mathrm{comb}}(v) = \frac{\#(\mathcal{E}_v^+) - \#(\mathcal{E}_v^-)}{\#(\mathcal{E}_v^+)} = \frac{\deg(v) - 2}{\deg(v) - 1}$$

for all $v \in \mathcal{V} \setminus \{o\}$. Therefore, $\mathrm{K}_{\mathrm{comb}}$ is nonnegative on $\mathcal{V}$ if there are no loose ends, that is, $\deg(v) \neq 1$ for all $v \in \mathcal{V}$. Let

$$\deg_*(\mathcal{V}) := \inf_{v \in \mathcal{V}} \deg(v), \qquad \deg_*^{\mathrm{ess}}(\mathcal{V}) := \liminf_{v \in \mathcal{V}} \deg(v).$$

Hence we easily get

$$\mathrm{K}_{\mathrm{comb}}(\mathcal{T}) = \frac{\deg_*(\mathcal{V}) - 2}{\deg_*(\mathcal{V}) - 1}, \qquad \mathrm{K}_{\mathrm{comb}}^{\mathrm{ess}}(\mathcal{T}) = \frac{\deg_*^{\mathrm{ess}}(\mathcal{V}) - 2}{\deg_*^{\mathrm{ess}}(\mathcal{V}) - 1},$$

and therefore we end up with the following estimate.

Lemma 8.1. *Assume* $\mathcal{T}$ *is a rooted tree without loose ends. Then*

$$\lambda_0(\mathbf{H}) \geq \frac{\mathrm{K}_{\mathrm{comb}}(\mathcal{T})^2}{4\,\ell^*(\mathcal{G})^2}, \qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) \geq \frac{\mathrm{K}_{\mathrm{comb}}^{\mathrm{ess}}(\mathcal{T})^2}{4\,\ell^*_{\mathrm{ess}}(\mathcal{G})^2}. \tag{8.1}$$

In particular, $\lambda_0(\mathbf{H}) > 0$ *if and only if* $\ell^*(\mathcal{G}) < \infty$ *and the spectrum of* $\mathbf{H}$ *is purely discrete if and only if* $\ell^*_{\mathrm{ess}}(\mathcal{G}) = 0$.

Proof. The proof immediately follows from Corollary 6.6, Remark 2.9(i) and the fact that the combinatorial curvature admits the following bound (take also into account Hypothesis 2.3)

$$\frac{1}{2} \le \mathrm{K}_{\mathrm{comb}}(\mathcal{T}) < 1. \qquad \square$$

Remark 8.2. *A few remarks are in order.*

(i) *In the case of regular metric trees (these are rooted trees with an additional symmetry – all the vertices from the same distance sphere have equal degrees as well as all the edges of the same generation are of the same length), the second claim in Lemma 8.1 was observed by M. Solomyak in* [62]. *In fact, under Hypothesis 2.3, conditions (5.1) and (5.5) of* [62] *hold true if and only if, respectively, $\ell^*(\mathcal{G}) < \infty$ and $\ell^*_{\mathrm{ess}}(\mathcal{G}) = 0$. However, the case of the Neumann Laplacian is considered in* [62], *and it follows that criteria for the positivity and discreteness for the Neumann and Dirichlet Laplacians coincide.*

(ii) *Let us mention that the positivity (however, without estimates) of a combinatorial isoperimetric constant for the type of trees considered in Lemma 8.1 is known (see* [65, Theorem 10.9]*)*

In the case of trees the estimates (8.1) can be improved, however, instead of providing these generalizations we are going to consider only one particular case.

Example 8.3 (Bethe lattices)**.** Fix $\beta \in \mathbb{Z}_{\ge 3}$ and consider the combinatorial graph, which is a rooted tree such that all vertices have degree β. This type of trees is called *Bethe lattices* (also known as *Cayley trees* or *homogeneous trees*) and they will be denoted by $\mathbb{T}_\beta$. Suppose that the corresponding metric graph is equilateral, that is, $|e| = 1$ for all $e \in \mathcal{E}$. By abusing the notation, we shall denote the corresponding metric graph by $\mathbb{T}_\beta$ too. Then one computes

$$\mathrm{K}_{\mathrm{comb}}(\mathbb{T}_\beta) = \mathrm{K}^{\mathrm{ess}}_{\mathrm{comb}}(\mathbb{T}_\beta) = \frac{\beta - 2}{\beta - 1} =: \mathrm{K}_\beta.$$

Noting that $\mathrm{K}_\beta \in [1/2, 1)$ and applying Lemma 8.1, we arrive at the following estimate

$$\lambda_0^{\mathrm{ess}}(\mathbb{T}_\beta) \ge \lambda_0(\mathbb{T}_\beta) \ge \frac{1}{4}\mathrm{K}_\beta^2. \tag{8.2}$$

On the other hand, it is straightforward to check that (see, e.g., [21])

$$\alpha(\mathbb{T}_\beta) = \mathrm{K}_{\mathrm{comb}}(\mathbb{T}_\beta) = \frac{\beta - 2}{\beta - 1}, \qquad \alpha_d(\mathbb{T}_\beta) = \frac{\beta - 2}{\beta}. \tag{8.3}$$

In particular, this implies that the equality holds in the second inequality in (4.5). Moreover, the spectra of both operators $\mathbf{H}$ and $\mathbf{h}$ can be computed explicitly (see, e.g., [62, Example 6.3] or [21, Theorem 1.14] together with Theorem 2.11) and, in particular,

$$\lambda_0(\mathbf{H}) = \lambda_0^{\mathrm{ess}}(\mathbf{H}) = \arccos^2\Big(\frac{2\sqrt{\beta - 1}}{\beta}\Big).$$

Comparing the last equality with the estimate (8.2), one can notice a gap between these estimates.

Let us mention that

$$\mu(\mathbb{T}_\beta) = \mu_o(\mathbb{T}_\beta) = \mu_*(\mathbb{T}_\beta) = \beta - 1,$$

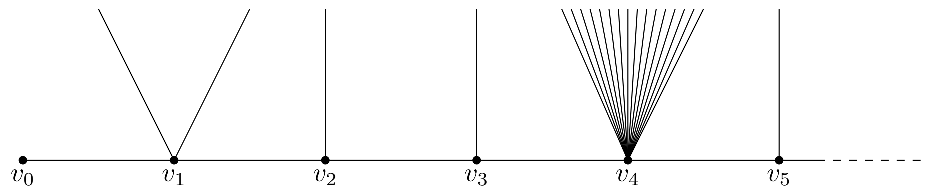

FIGURE 1. Tree with loose ends.

and thus the volume growth estimates (7.5) do not provide a reasonable upper bound for large values of β. $\Diamond$

Finally, we would like to mention that the absence of loose ends in Lemma 8.1 is essential as the next example shows.

Example 8.4 (A "sparse" tree with loose ends)**.** Consider the half-line $\mathbb{R}_{\geq 0}$ as an equilateral graph with vertices at the integers. Let us write v_n for the vertex placed at $n \in \mathbb{Z}_{\geq 0}$. Then, we will modify this graph by attaching edges to the vertices v_n with $n \geq 1$. More precisely, to the j^2-th vertex v_{j^2} with $j \in \mathbb{Z}_{\geq 1}$, we attach 2^{j^2} edges and to every other vertex v_n with $n \notin \{j^2\}_{j\geq 1}$, we attach exactly one edge (see Figure 1).

Clearly, we end up with a tree graph $\mathcal{T}$. For simplicity, we shall assume that the corresponding metric graph is equilateral, that is, $|e| = 1$ for all $e \in \mathcal{T}$. This tree is in a certain sense sparse and as a result it turns out that

$$\mu_*(\mathcal{T}) = 0,$$

and hence, by Theorem 7.1,

$$\lambda_0(\mathbf{H}) = \lambda_0^{\mathrm{ess}}(\mathbf{H}) = 0.$$

In fact, it is enough to show that $\mathrm{vol}_*(r) = 1$ for all $r > 1$. Namely, take $r > 1$ and set $j_r := 1+\lfloor (r+1)/2\rfloor$, where $\lfloor\cdot\rfloor$ is the usual floor function. Since $j_r^2-(j_r-1)^2 > r$, we get

$$1 \leq \mathrm{vol}_*(r) \leq \inf_{n\geq j_r} \frac{\mathrm{mes}(B_r(v_{n^2}))}{B_1(v_{n^2})} = \inf_{n\geq j_r} \frac{2^{n^2}+2r+2(r-1)}{2^{n^2}+2} = 1.$$

It is interesting to mention that in this case $\mu(\mathcal{T}) = \log(2) > 0$. Indeed,

$$2r-1+\sum_{k=1}^{\lfloor\sqrt{r}\rfloor-1}(2^{k^2}-1) \leq \mathrm{vol}_o(r) = \mathrm{mes}(B_r(v_0)) \leq 2r-1+\sum_{k=1}^{\lfloor\sqrt{r}\rfloor}(2^{k^2}-1)$$

and hence for all $r > 1$ we get

$$2^{(\lfloor\sqrt{r}\rfloor-1)^2} < \mathrm{vol}_o(r) \leq 2^{\lfloor\sqrt{r}\rfloor^2+1},$$

which implies the desired equality. $\Diamond$

8.2. **Antitrees.** Let $\mathcal{G}_d = (\mathcal{V},\mathcal{E})$ be a connected combinatorial graph. Fix a root vertex $o \in \mathcal{V}$ and then order the graph with respect to the combinatorial spheres S_n, $n \in \mathbb{Z}_{\geq 0}$ (notice that $S_0 = \{o\}$). The connected graph $\mathcal{G}_d$ is called an *antitree* if every vertex in S_n is connected to every vertex in S_{n+1} and there are no horizontal edges, i.e., there are no edges with all endpoints in the same sphere (see Figure 2). Clearly, an antitree is uniquely determined by the sequence $s_n := \#(S_n)$, $n \in \mathbb{Z}_{\geq 1}$.

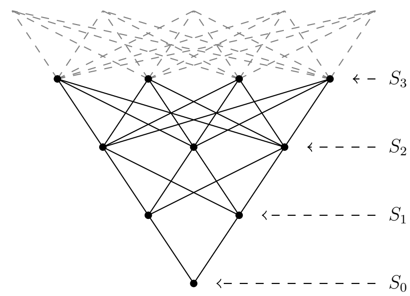

FIGURE 2. Example of an antitree with $s_n = n + 1$.

Let us denote antitrees by the letter $\mathcal{A}$ and also define the edge orientation according to the combinatorial ordering, that is, for every edge e its initial edge is the one in the smaller combinatorial sphere. It turns out that the curvatures of antitrees can be computed explicitly. Namely, define the following quantities:

$$\ell_n := \sup_{e\in\mathcal{E}_v^+ :\, v\in S_n} |e|, \tag{8.4}$$

and

$$\mathrm{K}_0 := 1, \qquad \mathrm{K}_{n+1} := 1 - \frac{s_n}{s_{n+2}} \tag{8.5}$$

for all $n \in \mathbb{Z}_{\geq 0}$.

Lemma 8.5. *If $\mathcal{A}$ is an antitree, then*

$$\mathrm{K}_{\mathrm{comb}}(\mathcal{A}) = \inf_{n\geq 0} \mathrm{K}_n, \qquad \mathrm{K}^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{A}) = \liminf_{n\to\infty} \mathrm{K}_n, \tag{8.6}$$

and

$$\mathrm{K}(\mathcal{A}) = \inf_{n\geq 0} \frac{\mathrm{K}_n}{\ell_n}, \qquad \mathrm{K}^{\mathrm{ess}}(\mathcal{A}) = \liminf_{n\to\infty} \frac{\mathrm{K}_n}{\ell_n}. \tag{8.7}$$

Proof. The proof follows by a direct inspection since $\mathrm{K}_{\mathrm{comb}}(v) = \mathrm{K}_n$ for all $v \in S_n$ and $n \in \mathbb{Z}_{\geq 0}$. $\square$

Combining Lemma 8.5 with the estimates for the corresponding isoperimetric constants (e.g., Corollary 6.6), we immediately end up with the estimates for $\lambda_0(\mathbf{H})$ and $\lambda_0^{\mathrm{ess}}(\mathbf{H})$. Let us demonstrate this by considering two examples.

Example 8.6 (Exponentially growing antitrees)**.** Fix $\beta \in \mathbb{Z}_{\geq 2}$ and let $\mathcal{A}_\beta$ be an antitree with sphere numbers $s_n = \beta^n$. Then $\mathrm{K}_0 = 1$ and

$$\mathrm{K}_n = 1 - \beta^{-2} \tag{8.8}$$

for all $n \in \mathbb{Z}_{\geq 1}$. Hence by Lemma 8.5

$$\frac{1-\beta^{-2}}{\ell^*(\mathcal{A}_\beta)} \leq \mathrm{K}(\mathcal{A}_\beta) \leq \frac{1}{\ell^*(\mathcal{A}_\beta)}$$

and

$$\mathrm{K}^{\mathrm{ess}}(\mathcal{A}_\beta) = \frac{1-\beta^{-2}}{\ell^*_{\mathrm{ess}}(\mathcal{A}_\beta)}.$$

Applying Lemmas 6.1 and 6.5 together with Theorem 3.4 and Lemma 2.8, we get

$$\frac{(1-\beta^{-2})^2}{4\,\ell^*(\mathcal{A}_\beta)^2} \le \lambda_0(\mathbf{H}_\beta) \le \frac{\pi^2}{\ell^*(\mathcal{A}_\beta)^2}, \tag{8.9}$$

and

$$\frac{(1-\beta^{-2})^2}{4\,\ell^*_{\mathrm{ess}}(\mathcal{A}_\beta)^2} \le \lambda_0^{\mathrm{ess}}(\mathbf{H}_\beta) \le \frac{\pi^2}{\ell^*_{\mathrm{ess}}(\mathcal{A}_\beta)^2}. \tag{8.10}$$

In particular, these bounds imply that the Kirchhoff Laplacian $\mathbf{H}_\beta$ is uniformly positive if and only if $\ell^*(\mathcal{A}_\beta) < \infty$. Moreover, its spectrum is purely discrete exactly when $\ell^*_{\mathrm{ess}}(\mathcal{A}_\beta) = 0$ (cf. Corollary 6.6).

Finally, let us compare these estimates with the volume growth estimates under the assumption that the tree is equilateral. In this case,

$$\mathrm{K}(\mathcal{A}_\beta) = \mathrm{K}^{\mathrm{ess}}(\mathcal{A}_\beta) = 1-\beta^{-2}.$$

On the other hand,

$$\mathrm{mes}(B_n(o)) = \sum_{k=0}^{n-1} \beta^{2k+1} = \beta\frac{\beta^{2n}-1}{\beta^2-1},$$

and then (7.4) implies that $\mu(\mathcal{A}_\beta) = 2\log(\beta)$. With a little more work one can show that

$$\mu_*(\mathcal{A}_\beta) = \mu(\mathcal{A}_\beta) = 2\log(\beta).$$

Indeed, it suffices to note that $\mu_*(\mathcal{A}_\beta) \le \mu(\mathcal{A}_\beta)$. Moreover, for all $x \in e_{u,v}$ where e connects S_n with S_{n+1}, $n \in \mathbb{Z}_{\ge 0}$ we have

$$\mathrm{mes}(B_1(x)) \le \mathrm{mes}(B_1(v)) = \beta^n + \beta^{n+2} = \beta^n(\beta^2+1)$$

and for all $r > 2$

$$\begin{aligned} \mathrm{mes}(B_r(x)) &\ge \mathrm{mes}(B_{\lfloor r\rfloor}(u)) = \mathrm{mes}(B_{n+\lfloor r\rfloor}(o)) - \mathrm{mes}(B_{n-\lfloor r\rfloor}(o)) \\ &\ge \mathrm{mes}(B_{n+\lfloor r\rfloor}(o)) - \mathrm{mes}(B_n(o)) = \sum_{k=n}^{n+\lfloor r\rfloor-1} \beta^{2k+1} = \beta^{2n+1}\frac{\beta^{2\lfloor r\rfloor}-1}{\beta^2-1}. \end{aligned}$$

Thus, we obtain

$$\mathrm{vol}_*(r) = \inf_{x\in\mathcal{G}} \frac{\mathrm{mes}(B_r(x))}{\mathrm{mes}(B_1(x))} \ge \inf_{n\ge 0} \frac{\beta^{2n+1}\frac{\beta^{2\lfloor r\rfloor}-1}{\beta^2-1}}{\beta^n(\beta^2+1)} = \frac{\beta^{2\lfloor r\rfloor+1}-\beta}{\beta^4-1},$$

which shows that $\mu_*(\mathcal{A}_\beta) \ge 2\log(\beta)$ and hence we are done.

Notice that the volume growth estimates (7.5) do not provide a reasonable upper bound for large values of β. ◊

Example 8.7 (Polynomially growing antitrees)**.** Fix $q \in \mathbb{Z}_{>0}$ and let $\mathcal{A}^q$ be the antitree with sphere numbers $s_n = (n+1)^q$, $n \ge 0$ (the case $q = 1$ is depicted on Figure 2). Then

$$\mathrm{K}_n = 1 - \frac{n^q}{(n+2)^q} = 1 - \Big(\frac{n}{n+2}\Big)^q = \frac{2q}{n} + \mathcal{O}(n^{-2}), \tag{8.11}$$

as $n \to \infty$. Hence, by Lemma 8.5,

$$\mathrm{K}_{\mathrm{comb}}(\mathcal{A}^q) = \mathrm{K}^{\mathrm{ess}}_{\mathrm{comb}}(\mathcal{A}^q) = 0$$

and

$$\mathrm{K}(\mathcal{A}^q) = \inf_{n\ge 0}\frac{1}{\ell_n}\left(1-\Big(\frac{n}{n+2}\Big)^q\right), \quad \mathrm{K}^{\mathrm{ess}}(\mathcal{A}^q) = \liminf_{n\to\infty}\frac{1}{\ell_n}\left(1-\Big(\frac{n}{n+2}\Big)^q\right).$$

Clearly, further analysis heavily depends on the behavior of the sequence $\{\ell_n\}$. Let us consider one particular case. Fix an $s \ge 0$ and assume now that

$$|e| = (n+1)^{-s}$$

for each edge e connecting S_n and S_{n+1}. Let us denote the corresponding Kirchhoff Laplacian by $\mathbf{H}_{q,s}$. It is not difficult to show by applying Theorem 2.2 that the corresponding pre-minimal operator is essentially self-adjoint whenever $s \le q+1$, however, $(\mathcal{V}_q, \varrho_0)$ is complete exactly when $s\in[0,1]$.

Remark 8.8. *In our forthcoming publication we shall show that the pre-minimal operator $\mathbf{H}_0$ is essentially self-adjoint exactly when the corresponding metric graph has infinite volume, that is, when $s \le 2q+1$. Moreover, in the case $s > 2q+1$, the deficiency indices of $\mathbf{H}_0$ are equal to 1 and one can describe all self-adjoint extensions of $\mathbf{H}_0$.*

Since $\ell_n = (n+1)^{-s}$ for all $n \in \mathbb{Z}_{\ge 0}$, we get

$$\ell^*(\mathcal{A}^q) = 1, \qquad \ell^*_{\mathrm{ess}}(\mathcal{A}^q) = \begin{cases} 1, & s=0\\ 0, & s>0\end{cases},$$

and

$$\mathrm{K}^{\mathrm{ess}}(\mathcal{A}^q) = \lim_{n\to\infty}(n+1)^s\left(1-\Big(\frac{n}{n+2}\Big)^q\right) = \begin{cases} 0, & s\in[0,1),\\ 2q, & s=1,\\ +\infty, & s>1.\end{cases} \tag{8.12}$$

In the case $s=1$, it is easy to show that the sequence $\{\mathrm{K}_n/\ell_n\}$ is strictly increasing and hence this is also true for all $s>1$. Hence

$$\mathrm{K}(\mathcal{A}^q) = \mathrm{K}(o) = 1, \quad s\ge 1.$$

Moreover, the corresponding isoperimetric constant is given by $\alpha(\mathcal{A}^q) = \mathrm{K}(\mathcal{A}^q) = 1$ (to see this just take the ball $B_1(o)$ as a subgraph $\mathcal{G}$ and then one gets $\alpha(\mathcal{A}^q)\le 1$, which together with (6.2) implies the equality).

Next let us compute $\mu(\mathcal{A}^q)$ assuming that $s\in[0,1]$ (otherwise we can't apply the result from Section 7). Set

$$r_n := \sum_{k=0}^{n-1}\ell_k = \sum_{k=0}^{n-1}\frac{1}{(1+k)^s} = (1+o(1))\times\begin{cases}\frac{n^{1-s}}{1-s}, & s\in[0,1),\\ \log(n), & s=1,\end{cases}$$

as $n\to\infty$. Then

$$\mathrm{vol}_o(r_n) = \sum_{k=0}^{n-1}\ell_k s_k s_{k+1} = \sum_{k=0}^{n-1}(k+1)^{q-s}(k+2)^q = \frac{n^{2q-s+1}}{2q-s+1}(1+o(1))$$

as $n\to\infty$. Therefore, it is not difficult to show that

$$\mu(\mathcal{A}^q) = \mu_o(\mathcal{A}^q) = \lim_{n\to\infty}\frac{\log(\mathrm{vol}_o(r_n))}{r_n} = \begin{cases} 0, & s\in[0,1),\\ 2q, & s=1.\end{cases} \tag{8.13}$$

Applying Theorem 7.1 together with Lemma 6.1 and Lemma 6.5, we end up with the following estimates.

Lemma 8.9. *Assume $q \in \mathbb{Z}_{\geq 1}$ and $s \in \mathbb{R}_{\geq 0}$. Then*

$$\lambda_0(\mathbf{H}_{q,s}) = \lambda_0^{\mathrm{ess}}(\mathbf{H}_{q,s}) = 0 \tag{8.14}$$

if and only if $s \in [0, 1)$. If $s \geq 1$, then the operator $\mathbf{H}_{q,s}$ is uniformly positive and

$$\frac{1}{4} \leq \lambda_0(\mathbf{H}_{q,s}) \leq \pi^2, \qquad\qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}_{q,s}) = \begin{cases} q^2, & s = 1, \\ +\infty, & s > 1. \end{cases} \tag{8.15}$$

Remark 8.10. *The exact value of $\lambda_0(\mathbf{H}_{q,s})$ for $s \geq 1$ or at least its asymptotic behavior with respect to q remains an open problem.* ♢

8.3. **Cayley graphs.** Suppose Γ is a finitely generated (infinite) group with the set of generators S. *The Cayley graph* $\mathcal{C}(\Gamma, S)$ of Γ with respect to S is the vertex set Γ and $u \sim v$ exactly when $u^{-1}v \in S$. This graph is connected, locally finite and regular ($\deg(v) = \#S$ for all $v \in \Gamma$). We assume that the unit element o does not belong to the set S (this excludes loops). The lattice $\mathbb{Z}^d$ is the standard example of a Cayley graph. Notice also that the Bethe lattice $\mathbb{T}_\beta$ is a Cayley graph if either $S = \{a_1, \dots, a_\beta \,|\, a_i^2 = o,\ i = 1, \dots, \beta\}$ or $\beta = 2N$ and $\Gamma = \mathbb{F}_N$ is a free group of N generators.

It is known that the positivity of a combinatorial isoperimetric constant α_{comb} is closely connected with the amenability of the group Γ (this is a variant of Følner's criterion, see, e.g., [65, Proposition 12.4]).

Theorem 8.11. *If $\mathcal{G}_d = \mathcal{C}(\Gamma, S)$ is the Cayley graph of a finitely generated group Γ, then $\alpha_{\mathrm{comb}}(\Gamma) = 0$ if and only if Γ is an amenable group.*

Notice that the class of amenable groups contains all Abelian groups, all subgroups of amenable groups, all solvable groups etc. In turn, the class of non-amenable groups includes countable discrete groups containing free subgroups of two generators. For further information on amenability and Cayley graphs we refer to [48, 50, 55, 56, 64, 65].

Combining Theorem 8.11 with Corollary 4.5 and Corollary 5.2, we arrive at the following result.

Lemma 8.12. *Let $\mathcal{G}_d$ be a Cayley graph $\mathcal{C}(\Gamma, S)$ of a finitely generated group Γ. Also, let $|\cdot|\colon \mathcal{E} \to \mathbb{R}_{>0}$ and $\mathcal{G} = (\mathcal{G}_d, |\cdot|)$ be a metric graph. Then:*

- (i) *If Γ is non-amenable, then $\lambda_0(\mathbf{H}) > 0$ if and only if $\ell^*(\mathcal{G}) < \infty$. Moreover, the spectrum of $\mathbf{H}$ is purely discrete if and only if $\ell^*_{\mathrm{ess}}(\mathcal{G}) = 0$.*
- (ii) *If Γ is amenable, then $\lambda_0(\mathbf{H}) = \lambda_0^{\mathrm{ess}}(\mathbf{H}) = 0$ whenever $\ell_*(\mathcal{G}) > 0$.*

Remark 8.13.
- (i) *If Γ is an amenable group, then the analysis of $\lambda_0(\mathbf{H})$ and $\lambda_0^{\mathrm{ess}}(\mathbf{H})$ in the case $\ell_*(\mathcal{G}) = 0$ remains an open (and, in our opinion, rather complicated) problem.*
- (ii) *The volume growth provides a number of amenability criteria. For example, groups of polynomial or subexponential growth are amenable. For further results and references we refer to* [56].
- (iii) *Using a completely different approach, the inequality $\lambda_0(\mathbf{H}) > 0$ was proved recently in* [14, Theorem 4.16] *for Cayley graphs of free groups under the additional symmetry assumption that edges in the same edge orbit have the same length.*

Appendix A. Cheeger's inequality for discrete Laplacians

Let $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ be an (unoriented) graph with countably infinite sets of vertices $\mathcal{V}$ and edges $\mathcal{E}$. Also, assume that Hypothesis 2.1 is satisfied. Let $m\colon \mathcal{V} \to \mathbb{R}_{>0}$ and $b\colon \mathcal{V} \times \mathcal{V} \to \mathbb{R}_{\geq 0}$ be weight functions such that $b(u,v) = b(v,u)$ for all $u, v \in \mathcal{V}$ and $b(u,v) \neq 0$ only if $u \sim v$. In fact, b can be considered as a weight function on the edge set $\mathcal{E}$. Usually, the triple $(\mathcal{V}, m, b)$ is called a *weighted graph*. With every such a triple one can associate a Laplace operator defined by the difference expression

$$(\tau f)(v) := \frac{1}{m(v)} \sum_{u \sim v} b(u,v)(f(v) - f(u)), \quad v \in \mathcal{V}. \tag{A.1}$$

Since the graph $\mathcal{G}_d$ is locally finite, τ is well defined on compactly supported functions and hence gives rise to a nonnegative symmetric pre-minimal operator in $\ell^2(\mathcal{V}; m)$. Let us denote its Friedrichs extension by $\mathbf{h}$.

The Cheeger inequality for $\mathbf{h}$ was proved recently in [5] by using the notion of intrinsic metrics on graphs (see Theorem 3.1 and Theorem 3.3 in [5]). The main aim of this section is to give a slight improvement to this estimate. Namely, let $d\colon \mathcal{E} \to \mathbb{R}_{>0}$ be a weight (or edge lengths). Similar to [5], we shall call d *intrinsic* on $\mathcal{G}_d$ (with respect to m and b) if the following inequality

$$\sum_{e \in \mathcal{E}_v} d(e)^2 b(e) \;\leq\; m(v) \tag{A.2}$$

holds for all $v \in \mathcal{V}$.

For every $X \subseteq \mathcal{V}$, we define its boundary edges by

$$\mathcal{E}_b(X) = \{e \in \mathcal{E} \mid e \text{ connects } X \text{ and } \mathcal{V} \backslash X\}.$$

For any $U \subseteq \mathcal{V}$, define

$$\alpha_d(U) := \inf_{\substack{X \subseteq U \\ X \text{ finite}}} \frac{(d \cdot b)(\mathcal{E}_b(X))}{m(X)}, \tag{A.3}$$

where for $X \subseteq \mathcal{V}$,

$$m(X) = \sum_{v \in X} m(v), \qquad (d \cdot b)(\mathcal{E}_b(X)) = \sum_{e \in \mathcal{E}_b(X)} d(e) b(e).$$

We define the isoperimetric constant with respect to d by

$$\alpha := \alpha_d(\mathcal{V}). \tag{A.4}$$

The isoperimetric constant at infinity is given by

$$\alpha_{\mathrm{ess}} := \sup_{\substack{X \subseteq \mathcal{V} \\ X \text{ finite}}} \alpha_d(\mathcal{V} \backslash X). \tag{A.5}$$

Theorem A.1. *If d is an intrinsic weight, then*

$$\lambda_0(\mathbf{h}) \geq \frac{1}{2}\alpha^2, \qquad \lambda_0^{\mathrm{ess}}(\mathbf{h}) \geq \frac{1}{2}\alpha_{\mathrm{ess}}^2. \tag{A.6}$$

Remark A.2. *As it was already mentioned, the Cheeger estimates for weighted graph Laplacians were proved in* [5]. *However, the definition of the isoperimetric constants in* [5] *uses* metrics *and hence one has to replace d in* (A.3) *by the corresponding path metric ϱ_d defined on $\mathcal{V}$ in a standard way*

$$\varrho_d(u,v) := \inf_{\mathcal{P} = \{v_0, \dots, v_n\}\colon\, v_0 = u \;\, v_n = v} \sum_k d(e_{v_{k-1}, v_k}). \tag{A.7}$$

Clearly, ϱ_d is intrinsic (in the sense of [5]*) if so is the weight d since*

$$\varrho_d(u, v) \le d(u, v) \tag{A.8}$$

for all $u \sim v$. Of course, in certain cases this leads to the same isoperimetric constant (e.g., if $\mathcal{G}_d$ is a tree), however, for graphs having a lot of cycles a construction of an intrinsic metric becomes a highly nontrivial task, which automatically implies complications in calculating the corresponding isoperimetric constant. On the other hand, to construct an intrinsic weight (in the sense of (A.2)*) is a rather simple task, in particular, for the weighted Laplacian* (2.29) *(see Remark A.4).*

The proof of Theorem A.1 is literally the same as of Theorem 3.1 and Theorem 3.3 from [5], however, we shall give it below for the sake of completeness.

Lemma A.3 (Co-area formulae)**.** *Let m and d be weight functions on $\mathcal{V}$ and $\mathcal{E}$, respectively. For any $f\colon \mathcal{V} \to \mathbb{R}_{\ge 0}$ and $t \ge 0$, let $\Omega_t := \Omega_t(f) = \{v \in \mathcal{V} |\ f(v) > t\}$. Then*

$$\sum_{v\in\mathcal{V}} f(v)m(v) = \int_0^\infty m(\Omega_t)\, dt, \tag{A.9}$$

$$\sum_{e\in\mathcal{E}} d(e)|f(e_i) - f(e_0)| = \int_0^\infty d(\mathcal{E}_b(\Omega_t))\, dt, \tag{A.10}$$

where the value $+\infty$ on both sides of the equation is allowed.

Proof. For an interval $I \subseteq \mathbb{R}$, let $\mathbb{1}_I(s)$ be its indicator function. Then

$$\begin{aligned}\sum_{v\in\mathcal{V}} f(v)m(v) &= \sum_{v\in\mathcal{V}} m(v) \int_0^{f(v)} dt = \sum_{v\in\mathcal{V}} m(v) \int_0^\infty \mathbb{1}_{[0,f(v))}(t)\, dt \\ &= \int_0^\infty \sum_{v\in\mathcal{V}} m(v)\mathbb{1}_{[0,f(v))}(t)\, dt = \int_0^\infty \sum_{v\in\Omega_t} m(v)\, dt = \int_0^\infty m(\Omega_t)\, dt.\end{aligned}$$

For every $e \in \mathcal{E}$, put $I_e := [\min\{f(e_0), f(e_i)\}, \max\{f(e_0), f(e_i)\}) \subset \mathbb{R}$. We have $t \in I_e$ if and only if $e \in \mathcal{E}_b(\Omega_t)$. Hence

$$\begin{aligned}\sum_{e\in\mathcal{E}} d(e)|f(e_i) - f(e_0)| &= \sum_{e\in\mathcal{E}} d(e) \int_{I_e} dt = \sum_{e\in\mathcal{E}} d(e) \int_0^\infty \mathbb{1}_{I_e}(t)\, dt \\ &= \int_0^\infty \sum_{e\in\mathcal{E}} d(e)\mathbb{1}_{I_e}(t)\, dt = \int_0^\infty \sum_{e\in\mathcal{E}_b(\Omega_t)} d(e)\, dt = \int_0^\infty d(\mathcal{E}_b(\Omega_t))\, dt. \qquad \square\end{aligned}$$

Proof of Theorem A.1. We start by proving the first estimate in (A.6). The Rayleigh quotient implies that it suffices to show that

$$2\, \mathbf{t}_{\mathbf{h}}[u] \ge \alpha^2 \|u\|^2_{\ell^2(\mathcal{V},m)} \tag{A.11}$$

holds for all real-valued u with finite support, where

$$\mathbf{t}_{\mathbf{h}}[u] = (\mathbf{h}u, u)_{\ell^2(\mathcal{V},m)} = \sum_{e\in\mathcal{E}} b(e)|u(e_i) - u(e_0)|^2$$

is the corresponding quadratic form. Let us now exploit Lemma A.3 with $f := u^2$. Notice that the set Ω_t is finite for all $t \ge 0$ and hence by (A.3) and (A.4) we have

$(d \cdot b)(\mathcal{E}_b(\Omega_t)) \geq \alpha\, m(\Omega_t)$ for all $t \geq 0$. Therefore we get from the co-area formulas

$$\begin{aligned}
\alpha \, \|u\|^2_{\ell^2(\mathcal{V},m)} &= \alpha \sum_{v\in\mathcal{V}} u(v)^2 m(v) = \alpha \int_0^\infty m(\Omega_t)\, dt \\
&\leq \int_0^\infty (d\cdot b)(\mathcal{E}_b(\Omega_t))\; dt = \sum_{e\in\mathcal{E}} d(e)b(e)|u(e_i)^2 - u(e_0)^2| \\
&= \sum_{e\in\mathcal{E}} \sqrt{b(e)}|u(e_i) - u(e_0)| \cdot d(e)\sqrt{b(e)}|u(e_i) + u(e_0)| \\
&\leq \mathfrak{t}_{\mathbf{h}}[u]^{1/2} \left(\sum_{e\in\mathcal{E}} d(e)^2 b(e)(u(e_i) + u(e_0))^2 \right)^{1/2}
\end{aligned}$$

by employing the Cauchy–Schwarz inequality in the last step. On the other hand,

$$\begin{aligned}
\sum_{e\in\mathcal{E}} d(e)^2 b(e)(u(e_i) + u(e_0))^2 &\leq 2\sum_{e\in\mathcal{E}} d(e)^2 b(e)(u(e_i)^2 + u(e_0)^2) \\
&= 2\sum_{v\in\mathcal{V}} u(v)^2 \sum_{e\in\mathcal{E}_v} d(e)^2 b(e) \leq 2\|u\|^2_{\ell^2(\mathcal{V},m)},
\end{aligned}$$

where we used (A.2) in the last step.

To get the second inequality, assume $X \subseteq \mathcal{V}$ finite. Let P denote the orthogonal projection onto the subspace of functions vanishing on X. Then $\mathbf{h}_{\mathcal{V}\setminus X} := P\mathbf{h}P$ with $\mathrm{dom}(\mathbf{h}_{\mathcal{V}\setminus X}) = \mathrm{dom}(\mathbf{h})$ is a relatively compact perturbation of $\mathbf{h}$. Thus we have

$$\lambda_0^{\mathrm{ess}}(\mathbf{h}) = \lambda_0^{\mathrm{ess}}(\mathbf{h}_{\mathcal{V}\setminus X}) \geq \lambda_0(\mathbf{h}_{\mathcal{V}\setminus X}) = \inf_{u\neq 0} \frac{\mathfrak{t}_{\mathbf{h}}[u]}{\|u\|_{\ell^2(\mathcal{V};m)}},$$

where the infimum is taken over all real-valued u with finite support which vanish on X. For such u, note that $\Omega_t(f)$ is contained in $\mathcal{V}\setminus X$. Hence (A.11) is valid with $\alpha(\mathcal{V}\setminus X)$ instead of α. Then $2\lambda_0^{\mathrm{ess}}(\mathbf{h}) \geq \alpha(\mathcal{V}\setminus X)^2$ and the second estimate follows. □

Remark A.4. *For the difference expression $\tau_{\mathcal{G}}$ defined in Section 2.5, the function m is given by* (2.10) *and the edge weight b is defined by $b(e) := 1/|e|$ for all $e \in \mathcal{E}$. Hence setting $d(e) := |e|$ for $e \in \mathcal{E}$, we conclude that $|\cdot|$ is intrinsic in the sense of* (A.2) *since*

$$\sum_{e\in\mathcal{E}_v} d(e)^2 b(e) = \sum_{e\in\mathcal{E}_v} |e|^2 \frac{1}{|e|} = \sum_{e\in\mathcal{E}_v} |e| = m(v)$$

for all $v \in \mathcal{V}$. Moreover, in this case we have

$$(d\cdot b)(\mathcal{E}_b(X)) = \sum_{e\in\mathcal{E}_b(X)} d(e)b(e) = \sum_{e\in\mathcal{E}_b(X)} |e|\frac{1}{|e|} = \#(\mathcal{E}_b(X)),$$

and hence (A.4) *and* (A.5) *coincide with* (4.2) *and* (4.3)*, respectively. In particular, Theorem A.1 implies the estimate* (4.4)*.*

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STRONG ISOPERIMETRIC INEQUALITY FOR TESSELLATING QUANTUM GRAPHS

NOEMA NICOLUSSI

Abstract. We investigate isoperimetric constants of infinite tessellating metric graphs. We introduce a curvature-like quantity, which plays the role of a metric graph analogue of discrete curvature notions for combinatorial tessellating graphs. Based on the definition in [26], we then prove a lower estimate and a criterium for positivity of the isoperimetric constant.

1. Introduction

Isoperimetric constants, which relate surface area and volume of sets, are among the most fundamental tools in spectral geometry of manifolds and graphs. They first appeared in this context in [7], where Cheeger obtained a lower bound on the spectral gap of Laplace–Beltrami operators. For discrete Laplacians on graphs, versions of Cheeger's inequality are known in various settings, e.g. [1, 2, 3, 9, 10, 13, 23, 30, 32]. They find application in many fields (such as the study of expander graphs and random walks on graphs, see [28] and [38] for more information) and consequently, there is a very large interest in graph isoperimetric constants.

In the case of *tessellating graphs* (i.e. edge graphs of tessellations of $\mathbb{R}^2$), they have been investigated using certain notions of *discrete curvature* (see for example [17, 24, 34, 37, 39]). On the other hand, the idea of plane graph curvature already appears earlier in several unrelated works [14, 20, 36] and was also employed to describe other geometric properties, for instance discrete analogues of the Gauss–Bonnet formula and the Bonnet–Myers theorem, e.g. [4, 8, 19, 22, 24, 36].

Another framework for isoperimetric constants are *metric graphs* $\mathcal{G}$, i.e. combinatorial graphs $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ with vertex set $\mathcal{V}$ and edge set $\mathcal{E}$, where each edge $e \in \mathcal{E}$ is identified with an interval $I_e = (0, |e|)$ of length $0 < |e| < \infty$. Topologically, $\mathcal{G}$ may be considered as a "network" of intervals glued together at the vertices. The analogue of the Laplace–Beltrami operator for metric graphs is the *Kirchhoff–Neumann Laplacian* $\mathbf{H}$ (also known as a *quantum graph*). It acts as an edgewise (negative) second derivative $f_e \mapsto -\frac{d^2}{dx_e^2} f_e$, $e \in \mathcal{E}$, and is defined on edgewise H^2-functions satisfying continuity and Kirchhoff conditions at the vertices (we refer to [5, 6, 11, 35] for more information and references; see also [12] for the case that $\mathcal{G}$ is infinite). A well-known result for *finite metric graphs* (i.e. $\mathcal{V}$ and $\mathcal{E}$ are

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finite sets) is a spectral gap estimate for $\mathbf{H}$ in terms of an isoperimetric constant due to Nicaise [33] (see also [25, 27]).

In this work, we are interested in *infinite metric graphs* (infinitely many vertices and edges). A notion of an isoperimetric constant $\alpha(\mathcal{G})$ in this context was introduced recently in [26] (see (2.5) below for a precise definition) together with the following Cheeger-type estimate

$$\frac{1}{4}\alpha(\mathcal{G})^2 \leq \lambda_0(\mathbf{H}) \leq \frac{\pi^2}{2\inf_{e\in\mathcal{E}}|e|}\alpha(\mathcal{G}), \tag{1.1}$$

which holds for every connected, simple, locally finite, infinite metric graph. Here $\lambda_0(\mathbf{H}) := \inf \sigma(\mathbf{H})$ is the bottom of the spectrum of $\mathbf{H}$.

However, let us stress that explicit computation of isoperimetric constants in general is a difficult problem (known to be NP-hard for combinatorial graphs [31]). Hence the question arises, whether one can find bounds on $\alpha(\mathcal{G})$ in terms of less complicated quantities. On the other hand, the definition of $\alpha(\mathcal{G})$ is purely combinatorial and moreover $\alpha(\mathcal{G})$ is related to the isoperimetric constant $\alpha_{\mathrm{comb}}(\mathcal{G}_d)$ of the combinatorial graph $\mathcal{G}_d$ (see [26] for further details). This strongly suggests to use discrete methods for further study. For combinatorial tessellating graphs, such tools are available in the form of discrete curvature and it is natural to ask whether similar techniques also apply to metric graphs. Moreover, the class of plane graphs contains important examples such as trees and edge graphs of regular tessellations.

Motivated by this, the subject of our paper are isoperimetric constants of *infinite tessellating metric graphs* (see Definition 2.1). Our main contribution is the definition of a *characteristic value* $c(\cdot)$ of the edges of a given metric graph (see (2.9)), which takes over the role of the classical discrete curvature (up to sign convention; as opposed to e.g. [17, 22, 24], our results on $\alpha(\mathcal{G})$ are formulated in terms of positive curvature). In the simple case of equilateral metric graphs (i.e. $|e| = 1$ for all $e \in \mathcal{E}$), c coincides with the characteristic edge value introduced by Woess in [37]. Moreover, for a finite tessellating metric graph (Corollary 3.9),

$$\sum_{e\in\mathcal{E}} -c(e)|e| = 1, \tag{1.2}$$

which can be interpreted as a metric graph analogue of the combinatorial Gauss–Bonnet formula known in the discrete case (see e.g. [22]).

In terms of these characteristic values, we then formulate our two main results: Theorem 3.1 contains a criterium for positivity of $\alpha(\mathcal{G})$ based on the averaged value of $c(\cdot)$ on large subgraphs $\widetilde{\mathcal{G}} \subset \mathcal{G}$. In Theorem 3.3, we obtain explicit lower bounds on $\alpha(\mathcal{G})$. A simplified version of this estimate is the following inequality:

$$\alpha(\mathcal{G}) \geq \inf_{e\in\mathcal{E}} c(e). \tag{1.3}$$

Theorem 3.3 can be interpreted as a metric graph analogue of the estimate in [24, Theorem 1] and a result by McKean in the manifold case [29].

Finally, we demonstrate the use of our theory by examples. First, we consider the case of equilateral (p, q)-regular graphs. Here, $\alpha(\mathcal{G})$ is closely related to $\alpha_{\mathrm{comb}}(\mathcal{G}_d)$ and hence can be computed explicitly. It turns out for large p and q, the estimate in Theorem 3.3 is quite close to the actual value. Second, we show how to construct an example where $\alpha(\mathcal{G})$ and $\alpha_{\mathrm{comb}}(\mathcal{G}_d)$ behave differently.

Let us finish the introduction by describing the structure of the paper. In Section 2, we recall a few basic notions and give a precise definition of infinite tessellating metric graphs. Moreover, we review the definition of $\alpha(\mathcal{G})$ and define the characteristic values. Section 3 contains our main results and proofs. In the final section, we consider examples.

2. Preliminaries

2.1. **(Combinatorial) planar graphs.** Let $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ be an infinite, unoriented graph with countably infinite sets of vertices $\mathcal{V}$ and edges $\mathcal{E}$. For a vertex $v \in \mathcal{V}$, we set

$$\mathcal{E}_v := \{e \in \mathcal{E} |\ e \text{ is incident to } v\} \tag{2.1}$$

and denote by $\deg(v) := \#\mathcal{E}_v$ the *combinatorial degree* of $v \in \mathcal{V}$. Throughout the paper, $\#A$ denotes the number of elements of a given set A. We will always assume that $\mathcal{G}_d$ is connected, simple (no loops or multiple edges) and locally finite ($\deg(v) < \infty$ for all $v \in \mathcal{V}$).

Moreover, we suppose that $\mathcal{G}_d$ is *planar* and consider a fixed planar embedding. Hence $\mathcal{G}_d$ can be regarded as a subset of the plane $\mathbb{R}^2$, which we assume to be closed. Denote by $\mathcal{T}$ the set of *faces* of $\mathcal{G}_d$, i.e. the closures of the connected components of $\mathbb{R}^2 \setminus \mathcal{G}_d$. Note that unbounded faces of $\mathcal{G}_d$ are included in $\mathcal{T}$ as well. Motivated by the next definition, we will refer to the elements $T \in \mathcal{T}$ as the *tiles* of $\mathcal{G}_d$.

Definition 2.1. A planar graph $\mathcal{G}_d$ is *tessellating* if the following additional conditions hold:

(i) $\mathcal{T}$ is locally finite, i.e. each compact subset K in $\mathbb{R}^2$ intersects only finitely many tiles.
(ii) Each bounded tile $T \in \mathcal{T}$ is a closed topological disc and its boundary ∂T consists of a finite cycle of at least three edges.
(iii) Each unbounded tile $T \in \mathcal{T}$ is a closed topological half-plane and its boundary ∂T consists of a (countably) infinite chain of edges.
(iv) Each edge $e \in \mathcal{E}$ is contained in the boundary of precisely two different tiles.
(v) Each vertex $v \in \mathcal{V}$ has degree ≥ 3.

Here, a subset $A \subseteq \mathbb{R}^2$ is called a closed topological disc (half-plane) if it is the image of the closed unit ball in $\mathbb{R}^2$ (the closed upper half-plane) under a homeomorphism $\phi\colon \mathbb{R}^2 \to \mathbb{R}^2$. For a tile $T \in \mathcal{T}$, we define

$$\mathcal{E}_T := \{e \in \mathcal{E} |\ e \subseteq \partial T\}, \qquad\qquad d_{\mathcal{T}}(T) := \#\mathcal{E}_T, \tag{2.2}$$

where the latter is called the *degree of a tile* $T \in \mathcal{T}$. Notice that according to Definition 2.1(ii), $d_{\mathcal{T}}(T) \geq 3$ for all $T \in \mathcal{T}$.

The above assumptions (i)–(v) imply that $\mathcal{T}$ is a *locally finite tessellation* of $\mathbb{R}^2$, i.e. a locally finite, countable family of closed subsets $T \subset \mathbb{R}^2$ such that the interiors are pairwise disjoint and $\bigcup_{T \in \mathcal{T}} T = \mathbb{R}^2$. In addition, $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ coincides with the edge graph of the tessellation in the following sense: by calling a connected component of the intersection of at least two tiles $T \in \mathcal{T}$ a $\mathcal{T}$-vertex, if it has only one point and a $\mathcal{T}$-edge otherwise, we recover the vertex and edge sets $\mathcal{V}$ and $\mathcal{E}$.

For a finite subgraph $\widetilde{\mathcal{G}} \subset \mathcal{G}_d$, let $\mathcal{F}(\widetilde{\mathcal{G}})$ be the set of *bounded faces* of $\widetilde{\mathcal{G}}$, i.e. the closures of all bounded, connected components of $\mathbb{R}^2 \backslash \widetilde{\mathcal{G}}$. By local finiteness, each bounded face of $\widetilde{\mathcal{G}}$ is a finite union of bounded tiles $T \in \mathcal{T}$. Moreover, define $\mathcal{P}(\widetilde{\mathcal{G}})$ as the set of tiles $T \in \mathcal{T}$ with $\partial T \subseteq \widetilde{\mathcal{G}}$. Note that always

$$\mathcal{P}(\widetilde{\mathcal{G}}) \subseteq \mathcal{F}(\widetilde{\mathcal{G}}).$$

2.2. **Metric graphs.** After assigning each edge $e \in \mathcal{E}$ a finite length $|e| \in (0, \infty)$, we obtain a *metric graph* $\mathcal{G} := (\mathcal{V}, \mathcal{E}, |\cdot|) = (\mathcal{G}_d, |\cdot|)$. Let us stress that in general $|e|$ is not related to the length of the Jordan arc in $\mathbb{R}^2$ representing the edge $e \in \mathcal{E}$. For a subgraph $\widetilde{\mathcal{G}} = (\widetilde{\mathcal{V}}, \widetilde{\mathcal{E}}) \subset \mathcal{G}$, define its *boundary vertices* by

$$\partial_{\mathcal{G}} \widetilde{\mathcal{G}} := \big\{ v \in \widetilde{\mathcal{V}} | \ \deg_{\widetilde{\mathcal{G}}}(v) < \deg(v) \big\}, \tag{2.3}$$

where $\deg_{\widetilde{\mathcal{G}}}(v)$ denotes the degree of a vertex $v \in \widetilde{\mathcal{V}}$ with respect to $\widetilde{\mathcal{G}}$. For a given finite subgraph $\widetilde{\mathcal{G}} \subset \mathcal{G}$ we then set

$$\deg(\partial_{\mathcal{G}} \widetilde{\mathcal{G}}) := \sum_{v \in \partial_{\mathcal{G}} \widetilde{\mathcal{G}}} \deg_{\widetilde{\mathcal{G}}}(v). \tag{2.4}$$

Following [26], the *isoperimetric constant* of a metric graph $\mathcal{G}$ is then defined by

$$\alpha(\mathcal{G}) := \inf_{\widetilde{\mathcal{G}}} \frac{\deg(\partial_{\mathcal{G}} \widetilde{\mathcal{G}})}{\operatorname{mes}(\widetilde{\mathcal{G}})} \in [0, \infty), \tag{2.5}$$

where the infimum is taken over all finite, connected subgraphs $\widetilde{\mathcal{G}} \subset \mathcal{G}$ and $\operatorname{mes}(\widetilde{\mathcal{G}})$ denotes the measure (the "total length") of $\widetilde{\mathcal{G}}$ with respect to the edge length function $|\cdot|$, $\operatorname{mes}(\widetilde{\mathcal{G}}) := \sum_{e \in \widetilde{\mathcal{E}}} |e|$. We will say that the metric graph $\mathcal{G}$ satisfies the *strong isoperimetric inequality* if $\alpha(\mathcal{G}) > 0$.

Recall that for a combinatorial graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ the *(combinatorial) isoperimetric constant* $\alpha_{\mathrm{comb}}(\mathcal{G}_d)$ is defined by (see, e.g., [10])

$$\alpha_{\mathrm{comb}}(\mathcal{G}_d) = \inf_{U \subset \mathcal{V}} \frac{\#\{e \in \mathcal{E} | \ e \text{ connects } U \text{ and } \mathcal{V} \setminus U\}}{\sum_{v \in U} \deg(v)}, \tag{2.6}$$

where the infimum is taken over all finite subsets $U \subset \mathcal{V}$. There is a close connection between $\alpha_{\mathrm{comb}}(\mathcal{G}_d)$ and $\alpha(\mathcal{G})$ and we refer for further details to [26].

We also need the following quantities. The *weight* $m(v)$ of a vertex $v \in \mathcal{V}$ is given by

$$m(v) = \sum_{e \in \mathcal{E}_v} |e|. \tag{2.7}$$

Clearly, $m(v)$ equals the measure (the "length") of the star $\mathcal{E}_v$. The *perimeter* $p(T)$ of a tile $T \in \mathcal{T}$ is defined as

$$p(T) := \begin{cases} \sum_{e \in \mathcal{E}_T} |e|, & T \in \mathcal{T} \text{ is bounded} \\ \infty, & T \in \mathcal{T} \text{ is unbounded} \end{cases}. \tag{2.8}$$

For every $e \in \mathcal{E}$, we define its *characteristic value* $c(e)$ by

$$c(e) := \frac{1}{|e|} - \sum_{v : v \in e} \frac{1}{m(v)} - \sum_{T : e \subseteq \partial T} \frac{1}{p(T)}. \tag{2.9}$$

Here we employ the convention that whenever ∞ appears in a denominator, the corresponding fraction $1/p$ has to be interpreted as zero if p is infinite. Let us mention that for equilateral metric graphs $\mathcal{G}$ (i.e. $|e| \equiv 1$ for all $e \in \mathcal{E}$), the characteristic value $c(e)$ coincides with the characteristic edge value introduced in [37] in the context of combinatorial graphs.

Finally, we need the following class of subgraphs of $\mathcal{G}$. A subgraph $\widetilde{\mathcal{G}} = (\widetilde{\mathcal{V}}, \widetilde{\mathcal{E}}) \subset \mathcal{G}$ is called *star-like*, if it can be written as a finite, connected union of stars. More precisely,

$$\widetilde{\mathcal{E}} = \bigcup_{v\in\widetilde{U}} \mathcal{E}_v$$

for some finite, connected vertex set $\widetilde{U} \subseteq \widetilde{\mathcal{V}}$.

Also, for a finite subgraph $\widetilde{\mathcal{G}} \subset \mathcal{G}$, we define its *interior graph* $\widetilde{\mathcal{G}}_{\rm int} = (\widetilde{\mathcal{V}}_{\rm int}, \widetilde{\mathcal{E}}_{\rm int})$ as the set of interior vertices $v \in \widetilde{\mathcal{V}}_{\rm int} := \widetilde{\mathcal{V}} \setminus \partial\widetilde{\mathcal{G}}$ together with all edges between such vertices. We say that $\widetilde{\mathcal{G}}$ is *complete*, if $\mathcal{F}(\widetilde{\mathcal{G}}_{\rm int}) = \mathcal{P}(\widetilde{\mathcal{G}}_{\rm int})$, or equivalently if every bounded face of $\widetilde{\mathcal{G}}_{\rm int}$ consists of exactly one tile $T \in \mathcal{T}$. Let us denote the class of star-like complete subgraphs by $\mathcal{S}(\mathcal{G})$.

3. Strong isoperimetric inequality for tessellating quantum graphs

Now we are in position to formulate our main results. Our first theorem relates the positivity of the isoperimetric constant with the positivity of the characteristic values of a metric graph.

Theorem 3.1. *Let $\mathcal{G} = (\mathcal{V}, \mathcal{E}, |\cdot|)$ be a tessellating metric graph having infinite volume,* $\mathrm{mes}(\mathcal{G}) = \sum_{e\in\mathcal{E}} |e| = \infty$. *If*

$$\ell^*(\mathcal{G}) := \sup_{e\in\mathcal{E}} |e| < \infty \tag{3.1}$$

and

$$\liminf_{\mathrm{mes}(\widetilde{\mathcal{G}})\to\infty} \frac{1}{\mathrm{mes}(\widetilde{\mathcal{G}})} \sum_{e\in\widetilde{\mathcal{E}}} c(e)|e| = \liminf_{\mathrm{mes}(\widetilde{\mathcal{G}})\to\infty} \frac{\sum_{e\in\widetilde{\mathcal{E}}} c(e)|e|}{\sum_{e\in\widetilde{\mathcal{E}}} |e|} > 0, \tag{3.2}$$

then $\alpha(\mathcal{G}) > 0$. Here $\liminf$ *is taken over all star-like complete subgraphs $\widetilde{\mathcal{G}} \in \mathcal{S}(\mathcal{G})$.*

Remark 3.2.

(i) Let us mention that (3.1) *is necessary for the strong isoperimetric inequality to hold for an arbitrary metric graph since (see, e.g.,* [26, Remark 3.3]*)*

$$\alpha(\mathcal{G}) \le \frac{2}{\ell^*(\mathcal{G})}. \tag{3.3}$$

(ii) If $\mathrm{mes}(\mathcal{G}) = \sum_{e\in\mathcal{E}} |e| < \infty$, *then the lower bound*

$$\alpha(\mathcal{G}) \ge \frac{2}{\mathrm{mes}(\mathcal{G})} > 0 \tag{3.4}$$

holds. In fact, if $\mathcal{G}$ is tessellating, then $\deg(\partial\widetilde{\mathcal{G}}) \ge 2$ *for every finite subgraph $\widetilde{\mathcal{G}} \subset \mathcal{G}$ and* (3.4) *follows immediately from* (2.5).

(iii) Theorem 3.1 can be seen as the analogue of [37, Theorem 1].

(iv) As we will see below, the proof of Theorem 3.1 implies the explicit estimate

$$\alpha(\mathcal{G}) \ge \min\Big\{\frac{2}{\ell^*(\mathcal{G})},\ \inf_{\widetilde{\mathcal{G}}\in\mathcal{S}} \frac{1}{\mathrm{mes}(\widetilde{\mathcal{G}})} \sum_{e\in\widetilde{\mathcal{E}}} c(e)|e|\Big\}, \tag{3.5}$$

however, the conditions in Theorem 3.1 are weaker than positivity of the right-hand side in (3.5).

The next result shows that pointwise estimates for the characteristic values also yield lower estimates for the isoperimetric constant. To this end, introduce the following quantities

$$M(\mathcal{G}) := \sup_{v\in\mathcal{V}} \frac{m(v)}{\inf_{e\in\mathcal{E}_v}|e|}, \qquad\qquad P(\mathcal{G}) := \sup_{T\in\mathcal{T}} \frac{p(T)}{\inf_{e\in\mathcal{E}_T}|e|}, \tag{3.6}$$

and set

$$K(\mathcal{G}) := 1 - \frac{1}{M(\mathcal{G})} - \frac{2}{P(\mathcal{G})} - \frac{1}{(M(\mathcal{G})-2)P(\mathcal{G})}. \tag{3.7}$$

Theorem 3.3. *Let $\mathcal{G} = (\mathcal{V}, \mathcal{E}, |\cdot|)$ be a tessellating metric graph. Suppose*

$$c_*(\mathcal{G}) := \inf_{e\in\mathcal{E}} c(e) > 0. \tag{3.8}$$

Then

$$\alpha(\mathcal{G}) \geq \frac{c_*(\mathcal{G})}{K(\mathcal{G})} > 0. \tag{3.9}$$

Theorem 3.3 can be considered as the metric graph analogue of the corresponding estimate for combinatorial graphs in [24, Theorem 1].

Remark 3.4. *The following obvious estimates*

$$M(\mathcal{G}) \geq \sup_{v\in\mathcal{V}} \deg(v) \geq 3, \qquad\qquad P(\mathcal{G}) \geq \sup_{T\in\mathcal{T}} d_{\mathcal{T}}(T) \geq 3, \tag{3.10}$$

imply that $K(\mathcal{G}) \leq 1$. Moreover, one can show that $K(\mathcal{G}) > 0$ if $c_*(\mathcal{G}) > 0$. Indeed, noting that

$$m(v) \leq \deg(v)\ell^*(\mathcal{G}), \qquad\qquad p(T) \leq d_{\mathcal{T}}(T)\ell^*(\mathcal{G}),$$

we easily get the rough estimate

$$c_*(\mathcal{G}) \leq \frac{1}{\ell^*(\mathcal{G})}\Big(1 - \frac{2}{\deg^*(\mathcal{G})} - \frac{2}{d^*_{\mathcal{T}}(\mathcal{G})}\Big), \tag{3.11}$$

where $\deg^*(\mathcal{G}) := \sup_{v\in\mathcal{V}} \deg(v)$ *and* $d^*_{\mathcal{T}}(\mathcal{G}) := \sup_{T\in\mathcal{T}} d_{\mathcal{T}}(T)$*. On the other hand,*

$$\begin{aligned} K(\mathcal{G}) &= \frac{1}{2}\Big(1 - \frac{2}{M(\mathcal{G})} - \frac{2}{P(\mathcal{G})}\Big) + \frac{1}{2} - \frac{1}{P(\mathcal{G})} - \frac{1}{(M(\mathcal{G})-2)P(\mathcal{G})} \\ &\geq \frac{1}{2}\Big(1 - \frac{2}{\deg^*(\mathcal{G})} - \frac{2}{d^*_{\mathcal{T}}(\mathcal{G})}\Big) + \frac{1}{2} - \frac{1}{d^*_{\mathcal{T}}(\mathcal{G})} - \frac{1}{(\deg^*(\mathcal{G})-2)d^*_{\mathcal{T}}(\mathcal{G})}. \end{aligned}$$

If $c_*(\mathcal{G}) > 0$, then so is the right-hand side in (3.11) *which implies*

$$\begin{aligned} K(\mathcal{G}) >& \frac{1}{2} - \frac{1}{d^*_{\mathcal{T}}(\mathcal{G})} - \frac{1}{(\deg^*(\mathcal{G})-2)d^*_{\mathcal{T}}(\mathcal{G})} \\ >& \frac{1}{\deg^*(\mathcal{G})} - \frac{1}{(\deg^*(\mathcal{G})-2)d^*_{\mathcal{T}}(\mathcal{G})} \geq 0. \end{aligned}$$

To prove Theorems 3.1 and 3.3, we first show that we can restrict in (2.5) to star-like complete subgraphs.

Lemma 3.5. *Let $\mathcal{G} = (\mathcal{V}, \mathcal{E}, |\cdot|)$ be a tessellating metric graph. Then*

$$\alpha(\mathcal{G}) = \min\Big\{\frac{2}{\ell^*(\mathcal{G})}, \alpha_{\mathcal{S}}(\mathcal{G})\Big\}, \tag{3.12}$$

where

$$\alpha_{\mathcal{S}}(\mathcal{G}) := \inf_{\widetilde{\mathcal{G}}\in\mathcal{S}} \frac{\deg(\partial\widetilde{\mathcal{G}})}{\mathrm{mes}(\widetilde{\mathcal{G}})}. \tag{3.13}$$

Proof. (i) First, we show that it suffices to consider subgraphs that are either star-like or consist of a single edge. Let $\widetilde{\mathcal{G}} = (\widetilde{\mathcal{V}}, \widetilde{\mathcal{E}})$ be a finite, connected subgraph of $\mathcal{G}$ and $\widetilde{\mathcal{V}}_{\text{int}} = \widetilde{\mathcal{V}} \setminus \partial\widetilde{\mathcal{G}}$. We split $\widetilde{\mathcal{V}}_{\text{int}} = \bigcup_{i=1}^n \mathcal{V}_i$ into a finite, disjoint union of connected vertex sets $\mathcal{V}_i$. Let $\mathcal{G}_i = (\mathcal{V}_i, \mathcal{E}_i) \subset \mathcal{G}$ be the subgraph with edge set

$$\mathcal{E}_i = \bigcup_{v \in \mathcal{V}_i} \mathcal{E}_v.$$

By construction, each $\mathcal{G}_i$ is star-like and each edge $e \in \mathcal{E}$ belongs to at most one $\mathcal{G}_i$. Let $\mathcal{E}_r = \widetilde{\mathcal{E}} \setminus \bigcup_{i=1}^n \mathcal{E}_i$ be the remaining edges. Then

$$\operatorname{mes}(\widetilde{\mathcal{G}}) = \sum_{i=1}^n \operatorname{mes}(\mathcal{G}_i) + \sum_{e \in \mathcal{E}_r} |e|.$$

Moreover, both vertices of an edge $e \in \mathcal{E}_r$ are in $\partial\widetilde{\mathcal{G}}$ and $\partial\mathcal{G}_i = \partial\widetilde{\mathcal{G}} \cap \mathcal{V}_i$. Hence

$$\deg(\partial\widetilde{\mathcal{G}}) = \sum_{v \in \partial\widetilde{\mathcal{G}}} \sum_{i=1}^n \deg_{\mathcal{G}_i}(v) + 2\#\mathcal{E}_r = \sum_{i=1}^n \deg(\partial\mathcal{G}_i) + 2\#\mathcal{E}_r.$$

This finally implies

$$\frac{\deg(\partial\widetilde{\mathcal{G}})}{\operatorname{mes}(\widetilde{\mathcal{G}})} = \frac{\sum_{i=1}^n \deg(\partial\mathcal{G}_i) + 2\#\mathcal{E}_r}{\sum_{i=1}^n \operatorname{mes}(\mathcal{G}_i) + \sum_{e \in \mathcal{E}_r} |e|} \geq \min_{\substack{i=1,\dots,n,\\ e \in \mathcal{E}_r}} \left\{ \frac{\deg(\partial\mathcal{G}_i)}{\operatorname{mes}(\mathcal{G}_i)}, \frac{2}{|e|} \right\}.$$

(ii) To complete the proof, it suffices to construct for every star-like subgraph $\widetilde{\mathcal{G}}$ a star-like, complete subgraph $\widehat{\mathcal{G}} \in \mathcal{S}(\mathcal{G})$ with $\widehat{\mathcal{G}} \supseteq \widetilde{\mathcal{G}}$ and $\deg(\partial\widetilde{\mathcal{G}}) \geq \deg(\partial\widehat{\mathcal{G}})$. Let $\widetilde{\mathcal{G}}_{\text{int}} = (\widetilde{\mathcal{V}}_{\text{int}}, \widetilde{\mathcal{E}}_{\text{int}})$ be the interior graph of $\widetilde{\mathcal{G}}$. Denote by $\mathcal{F}_0$ the set of bounded, open components of $\mathbb{R}^2 \setminus \widetilde{\mathcal{G}}_{\text{int}}$ and by $\mathcal{F} = \{F = \overline{f} | \, f \in \mathcal{F}_0\}$ the bounded faces of $\widetilde{\mathcal{G}}_{\text{int}}$. The idea is to add "edges contained in bounded faces". Define the subgraph $\widehat{\mathcal{G}} = (\widehat{\mathcal{V}}, \widehat{\mathcal{E}})$ by its edge set

$$\widehat{\mathcal{E}} = \widetilde{\mathcal{E}} \cup \bigcup_{v \in f :\, f \in \mathcal{F}_0} \mathcal{E}_v.$$

If an edge $e \in \mathcal{E}$ is incident to a vertex $v \in f$ with $f \in \mathcal{F}_0$, then its other vertex lies in $F = \overline{f}$. Hence $\deg_{\widehat{\mathcal{G}}}(v) = \deg_{\widetilde{\mathcal{G}}}(v)$ for every vertex v with $v \notin K := \bigcup_{F \in \mathcal{F}} F$. On the other hand, every vertex $v \in K$ belongs to $\widehat{\mathcal{G}}$ and satisfies $\deg_{\widehat{\mathcal{G}}}(v) = \deg_{\mathcal{G}}(v)$. Indeed, if $v \in F = \overline{f}$, then either $v \in f$ or $v \in \partial f \subseteq \widetilde{\mathcal{G}}_{\text{int}}$. This implies $\partial\widehat{\mathcal{G}} \subseteq \partial\widetilde{\mathcal{G}}$ and $\deg(\partial\widetilde{\mathcal{G}}) \geq \deg(\partial\widehat{\mathcal{G}})$. Moreover, $\widehat{\mathcal{E}} = \cup_{v \in \widehat{U}} \mathcal{E}_v$, where

$$\widehat{U} = \widetilde{\mathcal{V}}_{\text{int}} \cup \bigcup_{f \in \mathcal{F}_0} \{v \in \mathcal{V} | \, v \in f\}.$$

Also, $\widehat{U}$ is finite by local finiteness and connected since $\widetilde{\mathcal{G}}$ is star-like and $\partial f \subseteq \widetilde{\mathcal{G}}_{\text{int}}$ for $f \in \mathcal{F}_0$. It remains to show that $\widehat{\mathcal{G}}$ is complete. Let $\widehat{F}$ be a bounded face of the interior graph $\widehat{\mathcal{G}}_{\text{int}}$. Suppose $T \in \mathcal{T}$ with $T \subseteq \widehat{F}$. Then $T \subseteq \widehat{F} \subseteq F$ for some bounded face F of $\widetilde{\mathcal{G}}_{\text{int}}$. In particular, $e \subseteq K$ for every edge $e \subseteq \partial T$. But every vertex $v \in K$ belongs to $\widehat{\mathcal{G}}_{\text{int}}$, and hence $\partial T \subseteq \widehat{\mathcal{G}}_{\text{int}}$ and $\widehat{F} = T$ $\square$

Remark 3.6. *Combining* (3.12) *with* (3.3)*, one concludes that the inequality*

$$\frac{2}{\ell^*(\mathcal{G})} \leq \alpha_{\mathcal{S}}(\mathcal{G}) = \inf_{\widetilde{\mathcal{G}} \in \mathcal{S}} \frac{\deg(\partial\widetilde{\mathcal{G}})}{\operatorname{mes}(\widetilde{\mathcal{G}})} \tag{3.14}$$

implies that

$$\alpha(\mathcal{G}) = \frac{2}{\ell^*(\mathcal{G})}. \tag{3.15}$$

In Example 4.3, we provide an explicit construction of a graph satisfying (3.14)*.*

The next lemma contains the connection between $c(e)$ and $\alpha(\mathcal{G})$.

Lemma 3.7. *The following inequality*

$$\sum_{e\in\widetilde{\mathcal{E}}} c(e)|e| \leq \deg(\partial_{\mathcal{G}}\widetilde{\mathcal{G}}) \tag{3.16}$$

holds for any star-like, complete subgraph $\widetilde{\mathcal{G}} \in \mathcal{S}(\mathcal{G})$*.*

Proof. Let $\widetilde{\mathcal{G}}_{\text{int}} = (\widetilde{\mathcal{V}}_{\text{int}}, \widetilde{\mathcal{E}}_{\text{int}})$ be the interior graph and $\mathcal{E}^b := \widetilde{\mathcal{E}} \setminus \widetilde{\mathcal{E}}_{\text{int}}$ the remaining edges. Then

$$\begin{aligned}
\sum_{e\in\widetilde{\mathcal{E}}} c(e)|e| &= \sum_{e\in\widetilde{\mathcal{E}}} 1 - \sum_{v\in\widetilde{\mathcal{V}}} \frac{\operatorname{mes}(\mathcal{E}_v\cap\widetilde{\mathcal{E}})}{m(v)} - \sum_{T\in\mathcal{T}} \frac{\operatorname{mes}(\mathcal{E}_T\cap\widetilde{\mathcal{E}}_{\text{int}})}{p(T)} - \sum_{T\in\mathcal{T}} \frac{\operatorname{mes}(\mathcal{E}_T\cap\mathcal{E}^b)}{p(T)}\\
&= \#\mathcal{E}^b + \#\widetilde{\mathcal{E}}_{\text{int}} - \#\widetilde{\mathcal{V}}_{\text{int}} - \#\mathcal{P}(\widetilde{\mathcal{G}}_{\text{int}})\\
&\quad - \sum_{v\in\partial\widetilde{\mathcal{G}}} \frac{\operatorname{mes}(\mathcal{E}_v\cap\widetilde{\mathcal{E}})}{m(v)} - \sum_{T\in\mathcal{T},\mathcal{E}_T\not\subseteq\widetilde{\mathcal{E}}_{\text{int}}} \frac{\operatorname{mes}(\mathcal{E}_T\cap\widetilde{\mathcal{E}}_{\text{int}})}{p(T)} - \sum_{T\in\mathcal{T}} \frac{\operatorname{mes}(\mathcal{E}_T\cap\mathcal{E}^b)}{p(T)},
\end{aligned}$$

where $\mathcal{P}(\widetilde{\mathcal{G}}_{\text{int}})$ is the set of tiles $T \in \mathcal{T}$ with $\mathcal{E}_T \subseteq \widetilde{\mathcal{E}}_{\text{int}}$. By Euler's formula (see, e.g., [16])

$$\#\widetilde{\mathcal{E}}_{\text{int}} - \#\widetilde{\mathcal{V}}_{\text{int}} - \#\mathcal{F}(\widetilde{\mathcal{G}}_{\text{int}}) = -1,$$

Because $\widetilde{\mathcal{G}}$ is complete, $\mathcal{F}(\widetilde{\mathcal{G}}_{\text{int}}) = \mathcal{P}(\widetilde{\mathcal{G}}_{\text{int}})$ and $\sum |e|c(e)$ is equal to

$$\#\mathcal{E}^b - 1 - \sum_{v\in\partial\widetilde{\mathcal{G}}} \frac{\operatorname{mes}(\mathcal{E}_v\cap\widetilde{\mathcal{E}})}{m(v)} - \sum_{T\in\mathcal{T},\mathcal{E}_T\not\subseteq\widetilde{\mathcal{E}}_{\text{int}}} \frac{\operatorname{mes}(\mathcal{E}_T\cap\widetilde{\mathcal{E}}_{\text{int}})}{p(T)} - \sum_{T\in\mathcal{T}} \frac{\operatorname{mes}(\mathcal{E}_T\cap\mathcal{E}^b)}{p(T)}.$$

Since $\widetilde{\mathcal{G}}$ is star-like, there are no edges $e \in \widetilde{\mathcal{E}}$ with both vertices in $\partial\widetilde{\mathcal{G}}$. Therefore, $\#\mathcal{E}^b = \deg(\partial\widetilde{\mathcal{G}})$ and the proof is complete. ☐

Remark 3.8. *For future reference, observe that*

$$\begin{aligned}
&\sum_{v\in\partial\widetilde{\mathcal{G}}} \frac{\operatorname{mes}(\mathcal{E}_v\cap\widetilde{\mathcal{E}})}{m(v)} + \sum_{T\in\mathcal{T},\mathcal{E}_T\not\subseteq\widetilde{\mathcal{E}}_{\text{int}}} \frac{\operatorname{mes}(\mathcal{E}_T\cap\widetilde{\mathcal{E}}_{\text{int}})}{p(T)} + \sum_{T\in\mathcal{T}} \frac{\operatorname{mes}(\mathcal{E}_T\cap\mathcal{E}^b)}{p(T)}\\
&\qquad \geq \sum_{v\in\partial\widetilde{\mathcal{G}}} \frac{\deg_{\widetilde{\mathcal{G}}}(v)}{M(\mathcal{G})} + \sum_{T\in\mathcal{T},\mathcal{E}_T\not\subseteq\widetilde{\mathcal{E}}_{\text{int}}} \frac{\#(\mathcal{E}_T\cap\widetilde{\mathcal{E}}_{\text{int}})}{P(\mathcal{G})} + \sum_{T\in\mathcal{T}} \frac{\#(\mathcal{E}_T\cap\mathcal{E}^b)}{P(\mathcal{G})}.
\end{aligned}$$

This implies the following estimate

$$\begin{aligned}
\sum_{e\in\widetilde{\mathcal{E}}} c(e)|e| \leq{}& \deg(\partial\widetilde{\mathcal{G}})\Big(1 - \frac{1}{M(\mathcal{G})} - \frac{2}{P(\mathcal{G})}\Big)\\
&- \frac{1}{P(\mathcal{G})} \sum_{e\in\widetilde{\mathcal{E}}_{\text{int}}} \#\{T|\ e\in\mathcal{E}_T \ \textit{and}\ \mathcal{E}_T\not\subseteq\widetilde{\mathcal{E}}_{\text{int}}\}
\end{aligned} \tag{3.17}$$

for every star-like, complete subgraph $\widetilde{\mathcal{G}} \in \mathcal{S}(\mathcal{G})$*.*

Corollary 3.9. *Let $\mathcal{G} = (\mathcal{V}, \mathcal{E}, |\cdot|)$ be a finite tessellating metric graph, that is a finite graph satisfying all the assumptions of Section 2.1 except (iii) of Definition 2.1. Then*

$$\sum_{e\in\mathcal{E}} -c(e)|e| = 1. \tag{3.18}$$

Proof. By Euler's formula

$$\begin{aligned}\sum_{e\in\mathcal{E}} c(e)|e| &= \#\mathcal{E} - \sum_{v\in\mathcal{V}} \frac{\operatorname{mes}(\mathcal{E}\cap\mathcal{E}_v)}{m(v)} - \sum_{T\in\mathcal{T}} \frac{\operatorname{mes}(\mathcal{E}\cap\mathcal{E}_T)}{p(T)} \\ &= \#\mathcal{E} - \#\mathcal{V} - \#\mathcal{F}(\mathcal{G}) = -1.\end{aligned}$$

□

Remark 3.10. *Formula* (3.18) *can be seen as the analogue of the combinatorial Gauss–Bonnet formula known for combinatorial graphs (see* [22, Proposition 1]*). Let us also mention that the difference in the right-hand side arises from our convention $p(T) = \infty$ for unbounded $T \in \mathcal{T}$.*

Theorem 3.1 now follows from Lemma 3.5 and 3.7 together with the inequality $\deg(\partial\widetilde{\mathcal{G}}) \geq 1$ for $\widetilde{\mathcal{G}} \in \mathcal{S}(\mathcal{G})$. Moreover, we can already deduce (see (3.5) and (3.11)) the basic estimate

$$\alpha(\mathcal{G}) \geq c_*(\mathcal{G}). \tag{3.19}$$

By improving this bound further we finally obtain Theorem 3.3.

Proof of Theorem 3.3. We start by providing a basic inequality. By Remark 3.4, we have $K(\mathcal{G}) > 0$. Let $\deg^*(\mathcal{G}) := \sup_{v\in\mathcal{V}} \deg(v)$. Then using (3.10) and (3.11), a lengthy but straightforward calculation implies

$$\frac{c_*(\mathcal{G})}{K(\mathcal{G})} \leq \frac{\deg^*(\mathcal{G}) - 2}{\deg^*(\mathcal{G}) - 1} \frac{1}{\ell^*(\mathcal{G})}. \tag{3.20}$$

Hence by Lemma 3.5, it suffices to show that

$$\frac{\deg(\partial\widetilde{\mathcal{G}})}{\operatorname{mes}(\widetilde{\mathcal{G}})} \geq \frac{c_*(\mathcal{G})}{K(\mathcal{G})} \tag{3.21}$$

for every $\widetilde{\mathcal{G}} = (\widetilde{\mathcal{V}}, \widetilde{\mathcal{E}}) \in \mathcal{S}(\mathcal{G})$.

We will obtain (3.21) by induction over $\#\widetilde{\mathcal{V}}_{\text{int}}$. If $\#\widetilde{\mathcal{V}}_{\text{int}} = 1$, that is, $\widetilde{\mathcal{V}}_{\text{int}} = \{v\}$ for some $v \in \mathcal{V}$, then $\widetilde{\mathcal{G}}$ "consists of a single star". More precisely, $\widetilde{\mathcal{E}} = \mathcal{E}_v$ and (3.20) implies

$$\frac{\deg(\partial\widetilde{\mathcal{G}})}{\operatorname{mes}(\widetilde{\mathcal{G}})} \geq \frac{\deg(v)}{\deg(v)\ell^*(\mathcal{G})} \geq \frac{c_*(\mathcal{G})}{K(\mathcal{G})}.$$

Now suppose $\#\widetilde{\mathcal{V}}_{\text{int}} = n \geq 2$ and (3.21) holds for all $\widehat{\mathcal{G}} \in \mathcal{S}(\mathcal{G})$ with $\#\widehat{\mathcal{V}}_{\text{int}} < n$. We distinguish two cases:

(i) First, assume

$$\#\{u \in \partial\widetilde{\mathcal{G}} |\ u \text{ is connected to } v\} \leq \deg^*(\mathcal{G}) - 2$$

for all $v \in \widetilde{\mathcal{V}}_{\text{int}}$. In view of (3.17), define

$$\mathcal{E}_i := \{e \in \widetilde{\mathcal{E}}_{\text{int}} |\ \#\{T |\ e \in \mathcal{E}_T \text{ and } \mathcal{E}_T \not\subseteq \widetilde{\mathcal{E}}_{\text{int}}\} = i\}$$

for $i \in \{1,2\}$. Then

$$\sum_{e\in\widetilde{\mathcal{E}}_{\mathrm{int}}} \#\{T|\ e \in \mathcal{E}_T \text{ and } \mathcal{E}_T \not\subseteq \widetilde{\mathcal{E}}_{\mathrm{int}}\} = \#\mathcal{E}_1 + 2\#\mathcal{E}_2 = \sum_{v\in\widetilde{\mathcal{V}}_{\mathrm{int}}} \delta(v),$$

where $\delta(v) := \#(\mathcal{E}_v \cap \mathcal{E}_1)/2 + \#(\mathcal{E}_v \cap \mathcal{E}_2)$ for all $v \in \mathcal{V}$.

Now assume that $v \in \widetilde{\mathcal{V}}_{\mathrm{int}}$ and that v is connected to at least one vertex in $\partial\widetilde{\mathcal{G}}$. Since $\widetilde{\mathcal{G}}$ is star-like and $\#\widetilde{\mathcal{V}}_{\mathrm{int}} \geq 2$, v is connected to another vertex in $\widetilde{\mathcal{V}}_{\mathrm{int}}$ and hence there exists an interior edge $e \in \widetilde{\mathcal{E}}_{\mathrm{int}}$ incident to v. Going through the edges incident to v in counter-clockwise direction starting from e, denote by e_+ the "last" edge incident to v with $e_+ \in \widetilde{\mathcal{E}}_{\mathrm{int}}$. Define e_- analogously by going clockwise. Then $e_\pm \in \mathcal{E}_1 \cup \mathcal{E}_2$. Moreover, if $e_+ = e_-$, then $e = e_+ = e_- \in \mathcal{E}_2$. Thus $\delta(v) \geq 1$ for every such $v \in \widetilde{\mathcal{V}}_{\mathrm{int}}$. Since $\widetilde{\mathcal{G}}$ is star-like,

$$\begin{aligned}\sum_{v\in\widetilde{\mathcal{V}}_{\mathrm{int}}} \delta(v) &\geq \frac{1}{\deg^*(\mathcal{G})-2} \sum_{v\in\widetilde{\mathcal{V}}_{\mathrm{int}}} \#\{u \in \partial\widetilde{\mathcal{G}}|\ u \text{ is connected to } v\} \\ &\geq \frac{1}{M(\mathcal{G})-2}\deg(\partial\widetilde{\mathcal{G}}),\end{aligned}$$

and (3.21) follows from (3.17).

(ii) Assume that $\#\{u \in \partial\widetilde{\mathcal{G}}|\ u \text{ is connected to } v\} \geq \deg^*(\mathcal{G}) - 1$ for some vertex $v \in \widetilde{\mathcal{V}}_{\mathrm{int}}$. Since $\#\widetilde{\mathcal{V}}_{\mathrm{int}} \geq 2$, this implies $\deg(v) = \deg^*(\mathcal{G})$ and that v is connected to exactly one $w \in \widetilde{\mathcal{V}}_{\mathrm{int}}$. We "cut out" the $\deg^*(\mathcal{G}) - 1$ edges between v and $\partial\widetilde{\mathcal{G}}$ and define $\widehat{\mathcal{G}} = (\widehat{\mathcal{V}}, \widehat{\mathcal{E}})$ by its edge set

$$\widehat{\mathcal{E}} = \widetilde{\mathcal{E}} \setminus \{e \in \mathcal{E}|\ e \text{ connects } v \text{ and } \partial\widetilde{\mathcal{G}}\}.$$

Then $\widehat{\mathcal{G}}$ is again star-like and complete. Its interior graph $\widehat{\mathcal{G}}_{\mathrm{int}} = (\widehat{\mathcal{V}}_{\mathrm{int}}, \widehat{\mathcal{E}}_{\mathrm{int}})$ is given by $\widehat{\mathcal{V}}_{\mathrm{int}} = \widetilde{\mathcal{V}}_{\mathrm{int}} \setminus \{v\}$ and $\widehat{\mathcal{E}}_{\mathrm{int}} = \widetilde{\mathcal{E}}_{\mathrm{int}} \setminus \{e_{v,w}\}$, where $e_{v,w}$ is the edge between v and w. In particular, $\widehat{\mathcal{G}}$ satisfies (3.21).

Now assume (3.21) fails for $\widetilde{\mathcal{G}}$. Then

$$\deg(\partial\widetilde{\mathcal{G}})(\mathrm{mes}(\widetilde{\mathcal{G}}) - \mathrm{mes}(\widehat{\mathcal{G}})) \leq (\deg^*(\mathcal{G}) - 2)\mathrm{mes}(\widetilde{\mathcal{G}})$$

by (3.20). Consequently,

$$\begin{aligned}\frac{\deg(\partial\widehat{\mathcal{G}})}{\mathrm{mes}(\widehat{\mathcal{G}})} = \frac{\#\widehat{\mathcal{E}} - \#\widehat{\mathcal{E}}_{\mathrm{int}}}{\mathrm{mes}(\widehat{\mathcal{G}})} &= \frac{\#\widetilde{\mathcal{E}} - \#\widetilde{\mathcal{E}}_{\mathrm{int}} - \deg^*(\mathcal{G}) + 2}{\mathrm{mes}(\widehat{\mathcal{G}})} \\ &= \frac{\deg(\partial\widetilde{\mathcal{G}}) - \deg^*(\mathcal{G}) + 2}{\mathrm{mes}(\widehat{\mathcal{G}})} \leq \frac{\deg(\partial\widetilde{\mathcal{G}})}{\mathrm{mes}(\widetilde{\mathcal{G}})} < \frac{c_*(\mathcal{G})}{K(\mathcal{G})},\end{aligned}$$

which is a contradiction. $\square$

4. Examples

In this section, we illustrate the use of our results in three examples.

4.1. **(p,q)-regular graphs.** Let $p \in \mathbb{Z}_{\geq 3}$ and $q \in \mathbb{Z}_{\geq 3} \cup \{\infty\}$. A tessellating (combinatorial) graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ is called (p,q)-*regular*, if $\deg(v) = p$ for all $v \in \mathcal{V}$ and $d_{\mathcal{T}}(T) = q$ for all $T \in \mathcal{T}$. Let $\mathcal{G}_{p,q}$ denote both the corresponding combinatorial graph and the associated equilateral metric graph, that is, we put $|e| \equiv 1$ for all $e \in \mathcal{E}_{p,q} = \mathcal{E}(\mathcal{G}_{p,q})$. Notice that $\mathcal{G}_{p,\infty}$ is an infinite p-regular tree $\mathbb{T}_p$ (also known as a *Cayley tree* or a *Bethe lattice*).

Next, by (2.9), we get

$$c(e) = 1 - \frac{2}{p} - \frac{2}{q} =: c_{p,q}, \tag{4.1}$$

for all $e \in \mathcal{E}_{p,q}$, and the *vertex curvature* of the combinatorial graph $\mathcal{G}_{p,q}$ (see for example [8, 17, 37]) is given by

$$\kappa(v) = 1 - \frac{\deg(v)}{2} + \sum_{T: v\in T} \frac{1}{d_{\mathcal{T}}(T)} = 1 - \frac{p}{2} + \frac{p}{q} = -\frac{p}{2}\, c_{p,q}, \tag{4.2}$$

for all $v \in \mathcal{V}$.

Since strictly positive vertex curvature implies that $\mathcal{G}_d$ has only finitely many vertices (see [8, Theorem 1.7]), the characteristic value should satisfy $c_{p,q} \geq 0$. Clearly, $c_{p,q} = 0$ exactly when $(p,q) \in \{(4,4),(3,6),(6,3)\}$ and in these cases $\mathcal{G}_{p,q}$ is isomorphic to the square, hexagonal or triangle lattice in $\mathbb{R}^2$. If $c_{p,q} > 0$, then $\mathcal{G}_{p,q}$ is isomorphic to the edge graph of a tessellation of the Poincaré disc H^2 with regular q-gons of interior angle $2\pi/p$ (see [15, Remark 4.2.] and [21]). In the latter case, Theorem 3.3 implies $\alpha(\mathcal{G}_{p,q}) > 0$ and the estimate

$$\alpha(\mathcal{G}_{p,q}) \geq \frac{q(p-2)c_{p,q}}{q(p-1)c_{p,q}+1} = \frac{p-2}{p-1} \times \begin{cases} \frac{1}{1+(q(p-1)\,c_{p,q})^{-1}}, & q<\infty \\ 1, & q=\infty \end{cases}. \tag{4.3}$$

Notice that in the case $q = \infty$, equality holds true in (4.3) (see, e.g., [26, Example 8.3]).

It is well-known that (see [15, 18]),

$$\alpha_{\mathrm{comb}}(\mathcal{G}_{p,q}) = \frac{p-2}{p}\sqrt{1 - \frac{4}{(p-2)(q-2)}}. \tag{4.4}$$

By (a slight modification of) [26, Lemma 4.1],

$$\alpha(\mathcal{G}) = \frac{2\alpha_{\mathrm{comb}}(\mathcal{G}_d)}{\alpha_{\mathrm{comb}}(\mathcal{G}_d)+1} \tag{4.5}$$

for every equilateral metric graph $\mathcal{G} = (\mathcal{V},\mathcal{E},|\cdot|)$ with underlying combinatorial graph $\mathcal{G}_d = (\mathcal{V},\mathcal{E})$. Hence

$$\alpha(\mathcal{G}_{p,q}) = \frac{p-2}{p-1+\frac{p}{2}\left(\sqrt{\frac{(p-2)(q-2)}{pq-2(p+q)}}-1\right)} = \frac{p-2}{p-1} \times \begin{cases} \frac{1}{1+\delta(q(p-1)\,c_{p,q})^{-1}}, & q<\infty \\ 1, & q=\infty \end{cases}, \tag{4.6}$$

where

$$\delta := \frac{pq-2(p+q)}{2}\left(\sqrt{1+\frac{4}{pq-2(p+q)}}-1\right) \leq 1.$$

Comparing (4.6) with (4.3), we conclude that the error in the estimate (4.3) is uniformly of order $\frac{1}{(pq)^2}$.

Finally, let us mention that using (4.5), we can turn (4.3) into a lower estimate for $\alpha_{\mathrm{comb}}(\mathcal{G}_{p,q})$ as well. After a short calculation, we recover Theorem 1 from [24],

$$\alpha_{\mathrm{comb}}(\mathcal{G}_{p,q}) \geq \frac{p-2}{p}\left(1 - \frac{2}{(p-2)(q-2)-2}\right). \tag{4.7}$$

4.2. **Another example.** Denote by $\mathbb{Z}^2_+$ the square lattice of the upper half-plane, i.e. the combinatorial graph with vertex set $\mathbb{Z} \times \mathbb{Z}_{\geq 0}$ and two vertices connected if and only if they are connected in the square lattice $\mathbb{Z}^2 = \mathbb{Z} \times \mathbb{Z}$. Fix $k \in \mathbb{Z}_{\geq 3}$ and let $\mathcal{G}_k$ be the graph obtained from $\mathbb{Z}^2_+$ by attaching to each vertex $v \in \mathbb{Z} \times \{0\}$ an infinite k-regular tree (see Figure 1).

To assign edge lengths, we first define a partition of the edge set $\mathcal{E}_k$. We denote by $\mathcal{E}_{k,\mathrm{tree}}$ the set of edges $e \in \mathcal{E}_k$ belonging to one of the attached trees. Also, let

$$\mathcal{V}_n = \{(z,n) |\, z \in \mathbb{Z}\} = \mathbb{Z} \times \{n\}, \qquad n \in \mathbb{Z}_{\geq 0},$$

be the vertices on the "n-th horizontal line". For $n \in \mathbb{Z}_{\geq 0}$, we define $\mathcal{E}^+_{k,n}$ as the set of "vertical" edges between the n-th horizontal line $\mathcal{V}_n$ and the $(n+1)$-th horizontal line $\mathcal{V}_{n+1}$, and $\mathcal{E}^-_{k,n}$ as the set of "horizontal" edges connecting vertices in the n-th horizontal line $\mathcal{V}_n$ (see Figure 1). Finally, we equip $\mathcal{G}_k$ with edge lengths in the following way:

$$|e| = \begin{cases} 1, & e \in \mathcal{E}_{k,\mathrm{tree}} \\ \frac{1}{(2n+2)^2}, & e \in \mathcal{E}^-_{k,n} \\ \frac{1}{(2n+3)^2}, & e \in \mathcal{E}^+_{k,n} \end{cases}. \tag{4.8}$$

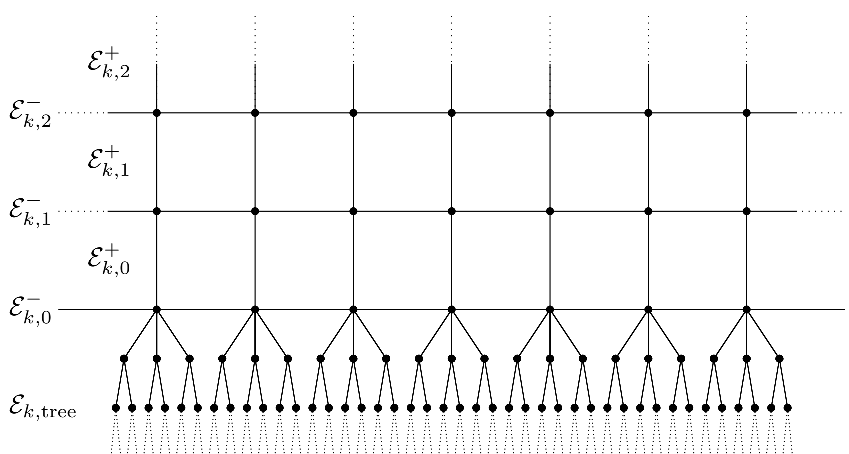

FIGURE 1. $\mathcal{G}_k$ for $k = 3$.

Now let us compute the characteristic values. First of all, for all $e \in \mathcal{E}_{k,\mathrm{tree}}$ we have the estimate

$$\inf_{e \in \mathcal{E}_{k,\mathrm{tree}}} c(e) = 1 - \frac{2}{k} = \frac{k-2}{k}.$$

Next, taking into account that $k \geq 3$, we get

$$c(e) = 4 - \frac{2}{k + 2\frac{1}{4} + \frac{1}{9}} - \frac{1}{\frac{1}{4} + 2\frac{1}{9} + \frac{1}{16}} = \frac{164}{77} - \frac{2}{k + \frac{11}{18}} > 1$$

for all $e \in \mathcal{E}^-_{k,0}$, and

$$c(e) = 9 - \frac{1}{k + 2\frac{1}{4} + \frac{1}{9}} - \frac{1}{\frac{1}{9} + \frac{1}{25} + 2\frac{1}{16}} - \frac{2}{\frac{1}{4} + 2\frac{1}{9} + \frac{1}{16}} = \frac{8955}{5467} - \frac{1}{k + \frac{11}{18}} > 1$$

for $e \in \mathcal{E}_{k,0}^+$. Moreover, after lengthy but straightforward calculations one can see that

$$c(e) > 1$$

for all $e \in \mathcal{E}_{k,n}^{\pm}$ with $n \geq 1$. Thus we obtain

$$c_*(\mathcal{G}_k) = \inf_{e \in \mathcal{E}_{k,\mathrm{tree}}} c(e) = \frac{k-2}{k} > 0, \tag{4.9}$$

and hence, by Theorem 3.3, $\alpha(\mathcal{G}_k) > 0$.

Now let us compute $K(\mathcal{G}_k)$. If $v \in \mathcal{V}_n$ with $n \geq 1$, then

$$\begin{aligned} \sup_{v \in \cup_{n \geq 1} \mathcal{V}_n} \frac{m(v)}{\inf_{e \in \mathcal{E}_v} |e|} &= \sup_{n \geq 1} (2n+3)^2 \left(\frac{1}{(2n+1)^2} + \frac{2}{(2n+2)^2} + \frac{1}{(2n+3)^2} \right) \\ &= \left(1 + \frac{2}{3}\right)^2 + 2\left(1 + \frac{1}{4}\right)^2 + 1 = \frac{497}{72} = 6.902\dot{7} \end{aligned}$$

For $v \in \mathcal{V}_0$, we obtain

$$\frac{m(v)}{\inf_{e \in \mathcal{E}_v} |e|} = 9\left(k + 2\frac{1}{4} + \frac{1}{9}\right) = 9k + \frac{11}{2}$$

Moreover, for the remaining vertices $v \in \mathcal{V}$ belonging to one of the attached trees,

$$\frac{m(v)}{\inf_{e \in \mathcal{E}_v} |e|} = k.$$

By assumption, $k \geq 3$ and hence $M(\mathcal{G}_k) = 9k + \frac{11}{2}$. In addition, $P(\mathcal{G}_k) = \infty$ since $\mathcal{T}$ contains unbounded tiles. Thus we obtain

$$K(\mathcal{G}_k) = 1 - \frac{1}{M(\mathcal{G}_k)} = \frac{18k+9}{18k+11}, \tag{4.10}$$

and Theorem 3.3 implies the lower estimate

$$\alpha(\mathcal{G}_k) \geq \frac{18k+11}{18k+9} \frac{k-2}{k}.$$

Our next goal is to derive an upper estimate. Denote by $\mathcal{T}$ the k-regular tree attached to the origin $o = (0,0) \in \mathbb{R}^2$. For $l \in \mathbb{Z}_{\geq 2}$, let $\widetilde{\mathcal{G}}_l$ be the subgraph consisting of all vertices in $\mathcal{T}$ that can be reached from o with a path using at most l edges and all edges between such vertices. Then it is straightforward to verify

$$\operatorname{mes}(\widetilde{\mathcal{G}}_l) = \sum_{j=0}^{l-1} k(k-1)^j = \frac{k((k-1)^l - 1)}{k-2}, \qquad \deg(\partial \widetilde{\mathcal{G}}_l) = k + k(k-1)^{l-1},$$

and as a consequence,

$$\lim_{l \to \infty} \frac{\deg(\partial \widetilde{\mathcal{G}}_l)}{\operatorname{mes}(\widetilde{\mathcal{G}}_l)} = \frac{k-2}{k-1} = \alpha(\mathbb{T}_k),$$

where $\mathbb{T}_k$ is the equilateral, k-regular tree (see Example 4.1 or [26, Example 8.3]). This implies the two-sided estimate

$$\frac{18k+11}{18k+9} \frac{k-2}{k} \leq \alpha(\mathcal{G}_k) \leq \frac{k-2}{k-1}.$$

In particular, $\alpha(\mathcal{G}_k) \to 1$ for $k \to \infty$.

Remark 4.1. *The two above examples demonstrate the use of Theorem 3.3 in two different situations. First of all, let us mention that by* [26, Corollary 4.4.] *the metric graph $\mathcal{G}$ satisfies the strong isoperimetric inequality if $\ell^*(\mathcal{G}) < \infty$ and the combinatorial isoperimetric constant $\alpha_{\mathrm{comb}}(\mathcal{G}_d)$ is positive,*

$$\alpha_{\mathrm{comb}}(\mathcal{G}_d) > 0.$$

In Example 4.1, the positivity of $\alpha_{\mathrm{comb}}(\mathcal{G}_{p,q})$ is known (see (4.4)*) and hence it is a priori clear that $\alpha(\mathcal{G}) > 0$. However, Example 4.1 shows that in certain situations Theorem 3.3 gives a good quantitative estimate.*

On the other hand, in Example 4.2 we have $\alpha_{\mathrm{comb}}(\mathcal{G}_k) = 0$ (since obviously $\alpha_{\mathrm{comb}}(\mathbb{Z}^2_+) = 0$), however, $\alpha(\mathcal{G}) > 0$. In particular, Theorem 3.3 shows that the isoperimetric constants of the combinatorial and metric graph behave differently.

4.3. **Non-equilateral p-regular trees.** We conclude with an example showing the use of Remark 3.6. For $p \in \mathbb{Z}_{\geq 6}$, let $\mathbb{T}_p$ be the equilateral, p-regular tree from Example 4.1. Fix an edge $\hat{e} \in \mathcal{E}(\mathbb{T}_p)$. In the following, we will consider $\mathbb{T}_p$ equipped with another choice of edge lengths. Define the metric graph $\mathcal{T}_p := (\mathbb{T}_p, |\cdot|)$ by assigning

$$|e| := \begin{cases} p, & e = \hat{e} \\ 1, & e \in \mathcal{E}(\mathbb{T}_p) \setminus \{\hat{e}\} \end{cases}.$$

Let $\widetilde{\mathcal{G}} \in \mathcal{S}(\mathcal{T}_p)$ be a star-like complete subgraph. If $\hat{e} \notin \widetilde{\mathcal{E}}$, then $\mathrm{mes}(\widetilde{\mathcal{G}}) = \#\widetilde{\mathcal{E}}$. If $\hat{e} \in \widetilde{\mathcal{E}}$, then $\widetilde{\mathcal{V}}_{\mathrm{int}} \neq \varnothing$ since $\widetilde{\mathcal{G}}$ is star-like. Hence

$$\mathrm{mes}(\widetilde{\mathcal{G}}) = \#\widetilde{\mathcal{E}} + p - 1 \leq 2\#\widetilde{\mathcal{E}}.$$

Thus we conclude from (4.6) and Lemma 3.5 that

$$\alpha_{\mathcal{S}}(\mathcal{T}_p) = \inf_{\widetilde{\mathcal{G}} \in \mathcal{S}} \frac{\deg(\partial\widetilde{\mathcal{G}})}{\mathrm{mes}(\widetilde{\mathcal{G}})} \geq \frac{1}{2} \inf_{\widetilde{\mathcal{G}} \in \mathcal{S}} \frac{\deg(\partial\widetilde{\mathcal{G}})}{\#\widetilde{\mathcal{E}}} = \frac{1}{2}\alpha(\mathbb{T}_p) = \frac{1}{2}\frac{p-2}{p-1} \geq \frac{2}{5}$$

for all $p \geq 6$. On the other hand, $\ell^*(\mathcal{T}_p) = p \geq 6$ by assumption. Hence Remark 3.6 implies

$$\alpha(\mathcal{T}_p) = \frac{2}{\ell^*(\mathcal{T}_p)} = \frac{2}{p}.$$

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QUANTUM GRAPHS ON RADIALLY SYMMETRIC ANTITREES

ALEKSEY KOSTENKO AND NOEMA NICOLUSSI

Abstract. We investigate spectral properties of Kirchhoff Laplacians on radially symmetric antitrees. This class of metric graphs admits a lot of symmetries, which enables us to obtain a decomposition of the corresponding Laplacian into the orthogonal sum of Sturm–Liouville operators. In contrast to the case of radially symmetric trees, the deficiency indices of the Laplacian defined on the minimal domain are at most one and they are equal to one exactly when the corresponding metric antitree has finite total volume. In this case, we provide an explicit description of all self-adjoint extensions including the Friedrichs extension.

Furthermore, using the spectral theory of Krein strings, we perform a thorough spectral analysis of this model. In particular, we obtain discreteness and trace class criteria, a criterion for the Kirchhoff Laplacian to be uniformly positive and provide spectral gap estimates. We show that the absolutely continuous spectrum is in a certain sense a rare event, however, we also present several classes of antitrees such that the absolutely continuous spectrum of the corresponding Laplacian is $[0, \infty)$.

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1. Introduction

This paper is devoted to one particular class of infinite quantum graphs, namely *Kirchhoff Laplacians on radially symmetric antitrees*. Antitrees appear in the study of *discrete Laplacians* on graphs at least since the 1980's (see [12] and also [11, Section 2]) and they attracted a considerable attention after the work of Wojciechowski [47]. More precisely, Wojciechowski used them in [47] (see also [30, §6] and [23]) to construct graphs of polynomial volume growth for which the combinatorial Laplacian is stochastically incomplete and the bottom of the essential spectrum is strictly positive, which is in sharp contrast to the manifold setting (cf. [9], [21], [22]). These apparent discrepancies were resolved later using the notion of intrinsic metrics, with antitrees appearing as key examples for certain thresholds (see [18, 24, 25, 29]). During the recent years, antitrees were also actively studied from other perspectives and we only refer to a brief selection of articles [1], [8], [11], [20], [42], where further references can be found.

In this paper, we consider antitrees from the perspective of quantum graphs and perform a detailed spectral analysis of the Kirchhoff Laplacian on radially symmetric antitrees. Our discussion includes characterization of self-adjointness and a complete description of self-adjoint extensions, spectral gap estimates and spectral types (discrete, singular and absolutely continuous spectrum).

Before proceeding further, let us first recall necessary definitions. Let $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ be a connected, simple (no loops or multiple edges) combinatorial graph. Fix a root vertex $o \in \mathcal{V}$ and then order the graph with respect to the combinatorial spheres S_n, $n \in \mathbb{Z}_{\geq 0}$ (notice that $S_0 = \{o\}$).

Definition 1.1. A connected simple rooted (infinite) graph $\mathcal{G}_d$ is called an *antitree* if every vertex in S_n, $n \geq 1$[1], is connected to all vertices in S_{n-1} and S_{n+1} and no vertices in S_k for all $|k - n| \neq 1$.

Notice that combinatorial antitrees admit radial symmetry and every antitree is uniquely determined by its sphere numbers $s_n = \#S_n$, $n \geq 0$ (see Figure 1).

If every edge of $\mathcal{G}_d$ is assigned a length $|e| \in (0, \infty)$, then $\mathcal{G} = (\mathcal{G}_d, |\cdot|)$ is called a *metric graph*. Upon identifying each edge e with the interval of length $|e|$, $\mathcal{G}$ may be considered as a "network" of intervals glued together at the vertices. In the following we shall denote combinatorial and metric antitrees by $\mathcal{A}_d$ and, respectively, $\mathcal{A}$. The analog of the Laplace–Beltrami operator for metric graphs is the *Kirchhoff Laplacian* $\mathbf{H}$ (or Kirchhoff–Neumann Laplacian, see Section 3.1), also called a *quantum graph*. It acts as an edgewise (negative) second derivative $f_e \mapsto -\frac{d^2}{dx_e^2} f_e$, $e \in \mathcal{E}$, and is defined on edgewise H^2-functions satisfying continuity and Kirchhoff conditions at the vertices (we refer to [2, 3, 15, 17, 32, 39] for more information and references).

Our approach employs the high degree of symmetry and this naturally demands symmetry assumptions also on the choice of edge lengths:

Hypothesis 1.2. *We shall assume that the metric antitree $\mathcal{A}$ is* radially symmetric*, that is, for each $n \geq 0$, all edges connecting combinatorial spheres S_n and S_{n+1} have the same length, say $\ell_n > 0$.*

One of our main motivations is Lemma 8.9 in [32]. More precisely, the symmetry of antitrees structure turned out useful in studying isoperimetric estimates and we

[1]By definition, the root o is connected to all vertices in S_1 and no vertices in S_k, $k \geq 2$.

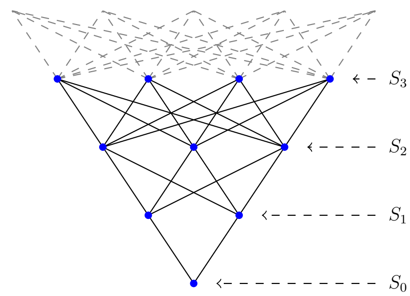

FIGURE 1. Antitree with sphere numbers $s_n = n + 1$.

were even able to compute explicitly the bottom of the essential spectrum of some (non-equilateral) quantum graphs (see [32, §8.2]). Despite an enormous interest in quantum graphs during the last two decades, to the best of our knowledge a detailed discussion of their spectral properties without further restrictions on edges lengths (for instance, one of the most common assumptions is $\inf_{e\in\mathcal{E}} |e| > 0$) has so far been obtained only for a few models and the most studied ones are *radially symmetric trees* (see e.g. [6, 10, 16, 36, 37, 44]). However, the assumption that $\mathcal{G}$ is a tree prevents many interesting phenomena to happen (for instance, by [32, Lemma 8.1], in this case the Kirchhoff Laplacian, actually, its Friedrichs extension, is boundedly invertible if and only if $\sup_{e\in\mathcal{E}} |e| < \infty$; in fact, this condition is only necessary in general [43]). Hence our goal in this work is to present a model which can be thoroughly analyzed but still exhibits in some sense rich spectral behavior.

Let us now briefly describe the content of the paper and our main results. To some extent we follow the approach developed by Naimark and Solomyak for radially symmetric trees (see [36, 37] and also [10, 43, 44]) and use some ideas from [8], where discrete Laplacians on radially symmetric "weighted" graphs have been analyzed. However, some modifications are necessary since comparing to [10, 37, 44] we are dealing with a completely different class of graphs (antitrees have a lot of cycles) and, in contrast to discrete Laplacians [8], we have to deal with unbounded operators (even when restricting to compact subsets of a metric graph) and in this case a search for *reducing subspaces* is a rather complicated task.[2]

First of all, the radial symmetry of $\mathcal{A}$ naturally hints to consider the space $\mathcal{F}_{\mathrm{sym}}$ of radially symmetric functions (w.r.t. the root $o \in \mathcal{V}$). It turns out that $\mathcal{F}_{\mathrm{sym}}$ is indeed reducing for the pre-minimal Kirchhoff Laplacian $\mathbf{H}_0$ (this means that $\mathbf{H}_0$ as well as its closure $\mathbf{H} = \overline{\mathbf{H}}_0$, the minimal Kirchhoff Laplacian, commutes with the orthogonal projection onto $\mathcal{F}_{\mathrm{sym}}$) and its restriction $\mathbf{H}_0 \upharpoonright \mathcal{F}_{\mathrm{sym}}$ is unitarily equivalent to a pre-minimal Sturm–Liouville operator H_0 defined in $L^2((0,\mathcal{L});\mu)$ by the differential expression

$$\tau := -\frac{1}{\mu(t)}\frac{d}{dt}\mu(t)\frac{d}{dt}, \qquad \mu(t) = \sum_{n\geq 0} s_n s_{n+1} \mathbb{1}_{[t_n,t_{n+1})}(t), \tag{1.1}$$

[2]After the submission of our paper we learned about the preprint [7] dealing with a similar decomposition in the general case of family preserving metric graphs, which includes antitrees as a particular example. However, the main focus of [7] is on the existence of a decomposition in a rather general situation, whereas in our work we use it mainly as a starting point for the spectral analysis.

and subject to the Neumann boundary condition at $x = 0$. Here $t_0 = 0$, $t_n = \sum_{k\le n-1} \ell_k$ for all $n \ge 1$ and $\mathcal{L} = \sum_{n\ge 0} \ell_n$ (see Section 3.2). Moreover, the remaining part of $\mathbf{H} = \overline{\mathbf{H}}_0$ decomposes into an infinite sum of self-adjoint (regular) Sturm–Liouville operators (see Theorem 3.5; its proof is given in Sections 2 and 3). This decomposition is the starting point of our analysis since it enables us to investigate $\mathbf{H}$ using the well-developed spectral theory of Sturm–Liouville operators. For example, this immediately provides a self-adjointness criterion together with a complete description of self-adjoint extensions of $\mathbf{H}$ (see Section 4). Namely, since all the summands in (3.18) except $\mathrm{H} = \overline{\mathrm{H}}_0$ are self-adjoint operators, we reduce the problem to the study of the operator H_0. Employing Weyl's limit point/limit circle classification, we obtain in Theorem 4.1 that deficiency indices of $\mathbf{H}$ are at most 1. Moreover, $\mathbf{H}$ is self-adjoint if and only if $\mathcal{A}$ has *infinite total volume*, i.e.

$$\mathrm{vol}(\mathcal{A}) := \sum_{e\in\mathcal{E}} |e| = \sum_{n\ge 0} s_n s_{n+1}\ell_n = \int_0^{\mathcal{L}} \mu(t)dt = \infty.$$

If $\mathcal{A}$ has finite total volume, $\mathrm{vol}(\mathcal{A}) < \infty$, all self-adjoint extensions can be described through a single boundary condition (in particular, this also provides a description of the domain of the Friedrichs extension). Moreover, all of their spectra are purely discrete and eigenvalues satisfy Weyl's law (see Corollary 5.1).

If $\mathrm{vol}(\mathcal{A}) = \infty$, i.e., $\mathbf{H}$ is self-adjoint, it was already observed in [32, Section 8.2] that $\sigma(\mathbf{H})$ is not necessarily discrete. In Section 5, we characterize the cases when $\mathbf{H}$ has purely discrete spectrum and when its resolvent $\mathbf{H}^{-1}$ belongs to the trace class (see Theorem 5.4 and Theorem 5.6). Let us stress that our main tool is the spectral theory of Krein strings [27] (see also [13]). More precisely, by a simple change of variables H can be transformed into the string form (see (5.12)) and then one simply needs to use the corresponding results from [26, 27]. Section 6 is devoted to *spectral estimates*, i.e., the investigation of the bottom of the spectrum $\lambda_0(\mathbf{H})$ of $\mathbf{H}$, $\lambda_0(\mathbf{H}) := \inf \sigma(\mathbf{H})$. This can be solved again by using the results of Kac and Krein from [26]. More precisely, we characterize the positivity of $\lambda_0(\mathbf{H})$ (Theorem 6.1 and Theorem 6.3) and derive two-sided estimates (Remark 6.2). Let us also mention at this point that the decomposition (3.18) indicates the way to compute the isoperimetric constant of a radially symmetric antitree (see Theorem 7.1) and hence it is interesting to compare Theorem 6.1 and Theorem 6.3 with the estimates obtained recently in [32] (see Remark 7.2).

To our best knowledge, the theory of Krein strings is applied in the context of quantum graphs for the first time. In fact, most of the analysis in Sections 5 and 6 can be performed with the help of Muckenhoupt inequalities [35] since the questions addressed in these sections allow a variational reformulation (in particular, Solomyak used this approach in [44] to investigate quantum graphs on radially symmetric trees). However, spectral theory of strings enables us to treat more subtle problems (like the study of the structure of the essential spectrum of $\mathbf{H}$). In Section 9, we employ the recent results from [4] and [14] on the absolutely continuous spectrum of strings to construct several classes of antitrees with absolutely continuous spectrum supported on $[0,\infty)$. For instance, if

$$\inf_{n\ge 0} \ell_n > 0, \qquad\qquad \sum_{n=1}^{\infty} \Big(\frac{s_{n+2}}{s_n} - 1\Big)^2 < \infty, \tag{1.2}$$

then $\sigma_{\mathrm{ac}}(\mathbf{H}) = [0,\infty)$ (see Theorem 9.6). Notice that to prove this claim we employ the analog of the Szegő theorem for strings recently established by Bessonov and Denisov [4]. Antitrees with polynomially growing sphere numbers satisfy the last assumption, however, it can be shown that in this case the usual trace class arguments do not apply (see Remark 9.4). Let us also emphasize that similar to the case of trees quantum graphs typically have purely singular spectrum in the case of antitrees (see Section 8). However, to the best of our knowledge, the only known examples of quantum graphs on trees having nonempty absolutely continuous spectrum are *eventually periodic radially symmetric trees* (see [16, Theorem 5.1]).

In the final section we demonstrate our results by considering two special classes of antitrees and complement the results of [32, Section 8.2]. In Section 10.1 we consider antitrees with exponentially increasing sphere numbers and demonstrate that in this case there are a lot of similarities with the spectral properties of quantum graphs on radially symmetric trees. Antitrees with polynomially increasing sphere numbers are treated in Section 10.2 and this class of quantum graphs exhibits a number of interesting phenomena. For example, one can show a transition from absolutely continuous spectrum supported on $[0,\infty)$ to purely discrete spectrum (see Corollary 10.7).

2. Decomposition of $L^2(\mathcal{A})$

2.1. **Auxiliary subspaces.** Let $\mathcal{A}$ be a metric radially symmetric antitree with sphere numbers $\{s_n\}_{n\geq 0}$ and lengths $\{\ell_n\}_{n\geq 0}$. Upon identifying every edge e with a copy of the interval $\mathcal{I}_e = [0,|e|]$ and considering $\mathcal{A}$ as the union of all edges glued together at certain endpoints, one can introduce the Hilbert space $L^2(\mathcal{A})$ of functions $f\colon \mathcal{A}\to\mathbb{C}$ as $L^2(\mathcal{A}) = \oplus_e L^2(e)$. Next, denote

$$t_n := \sum_{j=0}^{n-1} \ell_j, \qquad\qquad I_n := [t_n, t_{n+1}),$$

and let $\mathcal{H}_n := \mathbb{C}^{s_n s_{n+1}}$, $n\geq 0$. Notice that $s_n s_{n+1}$ is the number of edges in $\mathcal{E}_n^+$, where $\mathcal{E}_n^+$ is the set of edges connecting S_n with S_{n+1}. Enumerating the vertices in each sphere, let each entry a_{ij} of some $\mathbf{a} = (a_{ij})_{i,j}\in\mathcal{H}_n$ correspond to a coefficient of the edge $e\in\mathcal{E}_n^+$ connecting the i-th vertex of S_n with the j-th vertex of S_{n+1}. Moreover, we can identify each function $f\colon\mathcal{A}\to\mathbb{C}$ in a natural way with the sequence of functions $\mathbf{f} = (\mathbf{f}^n)_{n\geq 0}$ such that $\mathbf{f}^n\colon I_n\to\mathcal{H}_n$. In fact, $\mathbf{f}^n$ is given by

$$\mathbf{f}^n_{i,j}(t) := f(x_{ij}(t)), \quad t\in I_n, \tag{2.1}$$

where $x_{ij}(t)$ is the unique $x\in\mathcal{A}$, such that $|x| = t$ and x lies on the edge connecting the i-th vertex in S_n with the j-th vertex of S_{n+1}. Notice that the map

$$\begin{array}{rccc} U\colon & L^2(\mathcal{A}) & \to & \oplus_{n\geq 0} L^2(I_n;\mathcal{H}_n) \\ & f & \mapsto & \mathbf{f} = (\mathbf{f}^n)_{n\geq 0} \end{array} \tag{2.2}$$

is an isometric isomorphism since

$$\big(f,g\big)_{L^2(\mathcal{A})} = \sum_{n\geq 0}\int_{I^n} (\mathbf{f}^n(t),\mathbf{g}^n(t))_{\mathcal{H}_n}\, dt \tag{2.3}$$

for all $f, g \in L^2(\mathcal{A})$. Next we introduce the following subspaces:

$$\begin{aligned}
\mathcal{H}_n^{\text{sym}} &:= \big\{\mathbf{a} \in \mathcal{H}_n |\ a_{ij} = a_{11}\ \forall i, j\big\}, \\
\mathcal{H}_n^{+} &:= \Big\{\mathbf{a} \in \mathcal{H}_n |\ a_{ij} = a_{i1}\ \forall i, j, \text{ and } \sum_{i,j} a_{ij} = \sum_i a_{i1} = 0\Big\}, \\
\mathcal{H}_n^{-} &:= \Big\{\mathbf{a} \in \mathcal{H}_n |\ a_{ij} = a_{1j}\ \forall i, j, \text{ and } \sum_{i,j} a_{ij} = \sum_j a_{1j} = 0\Big\}, \\
\mathcal{H}_n^{0} &:= \Big\{\mathbf{a} \in \mathcal{H}_n |\ \sum_j a_{ij} = 0\ \forall i \text{ and } \sum_i a_{ij} = 0\ \forall j\Big\}.
\end{aligned}$$

It is straightforward to check that the above spaces are mutually orthogonal and their dimensions are given by

$$\begin{aligned}
&\dim(\mathcal{H}_n^{\text{sym}}) = 1, && \dim(\mathcal{H}_n^{0}) = (s_n - 1)(s_{n+1} - 1), \\
&\dim(\mathcal{H}_n^{+}) = s_n - 1, && \dim(\mathcal{H}_n^{-}) = s_{n+1} - 1.
\end{aligned}$$

Hence $\mathcal{H}_n$ admits the decomposition

$$\mathcal{H}_n = \begin{cases} \mathcal{H}_n^{\text{sym}} \oplus \mathcal{H}_n^{-}, & n = 0 \\ \mathcal{H}_n^{\text{sym}} \oplus \mathcal{H}_n^{+} \oplus \mathcal{H}_n^{-} \oplus \mathcal{H}_n^{0}, & n \geq 1 \end{cases}. \tag{2.4}$$

Notice that if $s_n = 1$ for some $n \geq 1$, then $\mathcal{H}_n^{+} = \mathcal{H}_n^{0} = \mathcal{H}_{n-1}^{0} = \mathcal{H}_{n-1}^{-} = \{0\}$.

One can also describe the above subspaces by identifying $\mathcal{H}_n$ with the tensor product $\mathbb{C}^{s_n} \otimes \mathbb{C}^{s_{n+1}}$. For example, setting

$$\mathbf{1}_{s_n} := \big(\underbrace{1, 1, \dots, 1}_{s_n}\big) \in \mathbb{C}^{s_n}, \qquad \mathbf{1}^n := \mathbf{1}_{s_n} \otimes \mathbf{1}_{s_{n+1}} \in \mathcal{H}_n, \tag{2.5}$$

for all $n \geq 0$, we get

$$\mathcal{H}_n^{\text{sym}} = \text{span}\{\mathbf{1}^n\}. \tag{2.6}$$

Moreover, denote

$$\omega_n := \mathrm{e}^{2\pi \mathrm{i}/s_n}, \quad n \geq 0,$$

and set

$$\mathbf{a}_{s_n}^j := \{\omega_n^j, \dots, \omega_n^{j(s_n-1)}, 1\} \in \mathbb{C}^{s_n}, \quad j \in \{1, \dots, s_n\}. \tag{2.7}$$

Notice that $\{\mathbf{a}_{s_n}^j\}_{j=1}^{s_n}$ forms an orthogonal basis in $\mathbb{C}^{s_n}$ for all $n \geq 0$. In particular, $\mathbf{a}_{s_n}^{s_n} = \mathbf{1}_{s_n}$ and $\|\mathbf{a}_{s_n}^j\|^2 = s_n$. Hence setting

$$\mathbf{a}_n^{i,j} := \mathbf{a}_{s_n}^i \otimes \mathbf{a}_{s_{n+1}}^j \in \mathcal{H}_n, \tag{2.8}$$

where $1 \leq i \leq s_n$ and $1 \leq j \leq s_{n+1}$, we easily get

$$\begin{aligned}
\mathcal{H}_n^{+} &= \text{span}\big\{\mathbf{a}_{s_n}^i \otimes \mathbf{1}_{s_{n+1}} |\ 1 \leq i < s_n\big\} = \text{span}\big\{\mathbf{a}_n^{i,s_{n+1}} |\ 1 \leq i < s_n\big\}, \\
\mathcal{H}_n^{-} &= \text{span}\big\{\mathbf{1}_{s_n} \otimes \mathbf{a}_{s_{n+1}}^j |\ 1 \leq j < s_{n+1}\big\} = \text{span}\big\{\mathbf{a}_n^{s_n,j} |\ 1 \leq j < s_{n+1}\big\}, \\
\mathcal{H}_n^{0} &= \text{span}\big\{\mathbf{a}_n^{i,j} |\ 1 \leq i < s_n,\ 1 \leq j < s_{n+1}\big\}.
\end{aligned} \tag{2.9}$$

Finally, observe that

$$\|\mathbf{a}_n^{i,j}\|^2 = s_n s_{n+1} \tag{2.10}$$

for all $1 \leq i \leq s_n$, $1 \leq j \leq s_{n+1}$ and $n \geq 0$.

2.2. **Definition of the subspaces.** The decomposition (2.4) naturally induces a decomposition of the Hilbert space $L^2(\mathcal{A})$. First consider the subspace

$$\mathcal{F}_{\rm sym} := \{f \in L^2(\mathcal{A}) |\, \mathbf{f}^n \colon I_n \to \mathcal{H}_n^{\rm sym},\ n \ge 0\}. \tag{2.11}$$

Clearly, it consists of functions which depend only on the distance to the root:

$$\mathcal{F}_{\rm sym} = \{f \in L^2(\mathcal{A}) |\, f(x) = f(y) \text{ if } |x| = |y|\}. \tag{2.12}$$

Moreover, its orthogonal complement is given by

$$\begin{aligned}\mathcal{F}_{\rm sym}^{\perp} &= \{f \in L^2(\mathcal{A}) |\, \mathbf{f}^n \colon I_n \to (\mathcal{H}_n^{\rm sym})^{\perp},\ n \ge 0\} \\ &= \Big\{f \in L^2(\mathcal{A}) |\, \sum_{e \in \mathcal{E}_n^+} f_e \equiv 0,\ n \ge 0\Big\}.\end{aligned} \tag{2.13}$$

Next we need to decompose $\mathcal{F}_{\rm sym}^{\perp}$. Set

$$\mathcal{F}_n^0 := \{f \in L^2(\mathcal{A}) |\, \mathbf{f}^n \colon I_n \to \mathcal{H}_n^0;\ \mathbf{f}^k \equiv 0,\ k \ne n\} \tag{2.14}$$

for all $n \ge 1$. Taking into account the definition of $\mathcal{H}_n^0$, it is not difficult to see that

$$\mathcal{F}_n^0 = \left\{ f \in L^2(\mathcal{A}) | \quad \begin{matrix} f \equiv 0 \text{ on } \mathcal{A} \setminus \mathcal{E}_n^+ \\ \sum_{e \in \mathcal{E}_v^+} f_e = \sum_{e \in \mathcal{E}_u^-} f_e \equiv 0\ \forall v \in S_n, u \in S_{n+1} \end{matrix} \right\}.$$

Here, for every $v \in \mathcal{V}$, $\mathcal{E}_v^+$ and $\mathcal{E}_v^-$ denote the edges connecting v with the next and, respectively, previous combinatorial spheres.

We need to be more careful with the remaining part since our aim is to find reducing subspaces for the quantum graph operator $\mathbf{H}$. For every $v \in \mathcal{V} \setminus o$, define the subspace $\widetilde{\mathcal{F}}_v$ consisting of functions which vanish away of $\mathcal{E}_v$, where $\mathcal{E}_v$ is the set of edges emanating from v. Moreover, on the corresponding star $\mathcal{E}_v$ they depend only on the distance to the root, that is,

$$\widetilde{\mathcal{F}}_v := \left\{ f \in L^2(\mathcal{A}) | \quad \begin{matrix} f \equiv 0 \text{ on } \mathcal{A} \setminus \mathcal{E}_v \\ f(x) = f(y) \text{ for a.e. } x, y \in \mathcal{E}_v, |x| = |y| \end{matrix} \right\}. \tag{2.15}$$

Notice that $\widetilde{\mathcal{F}}_v$ and $\widetilde{\mathcal{F}}_u$ are orthogonal for $u \ne v$ if u and v are not adjacent vertices. Next for all $n \ge 1$ consider the spaces

$$\widetilde{\mathcal{F}}_n := \bigoplus_{v \in S_n} \widetilde{\mathcal{F}}_v, \qquad n \ge 1, \tag{2.16}$$

and

$$\mathcal{F}_n := \widetilde{\mathcal{F}}_n \ominus \mathcal{F}_{\rm sym} = \Big\{ f \in \widetilde{\mathcal{F}}_n |\, \sum_{e \in \mathcal{E}_m^+} f_e \equiv 0,\ m \ge 0\Big\}. \tag{2.17}$$

Notice that with respect to the decomposition (2.4), we have

$$\mathcal{F}_n = \left\{ f \in L^2(\mathcal{A}) | \quad \begin{matrix} \mathbf{f}^{n-1} \colon I_{n-1} \to \mathcal{H}_{n-1}^-,\ \mathbf{f}^n \colon I_n \to \mathcal{H}_n^+ \\ \mathbf{f}^m \equiv 0,\ m \ne n-1, n \end{matrix} \right\}. \tag{2.18}$$

Thus, we arrive at the following result.

Lemma 2.1. *The Hilbert space $L^2(\mathcal{A})$ admits the decomposition*

$$L^2(\mathcal{A}) = \mathcal{F}_{\rm sym} \oplus \bigoplus_{n \ge 1} \mathcal{F}_n \oplus \bigoplus_{n \ge 1} \mathcal{F}_n^0. \tag{2.19}$$

Proof. The orthogonality of the subspaces in (2.19) follows directly from (2.3) and (2.4). Hence we only need to show that every $f \in L^2(\mathcal{A})$ is contained in the right hand side of (2.19). Since $L^2(\mathcal{A}) = \oplus_{e\in\mathcal{E}} L^2(e)$, it suffices to prove this claim in the case when f is zero except on a single edge $e \in \mathcal{E}$. Suppose that $e \in \mathcal{E}_n^+$ for some $n \geq 0$. Then for almost every $t \in I_n$ we have

$$\mathbf{f}^n(t) = \mathcal{P}_n^{\mathrm{sym}}(\mathbf{f}^n(t)) + \mathcal{P}_n^+(\mathbf{f}^n(t)) + \mathcal{P}_n^-(\mathbf{f}^n(t)) + \mathcal{P}_n^0(\mathbf{f}^n(t)) \in \mathcal{H}_n,$$

where $\mathcal{P}_n^j \colon \mathcal{H}_n \to \mathcal{H}_n^j$ is the orthogonal projection in $\mathcal{H}_n$ onto $\mathcal{H}_n^j$, $j \in \{\mathrm{sym}, +, -, 0\}$. Define $f_j \colon \mathcal{A} \to \mathbb{C}$ as the function identified with the sequence of functions $\mathbf{f}_j = (\mathbf{f}_j^k)_{k\geq 0}$ given by

$$\mathbf{f}_j^k(t) := P_k^j(\mathbf{f}^k(t)), \qquad j \in \{\mathrm{sym}, +, -, 0\},$$

for a.e. $t \in I_k$. Then $f_j \in L^2(\mathcal{A})$ for all $j \in \{\mathrm{sym}, +, -, 0\}$ and

$$f = f_{\mathrm{sym}} + f_+ + f_- + f_0.$$

Since $\mathbf{f}_j^k(t) \in \mathcal{H}_k^j$ for a.e. $t \in I_k$, we conclude that $f_{\mathrm{sym}} \in \mathcal{F}_{\mathrm{sym}}$, $f_0 \in \mathcal{F}_n^0$, $f_+ \in \mathcal{F}_n$ and $f_- \in \mathcal{F}_{n+1}$. $\square$

Our next aim is to write down explicit formulas for projections onto the subspaces in the decomposition (2.19). First, for any $\tilde{f} \in L^2(I_n)$ and $\mathbf{a} \in \mathcal{H}_n$, we set $\tilde{\mathbf{f}} := \tilde{f} \otimes \mathbf{a}$. Recalling that every function $f \colon \mathcal{A} \to \mathbb{C}$ can be identified via (2.2) with the sequence of vector-valued functions $\mathbf{f} = (\mathbf{f}^n)_{n\geq 0}$, we denote

$$\mathcal{F}_{\mathbf{a}}^n := \{f \in L^2(\mathcal{A}) |\, \mathbf{f}^n = f^n \otimes \mathbf{a},\ f^n \in L^2(I_n);\, \mathbf{f}^k \equiv 0,\ k \neq n\}. \tag{2.20}$$

Note that the orthogonal projection $P_{\mathbf{a}}^n$ of $L^2(\mathcal{A})$ onto $\mathcal{F}_{\mathbf{a}}^n$ is given by

$$(U(P_{\mathbf{a}}^n f))(t) := \begin{cases} 0, & t \notin I_n \\ \frac{1}{\|\mathbf{a}\|^2}(\mathbf{f}^n(t), \mathbf{a})_{\mathcal{H}_n}\mathbf{a}, & t \in I_n \end{cases}, \tag{2.21}$$

where U is the isometric isomorphism (2.2).

Combining the form of $P_{\mathbf{a}}^n$ with the decomposition (2.4) and (2.6), (2.9), we easily obtain the following result.

Lemma 2.2. *Let $\mathbf{1}^n \in \mathcal{H}_n$ and $\mathbf{a}_n^{i,j} \in \mathcal{H}_n$, $n \geq 0$ be given by* (2.5) *and* (2.8). *Then the orthogonal projections in the decomposition* (2.19) *are given by*

$$P_{\mathrm{sym}} = \sum_{n\geq 0} P_{\mathbf{1}^n}^n, \tag{2.22}$$

$$P_n^0 = \sum_{\substack{1\leq i<s_n \\ 1\leq j<s_{n+1}}} P_{\mathbf{a}_n^{i,j}}^n, \qquad n \geq 1, \tag{2.23}$$

$$P_n = \sum_{j=1}^{s_n-1} P_{\mathbf{a}_{n-1}^{s_{n-1},j}}^{n-1} + \sum_{i=1}^{s_n-1} P_{\mathbf{a}_n^{i,s_{n+1}}}^n, \qquad n \geq 1. \tag{2.24}$$

3. Reduction of the quantum graph operator

In this section, we show that each of the spaces in the above decomposition (2.19) is reducing for the quantum graph operator with Kirchhoff conditions and also obtain a description of the corresponding restrictions.

3.1. **Kirchhoff's Laplacian.** Let us briefly recall the definition of the Laplacian on a metric graph (for details we refer to [3, 17, 32]). Let $L^2(\mathcal{A})$ be the corresponding Hilbert space and the subspace of compactly supported L^2-functions will be denoted by $L^2_c(\mathcal{A})$. Moreover, denote by $H^2(\mathcal{A}\setminus\mathcal{V})$ the subspace of $L^2(\mathcal{A})$ consisting of edgewise H^2-functions, that is, $f\in H^2(\mathcal{A}\setminus\mathcal{V})$ if $f\in H^2(e)$ for every $e\in\mathcal{E}$, where $H^2(e)$ is the usual Sobolev space. The Kirchhoff (or Kirchhoff–Neumann) boundary conditions at every vertex $v\in\mathcal{V}$ are then given by

$$\begin{cases} f \text{ is continuous at } v \\ \sum_{e\in\mathcal{E}_v} f'_e(v) = 0 \end{cases}, \tag{3.1}$$

where

$$f_e(v) := \lim_{x_e\to v} f(x_e), \qquad\qquad f'_e(v) := \lim_{x_e\to v} \frac{f(x_e)-f_e(v)}{|x_e-v|}, \tag{3.2}$$

are well defined for all $f\in H^2(\mathcal{A}\setminus\mathcal{V})$ and every vertex $v\in\mathcal{V}$. Imposing these boundary conditions and restricting to compactly supported functions we get the pre-minimal operator $\mathbf{H}_0$ acting edgewise as the (negative) second derivative $f_e\mapsto -\frac{d^2}{dx_e^2}f_e$, $e\in\mathcal{E}$ on the domain

$$\mathrm{dom}(\mathbf{H}_0) = \{f\in H^2(\mathcal{A}\setminus\mathcal{V})\cap L^2_c(\mathcal{G})|\, f \text{ satisfies (3.1)},\ v\in\mathcal{V}\}. \tag{3.3}$$

The operator $\mathbf{H}_0$ is symmetric and its closure $\mathbf{H}=\overline{\mathbf{H}}_0$ is called *the minimal Kirchhoff Laplacian*.

First, we need the following simple but useful fact.

Lemma 3.1. *Let $f\in L^2(\mathcal{A})$ and $\mathbf{f}=Uf$ be given by (2.2). Then $f\in\mathrm{dom}(\mathbf{H}_0)$ if and only if $\mathbf{f}=(\mathbf{f}^n)_{n\geq 0}$ satisfies the following conditions:*

(i) $\mathbf{f}^n\equiv 0$ *for all sufficiently large n,*
(ii) $\mathbf{f}^n_{i,j}\in H^2(I_n)$ *for all $n\geq 0$,*
(iii) *for all $j\in\{1,\dots,s_1\}$*

$$\mathbf{f}^0_{1,j}(0+) = \mathbf{f}^0_{1,1}(0+), \qquad\qquad \sum_{j=1}^{s_1}(\mathbf{f}^0_{1,j})'(0+) = 0,$$

(iv) *for all $n\geq 1$,*

$$\begin{matrix} \mathbf{f}^n_{i,j}(t_n+) = \mathbf{f}^{n-1}_{k,i}(t_n-) \\ \sum_{j=1}^{s_{n+1}}(\mathbf{f}^n_{i,j})'(t_n+) = \sum_{k=1}^{s_{n-1}}(\mathbf{f}^{n-1}_{k,i})'(t_n-) \end{matrix}, \qquad i\in\{1,\dots,s_n\}.$$

Proof. The proof is straightforward. We only need to mention that (i) is equivalent to the fact that f is compactly supported; (ii) means that f belongs to the Sobolev space H^2 on each edge $e\in\mathcal{E}$; (iii) and (iv) are continuity and Kirchhoff's conditions at the vertices. ☐

3.2. **The subspace $\mathcal{F}_{\mathrm{sym}}$.** Set $\mathcal{I}_\mathcal{L}=[0,\mathcal{L})$, and define the length $\mathcal{L}$ and the weight function $\mu\colon\mathcal{I}_\mathcal{L}\to\mathbb{R}_{\geq 0}$ by

$$\mu(t) = \sum_{n\geq 0} s_n s_{n+1}\mathbb{1}_{I_n}(t), \quad t\in[0,\mathcal{L}); \qquad\qquad \mathcal{L}=\sum_{n\geq 0}\ell_n. \tag{3.4}$$

Consider the (pre-minimal) operator H_0 defined in $L^2(\mathcal{I}_\mathcal{L};\mu)$ by the Sturm–Liouville differential expression

$$\tau = -\frac{1}{\mu(t)}\frac{d}{dt}\mu(t)\frac{d}{dt}, \tag{3.5}$$

on the domain

$$\mathrm{dom}(\mathrm{H}_0) = \big\{f \in L^2_c(\mathcal{I}_\mathcal{L};\mu)|\, f,\ \mu f' \in AC(\mathcal{I}_\mathcal{L}),\ \tau f \in L^2(\mathcal{I}_\mathcal{L};\mu);\ f'(0)=0\big\}. \tag{3.6}$$

More concretely, H_0 acts as a negative second derivative and its domain $\mathrm{dom}(\mathrm{H}_0)$ consists of functions $f \in L^2(\mathcal{I}_\mathcal{L};\mu)$ having compact support in $\mathcal{I}_\mathcal{L}$, belonging to H^2 on every interval I_n and at each point t_n satisfying the boundary conditions

$$\begin{cases} f \text{ is continuous at } t_n, \\ s_{n-1}f'(t_n-) = s_{n+1}f'(t_n+). \end{cases} \tag{3.7}$$

Here we set $s_{-1} := 0$ in the case $n = 0$ for notational simplicity and the corresponding condition (3.7) reads as the Neumann boundary condition at $t = 0$.

Lemma 3.2. *The subspace $\mathcal{F}_{\mathrm{sym}}$ reduces the operator $\mathbf{H}_0$. Moreover, its restriction $\mathbf{H}_0 \restriction \mathcal{F}_{\mathrm{sym}}$ onto $\mathcal{F}_{\mathrm{sym}}$ is unitarily equivalent to the operator H_0.*

Proof. First let us show that $f_{\mathrm{sym}} := P_{\mathrm{sym}}f \in \mathrm{dom}(\mathbf{H}_0)$ for every $f \in \mathrm{dom}(\mathbf{H}_0)$. In fact, we need to show that $\mathbf{f}_{\mathrm{sym}} = Uf_{\mathrm{sym}}$ satisfies conditions (i)–(iv) of Lemma 3.1. Clearly, by continuity of f and (2.21), (2.22), $\mathbf{f}_{\mathrm{sym}}$ satisfies (i) and (ii). Moreover, both $(\mathbf{f}_{\mathrm{sym}})^n_{i,j}(t_n+)$ and $(\mathbf{f}_{\mathrm{sym}})^n_{k,m}(t_{n+1}-)$ depend only on $n \ge 0$. Since $\mathbf{f}$ satisfies both (iii) and (iv), we obtain that $(\mathbf{f}_{\mathrm{sym}})^0_{1,j}(0+)$ does not depend on j and

$$\begin{aligned}(\mathbf{f}_{\mathrm{sym}})^n_{i,j}(t_n+) &= \frac{1}{s_n s_{n+1}}\big(\mathbf{f}^n(t_n+), \mathbf{1}^n\big)_{\mathcal{H}_n} \\ &= \frac{1}{s_{n-1}s_n}\big(\mathbf{f}^{n-1}(t_n-), \mathbf{1}^{n-1}\big)_{\mathcal{H}_{n-1}} = (\mathbf{f}_{\mathrm{sym}})^{n-1}_{k,i}(t_n-)\end{aligned}$$

for all $i \in \{1,\dots,s_n\}$ and $n \ge 1$. Similarly,

$$\begin{aligned}\sum_{j=1}^{s_{n+1}}(\mathbf{f}'_{\mathrm{sym}})^n_{i,j}(t_n+) &= \frac{1}{s_n}\big((\mathbf{f}^n)'(t_n+), \mathbf{1}^n\big)_{\mathcal{H}_n} = \frac{1}{s_n}\sum_{i,j}(\mathbf{f}^n_{i,j})'(t_n+) \\ &= \frac{1}{s_n}\sum_{i=1}^{s_n}\sum_{j=1}^{s_{n+1}}(\mathbf{f}^n_{i,j})'(t_n+) = \frac{1}{s_n}\sum_{i=1}^{s_n}\sum_{k=1}^{s_{n-1}}(\mathbf{f}^{n-1}_{k,i})'(t_n-) \\ &= \frac{1}{s_n}\big((\mathbf{f}^{n-1})'(t_n-), \mathbf{1}^{n-1}\big)_{\mathcal{H}_{n-1}} = \sum_{k=1}^{s_{n-1}}(\mathbf{f}'_{\mathrm{sym}})^{n-1}_{k,i}(t_n-),\end{aligned} \tag{3.8}$$

which holds for all $i \in \{1,\dots,s_n\}$, $n \ge 1$. Moreover, for $n = 0$ we have

$$(\mathbf{f}'_{\mathrm{sym}})^0_{1,j}(0+) = \frac{1}{s_1}\sum_{m=1}^{s_1}(\mathbf{f}^0_{1,m})'(0+) = 0$$

for all $j \in \{1,\dots,s_1\}$. Hence $f_{\mathrm{sym}} = P_{\mathrm{sym}}f \in \mathrm{dom}(\mathbf{H}_0)$ for all $f \in \mathrm{dom}(\mathbf{H}_0)$. Noting that $\mathbf{H}_0$ is symmetric and $\mathcal{F}_{\mathrm{sym}}$ is clearly invariant for $\mathbf{H}_0$ we conclude that $\mathcal{F}_{\mathrm{sym}}$ is reducing for $\mathbf{H}_0$.

To prove the last claim, observe that the subspace $\mathcal{F}_{\mathrm{sym}}$ is isometrically isomorphic to the Hilbert space $L^2(\mathcal{I}_{\mathcal{L}};\mu)$. Indeed, for every $f \in \mathcal{F}_{\mathrm{sym}}$, set

$$\tilde{f}(t) := \frac{1}{s_n s_{n+1}} \sum_{e\in\mathcal{E}_n^+} f(x_e(t)) = \frac{1}{\|\mathbf{1}^n\|^2}(\mathbf{f}^n(t),\mathbf{1}^n)_{\mathcal{H}_n}, \qquad t \in I_n; \qquad n \geq 0, \tag{3.9}$$

where $x_e(t)$ is the unique point on e satisfying $|x_e(t)| = t$. Consider the map

$$U_s\colon \quad \begin{array}{ccc} \mathcal{F}_{\mathrm{sym}} & \to & L^2\big(\mathcal{I}_{\mathcal{L}};\mu\big) \\ f & \mapsto & \tilde{f} \end{array}. \tag{3.10}$$

Clearly, for every $f \in \mathcal{F}_{\mathrm{sym}}$, $\mathbf{f}^n(t) = \tilde{f}(t)\otimes \mathbf{1}^n$ for a.e. $t \in I_n$ and hence

$$\|\tilde{f}\|^2_{L^2(\mathcal{I}_{\mathcal{L}};\mu)} = \sum_{n\geq 0} s_n s_{n+1}\|\tilde{f}\|^2_{L^2(I_n)} = \sum_{n\geq 0}\|\mathbf{f}^n\|^2_{L^2(I_n;\mathcal{H}_n)} = \|\mathbf{f}\|^2 = \|f\|^2_{L^2(\mathcal{A})}.$$

It turns out that

$$\mathrm{H}_0 = U_s(\mathbf{H}_0 \restriction \mathcal{F}_{\mathrm{sym}})U_s^{-1}. \tag{3.11}$$

Indeed, $\mathbf{H}_0$ acts as the negative second derivative on every edge $e \in \mathcal{E}$ and hence for every $f \in \mathcal{F}_{\mathrm{sym}}$ we get

$$(U_s(\mathbf{H}_0 f))(t) = -\tilde{f}''(t), \qquad t \in I_n,$$

for all $n \geq 0$. Therefore, it remains to show that $U_s(\mathcal{F}_{\mathrm{sym}} \cap \mathrm{dom}(\mathbf{H}_0)) = \mathrm{dom}(\mathrm{H}_0)$. In fact, we only need to show that every $\tilde{f} = U_s f$ with $f \in \mathcal{F}_{\mathrm{sym}}$ satisfies (3.7) if and only if $f \in \mathrm{dom}(\mathbf{H}_0)$. Indeed, by (3.9) and continuity of f, $\tilde{f}(t_n+) = \tilde{f}(t_n-)$ for all $n \geq 1$ if $f \in \mathcal{F}_{\mathrm{sym}} \cap \mathrm{dom}(\mathbf{H}_0)$. Moreover, similar to (3.8) one checks that

$$s_{n+1}\tilde{f}'(t_n+) = s_{n-1}\tilde{f}'(t_n-), \qquad n \geq 0,$$

exactly when $f \in \mathcal{F}_{\mathrm{sym}} \cap \mathrm{dom}(\mathbf{H}_0)$. This finishes the proof of Lemma 3.2. $\square$

3.3. **Restriction to $\mathcal{F}_n^0$.** Our next aim is to show that each $\mathcal{F}_n^0$, $n \geq 1$, is a reducing subspace for $\mathbf{H}_0$ and its restriction is unitarily equivalent to $(s_n-1)(s_{n+1}-1)$ copies of $\mathbf{h}_n$, the second derivative with the Dirichlet boundary conditions on $L^2(I_n)$,

$$\mathbf{h}_n := -\frac{d^2}{dt^2}, \quad \mathrm{dom}(\mathbf{h}_n) = \{f \in H^2(I_n) |\, f(t_n+) = f(t_{n+1}-) = 0\}. \tag{3.12}$$

By Lemma 2.2, this will be a consequence of the following lemma.

Lemma 3.3. *Let $n \geq 1$ be such that $s_n > 1$ and $s_{n+1} > 1$. Then each of the subspaces $\mathcal{F}^n_{\mathbf{a}}$, where $\mathbf{a} = \mathbf{a}_n^{i,j}$ with $1 \leq i < s_n$ and $1 \leq j < s_{n+1}$, is reducing for the operator $\mathbf{H}_0$. The restricted operator $\mathbf{H}_0 \restriction \mathcal{F}^n_{\mathbf{a}}$ is unitarily equivalent to the operator $\mathbf{h}_n$ defined by* (3.12).

Proof. Clearly, $\mathcal{F}^n_{\mathbf{a}}$ is invariant for $\mathbf{H}_0$. Since $\mathbf{H}_0$ is symmetric, we only have to prove that $\tilde{f} := P^n_{\mathbf{a}} f \in \mathrm{dom}(\mathbf{H}_0)$ whenever $f \in \mathrm{dom}(\mathbf{H}_0)$. In fact, we need to show that $\tilde{\mathbf{f}} := U(P^n_{\mathbf{a}} f)$ given by (2.21) satisfies conditions (i)–(iv) of Lemma 3.1. Conditions (i) and (ii) are obviously satisfied since $f \in \mathrm{dom}(\mathbf{H}_0)$ and by the definition of $U(P^n_{\mathbf{a}} f)$. Since $\tilde{\mathbf{f}}^m = 0$ for all $m \neq n$ and $n \geq 1$, (iii) clearly holds and, moreover, we need to verify (iv) only at t_n and t_{n+1}.

Let us start with continuity. Suppose $\mathbf{a} = \mathbf{a}_n^{i,j}$ for some $1 \leq i < s_n$ and $1 \leq j < s_{n+1}$. First observe that

$$\tilde{\mathbf{f}}^n_{k,m}(t_n+) = \tilde{\mathbf{f}}^n_{k,m}(t_{n+1}-) = 0$$

for all $k \in \{1, \dots, s_n\}$ and $m \in \{1, \dots, s_{n+1}\}$. Indeed,

$$\lim_{t \to t_n+} (\mathbf{f}^n(t), \mathbf{a})_{\mathcal{H}_n} = (\mathbf{f}^n(t_n+), \mathbf{a})_{\mathcal{H}_n} = \sum_{k=1}^{s_n} \mathbf{f}^n_{k,1}(t_n+)\omega_n^{-ik} \sum_{m=1}^{s_{n+1}} \omega_{n+1}^{-jm} = 0.$$

Here we employed the continuity of f, $\mathbf{f}^n_{k,j}(t_n+) = \mathbf{f}^n_{k,1}(t_n+)$ for all $j \in \{1, \dots, s_{n+1}\}$, together with (2.8). This shows that $\tilde{\mathbf{f}}$ satisfies the first condition in (iv).

Next observe that

$$\sum_{m=1}^{s_{n+1}} (\tilde{\mathbf{f}}^n_{k,m})'(t_n+) = \frac{\omega_n^{ik}}{s_n s_{n+1}} ((\mathbf{f}^n)'(t_n+), \mathbf{a})_{\mathcal{H}_n} \sum_{m=1}^{s_{n+1}} \omega_{n+1}^{jm} = 0$$

for all $k \in \{1, \dots, s_n\}$. Since $(\tilde{\mathbf{f}}^{n-1})' = 0$, $\tilde{\mathbf{f}}$ satisfies (iv) at t_n. Similar arguments shows that (iv) holds true at t_{n+1} as well. This finishes the proof of the inclusion $\tilde{f} = P^n_{\mathbf{a}} f \in \operatorname{dom}(\mathbf{H}_0)$.

Finally, noting that

$$\begin{array}{cccc} U^n_{\mathbf{a}}\colon & L^2(I_n) & \to & \mathcal{F}^n_{\mathbf{a}} \\ & f & \mapsto & f \cdot \frac{\mathbf{a}}{\|\mathbf{a}\|} \end{array} \tag{3.13}$$

establishes an isometric isomorphism of $L^2(I_n)$ onto $\mathcal{F}^n_{\mathbf{a}}$, it is straightforward to verify the last claim and we left it to the reader. $\square$

3.4. **Restriction to $\mathcal{F}_n$.** Next, we show that $\mathcal{F}_n$, $n \geq 1$ is reducing for $\mathbf{H}_0$ as well and the corresponding restriction is unitarily equivalent to $s_n - 1$ copies of the operator $\widetilde{\mathbf{h}}_n$ defined by

$$\widetilde{\tau}_n = -\frac{1}{\mu(t)} \frac{d}{dt} \mu(t) \frac{d}{dt},$$

on $L^2((t_{n-1}, t_{n+1}); \mu)$ and equipped with Dirichlet conditions at the endpoints. Here the weight function μ is defined by (3.4). The domain of $\widetilde{\mathbf{h}}_n$ admits a very simple description since inside I_{n-1} and I_n the differential expression $\widetilde{\tau}_n$ reduces to the negative second derivative and hence $\operatorname{dom}(\widetilde{\mathbf{h}}_n)$ consists of functions which are H^2 in I_{n-1} and I_n, satisfy the Dirichlet conditions at t_{n-1} and t_{n+1} and also the following coupling conditions at t_n:

$$\begin{cases} f(t_n+) = f(t_n-) \\ s_{n-1} f'(t_n-) = s_{n+1} f'(t_n+) \end{cases}. \tag{3.14}$$

Recall that $\mathcal{F}_n = \operatorname{ran}(P_n)$, where the projection P_n is given by (2.24). By (2.8) and (2.5),

$$\mathbf{a}_{n-1}^{s_{n-1},j} = \mathbf{1}_{s_{n-1}} \otimes \mathbf{a}^j_{s_n}, \qquad \mathbf{a}_n^{j,s_{n+1}} = \mathbf{a}^j_{s_n} \otimes \mathbf{1}_{s_{n+1}},$$

and hence

$$P_n = \sum_{j=1}^{s_n - 1} \big(P^{n-1}_{\mathbf{1}_{s_{n-1}} \otimes \mathbf{a}^j_{s_n}} + P^n_{\mathbf{a}^j_{s_n} \otimes \mathbf{1}_{s_{n+1}}} \big). \tag{3.15}$$

Denoting the summands in (3.15) by $\widetilde{P}^j_n$, $j \in \{1, \dots, s_n - 1\}$, we set

$$\widetilde{\mathcal{F}}^j_n := \operatorname{ran}(\widetilde{P}^j_n) = \mathcal{F}^{n-1}_{\mathbf{1}_{s_{n-1}} \otimes \mathbf{a}^j_{s_n}} \oplus \mathcal{F}^n_{\mathbf{a}^j_{s_n} \otimes \mathbf{1}_{s_{n+1}}}. \tag{3.16}$$

Since $\mathcal{F}_n = \bigoplus_{j=1}^{s_n - 1} \widetilde{\mathcal{F}}^j_n$, these claims will follow from the following lemma:

Lemma 3.4. *Every subspace $\widetilde{\mathcal{F}}_n^j$ with $n \geq 1$ and $j \in \{1, \dots, s_n - 1\}$, is reducing for the operator $\mathbf{H}_0$. Moreover, its restriction onto $\widetilde{\mathcal{F}}_n^j$ is unitarily equivalent to $\widetilde{\mathbf{h}}_n$.*

Proof. Since $\widetilde{\mathcal{F}}_n^j$ is invariant for $\mathbf{H}_0$ and $\mathbf{H}_0$ is symmetric, we only need to show that for every $f \in \mathrm{dom}(\mathbf{H}_0)$ its projection $\tilde{f} := \widetilde{P}_n^j f$ onto $\widetilde{\mathcal{F}}_n^j$ also belongs to $\mathrm{dom}(\mathbf{H}_0)$. Following step by step the proof of Lemma 3.3, we only need to show that $\tilde{\mathbf{f}} := U\tilde{f}$ satisfies condition (iv) of Lemma 3.1 at t_n.

First observe that by (2.21)

$$\tilde{\mathbf{f}}(t) = \begin{cases} \tilde{f}_{n-1}(t)(\mathbf{1}_{s_{n-1}} \otimes \mathbf{a}_{s_n}^j), & t \in I_{n-1} \\ \tilde{f}_n(t)(\mathbf{a}_{s_n}^j \otimes \mathbf{1}_{s_{n+1}}), & t \in I_n \end{cases} \tag{3.17}$$

where

$$\tilde{f}_{n-1}(t) = \frac{1}{s_{n-1}s_n}(\mathbf{f}^{n-1}(t), \mathbf{a}_{n-1}^{s_{n-1},j})_{\mathcal{H}_{n-1}}, \quad \tilde{f}_n(t) = \frac{1}{s_n s_{n+1}}(\mathbf{f}^n(t), \mathbf{a}_n^{j,s_{n+1}})_{\mathcal{H}_n}.$$

Notice that

$$\tilde{f}_{n-1}(t_n-) = \frac{1}{s_{n-1}s_n}\sum_{k=1}^{s_{n-1}}\sum_{m=1}^{s_n} \mathbf{f}_{k,m}^{n-1}(t_n-)\omega_n^{-jm} = \frac{1}{s_n}\sum_{m=1}^{s_n} \mathbf{f}_{1,m}^{n-1}(t_n-)\omega_n^{-jm}$$

and

$$\tilde{f}_n(t_n+) = \frac{1}{s_n s_{n+1}}\sum_{m=1}^{s_n}\sum_{k=1}^{s_{n+1}} \mathbf{f}_{m,k}^{n}(t_n+)\omega_n^{-jm} = \frac{1}{s_n}\sum_{m=1}^{s_n} \mathbf{f}_{m,1}^{n}(t_n+)\omega_n^{-jm}.$$

However, by Lemma 3.1,

$$\mathbf{f}_{1,m}^{n-1}(t_n-) = \mathbf{f}_{m,1}^{n}(t_n+), \qquad m \in \{1, \dots, s_n\},$$

and hence we get

$$\begin{aligned} \tilde{\mathbf{f}}_{1,k}^{n-1}(t_n-) &= \frac{\omega_n^{jk}}{s_n}\sum_{m=1}^{s_n} \mathbf{f}_{1,m}^{n-1}(t_n-)\omega_n^{-jm} \\ &= \frac{\omega_n^{jk}}{s_n}\sum_{m=1}^{s_n} \mathbf{f}_{m,1}^{n}(t_n+)\omega_n^{-jm} = \tilde{\mathbf{f}}_{k,1}^{n}(t_n+) \end{aligned}$$

for all $k \in \{1, \dots, s_n\}$. This shows that $\tilde{\mathbf{f}}$ satisfies the first equality in condition (iv) of Lemma 3.1. Let us check the second one. However, we have

$$\begin{aligned} \sum_{k=1}^{s_{n-1}} (\tilde{\mathbf{f}}_{k,m}^{n-1})'(t_n-) &= \sum_{k=1}^{s_{n-1}} \tilde{f}_{n-1}'(t_n-)\omega_n^{jm} = s_{n-1}\tilde{f}_{n-1}'(t_n-)\omega_n^{jm} \\ &= \frac{\omega_n^{jm}}{s_n}\sum_{l=1}^{s_n}\omega_n^{-jl}\sum_{k=1}^{s_{n-1}}(\mathbf{f}_{k,l}^{n-1})'(t_n-) \\ &= \frac{\omega_n^{jm}}{s_n}\sum_{l=1}^{s_n}\omega_n^{-jl}\sum_{k=1}^{s_{n+1}}(\mathbf{f}_{l,k}^{n})'(t_n+) = s_{n+1}\tilde{f}_n'(t_n+)\omega_n^{jm} \\ &= \sum_{k=1}^{s_{n+1}} \tilde{f}_n'(t_n+)\omega_n^{jm} = \sum_{k=1}^{s_{n+1}}(\tilde{\mathbf{f}}_{m,k}^{n})'(t_n+). \end{aligned}$$

This shows that $\tilde{\mathbf{f}}$ satisfies all the conditions of Lemma 3.1 and hence $\tilde{f} \in \mathrm{dom}(\mathbf{H}_0)$.

It remains to notice that the map $U_n^j\colon L^2((t_{n-1}, t_{n+1}); \mu) \to \widetilde{\mathcal{F}}_n^j$ defined by (3.17) is an isometric isomorphism and $(U_n^j)^{-1}(\mathbf{H}_0 \restriction \widetilde{\mathcal{F}}_n^j)U_n^j = \widetilde{\mathbf{h}}_n$. $\square$

3.5. **The decomposition of the operator H.** Combining the results of Sections 3.2–3.4, we arrive at the following decomposition of quantum graph operators on radially symmetric anti-trees.

Theorem 3.5. *Let $\mathcal{A}$ be an infinite radially symmetric antitree. The decomposition* (2.19) *reduces the operator* $\mathbf{H}$*. Moreover, with respect to this decomposition,* $\mathbf{H}$ *is unitarily equivalent to the following orthogonal sum of Sturm–Liouville operators*

$$\mathrm{H} \oplus \bigoplus_{n\geq 1} \Big(\oplus_{j=1}^{(s_n-1)(s_{n+1}-1)} \mathbf{h}_n \Big) \oplus \bigoplus_{n\geq 1} \Big(\oplus_{j=1}^{s_n-1} \widetilde{\mathbf{h}}_n \Big), \tag{3.18}$$

where $\mathrm{H} = \overline{\mathrm{H}_0}$ *and the operators* H_0*,* $\mathbf{h}_n$ *and* $\widetilde{\mathbf{h}}_n$ *are defined in Sections 3.2, 3.3 and 3.4, respectively.*

4. Self-adjointness

Theorem 3.5 reduces the spectral analysis of quantum graph operators on radially symmetric antitrees to the analysis of certain classes of Sturm–Liouville operators. Moreover, the Sturm–Liouville operators $\mathbf{h}_n$ and $\widetilde{\mathbf{h}}_n$ in the decomposition (3.18) are self-adjoint for all $n \geq 1$ and their spectra can be computed explicitly. This enables us to perform a rather detailed study of spectral properties of the operator $\mathbf{H} = \overline{\mathbf{H}_0}$. We begin with the characterization of self-adjoint extensions of the operator $\mathbf{H}$.

Theorem 4.1. *Let $\mathcal{A}$ be an infinite radially symmetric antitree. Then:*

(i) The operator $\mathbf{H}$ *is self-adjoint if and only if the total volume of* $\mathcal{A}$ *is infinite,*

$$\mathrm{vol}(\mathcal{A}) := \sum_{e\in\mathcal{E}(\mathcal{A})} |e| = \sum_{n\geq 0} s_n s_{n+1} \ell_n = \infty. \tag{4.1}$$

(ii) If $\mathrm{vol}(\mathcal{A}) < \infty$*, then the deficiency indices of* $\mathbf{H}$ *equal* 1 *and self-adjoint extensions of* $\mathbf{H}$ *form a one-parameter family* $\mathbf{H}_\theta := \mathbf{H}^* \restriction \mathrm{dom}(\mathbf{H}_\theta)$*,* $\theta \in [0, \pi)$*, where*

$$\mathrm{dom}(\mathbf{H}_\theta) = \{f \in \mathrm{dom}(\mathbf{H}^*) |\ \cos(\theta) f(\mathcal{L}) + \sin(\theta) f'(\mathcal{L}) = 0\},$$

where

$$f(\mathcal{L}) := \lim_{t\to\mathcal{L}} (U_s P_{\mathrm{sym}} f)(t), \tag{4.2}$$

$$f'(\mathcal{L}) := \lim_{t\to\mathcal{L}} \mu(t)(U_s P_{\mathrm{sym}} f)'(t), \tag{4.3}$$

and the operators P_{sym} *and* U_s *are given, respectively, by* (2.22) *and* (3.10).

Proof. (i) By Theorem 3.5, the operator $\mathbf{H}$ is self-adjoint only if so are the operators on the right-hand side in the decomposition (3.18). However, both $\mathbf{h}_n$ and $\widetilde{\mathbf{h}}_n$ are self-adjoint for all $n \geq 1$. The self-adjointness criterion for $\mathrm{H} = \overline{\mathrm{H}_0}$ follows from the standard limit point/limit circle classification (see, e.g., [46]). Namely, the equation $\tau y = 0$ with τ given by (3.5), has two linearly independent solutions

$$y_1(t) \equiv 1, \qquad\qquad y_2(t) = \int_0^t \frac{ds}{\mu(s)}.$$

Now one simply needs to verify whether or not both solutions y_1 and y_2 belong to $L^2(\mathcal{I}_\mathcal{L};\mu)$. Clearly, $y_1 \in L^2(\mathcal{I}_\mathcal{L};\mu)$ exactly when the series in (4.1) converges. Moreover, it is straightforward to check that $y_2 \in L^2(\mathcal{I}_\mathcal{L};\mu)$ if and only if the series

$$\sum_{n\ge 0} s_n s_{n+1}\ell_n\Big(\sum_{k\le n}\frac{\ell_k}{s_k s_{k+1}}\Big)^2 \tag{4.4}$$

converges. Since $s_n s_{n+1} \ge 1$ for all $n \ge 0$, this series converges exactly when the series in (4.1) converges. The Weyl alternative finishes the proof of (i).

(ii) The above considerations imply that the deficiency indices of $\mathbf{H}$ and H coincide. However, the deficiency indices of H are at most 1. Thus, if the operator H is not self-adjoint, its deficiency indices equal 1. Moreover, one can easily describe all self-adjoint extensions of H. First of all, for every $g \in \mathrm{dom}(\mathrm{H}_0^*) = \mathrm{dom}(\mathrm{H}^*)$ the following limits

$$\lim_{t\to\mathcal{L}} W_t(g,y_1), \qquad\qquad \lim_{t\to\mathcal{L}} W_t(g,y_2)$$

exist and are finite (see, e.g., [46]). Here $W_t(g,h) = g(t)(\mu h')(t) - (\mu g')(t)h(t)$ is the modified Wronskian. Thus for every $g \in \mathrm{dom}(\mathrm{H}_0^*)$ the following limits

$$g(\mathcal{L}) := \lim_{t\to\mathcal{L}} g(t), \qquad\qquad g'_\mu(\mathcal{L}) := \lim_{t\to\mathcal{L}} \mu(t)g'(t) \tag{4.5}$$

exist and are finite. Hence self-adjoint extensions of H form a one-parameter family

$$\mathrm{dom}(\mathrm{H}(\theta)) = \big\{g \in \mathrm{dom}(\mathrm{H}_0^*)|\ \cos(\theta)g(\mathcal{L}) + \sin(\theta)g'_\mu(\mathcal{L}) = 0\big\}, \quad \theta \in [0,\pi).$$

It remains to use (3.11) and (2.22). $\square$

Remark 4.2. Let us mention that in the case $\mathrm{vol}(\mathcal{A}) < \infty$ the Friedrichs extension of $\mathbf{H}$ coincides with the operator $\mathbf{H}_\theta$ with $\theta = 0$. Moreover, it is possible to show that in fact the limits in (4.2) and (4.3) coincide with

$$\lim_{|x|\to\mathcal{L}} f(x), \qquad\qquad \lim_{t\to\mathcal{L}} \sum_{|x|=t} f'(x)$$

for every f in the domain of $\mathbf{H}^*$. In particular, this would imply that the Friedrichs extension of $\mathbf{H}$ is simply given as the restriction of $\mathbf{H}^*$ to functions vanishing at $\mathcal{L}$. Let us also mention that $\mathbf{H}^* = \mathbf{H}_0^*$ in fact coincides with the maximal operator, that is $\mathrm{dom}(\mathbf{H}^*)$ consists of functions $f \in L^2(\mathcal{A}) \cap H^2(\mathcal{A}\setminus\mathcal{V})$ satisfying boundary conditions (3.1) for all $v \in \mathcal{V}$ and such that $f'' \in L^2(\mathcal{A})$.

5. Discreteness

As an immediate corollary of Theorem 4.1 we obtain the following result.

Corollary 5.1. *If* $\mathrm{vol}(\mathcal{A}) < \infty$*, then the spectrum of each self-adjoint extension* $\mathbf{H}_\theta$ *of* $\mathbf{H}$ *is purely discrete and, moreover,*

$$N(\lambda;\mathbf{H}_\theta) = \frac{\mathrm{vol}(\mathcal{A})}{\pi}\sqrt{\lambda}(1+o(1)), \quad \lambda\to\infty, \tag{5.1}$$

for all $\theta \in [0,\pi)$.

Here $N(\lambda;A)$ is the eigenvalue counting function of a (bounded from below) self-adjoint operator A with purely discrete spectrum. Namely,

$$N(\lambda;A) = \#\{k\colon \lambda_k(A) \le \lambda\},$$

where $\{\lambda_k(A)\}_{k\geq 0}$ are the eigenvalues of A (counting multiplicities) ordered in the increasing order.

Proof. By Theorem 3.5,

$$\sigma(\mathbf{H}_\theta) = \sigma(\mathrm{H}(\theta)) \cup \overline{\cup_{n\geq 1}\sigma(\mathbf{h}_n)} \cup \overline{\cup_{n\geq 1}\sigma(\widetilde{\mathbf{h}}_n)}. \tag{5.2}$$

Since $s_n \geq 1$ for all $n \geq 1$, $\mathrm{vol}(\mathcal{A}) < \infty$ implies that $\ell_n = o(1)$ as $n \to \infty$ and hence both sets $\cup_{n\geq 1}\sigma(\mathbf{h}_n)$ and $\cup_{n\geq 1}\sigma(\widetilde{\mathbf{h}}_n)$ have no finite accumulation points. It remains to note that the spectrum of $\mathrm{H}(\theta)$ is discrete in this case as well.

According to the decomposition (3.18), we clearly have

$$N(\lambda;\mathbf{H}_\theta) = N(\lambda;\mathrm{H}(\theta)) + \sum_{n\geq 1}(s_n-1)(s_{n+1}-1)N(\lambda;\mathbf{h}_n) + \sum_{n\geq 1}(s_n-1)N(\lambda;\widetilde{\mathbf{h}}_n).$$

It is well known that (cf., e.g., [19, Chapter 6.7])

$$N(\lambda;\mathrm{H}(\theta)) = \frac{\mathcal{L}}{\pi}\sqrt{\lambda}(1+o(1)), \quad \lambda\to\infty,$$

for all $\theta \in [0,\pi)$. Taking into account that

$$\sigma(\mathbf{h}_n) = \left\{\frac{\pi^2 k^2}{\ell_n^2}\right\}_{k\geq 1}, \tag{5.3}$$

we clearly have

$$N(\lambda;\mathbf{h}_n) = \left\lfloor \frac{\ell_n}{\pi}\sqrt{\lambda}\right\rfloor \tag{5.4}$$

for all $\lambda \geq 0$, where $\lfloor\cdot\rfloor$ is the usual floor function. Moreover,

$$\left\lfloor \frac{\ell_{n-1}}{\pi}\sqrt{\lambda}\right\rfloor + \left\lfloor \frac{\ell_n}{\pi}\sqrt{\lambda}\right\rfloor \leq N(\lambda;\widetilde{\mathbf{h}}_n) \leq \left\lfloor \frac{\ell_{n-1}}{\pi}\sqrt{\lambda}+\frac{1}{2}\right\rfloor + \left\lfloor \frac{\ell_n}{\pi}\sqrt{\lambda}+\frac{1}{2}\right\rfloor, \tag{5.5}$$

for all $\lambda > 0$. The latter follows by employing the standard Dirichlet–Neumann bracketing, that is, one can estimate the eigenvalues of $\widetilde{\mathbf{h}}_n$ via the eigenvalues of the operators $\widetilde{\mathbf{h}}_n^D$ and $\widetilde{\mathbf{h}}_n^N$ subject to Dirichlet, respectively, Neumann boundary conditions at t_n:

$$\lambda_k(\widetilde{\mathbf{h}}_n^N) \leq \lambda_k(\widetilde{\mathbf{h}}_n) \leq \lambda_k(\widetilde{\mathbf{h}}_n^D), \quad k\geq 1. \tag{5.6}$$

Combining (5.4) with (5.5) and using a very simple estimate (see Lemma 5.2 below), we immediately arrive at (5.1). $\square$

Lemma 5.2. *Let $\{a_n\}_{n\geq 1}$ and $\{b_n\}_{n\geq 1}$ be nonnegative sequences such that $\lim_n b_n = 0$ and $\sum_n a_n b_n < \infty$. Then for every $\alpha\in[0,1)$,*

$$\lim_{\lambda\to\infty}\sum_{n\geq 1} a_n \frac{|b_n\lambda - \lfloor b_n\lambda+\alpha\rfloor|}{\lambda} = 0. \tag{5.7}$$

Proof. Indeed,

$$\sum_{n\geq 1} a_n \frac{|b_n\lambda - \lfloor b_n\lambda+\alpha\rfloor|}{\lambda} = \sum_{n:\, b_n<\frac{1-\alpha}{\lambda}} + \sum_{n:\, b_n\geq\frac{1-\alpha}{\lambda}} a_n \frac{|b_n\lambda - \lfloor b_n\lambda+\alpha\rfloor|}{\lambda}.$$

The first summand can be estimated as follows

$$\sum_{n:\, b_n<\frac{1-\alpha}{\lambda}} a_n \frac{|b_n\lambda - \lfloor b_n\lambda+\alpha\rfloor|}{\lambda} = \sum_{n:\, b_n<\frac{1-\alpha}{\lambda}} a_n b_n = o(1),$$

as $\lambda \to \infty$. Moreover, we have

$$\sum_{n\colon b_n \geq \frac{1-\alpha}{\lambda}} a_n \frac{\lfloor b_n\lambda - \lfloor b_n\lambda + \alpha \rfloor \rfloor}{\lambda} \leq \sum_{n\colon b_n \geq \frac{1-\alpha}{\lambda}} a_n \frac{1}{\lambda} = o(1),$$

as $\lambda \to \infty$, which proves the claim. $\square$

Remark 5.3. We are not aware (except a few special cases) of a closed form of eigenvalues of $\widetilde{\mathbf{h}}_n$. It is not difficult to show that $\sigma(\widetilde{\mathbf{h}}_n)$ consists of simple positive eigenvalues $\{\widetilde{\lambda}_k\}_{k\geq 1}$ satisfying (5.5) and even to express $\sigma(\widetilde{\mathbf{h}}_n)$ with the help of the *arctangent function with two arguments*, although this does not lead to a closed formula.

In the case $\mathrm{vol}(\mathcal{A}) = \infty$, the spectrum of $\mathbf{H}$ may have a rather complicated structure. In particular, it may not be purely discrete. The next result provides a criterion for $\mathbf{H}$ to have purely discrete spectrum. Set

$$\mathcal{L}_\mu := \int_0^{\mathcal{L}} \frac{dx}{\mu(x)} = \sum_{n\geq 0} \frac{\ell_n}{s_n s_{n+1}}. \tag{5.8}$$

Theorem 5.4. *Let $\mathcal{A}$ be an infinite radially symmetric antitree with $\mathrm{vol}(\mathcal{A}) = \infty$. Then the spectrum of $\mathbf{H}$ is discrete if and only if the following conditions are satisfied:*

(i) $\ell_n \to 0$ *as* $n \to \infty$,
(ii) $\mathcal{L}_\mu < \infty$, *and*
(iii)

$$\lim_{n\to\infty} \sum_{k=0}^{n} s_k s_{k+1} \ell_k \sum_{k\geq n} \frac{\ell_k}{s_k s_{k+1}} = 0. \tag{5.9}$$

Proof. Denote

$$\mathbf{H}^1 := \bigoplus_{n\geq 1} \Big(\oplus_{j=1}^{(s_n-1)(s_{n+1}-1)} \mathbf{h}_n \Big), \qquad \mathbf{H}^2 := \bigoplus_{n\geq 1} \Big(\oplus_{j=1}^{s_n-1} \widetilde{\mathbf{h}}_n \Big). \tag{5.10}$$

By Theorem 4.1(i), $\mathbf{H}$ is self-adjoint and hence (3.18) implies that

$$\sigma(\mathbf{H}) = \sigma(\mathrm{H}) \cup \sigma(\mathbf{H}^1) \cup \sigma(\mathbf{H}^2) = \sigma(\mathrm{H}) \cup \overline{\big(\cup_{n\geq 1} \sigma(\mathbf{h}_n) \big)} \cup \overline{\big(\cup_{n\geq 1} \sigma(\widetilde{\mathbf{h}}_n) \big)}. \tag{5.11}$$

Thus the spectrum of $\mathbf{H}$ is discrete if and only if the spectra of all three operators H, $\mathbf{H}^1$ and $\mathbf{H}^2$ are discrete.

In order to investigate the operator H, we need to transform it to the Krein string form by using a suitable change of variables ($x \mapsto \int_0^x \frac{ds}{\mu(s)}$) and then to apply the Kac–Krein criterion [26]. To be more precise, it is straightforward to verify that H is unitarily equivalent to the operator $\widetilde{\mathrm{H}}$ defined in the Hilbert space $L^2([0, \mathcal{L}_\mu); \widetilde{\mu})$ by the differential expression

$$\widetilde{\tau} = -\frac{1}{\widetilde{\mu}(x)} \frac{d^2}{dx^2} \tag{5.12}$$

and subject to the Neumann boundary condition at $x = 0$. Here

$$\widetilde{\mu} := \mu^2 \circ g^{-1}, \tag{5.13}$$

where g^{-1} is the inverse of the function $g\colon [0,\mathcal{L}) \to [0,\mathcal{L}_\mu)$ given by

$$g(x) = \int_0^x \frac{ds}{\mu(s)}, \qquad \mathcal{L}_\mu := g(\mathcal{L}) = \int_0^{\mathcal{L}} \frac{ds}{\mu(s)}. \tag{5.14}$$

Notice that g is strictly increasing and locally absolutely continuous on $[0,\mathcal{L})$ and maps $[0,\mathcal{L})$ onto $[0,\mathcal{L}_\mu)$. Hence its inverse $g^{-1}\colon [0,\mathcal{L}_\mu) \to [0,\mathcal{L})$ is also strictly increasing and locally absolutely continuous on $[0,\mathcal{L}_\mu)$.

Applying the Kac–Krein criterion (see [26], [27, §11.9]), we conclude that H has purely discrete spectrum if and only if $\mathcal{L}_\mu < \infty$ and

$$\lim_{x\to\mathcal{L}} \Phi(x) = 0, \tag{5.15}$$

where $\Phi\colon [0,\mathcal{L}) \to \mathbb{R}_{\geq 0}$ is given by

$$\Phi(x) := \int_0^x \mu(s)ds \cdot \int_x^{\mathcal{L}} \frac{ds}{\mu(s)}, \quad x \in [0,\mathcal{L}). \tag{5.16}$$

First of all, observe that

$$\Phi(x) \leq \int_0^{t_{n+1}} \mu(s)ds \cdot \int_{t_n}^{\mathcal{L}} \frac{ds}{\mu(s)} = \sum_{k=0}^{n} s_k s_{k+1}\ell_k \sum_{k\geq n} \frac{\ell_k}{s_k s_{k+1}}$$

for all $x \in [t_n, t_{n+1})$ and hence sufficiency of (5.9) follows. Moreover, straightforward calculations show that

$$\begin{aligned}\Phi\Big(\frac{t_n + t_{n+1}}{2}\Big) &= \Big(\sum_{k=0}^{n-1} s_k s_{k+1}\ell_k + s_n s_{n+1}\frac{\ell_n}{2}\Big)\Big(\sum_{k\geq n+1} \frac{\ell_k}{s_k s_{k+1}} + \frac{\ell_n}{2 s_n s_{n+1}}\Big)\\ &\geq \frac{1}{4}\sum_{k=0}^{n} s_k s_{k+1}\ell_k \sum_{k\geq n} \frac{\ell_k}{s_k s_{k+1}},\end{aligned}$$

which implies the necessity of (5.9). Notice also that the right-hand side in the last inequality is strictly greater than $\frac{1}{4}\ell_n^2$, which also implies (i).

It remains to note that the spectra of the operators $\mathbf{H}^1$ and $\mathbf{H}^2$ are discrete if condition (i) is satisfied (see (5.3) and (5.4)). □

Remark 5.5. Let us mention that in fact both conditions (i) and (ii) in Theorem 5.4 follow from (iii).

If $\mathrm{vol}(\mathcal{A}) = \infty$ and the corresponding Hamiltonian $\mathbf{H}$ has purely discrete spectrum, it follows from the proof of Weyl's law (5.1) that $\frac{N(\lambda;\mathbf{H})}{\sqrt{\lambda}} \to \infty$ as $\lambda \to \infty$. However, we can characterize radially symmetric antitress such that the resolvent of the corresponding quantum graph operator $\mathbf{H}$ belongs to the trace class.

Theorem 5.6. *Let $\mathcal{A}$ be an infinite radially symmetric antitree with* $\mathrm{vol}(\mathcal{A}) = \infty$. *Also, let the spectrum of* $\mathbf{H}$ *be purely discrete. Then*[3]

$$\sum_{\lambda\in\sigma(\mathbf{H})} \frac{1}{\lambda} < \infty \tag{5.17}$$

if and only if

$$\sum_{n\geq 1} s_n s_{n+1}\ell_n^2 < \infty, \tag{5.18}$$

[3]The summation in (5.17) is according to multiplicities.

and

$$\sum_{n\geq 0} \frac{\ell_n}{s_n s_{n+1}} \sum_{k=0}^{n-1} s_k s_{k+1} \ell_k < \infty. \tag{5.19}$$

Proof. As in the proof of Theorem 5.4, observe that the spectrum of $\mathbf{H}$ consists of three sets of eigenvalues. Let us denote the second and the third summands in (3.18) by $\mathbf{H}^1$ and $\mathbf{H}^2$, respectively. The spectrum of the self-adjoint operator $\mathbf{h}_n$ is given by (5.3) and hence

$$\sum_{\lambda\in\sigma(\mathbf{H}^2)} \frac{1}{\lambda} = \sum_{n\geq 1}(s_n-1)(s_{n+1}-1)\sum_{k\geq 1}\frac{\ell_n^2}{\pi^2 k^2} = \frac{1}{6}\sum_{n\geq 1}(s_n-1)(s_{n+1}-1)\ell_n^2. \tag{5.20}$$

Similarly, using the Dirichlet–Neumann bracketing (5.6), we get

$$\begin{aligned}
\sum_{\lambda\in\sigma(\mathbf{H}^1)} \frac{1}{\lambda} &\leq \sum_{n\geq 1}(s_n-1)\sum_{\lambda\in\sigma(\widetilde{\mathbf{h}}_n^N)}\frac{1}{\lambda}\\
&= \sum_{n\geq 1}(s_n-1)\sum_{k\geq 1}\frac{\ell_{n-1}^2}{\pi^2(k-1/2)^2} + \frac{\ell_n^2}{\pi^2(k-1/2)^2}\\
&= \frac{1}{2}\sum_{n\geq 1}(s_n-1)(\ell_{n-1}^2+\ell_n^2) \leq \frac{1}{2}\sum_{n\geq 0}(s_n+s_{n+1}-2)\ell_n^2.
\end{aligned}$$

Using the Dirichlet eigenvalues, one can prove a similar bound from below. Moreover, combining the latter with (5.18) implies that the resolvents of both $\mathbf{H}_1$ and $\mathbf{H}_2$ belong to the trace class exactly when

$$\sum_{n\geq 1}(s_n s_{n+1}-1)\ell_n^2 < \infty. \tag{5.21}$$

Next observe that $0 \in \sigma(\mathrm{H})$ exactly when $\mathbb{1} \in L^2(\mathcal{I}_\mathcal{L};\mu)$, which is equivalent to $\mathrm{vol}(\mathcal{A}) < \infty$. Thus 0 is not an eigenvalue of $\mathbf{H}$ whenever $\mathrm{vol}(\mathcal{A}) = \infty$. Finally, applying M. G. Krein's theorem to the operator H (see [26], [27, §11.10]), we conclude that H^{-1} is trace class if and only if $\mathcal{L}_\mu < \infty$ and

$$\int_0^\mathcal{L} \frac{1}{\mu(x)}\int_0^x \mu(s)ds\,dx < \infty. \tag{5.22}$$

However, using (3.4), we get

$$\begin{aligned}
\int_0^\mathcal{L} \frac{1}{\mu(x)}\int_0^x \mu(s)ds\,dx &= \sum_{n\geq 0}\int_{t_n}^{t_{n+1}} \frac{1}{\mu(x)}\int_0^x \mu(s)ds\,dx\\
&= \sum_{n\geq 0}\frac{1}{s_n s_{n+1}}\int_{t_n}^{t_{n+1}}\Big(\sum_{k=0}^{n-1} s_k s_{k+1}\ell_k + s_n s_{n+1}(x-t_n)\Big)dx\\
&= \sum_{n\geq 0}\frac{\ell_n}{s_n s_{n+1}}\sum_{k=0}^{n-1} s_k s_{k+1}\ell_k + \frac{1}{2}\sum_{n\geq 0}\ell_n^2.
\end{aligned}$$

Notice that the latter in particular shows that $\{\ell_n\}_{n\geq 0} \in \ell^2$ and combining this fact with (5.21) we arrive at (5.18). This completes the proof. $\square$

Remark 5.7. Using the same arguments and the results from [28, 41] one would be able to characterize radially symmetric antitrees such that the resolvent of the corresponding Kirchhoff Laplacian belongs to the Schatten–von Neumann ideal $\mathfrak{S}_p$, $p \in (1, \infty)$ (and even to other trace ideals), however, these results look cumbersome and we decided not to include them.

6. Spectral gap estimates

We restrict our discussion to the case $\mathrm{vol}(\mathcal{A}) = \infty$ for several reasons. Of course, the main one is the fact that in this case $\mathbf{H}_0$ is essentially self-adjoint and this simplifies some considerations. However, for finite volume metric graphs the corresponding estimates remain to be true for the Friedrichs extension of $\mathbf{H}_0$.

Theorem 6.1. *Let $\mathcal{A}$ be an infinite radially symmetric antitree with* $\mathrm{vol}(\mathcal{A}) = \infty$. *Then the bottom of the spectrum $\lambda_0(\mathbf{H}) = \inf \sigma(\mathbf{H})$ of $\mathbf{H}$ is strictly positive if and only if the following conditions are satisfied:*

(i) $\ell^*(\mathcal{A}) = \sup_{n \geq 0} \ell_n < \infty$,

(ii) $\mathcal{L}_\mu = \sum_{n \geq 0} \frac{\ell_n}{s_n s_{n+1}} < \infty$, *and*

(iii)
$$C(\mathcal{L}) := \sup_{x \in (0, \mathcal{L})} \int_0^x \mu(s) ds \cdot \int_x^{\mathcal{L}} \frac{ds}{\mu(s)} < \infty. \tag{6.1}$$

Moreover, we have the following estimate
$$\frac{1}{4C(\mathcal{L})} \leq \lambda_0(\mathbf{H}) \leq \frac{1}{C(\mathcal{L})}. \tag{6.2}$$

Proof. Since $\mathrm{vol}(\mathcal{A}) = \infty$, the operator $\mathbf{H}$ is self-adjoint by Theorem 4.1. Moreover, by Theorem 3.5, we have
$$\lambda_0(\mathbf{H}) = \min\{\lambda_0(\mathrm{H}), \lambda_0(\mathbf{H}^1), \lambda_0(\mathbf{H}^2)\}, \tag{6.3}$$
where $\mathbf{H}^1$ and $\mathbf{H}^2$ are given by (5.10). Observe that
$$\lambda_0(\mathbf{H}) = \lambda_0(\mathrm{H}). \tag{6.4}$$
Indeed, it suffices to compare the domains of H_0 and $\mathbf{h}_n$, $\widetilde{\mathbf{h}}_n$ and then exploit the Rayleigh quotient. For instance,
$$\lambda_0(\mathrm{H}) = \inf_{\substack{f \in \mathrm{dom}(\mathrm{H}_0) \\ f \neq 0}} \frac{(\mathrm{H}f, f)_{L^2(\mathcal{I}_\mathcal{L};\mu)}}{\|f\|^2_{L^2(\mathcal{I}_\mathcal{L};\mu)}} \leq \inf_{\substack{f \in \mathrm{dom}(\mathrm{H}_0) \\ \mathrm{supp}(f) \subset [t_{n-1}, t_{n+1}]}} \frac{(\mathrm{H}f, f)_{L^2(\mathcal{I}_\mathcal{L};\mu)}}{\|f\|^2_{L^2(\mathcal{I}_\mathcal{L};\mu)}}$$
$$\leq \inf_{\substack{f \in \mathrm{dom}(\widetilde{\mathbf{h}}_n) \\ f \neq 0}} \frac{(\widetilde{\mathbf{h}}_n f, f)_{L^2(I_{n-1} \cup I_n;\mu)}}{\|f\|^2_{L^2(I_{n-1} \cup I_n;\mu)}} = \lambda_0(\widetilde{\mathbf{h}}_n).$$

The operator H can be studied in the framework of Krein strings, however, we need to apply the Kac–Krein criteria [26] to the *dual string* since both Corollary 1.1 and Remark 2.2 in [26] are stated subject to the Dirichlet boundary condition at $x = 0$. For a detailed discussion of dual strings we refer to [27, §12] and the desired connection is [27, equality (12.6)][4]. More precisely, assuming $\mathcal{L}_\mu < \infty$ and

[4]This statement can be seen as the analog of the *abstract commutation*: for a closed operator A acting in a Hilbert space $\mathfrak{H}$, the operators $(A^*A) \restriction_{\ker(A)^\perp}$ and $(AA^*) \restriction_{\ker(A^*)^\perp}$ are unitarily equivalent.

then applying Theorem 1 from [26], we get the estimate

$$x\left(M^{-1}(\infty) - M^{-1}(x)\right) \le \frac{1}{\lambda_0(\mathrm{H})}, \tag{6.5}$$

which holds for all $x > 0$. Here M^{-1} denotes the inverse to the function $M\colon [0, \mathcal{L}_\mu) \to [0, \infty)$ defined by (see also (5.13) and (5.14))

$$M(x) := \int_0^x \widetilde{\mu}(s)ds = \int_0^x (\mu^2 \circ g^{-1})(s)ds = \int_0^{g^{-1}(x)} \mu(s)ds. \tag{6.6}$$

Notice that M is a strictly increasing and absolutely continuous function mapping $[0, \mathcal{L}_\mu)$ onto $[0, \infty)$ (the latter follows from the assumption $\mathrm{vol}(\mathcal{A}) = \infty$). Thus (6.5) is equivalent to

$$M(x)\,(\mathcal{L}_\mu - x) \le \frac{1}{\lambda_0(\mathrm{H})}, \qquad x \in (0, \mathcal{L}_\mu). \tag{6.7}$$

By changing variables, we end up with the following estimate

$$\sup_{x\in(0,\mathcal{L})} \int_0^x \mu(s)ds \cdot \int_x^{\mathcal{L}} \frac{ds}{\mu(s)} \le \frac{1}{\lambda_0(\mathrm{H})}. \tag{6.8}$$

Applying Theorem 3 from [26] and using the same arguments, we end up with the lower bound

$$\frac{1}{4\lambda_0(\mathrm{H})} \le \sup_{x\in(0,\mathcal{L})} \int_0^x \mu(s)ds \cdot \int_x^{\mathcal{L}} \frac{ds}{\mu(s)}. \tag{6.9}$$

Taking into account [26, Remark 2.2], we conclude that the condition $\mathcal{L}_\mu < \infty$ is also necessary for the positivity of $\lambda_0(\mathrm{H})$. It remains to note that the necessity of (i) follows from (iii). Indeed, assuming the converse, that is, there is a sequence of lengths ℓ_{n_k} tending to infinity, and then choosing x_{n_k} as the middle points of the corresponding intervals, one immediately concludes that $C(\mathcal{L}) = \infty$ by evaluating (6.1) at x_{n_k}. $\square$

Remark 6.2. Arguing as in the proof of Theorem 5.4 one can show that conditions (i)–(iii) in Theorem 6.1 can be replaced by the single condition

$$\sup_{n\ge 0} \sum_{k=0}^{n} s_k s_{k+1} \ell_k \sum_{k\ge n} \frac{\ell_k}{s_k s_{k+1}} < \infty. \tag{6.10}$$

However, this expression provides only an upper bound on $C(\mathcal{L})$:

$$\sup_{n\ge 0} \sum_{k=0}^{n} s_k s_{k+1} \ell_k \sum_{k\ge n+1} \frac{\ell_k}{s_k s_{k+1}} \le C(\mathcal{L}) \le \sup_{n\ge 0} \sum_{k=0}^{n} s_k s_{k+1} \ell_k \sum_{k\ge n} \frac{\ell_k}{s_k s_{k+1}}. \tag{6.11}$$

Since 0 is not an eigenvalue of $\mathbf{H}$ if $\mathrm{vol}(\mathcal{A}) = \infty$, $\lambda_0(\mathbf{H}) > 0$ is equivalent to $\lambda_0^{\mathrm{ess}}(\mathbf{H}) > 0$, where $\lambda_0^{\mathrm{ess}}(\mathbf{H})$ denotes the bottom of the essential spectrum of $\mathbf{H}$, $\lambda_0^{\mathrm{ess}}(\mathbf{H}) := \inf \sigma_{\mathrm{ess}}(\mathbf{H})$. Thus Theorem 6.1 also provides a criterion for $\lambda_0^{\mathrm{ess}}(\mathbf{H})$ to be strictly positive. Moreover, by employing Glazman's decomposition principle one can prove a similar to (6.1) bound on $\lambda_0^{\mathrm{ess}}(\mathbf{H})$.

Theorem 6.3. *Let $\mathcal{A}$ be an infinite radially symmetric antitree with* $\mathrm{vol}(\mathcal{A}) = \infty$*. Then $\lambda_0^{\mathrm{ess}}(\mathbf{H}) > 0$ if and only if* (6.10) *holds true. Moreover,*

$$\frac{1}{4C_{\mathrm{ess}}(\mathcal{L})} \le \lambda_0^{\mathrm{ess}}(\mathbf{H}) \le \frac{1}{C_{\mathrm{ess}}(\mathcal{L})}, \tag{6.12}$$

where the constant $C_{\text{ess}}(\mathcal{L})$ *is given by*

$$C_{\text{ess}}(\mathcal{L}) = \lim_{x\to\mathcal{L}} \sup_{y\in(x,\mathcal{L})} \int_x^y \mu(s)ds \cdot \int_y^{\mathcal{L}} \frac{ds}{\mu(s)}. \tag{6.13}$$

A few remarks are in order.

Remark 6.4.
(i) The equality $C_{\text{ess}}(\mathcal{L}) = 0$ implies Theorem 5.4.
(ii) One can prove Theorem 6.1 avoiding the use of the Kac–Krein results [26]. Namely, with the help of the Rayleigh quotient, one can rewrite the inequality $\lambda_0(\mathrm{H}) > 0$ as a variational problem and then apply Muckenhoupt's inequalities (see, e.g., [33, §1.3.1], [35]). In particular, M. Solomyak employed this approach in the study of quantum graph operators on radially symmetric trees (see [44, §5]).
(iii) It is interesting to compare Theorems 6.1 and 6.3 with volume growth estimates (cf. [45]). For instance, by [32, Theorem 7.1],

$$\lambda_0(\mathbf{H}) \le \lambda_0^{\text{ess}}(\mathbf{H}) \le \frac{1}{4}\mathrm{v}(\mathcal{A})^2, \tag{6.14}$$

where

$$\mathrm{v}(\mathcal{A}) := \liminf_{n\to\infty} \frac{1}{\sum_{k=0}^n \ell_k} \log\Big(\sum_{k=0}^n s_k s_{k+1}\ell_k\Big). \tag{6.15}$$

However, this result applies only if $\mathcal{L} = \sum_{n\ge 0} \ell_n = \infty$.

7. Isoperimetric constant

Recall that [32, §3] the *isoperimetric constant* $\alpha(\mathcal{G})$ of a metric graph $\mathcal{G}$ is

$$\alpha(\mathcal{G}) := \inf_{\widetilde{\mathcal{G}}} \frac{\deg_{\mathcal{G}}(\partial\widetilde{\mathcal{G}})}{\mathrm{vol}(\widetilde{\mathcal{G}})}, \tag{7.1}$$

where the infimum is taken over all finite connected subgraphs $\widetilde{\mathcal{G}} = (\widetilde{\mathcal{V}}, \widetilde{\mathcal{E}})$. Here

$$\partial\widetilde{\mathcal{G}} = \{v \in \widetilde{\mathcal{V}} |\ \deg_{\widetilde{\mathcal{G}}}(v) < \deg_{\mathcal{G}}(v)\},$$

is the *boundary* of $\widetilde{\mathcal{G}}$ and

$$\deg_{\mathcal{G}}(\partial\widetilde{\mathcal{G}}) := \sum_{v\in\partial\widetilde{\mathcal{G}}} \deg_{\widetilde{\mathcal{G}}}(v), \qquad \mathrm{vol}(\widetilde{\mathcal{G}}) := \sum_{e\in\widetilde{\mathcal{E}}} |e|. \tag{7.2}$$

Computation of the isoperimetric constant is known to be an NP-hard problem, however, due to the presence of symmetries, we are able to find $\alpha(\mathcal{A})$ for radially symmetric antitrees.

Theorem 7.1. *The isoperimetric constant of a radially symmetric antitree* $\mathcal{A}$ *is*

$$\alpha(\mathcal{A}) = \inf_{n\ge 0} \frac{s_n s_{n+1}}{\sum_{k=0}^n s_k s_{k+1}\ell_k}. \tag{7.3}$$

Proof. The decomposition obtained in Theorem 3.5 suggests to take the infimum in (7.1) only over radially symmetric subgraphs. Namely, choosing $\mathcal{A}_n$ for every $n \ge 0$ as the subgraph consisting of all edges between the root o and the combinatorial sphere S_{n+1}, we have $\partial\mathcal{A}_n = S_{n+1}$ and $\deg_{\mathcal{A}_n}(v) = s_n$ for all vertices $v \in S_{n+1}$. Hence by (7.1) we get

$$\alpha(\mathcal{A}) \le \frac{\deg(\partial\mathcal{A}_n)}{\mathrm{vol}(\mathcal{A}_n)} = \frac{s_n s_{n+1}}{\sum_{k\le n} s_k s_{k+1}\ell_k}. \tag{7.4}$$

Thus it remains to show that indeed it suffices to restrict the infimum in (7.1) to the family $\{\mathcal{A}_n\}_{n\geq 0}$. Observe that $\{\mathcal{A}_n\}_{n\geq 0}$ is a net, that is, for every finite connected subgraph $\widetilde{\mathcal{A}}$ of $\mathcal{A}$ there is $n \geq 0$ such that $\widetilde{\mathcal{A}}$ is a subgraph of $\mathcal{A}_n$. Hence we will proceed by induction in n.

Let us start with subgraphs $\widetilde{\mathcal{A}} \subsetneq \mathcal{A}_0$. Then $\widetilde{\mathcal{A}}$ consists of $m < s_0 s_1$ edges of $\mathcal{E}_0^+$ and $\mathrm{vol}(\widetilde{\mathcal{A}}) = m\ell_0$. Moreover, for all vertices of $\widetilde{\mathcal{A}}$, $\deg_{\widetilde{\mathcal{A}}}(v) < \deg_{\mathcal{A}}(v)$ and hence $\deg(\partial\widetilde{\mathcal{A}}) = 2m$, which implies

$$\frac{\deg(\partial\widetilde{\mathcal{A}})}{\mathrm{vol}(\widetilde{\mathcal{A}})} = \frac{2m}{m\ell_0} = \frac{2}{\ell_0} > \frac{\deg(\partial\mathcal{A}_0)}{\mathrm{vol}(\mathcal{A}_0)} = \frac{1}{\ell_0}.$$

Take $n \geq 1$ and assume that

$$\frac{\deg(\partial\widetilde{\mathcal{A}})}{\mathrm{vol}(\widetilde{\mathcal{A}})} \geq \inf_{k\leq n-1} \frac{\deg(\partial\mathcal{A}_k)}{\mathrm{vol}(\mathcal{A}_k)} = \inf_{k\leq n-1} \frac{s_k s_{k+1}}{\sum_{j\leq k} s_j s_{j+1}\ell_j} \tag{7.5}$$

holds for all connected subgraphs $\widetilde{\mathcal{A}} \subseteq \mathcal{A}_{n-1}$. Take now a connected subgraph $\widetilde{\mathcal{A}} \subseteq \mathcal{A}_n$ such that $\widetilde{\mathcal{A}} \nsubseteq \mathcal{A}_{n-1}$. The latter in particular implies that $\mathcal{V}(\widetilde{\mathcal{A}}) \cap S_n \neq \emptyset$ and $\mathcal{V}(\widetilde{\mathcal{A}}) \cap S_{n+1} \neq \emptyset$. We can also assume that $\mathcal{V}(\widetilde{\mathcal{A}}) \cap S_{n-1} \neq \emptyset$ since otherwise $\mathcal{E}(\widetilde{\mathcal{A}}) \subseteq \mathcal{E}_n^+$ and hence in this case

$$\frac{\deg(\partial\widetilde{\mathcal{A}})}{\mathrm{vol}(\widetilde{\mathcal{A}})} = \frac{2}{\ell_n} > \frac{s_n s_{n+1}}{\sum_{k\leq n} s_k s_{k+1}\ell_k} = \frac{\deg(\partial\mathcal{A}_n)}{\mathrm{vol}(\mathcal{A}_n)}. \tag{7.6}$$

Let us first show that without loss of generality we can take $\widetilde{\mathcal{A}}$ such that each edge $e \in \mathcal{E}(\widetilde{\mathcal{A}})$ contains at least one vertex in $\mathcal{V}_{\mathrm{int}}(\widetilde{\mathcal{A}}) := \mathcal{V}(\widetilde{\mathcal{A}}) \setminus \partial\widetilde{\mathcal{A}}$. Indeed, if not, consider the induced subgraph $\widetilde{\mathcal{A}}_{\mathrm{int}}$, which we can split into a finite disjoint union of connected subgraphs $\{\widetilde{\mathcal{A}}_j\}$. In particular, $\widetilde{\mathcal{V}}_{\mathrm{int}} = \cup_j \mathcal{V}(\widetilde{\mathcal{A}}_j)$. Let $\mathcal{G}_j$ be the star-like subgraphs of $\mathcal{A}$ with edge sets $\mathcal{E}(\mathcal{G}_j) = \cup_{v\in\mathcal{V}(\widetilde{\mathcal{A}}_j)}\mathcal{E}_v$. By construction, $\mathcal{G}_j \subseteq \mathcal{A}_n$ and each edge of $\mathcal{G}_j$ contains a vertex from $\mathcal{V}(\mathcal{G}_j) \setminus \partial\mathcal{G}_j = \mathcal{V}(\widetilde{\mathcal{A}}_j)$. Moreover, let $\mathcal{E}_r = \mathcal{E}(\widetilde{\mathcal{A}}) \setminus \cup_j\mathcal{E}(\mathcal{G}_j)$ be the remaining edges of $\widetilde{\mathcal{A}}$. Then it is straightforward to verify (see also [38, proof of Lemma 3.5]) that

$$\frac{\deg(\partial\widetilde{\mathcal{A}})}{\mathrm{vol}(\widetilde{\mathcal{A}})} = \frac{\sum_j \deg(\partial\mathcal{G}_j) + 2\#\mathcal{E}_r}{\sum_j \mathrm{vol}(\mathcal{G}_j) + \sum_{e\in\mathcal{E}_r}|e|} \geq \min_{j,e\in\mathcal{E}_r}\left\{\frac{\deg(\partial\mathcal{G}_j)}{\mathrm{vol}(\mathcal{G}_j)}, \frac{2}{|e|}\right\}.$$

Taking into account (7.6), this proves the claim.

Consider a new graph $\widetilde{\mathcal{A}}'$ obtained from $\widetilde{\mathcal{A}}$ by adding all possible edges connecting S_n with S_{n-1} and S_{n+1} such that the new graph $\widetilde{\mathcal{A}}'$ is connected. By construction, $\widetilde{\mathcal{A}}' \subseteq \mathcal{A}_n$. Moreover, $S_{n+1} \subseteq \partial\widetilde{\mathcal{A}}'$ and $\deg_{\widetilde{\mathcal{A}}'}(v) = s_n$ for all $v \in S_{n+1}$. Hence

$$\frac{\deg(\partial\widetilde{\mathcal{A}}')}{\mathrm{vol}(\widetilde{\mathcal{A}}')} \geq \frac{s_n s_{n+1}}{\mathrm{vol}(\mathcal{A}_n)} = \frac{\deg(\partial\mathcal{A}_n)}{\mathrm{vol}(\mathcal{A}_n)}.$$

We also need another subgraph $\widetilde{\mathcal{A}}''$ of $\widetilde{\mathcal{A}}$ obtained by removing the edges of $\widetilde{\mathcal{A}}$ connecting S_{n+1} with $S_n \setminus \partial\widetilde{\mathcal{A}}$ and also $S_n \setminus \partial\widetilde{\mathcal{A}}$ with the vertices in $S_{n-1} \cap \partial\widetilde{\mathcal{A}}$. The obtained graph $\widetilde{\mathcal{A}}''$ is a connected subgraph of $\mathcal{A}_{n-1}$ and hence satisfies the induction hypothesis (7.5). Our aim is to show that

$$\frac{\deg(\partial\widetilde{\mathcal{A}})}{\mathrm{vol}(\widetilde{\mathcal{A}})} \geq \min\Big\{\frac{\deg(\partial\widetilde{\mathcal{A}}')}{\mathrm{vol}(\widetilde{\mathcal{A}}')}, \frac{\deg(\partial\widetilde{\mathcal{A}}'')}{\mathrm{vol}(\widetilde{\mathcal{A}}'')}\Big\}, \tag{7.7}$$

Denoting $M := \#(S_n \cap \widetilde{\mathcal{V}}_{\mathrm{int}})$ and $N := \#(S_{n-1} \cap \partial\widetilde{\mathcal{A}})$, we get

$$\mathrm{vol}(\widetilde{\mathcal{A}}') = \mathrm{vol}(\widetilde{\mathcal{A}}) + (s_n - M)s_{n+1}\ell_n + (s_n - M)N\ell_{n-1}, \tag{7.8}$$

and

$$\mathrm{vol}(\widetilde{\mathcal{A}}'') = \mathrm{vol}(\widetilde{\mathcal{A}}) - Ms_{n+1}\ell_n - MN\ell_{n-1}. \tag{7.9}$$

Moreover, a careful inspection shows that

$$\deg(\partial\widetilde{\mathcal{A}}') \le \deg(\partial\widetilde{\mathcal{A}}) + (s_n - M)(s_{n+1} - s_{n-1} + 2N), \tag{7.10}$$

and

$$\deg(\partial\widetilde{\mathcal{A}}) = \deg(\partial\widetilde{\mathcal{A}}'') + M(s_{n+1} - s_{n-1} + 2N). \tag{7.11}$$

Now observe that if (7.7) fails to hold, then (7.9) and (7.11) would imply

$$\frac{s_{n+1} + 2N - s_{n-1}}{s_{n+1}\ell_n + N\ell_{n-1}} < \frac{\deg(\partial\widetilde{\mathcal{A}})}{\mathrm{vol}(\widetilde{\mathcal{A}})}, \tag{7.12}$$

and, moroever, (7.8) and (7.10) lead to

$$\frac{s_{n+1} + 2N - s_{n-1}}{s_{n+1}\ell_n + N\ell_{n-1}} > \frac{\deg(\partial\widetilde{\mathcal{A}})}{\mathrm{vol}(\widetilde{\mathcal{A}})}. \tag{7.13}$$

This contradiction proves (7.7) and hence finishes the proof of (7.3). □

Remark 7.2. A few remarks are in order.

(i) By the Cheeger-type estimate [32, Theorem 3.4], we have

$$\lambda_0(\mathbf{H}) \ge \frac{1}{4}\alpha(\mathcal{A})^2. \tag{7.14}$$

Comparing (7.14) and (7.3) with (6.2) and (6.11), we conclude that positivity of the isoperimetric constant is indeed only sufficient for $\lambda_0(\mathbf{H}) > 0$. For example, $\alpha(\mathcal{A}) = 0$ whenever $\mathrm{vol}(\mathcal{A}) = \infty$ and $\{s_n s_{n+1}\}_{n\ge 0}$ has a bounded subsequence.

(ii) The isoperimetric constant $\alpha(\mathcal{A})$ measures the ratio of the number of boundary points of $\mathcal{A}_n$ to the volume of $\mathcal{A}_n$ and thus provides a lower bound for $\lambda_0(\mathbf{H})$. The volume growth estimate (6.14) provides an upper bound by relating the exponential growth of the volume of $\mathcal{A}_n$ with respect to its diameter. Notice that the volume of the subgraph $\mathcal{A}_n$ also appears in (6.10)–(6.11). The meaning of the other quantity in (6.11), namely, of $\sum_{k\ge n} \frac{\ell_k}{s_k s_{k+1}}$, which however provides two-sided estimates, remains unclear to us.

8. Singular spectrum

Using the isometric isomorphism $U_\mu\colon f \mapsto \sqrt{\mu} f$ between Hilbert spaces $L^2(\mathcal{I}_\mathcal{L};\mu)$ and $L^2(\mathcal{I}_\mathcal{L})$, it is straightforward to check that the pre-minimal operator H_0 defined in Section 3.2 is unitarily equivalent to the operator $\widetilde{\mathrm{H}}_0$ defined in $L^2(\mathcal{I}_\mathcal{L})$ by

$$\widetilde{\mathrm{H}}_0 f = -f'', \quad f \in \mathrm{dom}(\widetilde{\mathrm{H}}_0) = U_\mu(\mathrm{dom}(\mathrm{H}_0))$$

$$\mathrm{dom}(\widetilde{\mathrm{H}}_0) = \big\{ f \in L^2_c(\mathcal{I}_\mathcal{L}) |\, \frac{1}{\sqrt{\mu}} f, \sqrt{\mu} f' \in AC(\mathcal{I}_\mathcal{L}),\ f'(0) = 0,\ f'' \in L^2(\mathcal{I}_\mathcal{L}) \big\}.$$

Since μ is piece-wise constant on $(0, \mathcal{L})$, the domain of $\widetilde{\mathrm{H}}_0$ consists of compactly supported functions $f \in L^2_c(\mathcal{I}_\mathcal{L})$ such that $f \in H^2(I_n)$ for all $n \geq 0$ and also satisfying the following boundary conditions

$$f'(0) = 0; \qquad f(t_n+) = \sqrt{\frac{s_{n+1}}{s_{n-1}}} f(t_n-), \quad f'(t_n+) = \sqrt{\frac{s_{n-1}}{s_{n+1}}} f'(t_n-),$$

for all $n \geq 1$. Denote the closure of $\widetilde{\mathrm{H}}_0$ by $\widetilde{\mathrm{H}}$. The operator $\widetilde{\mathrm{H}}$ has actively been studied since its spectral properties play a crucial role in understanding spectral properties of Kirchhoff Laplacians on radial metric trees (let us only mention [6, 16]). It turns out that one can immediately apply most of the results from [6] and [16] in order to prove the corresponding spectral properties of Kirchhoff Laplacians on radially symmetric antitrees. However, we need the following assumptions on the geometry of metric antitrees:

Hypothesis 8.1. *There is a positive lower bound on the edge lengths,* $\ell_*(\mathcal{A}) := \inf_{n\geq 0} \ell_n > 0$*, and sphere numbers are such that*

$$\liminf_{n\geq 0} \frac{s_{n+2}}{s_n} > 1. \tag{8.1}$$

In this case clearly $\mathcal{L} = \sum_{n\geq 0} \ell_n = \infty$ and hence both operators H and $\widetilde{\mathrm{H}}$ are self-adjoint. The next result is the analog of [6, Theorem 2].

Theorem 8.2. *Assume Hypothesis 8.1. If in addition*

$$\sup_{n\geq 0} \ell_n = \infty, \tag{8.2}$$

then $\sigma(\mathbf{H}) = \mathbb{R}_{\geq 0}$ *and* $\sigma_{\mathrm{ac}}(\mathbf{H}) = \emptyset$*.*

Proof. By Theorem 3.5, it suffices to show that $\sigma(\widetilde{\mathrm{H}}) = \mathbb{R}_{\geq 0}$ and $\sigma_{\mathrm{ac}}(\widetilde{\mathrm{H}}) = \emptyset$ since $\widetilde{\mathrm{H}} = U_\mu \mathrm{H} U_\mu^{-1}$. However, the latter follows from [6, Theorem 6]. □

Moreover, using the results from [31, §4] and arguing as in the proof of [34, Theorem 1] (see also [17, Theorem 5.20]), one can prove the following statement.

Theorem 8.3. *Assume Hypothesis 8.1. If in addition*

$$\sup_{n\geq 0} \frac{s_{n+2}}{s_n} = \infty, \tag{8.3}$$

then $\sigma_{\mathrm{ac}}(\mathbf{H}) = \emptyset$*.*

In contrast to radially symmetric trees, antitrees always have a rather rich point spectrum (see Theorem 3.5). Moreover, under the assumptions of Hypothesis 8.1 this point spectrum is not a discrete subset, that is, it has finite accumulation points (see Remark 5.3). On the other hand, similar to [6, Theorem 7], we can construct a class of antitrees such that $\sigma(\mathrm{H})$ is purely singular continuous. Moreover, it is possible to show that under the assumption $\ell_*(\mathcal{A}) > 0$ this situation is in a certain sense typical (cf. [6, Theorems 4 and 8]). Let us only mention the following Remling-type result (cf. [40, Theorem 1.1]).

Theorem 8.4. *Assume Hypothesis 8.1. Also, assume that the sets* $\{\ell_n\}_{n\geq 0}$ *and* $\{\frac{s_{n+2}}{s_n}\}_{n\geq 0}$ *are finite. Then* $\sigma_{\mathrm{ac}}(\mathbf{H}) \neq \emptyset$ *if and only if the sequence* $\{(\ell_n, \frac{s_{n+2}}{s_n})\}_{n\geq 0}$ *is eventually periodic.*

The proof is again omitted since it is analogous to that of [16, Theorem 5.1].

9. Absolutely continuous spectrum

The decomposition (3.18) shows that

$$\sigma_{\mathrm{ac}}(\mathbf{H}) = \sigma_{\mathrm{ac}}(\mathrm{H}) \tag{9.1}$$

and both have multiplicity at most 1. The results of the previous section show that antitrees with nonempty absolutely continuous spectrum is a rare event. Our main aim in this section is to apply two recent result from [4] and [14] on the absolutely continuous spectrum of Krein and generalized indefinite strings, respectively, in order to construct several classes of antitrees with rich absolutely continuous spectra, however, which are not eventually periodic in the sense of Theorem 8.4. We begin with the following result.

Theorem 9.1. *Let $\mathcal{A}$ be an infinite radially symmetric antitree such that*

$$\mathcal{L} = \sum_{n\ge 0} \ell_n = \infty.$$

Also, let μ be the function given by (3.4)*. If*

$$\sum_{n\ge 0} \left(\int_n^{n+2} \mu(x)dx \int_n^{n+2} \frac{dx}{\mu(x)} - 4 \right) < \infty, \tag{9.2}$$

then $\sigma_{\mathrm{ac}}(\mathbf{H}) = \mathbb{R}_{\ge 0}$.

Proof. We only need to use Theorem 2 from [4]. Indeed, as we know (see the proof of Theorem 6.1), the operator H is unitarily equivalent to the Krein string operator $\widetilde{\mathrm{H}}$ given by (5.12)–(5.14). Applying now Theorem 2 from [4] to the operator $\widetilde{\mathrm{H}}$, after straightforward calculations the corresponding condition (1.9) from [4] turns into (9.2). □

Remark 9.2. Let us mention that in Theorem 9.1, upon suitable modifications of [4, Theorem 2], one can replace the intervals $(n, n+2)$ by intervals $\mathcal{I}_n$, $n \ge 0$ which "asymptotically" behave like $(n, n+2)$ (actually, by intervals with lengths uniformly bounded from above as well as by a positive constant from below and satisfying a suitable overlapping property [5]), however, one has to replace 4 by a square of the length of the corresponding interval:

$$\sum_{n\ge 0} \left(\int_{\mathcal{I}_n} \mu(x)dx \int_{\mathcal{I}_n} \frac{dx}{\mu(x)} - |\mathcal{I}_n|^2 \right) < \infty. \tag{9.3}$$

Let us first demonstrate the above result by considering an example of equilateral antitrees and then we shall extend it to a much wider setting (see Theorem 9.6 below).

Corollary 9.3 (Equilateral antitrees)**.** *Let $\mathcal{A}$ be an infinite radially symmetric antitree with $\ell_n = \ell > 0$ for all $n \ge 0$. If*

$$\sum_{n\ge 0} \left(\frac{s_{n+2}}{s_n} - 1 \right)^2 < \infty, \tag{9.4}$$

then $\sigma_{\mathrm{ac}}(\mathbf{H}) = \mathbb{R}_{\ge 0}$.

Proof. Setting $\mathcal{I}_n = (\ell n, \ell(n+2))$, $n \geq 0$, straightforward calculations show that

$$\begin{aligned}\int_{\mathcal{I}_n} \mu(x)dx \int_{\mathcal{I}_n} \frac{dx}{\mu(x)} - |\mathcal{I}_n|^2 \\ &= (s_n s_{n+1} + s_{n+1}s_{n+2})\Big(\frac{1}{s_n s_{n+1}} + \frac{1}{s_{n+1}s_{n+2}}\Big)\ell^2 - 4\ell^2 \\ &= \frac{(s_{n+2}+s_n)^2}{s_n s_{n+2}}\ell^2 - 4\ell^2 = \ell^2 \frac{(s_{n+2}-s_n)^2}{s_n s_{n+2}} = \ell^2 \frac{s_n}{s_{n+2}}\Big(\frac{s_{n+2}}{s_n} - 1\Big)^2.\end{aligned}$$

Theorem 9.1 and Remark 9.2 complete the proof. □

Remark 9.4. First of all, Corollary 9.3 demonstrates that (8.1) is essential for the results of Section 8. Let us also mention that it is possible to show by using the results of [31, §4.2] that the stronger condition

$$\sum_{n\geq 0} \Big|\frac{s_{n+2}}{s_n} - 1\Big| < \infty \tag{9.5}$$

holds exactly when the operator $\widetilde{\mathrm{H}}$ considered in Section 8 is a trace class perturbation (in the resolvent sense) of the free Hamiltonian $-\frac{d^2}{dx^2}$ acting in $L^2(\mathbb{R}_+)$ and hence in this case the Birman–Krein theorem implies $\sigma_{\mathrm{ac}}(\mathrm{H}) = \mathbb{R}_{\geq 0}$. However, (9.5) does not hold already for polynomially growing equilateral antitrees, e.g., take $s_n = n+1$ (see also Section 10.2). Moreover, (9.4) is equivalent to the fact that $\widetilde{\mathrm{H}}$ is a Hilbert–Schmidt class perturbation (in the resolvent sense) of the free Hamiltonian.

The rather strong assumption that $\mathcal{A}$ is equilateral can indeed be replaced by $\ell_*(\mathcal{A}) > 0$. In order to do this, it will turn out useful to rewrite (9.2). Let

$$\mathcal{M} := \operatorname{ran}(\mu) = \{s_n s_{n+1} :\ n \in \mathbb{Z}_{\geq 0}\} \tag{9.6}$$

be the image of the function μ defined in (3.4). For every $s \in \mathcal{M}$, we set

$$\mathcal{I}_s := \mu^{-1}(\{s\}) = \{x \in [0,\infty) :\ \mu(x) = s\}, \tag{9.7}$$

that is, $\mathcal{I}_s$ is the preimage of $\{s\} \in \mathcal{M}$ with respect to μ.

Lemma 9.5. *Let $\mathcal{A}$ be an infinite radially symmetric antitree with $\mathcal{L} = \infty$. Then*

$$\sum_{n\geq 0}\Big(\int_n^{n+2} \mu(x)dx \int_n^{n+2} \frac{dx}{\mu(x)} - 4\Big) = \frac{1}{2}\sum_{n\geq 0}\sum_{s\in\mathcal{M}}\sum_{\xi\neq s} |\mathcal{I}_s^n||\mathcal{I}_\xi^n| \frac{(s-\xi)^2}{s\xi}, \tag{9.8}$$

where $|\mathcal{I}_s^n|$ is the Lebesgue measure of $\mathcal{I}_s^n := \mathcal{I}_s \cap (n, n+2)$.

Proof. For every fixed $n \in \mathbb{Z}_{\geq 0}$, we clearly have

$$\begin{aligned}\int_n^{n+2} \mu(x)dx \int_n^{n+2} \frac{dx}{\mu(x)} &= \Big(\sum_{s\in\mathcal{M}} s|\mathcal{I}_s^n|\Big)\Big(\sum_{\xi\in\mathcal{M}} \frac{1}{\xi}|\mathcal{I}_\xi^n|\Big) \\ &= \sum_{s\in\mathcal{M}}\sum_{\xi\neq s} |\mathcal{I}_s^n||\mathcal{I}_\xi^n|\frac{s}{\xi} + \sum_{s\in\mathcal{M}} |\mathcal{I}_s^n|^2 \\ &= \frac{1}{2}\sum_{s\in\mathcal{M}}\sum_{\xi\neq s} |\mathcal{I}_s^n||\mathcal{I}_\xi^n|\Big(\frac{\xi}{s} + \frac{s}{\xi}\Big) + \sum_{s\in\mathcal{M}} |\mathcal{I}_s^n|^2.\end{aligned}$$

Moreover, by construction

$$\sum_{s\in\mathcal{M}} |\mathcal{I}_s^n| = 2, \tag{9.9}$$

and hence

$$\sum_{s\in\mathcal{M}} |\mathcal{I}_s^n|^2 - 4 = \sum_{s\in\mathcal{M}} |\mathcal{I}_s^n|(|\mathcal{I}_s^n| - 2) = -\sum_{s\in\mathcal{M}}\sum_{\xi\neq s} |\mathcal{I}_s^n||\mathcal{I}_\xi^n|.$$

Combining the last two equalities, we get

$$\begin{aligned}\int_n^{n+2} \mu(x)dx \int_n^{n+2} \frac{dx}{\mu(x)} - 4 &= \frac{1}{2}\sum_{s\in\mathcal{M}}\sum_{\xi\neq s} |\mathcal{I}_s^n||\mathcal{I}_\xi^n| \left(\frac{\xi}{s} + \frac{s}{\xi} - 2\right) \\ &= \frac{1}{2}\sum_{s\in\mathcal{M}}\sum_{\xi\neq s} |\mathcal{I}_s^n||\mathcal{I}_\xi^n| \frac{(s-\xi)^2}{s\xi},\end{aligned}$$

which completes the proof. □

Theorem 9.6. *Let $\mathcal{A}$ be an infinite radially symmetric antitree with sphere numbers satisfying* (9.4). *If*

$$\ell_*(\mathcal{A}) = \inf_{n\geq 0} \ell_n > 0,$$

then $\sigma_{\mathrm{ac}}(\mathbf{H}) = \mathbb{R}_{\geq 0}$.

Proof. Suppose $\ell_*(\mathcal{A}) \geq 2$. Then, by Lemma 9.5, for every $n \in \mathbb{Z}_{\geq 0}$, we get

$$\begin{aligned}\int_n^{n+2} \mu(x)dx \int_n^{n+2} \frac{dx}{\mu(x)} - 4 &= \frac{1}{2}\sum_{s\in\mathcal{M}}\sum_{\xi\neq s} |\mathcal{I}_s^n||\mathcal{I}_\xi^n| \frac{(s-\xi)^2}{s\xi} \\ &\leq \sum_{s\in\mathcal{M}_n}\sum_{\xi\neq s} |\mathcal{I}_\xi^n| \frac{(s-\xi)^2}{s\xi},\end{aligned}$$

where $\mathcal{M}_n := \mu\big((n, n+2)\big) = \{s_k s_{k+1} \colon (n, n+2) \cap I_k \neq \varnothing\}$. Since $\ell_k \geq 2$ for all $k \geq 0$ by assumption, μ is either constant on $(n, n+2)$ or attains precisely two different values. In the first case, the righthand side is equal to zero. In the second, we obviously get the estimate

$$\int_n^{n+2} \mu(x)dx \int_n^{n+2} \frac{dx}{\mu(x)} - 4 \leq 2 \sum_{t_k\in(n,n+2)} \frac{(s_{k+1} - s_{k-1})^2}{s_{k-1}s_{k+1}}.$$

Thus we end up with the following bound

$$\begin{aligned}\sum_{n\geq 0}\left(\int_n^{n+2} \mu(x)dx \int_n^{n+2} \frac{dx}{\mu(x)} - 4\right) &\leq 2\sum_{n\geq 0}\sum_{t_k\in(n,n+2)} \frac{(s_{k+1} - s_{k-1})^2}{s_{k-1}s_{k+1}} \\ &\leq 4\sum_{n\geq 0} \frac{(s_{n+2} - s_n)^2}{s_n s_{n+2}} < \infty,\end{aligned}$$

which proves the claim by applying Theorem 9.1.

It remains to note that the general case $\ell_*(\mathcal{A}) > 0$ can be reduced to the one with $\ell_*(\mathcal{A}) \geq 2$ by using the standard scaling argument (see also Remark 9.2). □

In fact, one can extend the above result to the case when lengths do not admit a strictly positive lower bound. However, in this case one has to modify (9.4) in an appropriate way.

Lemma 9.7. *Let $\mathcal{A}$ be an infinite radially symmetric antitree with $\mathcal{L} = \infty$. Also, let $\ell_n \leq 1$ for all $n \geq 0$ and $\ell_n = o(1)$ as $n \to \infty$. If $\{s_n\}_{n\geq 0}$ is a nondecreasing sequence such that*

$$\sum_{n\geq 0} \left(\frac{s_{m(n+2)}}{s_{m(n)}} - 1\right)^2 < \infty, \tag{9.10}$$

then $\sigma_{\mathrm{ac}}(\mathbf{H}) = \mathbb{R}_{\geq 0}$.

Here for each $n \in \mathbb{Z}_{\geq 0}$ the natural number $m(n)$ is defined by

$$t_{m(n)} \leq n < t_{m(n)+1}, \qquad t_n = \sum_{k=0}^{n-1} \ell_k. \tag{9.11}$$

Proof. Set $\mathcal{I}_n := (t_{m(n)}, t_{m(n+2)+1})$, $n \geq 0$. By construction $(n, n+2) \subseteq \mathcal{I}_n$ for all $n \geq 0$ and $|\mathcal{I}_n \setminus (n, n+2)| = o(1)$ as $n \to \infty$. Thus, by Theorem 9.1 and Remark 9.2, it suffices to show that

$$\sum_{n\geq 0} \underbrace{\left(\int_{t_{m(n)}}^{t_{m(n+2)+1}} \mu(x)dx \int_{t_{m(n)}}^{t_{m(n+2)+1}} \frac{dx}{\mu(x)} - (t_{m(n+2)+1} - t_{m(n)})^2\right)}_{=:R_n} < \infty. \tag{9.12}$$

Since μ is given by (3.4), we get

$$\begin{aligned}
R_n &= \sum_{k=m(n)}^{m(n+2)} s_k s_{k+1} \ell_k \sum_{k=m(n)}^{m(n+2)} \frac{\ell_k}{s_k s_{k+1}} - \Big(\sum_{k=m(n)}^{m(n+2)} \ell_k\Big)^2 \\
&= \sum_{k,j=m(n)}^{m(n+2)} \ell_k \ell_j \Big(\frac{s_j s_{j+1}}{s_k s_{k+1}} - 1\Big) \\
&= 2 \sum_{m(n)\leq k<j\leq m(n+2)} \ell_k \ell_j \frac{(s_j s_{j+1} - s_k s_{k+1})^2}{s_k s_{k+1} s_j s_{j+1}} \\
&\leq 2 \sum_{m(n)\leq k<j\leq m(n+2)} \ell_k \ell_j \frac{(s^2_{m(n+2)+1} - s^2_{m(n)})^2}{s^4_{m(n)}} \\
&\lesssim 2 \sup_{k\geq 0} |\mathcal{I}_k|^2 \left(\frac{s^2_{m(n+2)}}{s^2_{m(n)}} - 1\right)^2 \lesssim \left(\frac{s_{m(n+2)}}{s_{m(n)}} - 1\right)^2
\end{aligned}$$

for all $n \geq 0$ if $\frac{s_{m(n+2)}}{s_{m(n)}} = 1 + o(1)$. $\square$

Remark 9.8. In fact, the assumptions on lengths that $\ell_n \leq 1$ for all $n \geq 0$ and $\ell_n = o(1)$ as $n \to \infty$ as well as monotonicity of sphere numbers are superfluous and we need them for simplicity only. Of course, one can considerably weaken them, however, the analysis becomes more involved and cumbersome.

We finish this section with another result based on [14], which also allows to construct antitrees with absolutely continuous spectrum supported on $\mathbb{R}_{\geq 0}$.

Theorem 9.9. *Let $\mathcal{A}$ be an infinite radially symmetric antitree such that* $\mathrm{vol}(\mathcal{A}) = \infty$ *and $\mathcal{L}_\mu = \infty$. If there are constants $a \in \mathbb{R}$ and $b \in \mathbb{R}_{>0}$ such that*

$$\int_0^{\mathcal{L}} \frac{1}{\mu(x)} \Big| \int_0^x \Big(\mu(s) - \frac{b}{\mu(s)}\Big) ds - a \Big|^2 dx < \infty, \tag{9.13}$$

where μ is given by (3.4)*, then* $\sigma_{\mathrm{ac}}(\mathbf{H}) = \mathbb{R}_{\geq 0}$.

Proof. As in the proof of Theorem 9.1, we know that the operator H is unitarily equivalent to the operator $\widetilde{\mathrm{H}}$. By Theorem 3.1 from [14], $\sigma_{\mathrm{ac}}(\widetilde{\mathrm{H}}) = [0,\infty)$ if there are constants $a \in \mathbb{R}$ and $b \in \mathbb{R}_{>0}$ such that

$$\int_0^\infty |M(x) - a - bx|^2\, dx < \infty,$$

where M is defined by (6.6). Straightforward calculations finish the proof. $\square$

Remark 9.10. For a string operator defined by (5.12), Theorem 9.1 and Theorem 9.9 also imply that the entropy, respectively, some sort of relative entropy of the corresponding spectral measure is finite (see [4] for details). However, the meaning of this fact for the corresponding quantum graph operator $\mathbf{H}$ is unclear to us.

10. Examples

10.1. **Exponentially growing antitrees.** Fix $\beta \in \mathbb{Z}_{\geq 2}$ and let $\mathcal{A}_\beta$ be the antitree with sphere numbers $s_n = \beta^n$, $n \geq 0$ (cf. [32, Example 8.6]). Suppose that $\{\ell_n\}_{n\geq 0}$ are the lengths. Notice that

$$\mathrm{vol}(\mathcal{A}_\beta) = \sum_{n\geq 0} \beta^{2n+1}\ell_n. \tag{10.1}$$

Then the basic spectral properties of the corresponding quantum graph operator are contained in the following proposition.

Proposition 10.1. *Let $\mathbf{H}^\beta$ be the quantum graph operator associated with the antitree $\mathcal{A}_\beta$. Then:*

(i) The operator $\mathbf{H}^\beta$ is self-adjoint if and only if the series in (10.1) *diverges.*
(ii) If $\mathrm{vol}(\mathcal{A}_\beta) < \infty$, then deficiency indices of $\mathbf{H}^\beta$ are equal to 1*. Moreover, the spectra of self-adjoint extensions of $\mathbf{H}^\beta$ are purely discrete and eigenvalues admit the standard Weyl asymptotic* (5.1).

Assume in addition that $\mathrm{vol}(\mathcal{A}_\beta) = \infty$.

(iii) The spectrum of $\mathbf{H}^\beta$ is purely discrete if and only if $\ell_n = o(1)$ as $n \to \infty$.
(iv) The resolvent of $\mathbf{H}^\beta$ belongs to the trace class if and only if

$$\sum_{n\geq 0} \beta^{2n}\ell_n^2 < \infty. \tag{10.2}$$

(v) $\mathbf{H}^\beta$ is positive definite if and only if $\ell^*(\mathcal{A}_\beta) < \infty$. Moreover, in this case

$$\frac{1}{4C} \leq \lambda_0(\mathbf{H}^\beta) \leq \frac{1}{C}, \qquad \frac{1}{4C_{\mathrm{ess}}} \leq \lambda_0^{\mathrm{ess}}(\mathbf{H}^\beta) \leq \frac{1}{C_{\mathrm{ess}}}, \tag{10.3}$$

where

$$\sup_{n\geq 0} \sum_{k=0}^{n} \beta^{2k}\ell_k \sum_{k\geq n+1} \frac{\ell_k}{\beta^{2k}} \leq C \leq \sup_{n\geq 0} \sum_{k=0}^{n} \beta^{2k}\ell_k \sum_{k\geq n} \frac{\ell_k}{\beta^{2k}}, \tag{10.4}$$

and

$$\lim_{m\to\infty} \sup_{n\geq m} \sum_{k=m}^{n} \beta^{2k}\ell_k \sum_{k\geq n+1} \frac{\ell_k}{\beta^{2k}} \leq C_{\mathrm{ess}} \leq \lim_{m\to\infty} \sup_{n\geq m} \sum_{k=m}^{n} \beta^{2k}\ell_k \sum_{k\geq n} \frac{\ell_k}{\beta^{2k}}. \tag{10.5}$$

Proof. Items (i) and (ii) follow from Theorem 4.1 and Corollary 5.1.

(iii) Applying Theorem 5.4 (see also Remark 5.5), we only need to show that $\ell_n = o(1)$ as $n \to \infty$ is sufficient for the discreteness. Indeed, we can estimate

$$\begin{aligned}\sum_{k=0}^{n} \beta^{2k} \ell_k \sum_{k\ge n} \frac{\ell_k}{\beta^{2k}} &\le \ell^*(\mathcal{A}_\beta) \sup_{k\ge n} \ell_k \sum_{k=0}^{n} \beta^{2k} \sum_{k\ge n} \frac{1}{\beta^{2k}} \\ &= \ell^*(\mathcal{A}_\beta) \sup_{k\ge n} \ell_k \frac{\beta^{2n+2}-1}{\beta^{2n+2}} \Big(\frac{\beta^2}{\beta^2-1}\Big)^2 < \frac{\ell^*(\mathcal{A}_\beta)}{(1-\beta^{-2})^2} \sup_{k\ge n} \ell_k,\end{aligned} \tag{10.6}$$

where $\ell^*(\mathcal{A}_\beta) = \sup_{n\ge 0} \ell_n$. Hence (5.9) is satisfied if $\ell_n = o(1)$.

(iv) Clearly, (10.2) coincides with condition (i) of Theorem 5.6 and hence it is necessary. Applying the Cauchy–Schwarz inequality, we get the following estimate:

$$\begin{aligned}\sum_{n\ge 0} \frac{\ell_n}{s_n s_{n+1}} \sum_{k=0}^{n-1} s_k s_{k+1} \ell_k &= \sum_{n\ge 0} \frac{\ell_n}{\beta^{2n}} \sum_{k=0}^{n-1} \beta^{2k} \ell_k \\ &\le \sum_{n\ge 0} \frac{\ell_n}{\beta^{2n}} \Big(\sum_{k=0}^{n-1} \beta^{2k} \ell_k^2 \sum_{k=0}^{n-1} \beta^{2k}\Big)^{1/2} = \sum_{n\ge 0} \frac{\ell_n}{\beta^{2n}} \Big(\frac{\beta^{2n}-1}{\beta^2-1} \sum_{k=0}^{n-1} \beta^{2k} \ell_k^2\Big)^{1/2} \\ &< \sum_{n\ge 0} \frac{\ell_n}{\beta^{n}} \Big(\sum_{k=0}^{n-1} \beta^{2k} \ell_k^2\Big)^{1/2} < \frac{\ell^*(\mathcal{A}_\beta)}{\beta-1} \Big(\sum_{k\ge 0} \beta^{2k} \ell_k^2\Big)^{1/2}.\end{aligned}$$

Therefore, (10.2) implies condition (ii) of Theorem 5.6, which proves the claim.

(v) immediately follows from (10.6), Theorem 6.1, Theorem 6.3 and Remark 6.2. ☐

Remark 10.2.

(i) Both the discreteness and uniform positivity criteria for $\mathbf{H}^\beta$ were obtained in [32, Example 8.6]. Notice that these results are a consequence of the positivity of the combinatorial isoperimetric constant in this case (see [32]). Moreover, using the rough estimate (10.6), one would be able to recover the lower bounds (8.9) and (8.10) from [32].

(ii) It is impossible to apply Theorem 9.1 and Theorem 9.9 to $\mathcal{A}_\beta$ (this either can be seen from Proposition 10.1(v) or one can prove that both conditions (9.2) and (9.13) are always violated if sphere numbers grow exponentially).

(iii) Since the sphere numbers of $\mathcal{A}_\beta$ satisfy

$$\frac{s_{n+2}}{s_n} = \beta^2$$

for all $n \ge 0$, we can apply the results of Section 8. Namely, under the additional assumption $\ell_*(\mathcal{A}_\beta) > 0$, we conclude that the absolutely continuous spectrum of $\mathbf{H}$ is in general empty. In particular, it is always the case if $\ell^*(\mathcal{A}_\beta) = \infty$ (Theorem 8.2). Moreover, assuming that $\{\ell_n\}_{n\ge 0}$ is a finite set, by Theorem 8.4, $\sigma_{\mathrm{ac}}(\mathbf{H}) \neq \emptyset$ would imply that the sequence $\{\ell_n\}_{n\ge 0}$ is eventually periodic.

(iv) Notice that the isoperimetric constant is given by (see (7.3))

$$\frac{1}{\alpha(\mathcal{A}_\beta)} = \sup_{n\ge 0} \frac{1}{\beta^{2n}} \sum_{k=0}^{n} \beta^{2k} \ell_k.$$

10.2. **Polynomially growing antitrees.** Fix $q \in \mathbb{Z}_{\geq 1}$ and let $\mathcal{A}^q$ be the antitree with sphere numbers $s_n = (n+1)^q$, $n \geq 0$ (the case $q = 1$ is depicted in Figure 1). Suppose that $\{\ell_n\}_{n\geq 0}$ are the lengths. Notice that

$$\mathrm{vol}(\mathcal{A}^q) = \sum_{n\geq 0} (n+1)^q (n+2)^q \ell_n. \tag{10.7}$$

Then the basic spectral properties of the corresponding quantum graph operator are contained in the following proposition.

Proposition 10.3. *Let $\mathbf{H}^q$ be the quantum graph operator associated with the antitree $\mathcal{A}^q$. Then:*

(i) The operator $\mathbf{H}^q$ is self-adjoint if and only if

$$\sum_{n\geq 0} n^{2q} \ell_n = \infty. \tag{10.8}$$

(ii) If the series in (10.8) *converges, then deficiency indices of $\mathbf{H}^q$ are equal to* 1*. Moreover, the spectra of self-adjoint extensions of $\mathbf{H}^q$ are purely discrete and eigenvalues admit the standard Weyl asymptotic* (5.1).

Assume in addition that (10.8) *is satisfied, that is, $\mathbf{H}^q$ is self-adjoint.*

(iii) The spectrum of $\mathbf{H}^q$ is purely discrete if and only if

$$\lim_{n\to\infty} \sum_{k=0}^{n} k^{2q} \ell_k \sum_{k\geq n} \frac{\ell_k}{k^{2q}} = 0. \tag{10.9}$$

In particular, the spectrum is purely discrete if $\ell_n = o(n^{-1})$ as $n \to \infty$.

(iv) The resolvent of $\mathbf{H}^q$ belongs to the trace class if and only if

$$\sum_{n\geq 0} n^{2q} \ell_n^2 < \infty. \tag{10.10}$$

(v) $\mathbf{H}^q$ is positive definite if and only if

$$\sup_{n\geq 1} \sum_{k=0}^{n} k^{2q} \ell_k \sum_{k\geq n} \frac{\ell_k}{k^{2q}} < \infty. \tag{10.11}$$

In particular, $\lambda_0(\mathbf{H}^q) > 0$ if $\ell_n = \mathcal{O}(n^{-1})$ as $n \to \infty$.

(vi) If $\ell_*(\mathcal{A}^q) > 0$, then $\sigma_{\mathrm{ac}}(\mathbf{H}^q) = \mathbb{R}_{\geq 0}$.

Proof. (i) and (ii) follow immediately from Theorem 4.1 and Corollary 5.1 since $\mathrm{vol}(\mathcal{A}^q) = \infty$ exactly when (10.8) is satisfied.

(iii) Applying Theorem 5.4 (see also Remark 5.5), we conclude that in the case (10.8), the operator $\mathbf{H}$ has purely discrete spectrum if and only if

$$\lim_{n\to\infty} \sum_{k=0}^{n} (k^2+3k+2)^q \ell_k \sum_{k\geq n} \frac{\ell_k}{(k^2+3k+2)^q} = 0.$$

It is not difficult to show that the latter is equivalent to (10.9). Moreover, (10.9) holds true whenever $\ell_n = o(n^{-1})$ as $n \to \infty$ since

$$\sum_{k=0}^{n} k^{2q-1} = \frac{n^{2q}}{2q}(1+o(1)), \qquad \sum_{k\geq n} \frac{1}{k^{2q+1}} = \frac{n^{-2q}}{2q}(1+o(1)).$$

(iv) First observe that (5.18) is equivalent to (10.10). Moreover, (10.10) implies also (5.19). Indeed, we get

$$
\begin{aligned}
\sum_{n\ge 0}\frac{\ell_n}{(n^2+3n+2)^q}\sum_{k=0}^{n-1}(k^2+3k+2)^q\ell_k &< \sum_{n\ge 0}\frac{\ell_n}{(n+1)^{2q}}\sum_{k=0}^{n-1}(k+2)^{2q}\ell_k\\
&\le \sum_{n\ge 0}\frac{\ell_n}{(n+1)^{2q}}\Big(\sum_{k=0}^{n-1}(k+2)^{2q}\ell_k^2\sum_{k=0}^{n-1}(k+2)^{2q}\Big)^{1/2}\\
&\lesssim \sum_{n\ge 0}\frac{\ell_n}{(n+1)^{2q}}\Big((n+1)^{2q+1}\sum_{k=0}^{n-1}(k+2)^{2q}\ell_k^2\Big)^{1/2}\\
&< \Big(\sum_{k\ge 0}(k+2)^{2q}\ell_k^2\Big)^{1/2}\sum_{n\ge 0}\frac{\ell_n}{(n+1)^{q-1/2}}\\
&< \sum_{k\ge 0}(k+2)^{2q}\ell_k^2\Big(\sum_{n\ge 1}\frac{1}{n^{4q-1}}\Big)^{1/2},
\end{aligned}
$$

where the second and the last inequalities we obtained by applying the Cauchy–Schwarz inequality. It remains to use Theorem 5.6.

(v) follows by applying Theorem 6.1 (see also Remark 6.2).

(vi) Since

$$
\sum_{n\ge 0}\Big(\frac{s_{n+2}}{s_n}-1\Big)^2=\sum_{n\ge 1}\Big(\frac{(n+2)^q}{n^q}-1\Big)^2\lesssim\sum_{n\ge 1}\frac{1}{n^2}=\frac{\pi^2}{6},
$$

the claim is immediate from Theorem 9.6. □

Remark 10.4. A few remarks are in order.

(i) The antitree $\mathcal{A}^q$ and the corresponding Kirchhoff Laplacian $\mathbf{H}$ have been considered in [32, Example 8.7]. The analysis of spectral properties (in particular, spectral estimates) is a rather delicate task in this case since the combinatorial isoperimetric constant of $\mathcal{A}^q$ is equal to 0. We were able to describe basic spectral properties of $\mathbf{H}^q$ only due to the presence of radial symmetry. Spectral properties of Kirchhoff Laplacians without radial symmetry seems to be a rather complicated problem − even the self-adjointness problem (modulo some recent criteria obtained in [17]) is unclear to us at the moment.

(ii) It can be demonstrated by examples that the conditions $\ell_n = o(n^{-1})$ (resp., $\ell_n = \mathcal{O}(n^{-1})$) as $n\to\infty$ are not necessary for the discreteness (resp., positivity). However, they are in a certain sense sharp (see [32, Lemma 8.9] and also Example 10.6 below).

(iii) Since $s_{n+2} = s_n(1 + o(1))$, we can't apply the results of Section 8 (see Hypothesis 8.1). Moreover, Proposition 10.3(vi) shows that in general $\mathbf{H}^q$ has absolutely continuous spectrum supported on $\mathbb{R}_{\ge 0}$. However, Theorem 9.1 is a consequence of [4, Theorem 2], which allows a presence of a rather rich singular (continuous) spectrum.

We can also improve Proposition 10.3(vi) by allowing arbitrarily small lengths.

Corollary 10.5. *Suppose $\ell_n \le 1$ for all $n \ge 0$ and $\ell_n = o(1)$ as $n \to \infty$. If*

$$\sum_{n\ge 0}\left(\frac{m(n+2)}{m(n)} - 1\right)^2 < \infty, \qquad (10.12)$$

then $\sigma_{\mathrm{ac}}(\mathbf{H}^q) = \mathbb{R}_{\ge 0}$. Here $m(n)$ is defined as in Lemma 9.7.

Proof. We need to apply Lemma 9.7 and notice that in this case

$$\frac{s_{m(n+2)}}{s_{m(n)}} - 1 = \left(\frac{m(n+2)+1}{m(n)+1}\right)^q - 1 \approx \frac{m(n+2)}{m(n)} - 1,$$

as $n \to \infty$. □

Example 10.6. Fix $s \ge 0$. Let the lengths of the metric antitree $\mathcal{A}^q$ be given by

$$\ell_n = \frac{1}{(n+1)^s}, \qquad n \ge 0. \qquad (10.13)$$

Denote the corresponding Kirchhoff Laplacian by $\mathbf{H}^{q,s}$. Applying Proposition 10.3 and Corollary 10.5, we end up with the following description of the spectral properties of $\mathbf{H}^{q,s}$.

Corollary 10.7. *(i) $\mathbf{H}^{q,s}$ is self-adjoint if and only if $s \in [0, 2q+1]$. If $s > 2q+1$, then then deficiency indices of $\mathbf{H}^{q,s}$ are equal to* 1. *Moreover, in this case the spectra of self-adjoint extensions $\mathbf{H}^{q,s}_\theta$ of $\mathbf{H}^{q,s}$ are purely discrete and eigenvalues admit the standard Weyl asymptotic*

$$\lim_{\lambda\to\infty} \frac{N(\lambda; \mathbf{H}^{q,s}_\theta)}{\sqrt{\lambda}} = \frac{1}{\pi}\sum_{k=0}^{q}\binom{q}{k}\zeta(s-2q+k), \qquad (10.14)$$

where ζ is the Riemann zeta function.

Assume in addition that $s \in [0, 2q+1]$, that is, $\mathbf{H}^q$ is self-adjoint.

(ii) The spectrum of $\mathbf{H}^{q,s}$ is purely discrete if and only if $s \in (1, 2q+1]$. Moreover, the resolvent of $\mathbf{H}^{q,s}$ belongs to the trace class if and only if $s \in (q+1/2, 2q+1]$.

(iii) $\mathbf{H}^{q,s}$ is positive definite if and only if $s \in [1, 2q+1]$.

(iv) If $s \in [0,1)$, then $\sigma_{\mathrm{ac}}(\mathbf{H}^{q,s}) = \mathbb{R}_{\ge 0}$.

We leave its proof to the reader and finish this section with a few remarks.

Remark 10.8. Corollary 10.7 complements the results obtained in [32, Example 8.7]. Moreover, items (ii) and (iii) demonstrate sharpness of sufficient conditions obtained in Proposition 10.3(iii) and (v). Let us only mention that the question on the structure of the essential spectrum of $\mathbf{H}^{q,1}$ as well as on the structure of the singular spectrum of $\mathbf{H}^{q,s}$ with $s \in [0,1]$ remains open.

Remark 10.9. In conclusion let us mention that choosing slightly different lengths

$$\ell_n = \frac{(n+1)^{q-s}}{(n+2)^q}, \quad n \ge 0,$$

and denoting the corresponding operator by $\widetilde{\mathbf{H}}^{q,s}$, we obtain

$$\lim_{\lambda\to\infty} \frac{N(\lambda; \widetilde{\mathbf{H}}^{q,s}_\theta)}{\sqrt{\lambda}} = \frac{1}{\pi}\zeta(s-2q), \quad s > 2q+1. \qquad (10.15)$$

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SELF-ADJOINT AND MARKOVIAN EXTENSIONS OF INFINITE QUANTUM GRAPHS

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Abstract. We investigate the relationship between one of the classical notions of boundaries for infinite graphs, *graph ends*, and self-adjoint extensions of the minimal Kirchhoff Laplacian on a metric graph. We introduce the notion of *finite volume* for ends of a metric graph and show that finite volume graph ends is the proper notion of a boundary for Markovian extensions of the Kirchhoff Laplacian. In contrast to manifolds and weighted graphs, this provides a transparent geometric characterization of the uniqueness of Markovian extensions, as well as of the self-adjointness of the Gaffney Laplacian — the underlying metric graph does not have finite volume ends. If however finitely many finite volume ends occur (as is the case of tessellating graphs or Cayley graphs of amenable finitely generated countable groups), we provide a complete description of Markovian extensions upon introducing a suitable notion of traces of functions and normal derivatives on the set of graph ends.

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1. Introduction

This paper is concerned with developing extension theory for infinite *quantum graphs*. Quantum graphs are Schrödinger operators on *metric graphs*, that is combinatorial graphs where edges are considered as intervals with certain lengths. Motivated by a vast amount of applications in chemistry and physics, they have become a popular subject in the last decades (we refer to [8, 9, 24, 63] for an overview and further references). From the perspective of Dirichlet forms, quantum graphs play an important role as an intermediate setting between Laplacians on Riemannian manifolds and difference Laplacians on weighted graphs. On the one hand, being locally one-dimensional, quantum graphs allow to simplify considerations of complicated geometries. On the other hand, there is a close relationship between random walks on graphs and Brownian motion on metric graphs, however, in contrast to the discrete case, the corresponding quadratic form in the metric case is a strongly local Dirichlet form and in this situation more tools are available (see [7, 26, 60, 61] for various manifestations of this point of view). Let us also mention that metric graphs can be seen as non-Archimedean analogues of Riemann surfaces, which finds numerous applications in algebraic geometry (see [2, 5, 6, 67] for further references).

The most studied quantum graph operator is the *Kirchhoff Laplacian*, which provides the analog of the Laplace–Beltrami operator in the setting of metric graphs. Its spectral properties are crucial in connection with the heat equation and the Schrödinger equation and any further analysis usually relies on the *self-adjointness of the Laplacian*. Whereas on finite metric graphs the Kirchhoff Laplacian is always self-adjoint, the question is more subtle for *graphs with infinitely many edges*. For instance, a uniform lower bound for the edge lengths guarantees self-adjointness (see [9, 63]), but this commonly used condition is independent of the combinatorial graph structure and clearly excludes a number of interesting cases (the so-called *fractal metric graphs*). Moreover, most of the results on strongly local Dirichlet forms require completeness of a given metric space w.r.t. the "intrinsic" metric (cf., e.g., [71]), which coincides with the natural path (geodesic) metric in the case of metric graphs. Geodesic completeness (w.r.t. the natural path metric) guarantees self-adjointness of the (minimal) Kirchhoff Laplacian, however, this result is far from being optimal (see [25, §4] and also Section 2.4 below). The search for self-adjointness criteria for infinite quantum graphs is an open and – in our opinion – rather difficult problem.

If the (minimal) Kirchhoff Laplacian is not self-adjoint, the natural next step is to ask for a description of its self-adjoint extensions, which corresponds to possible descriptions of the system in quantum mechanics or, if we speak about Markovian extensions, possible descriptions of Brownian motions. Naturally, this question is tightly related to finding appropriate boundary notions for infinite graphs. Our goal in this paper is to investigate the connection between extension theory and one particular notion, namely *graph ends*, a concept which goes back to the work of Freudenthal [28] and Halin [36] and provides a rather refined way of compactifying graphs. However, the definition of graph ends is purely combinatorial and naturally must be modified to capture the additional metric structure of our setting. Based on the correspondence between graph ends and topological ends of metric graphs, we introduce the concept of *ends of finite volume*. First of all, it turns out that finite volume ends play a crucial role in describing Sobolev spaces H^1 and H^1_0 on metric graphs. More specifically, we show that the presence of finite volume ends is the only reason for the strict inclusion $H^1_0 \subsetneq H^1$ to hold. This in particular provides a surprisingly transparent geometric characterization of the uniqueness of Markovian extensions of the minimal Kirchhoff Laplacian as well as the self-adjointness of the so-called *Gaffney Laplacian* (we are not aware of its analogs either in the manifold setting or in the context of weighted graph Laplacians, cf. [33, 35, 43, 50, 56, 57]). As yet another manifestation of the fact that finite volume graph ends represent the proper boundary for Markovian extensions of the Kirchhoff Laplacian, we provide a complete description of *all finite energy extensions* (i.e., self-adjoint extensions with domains contained in H^1, and all Markovian extensions clearly satisfy this condition), however, under the additional assumption that there are only finitely many finite volume ends. Let us stress that this class of graphs includes a wide range of interesting models (Cayley graphs of a large class of finitely generated countable groups, tessellating graphs, rooted antitrees etc. have exactly one end and in this case there are no finite volume ends exactly when the total volume of the corresponding metric graph is infinite). Moreover, we emphasize that in all those cases the dimension of the space of finite energy extensions is equal to the number of finite volume ends, however, for deficiency indices, i.e., the dimension of the space of self-adjoint extensions, this only gives a lower bound (for example, for Cayley graphs the dimension of the space of finite energy extensions is independent of the choice of a generating set, although deficiency indices do depend on this choice in a rather nontrivial way). On the other hand, it may happen that these dimensions coincide. The latter holds only if the maximal domain is contained in H^1, that is, if every self-adjoint extension is a finite energy extension. This is further equivalent to the validity of a certain non-trivial Sobolev-type inequality (see (1.1) below). The appearance of this condition demonstrates the mixed dimensional behavior of infinite quantum graphs since the analogous estimate holds true in the one-dimensional situation, but usually fails in the PDE setting.

Let us now sketch the structure of the article and describe its content and our results in greater details.

Section 2 is of preliminary character where we collect basic notions and facts about graphs and metric graphs (Section 2.1); graph ends (Section 2.2); the minimal and maximal Kirchhoff Laplacians (Section 2.3); deficiency indices and their connection with the spaces of L^2 harmonic and λ-harmonic functions (Section 2.4).

The core of the paper is Section 3, where we discuss Sobolev spaces $H^1(\mathcal{G})$ and $H^1_0(\mathcal{G})$ and introduce the set of finite volume ends $\mathfrak{C}_0(\mathcal{G})$ (Definition 3.7). We show that $\mathfrak{C}_0(\mathcal{G})$ is the proper boundary for H^1 functions, which can also be seen as an ideal boundary by applying C^*-algebras techniques (see Remark 3.13). The central result of this section is Theorem 3.11, which shows that $H^1(\mathcal{G}) = H^1_0(\mathcal{G})$ if and only if there are no finite volume ends. The latter also leads to a surprisingly transparent geometric characterization of the uniqueness of Markovian extensions of the Kirchhoff Laplacian (Corollary 5.5) as well as the self-adjointness of the Gaffney Laplacian (Remark 5.6(ii)).

The next Section 4 contains further applications of the above considerations. Namely, Theorem 4.1 demonstrates that deficiency indices of the minimal Kirchhoff Laplacian can be estimated from below by the number of finite volume ends. This estimate is sharp (e.g., if there are infinitely many finite volume ends) and we also find necessary and sufficient conditions for the equality to hold. In particular, if $\#\mathfrak{C}_0(\mathcal{G}) < \infty$, the latter is equivalent to the validity of the following Sobolev-type inequality (see Remark 4.2)

$$\|f'\|_{L^2(\mathcal{G})} \le C(\|f\|_{L^2(\mathcal{G})} + \|f''\|_{L^2(\mathcal{G})}) \tag{1.1}$$

for all f in the maximal domain of the Kirchhoff Laplacian. Metric graphs are locally one-dimensional and the corresponding inequality is trivially satisfied in the one-dimensional case, however, globally infinite metric graphs are more complex and hence (1.1) rather resembles the multi-dimensional setting of PDEs (in particular, (1.1) does not hold true if $\mathcal{G}$ has a *non-free* finite volume end, see Proposition 4.9).

In the next sections, we focus on a particular class of self-adjoint extensions whose domains are contained in H^1 (we call them *finite energy extensions*). These extensions have good properties and their importance stems from the fact that they contain the class of Markovian extensions (they also arise as self-adjoint restrictions of the Gaffney Laplacian). In Section 5 we show that (under some additional mild assumptions) their *resolvents and heat semigroups* are *integral operators* with continuous, bounded kernels and they belong to the trace class if $\mathcal{G}$ has finite total volume (Theorems 5.1 and 5.2).

In Section 6 we proceed further and show that finite volume ends is the proper boundary for this class of extensions. Namely, under the additional and rather restrictive assumption of *finitely many ends with finite volume*, in Sections 6.1–6.2, we introduce a suitable notion of a *normal derivative* at graph ends (as a by-product, this also gives an explicit description of the domain of the Neumann extension, see Corollary 6.7). Section 6.3 contains a complete description of finite energy extensions and also of Markovian extensions (Theorem 6.11). Let us stress that the case of infinitely many ends is incomparably more complicated and will be the subject of future work.

In general, inequality in (1.1) is difficult to verify/contradict and even simple examples can exhibit rather complicated behavior (see Appendix B). The main and in fact the only reason for (1.1) fail to hold is the presence of L^2 harmonic functions having infinite energy, that is, not belonging to H^1. Moreover, in order to compute deficiency indices of the Kirchhoff Laplacian one, roughly speaking, needs to find the dimension of the space of L^2 harmonic functions and description of self-adjoint extensions requires a thorough understanding of the behavior of L^2 harmonic functions at "infinity". Dictated by a distinguished role of harmonic functions in analysis, there is an enormous amount of literature dedicated to various classes of harmonic functions (positive, bounded etc.), which is further related to different notions of boundaries (metric completion, Poisson and Martin boundaries, Royden and Kuramochi boundaries etc.) and search for a suitable notion in this context (namely, L^2 harmonic functions) is a highly nontrivial problem, which seems not to be very well studied either in the context of *incomplete* manifolds (cf. [56, 57]) or in the case of weighted graphs (see [37, 43]). We further illustrate this by considering the case of rooted *antitrees*, a special class of infinite graphs with a particularly high degree of symmetry (see Section 7). Infinite rooted antitrees have exactly one graph end, which makes them a good toy model for our purposes. The above considerations show that the space of finite energy L^2 harmonic functions is nontrivial only if a given metric antitree has finite total volume and in this case the only such functions are constants. However, adjusting lengths in a suitable way for a concrete polynomially growing antitree (Figure 1) we can make the space of L^2 harmonic functions as large as we please (even infinite dimensional!).

Notation. $\mathbb{Z}$, $\mathbb{R}$, $\mathbb{C}$ have their usual meaning; $\mathbb{Z}_{\geq a} := \mathbb{Z} \cap [a, \infty)$.
z^* denotes the complex conjugate of $z \in \mathbb{C}$.
For a given set S, $\#S$ denotes its cardinality if S is finite; otherwise we set $\#S = \infty$.
If it is not explicitly stated otherwise, we shall denote by (x_n) a sequence $(x_n)_{n=0}^{\infty}$.
$C_b(X)$ is the space of bounded, continuous functions on a locally compact space X.
$C_0(X)$ is the space of continuous functions vanishing at infinity.
For a finite or countable set X, $C(X)$ is the set of complex-valued functions on X.
$\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ is a discrete graph (satisfying Hypothesis 2.1).
$\mathcal{G} = (\mathcal{G}_d, |\cdot|)$ is a metric graph.
ϱ is the natural (geodesic) path metric on $\mathcal{G}$.
ϱ_m is the star metric on $\mathcal{V}$ corresponding to the star weight m.
$\Omega(\mathcal{G}_d)$ denotes the graph ends of $\mathcal{G}_d$.
$\mathfrak{C}(\mathcal{G})$ denotes the topological ends of the corresponding metric graph $\mathcal{G}$.
$\mathfrak{C}_0(\mathcal{G})$ stays for the finite volume topological ends of $\mathcal{G}$.
$\widehat{\mathcal{G}}$ is the end (Freudenthal) compactification of $\mathcal{G}$.
$\mathbf{H}_0^0$ is the pre-minimal Kirchhoff Laplacian on $\mathcal{G}$.
$\mathbf{H}_0$ is the minimal Kirchhoff Laplacian, the closure of $\mathbf{H}_0^0$ in $L^2(\mathcal{G})$.
$\mathrm{n}_{\pm}(\mathbf{H}_0)$ are the deficiency indices of $\mathbf{H}_0$.
$\mathbf{H}_F$ and $\mathbf{H}_N$ are Friedrichs and Neumann extensions of $\mathbf{H}_0$, respectively.
$\mathbf{H}$ is the maximal Kirchhoff Laplacian on $\mathcal{G}$.

2. Quantum graphs

2.1. **Combinatorial and metric graphs.** In what follows, $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ will be an unoriented graph with countably infinite sets of vertices $\mathcal{V}$ and edges $\mathcal{E}$. For two vertices u, $v \in \mathcal{V}$ we shall write $u \sim v$ if there is an edge $e_{u,v} \in \mathcal{E}$ connecting u with v. For every $v \in \mathcal{V}$, we denote the set of edges incident to the vertex v by $\mathcal{E}_v$ and

$$\deg_{\mathcal{G}}(v) := \#\{e | \, e \in \mathcal{E}_v\} \tag{2.1}$$

is called *the degree* (*valency* or *combinatorial degree*) of a vertex $v \in \mathcal{V}$. When there is no risk of confusion which graph is involved, we shall write deg instead of $\deg_{\mathcal{G}}$. *A path* $\mathcal{P}$ of length $n \in \mathbb{Z}_{\geq 0} \cup \{\infty\}$ is a sequence of vertices $(v_0, v_1, \dots, v_n)$ such that $v_{k-1} \sim v_k$ for all $k \in \{1, \dots, n\}$.

The following assumption is imposed throughout the paper.

Hypothesis 2.1. *$\mathcal{G}_d$ is* locally finite *($\deg(v) < \infty$ for every $v \in \mathcal{V}$),* connected *(for any two vertices $u, v \in \mathcal{V}$ there is a path connecting u and v), and* simple *(there are no loops or multiple edges).*

Assigning to each edge $e \in \mathcal{E}$ a finite length $|e| \in (0, \infty)$ turns $\mathcal{G}_d$ into a *metric graph* $\mathcal{G} := (\mathcal{V}, \mathcal{E}, |\cdot|) = (\mathcal{G}_d, |\cdot|)$. The latter equips $\mathcal{G}$ with a (natural) topology and metric. More specifically (see, e.g., [38, Chapter 1.1]), a metric graph $\mathcal{G}$ can be considered as a topological space. Namely, a metric graph $\mathcal{G}$ is a Hausdorff topological space with countable base such that each point $x \in \mathcal{G}$ has a neighbourhood

$\mathcal{E}_x(r)$ homeomorphic to a star-shaped set $\mathcal{E}(\deg(x), r_x)$ of degree $\deg(x) \geq 1$,

$$\mathcal{E}(\deg(x), r_x) := \{z = r\mathrm{e}^{2\pi\mathrm{i}k/\deg(x)} | \, r \in [0, r_x), \; k = 1, \dots, \deg(x)\} \subset \mathbb{C}.$$

By assigning each edge a direction, every edge $e \in \mathcal{E}$ can be identified with a copy of the interval $\mathcal{I}_e = [0, |e|]$; moreover, the ends of the edges that correspond to the same vertex v are identified as well. Thus, $\mathcal{G}$ can be equipped with *the natural path metric* ϱ (the distance between two points $x, y \in \mathcal{G}$ is defined as the length of the "shortest" path connecting x and y).

Sometimes, we will consider $\mathcal{G}_d$ as a rooted graph with a fixed root $o \in \mathcal{V}$. In this case we denote by S_n, $n \in \mathbb{Z}_{\geq 0}$ the n-th combinatorial sphere with respect to the order induced by o (notice that $S_0 = \{o\}$).

2.2. **Graph ends.** One possible definition of a boundary for an infinite graph is the notion of the so-called *graph ends* (see [28, 36] and [73, §21]).

Definition 2.1. A sequence of distinct vertices $(v_n)_{n \in \mathbb{Z}_{\geq 0}}$ (resp., $(v_n)_{n \in \mathbb{Z}}$) such that $v_n \sim v_{n+1}$ for all $n \in \mathbb{Z}_{\geq 0}$ (resp., for all $n \in \mathbb{Z}$) is called a *ray* (resp., *double ray*). Subrays of a ray/double ray are called *tails*.

Two rays $\mathcal{R}_1, \mathcal{R}_2$ are called *equivalent* – and we write $\mathcal{R}_1 \sim \mathcal{R}_2$ – if there is a third ray containing infinitely many vertices of both $\mathcal{R}_1$ and $\mathcal{R}_2$.[1] An equivalence class of rays is called a *graph end of* $\mathcal{G}_d$ and the set of graph ends will be denoted by $\Omega(\mathcal{G}_d)$. Moreover, we will write $\mathcal{R} \in \omega$ whenever $\mathcal{R}$ is a ray belonging to the end $\omega \in \Omega(\mathcal{G}_d)$.

An important feature of graph ends is their relation to topological ends of a metric graph $\mathcal{G}$.

Definition 2.2. Consider sequences $\mathcal{U} = (U_n)_{n=0}^{\infty}$ of non-empty open connected subsets of $\mathcal{G}$ with compact boundaries and such that $U_{n+1} \subseteq U_n$ for all $n \geq 0$ and $\bigcap_{n \geq 0} \overline{U_n} = \emptyset$. Two such sequences $\mathcal{U}$ and $\mathcal{U}'$ are called *equivalent* if for all $n \geq 0$ there exist j and k such that $U_n \supseteq U_j'$ and $U_n' \supseteq U_k$. An equivalence class γ of sequences is called a *topological end* of $\mathcal{G}$ and $\mathfrak{C}(\mathcal{G})$ denotes the set of topological ends of $\mathcal{G}$.

For locally finite graphs, there is a bijection between topological ends of a metric graph $\mathfrak{C}(\mathcal{G})$ and graph ends $\Omega(\mathcal{G}_d)$ of the underlying combinatorial graph $\mathcal{G}_d$ (see [73, §21], [21, §8.6 and also p.277–278]; for the case of graphs which are not locally finite see [16, 22]).

Theorem 2.3. *For every topological end $\gamma \in \mathfrak{C}(\mathcal{G})$ of a locally finite metric graph $\mathcal{G} = (\mathcal{G}_d, |\cdot|)$ there exists a unique graph end $\omega_\gamma \in \Omega(\mathcal{G}_d)$ such that for every sequence $\mathcal{U}$ representing γ, each U_n contains a ray from ω_γ. Moreover, the map $\gamma \mapsto \omega_\gamma$ is a bijection between $\mathfrak{C}(\mathcal{G})$ and $\Omega(\mathcal{G}_d)$.*

Therefore, we may identify topological ends of a metric graph $\mathcal{G}$ and graph ends of the underlying graph $\mathcal{G}_d$. We will simply speak of the *ends* of $\mathcal{G}$. One obvious advantage of this identification is the fact that the definition of $\Omega(\mathcal{G}_d)$ is purely combinatorial and does not depend on edge lengths.

[1] Equivalently, $\mathcal{R}_1 \sim \mathcal{R}_2$ if and only if $\mathcal{R}_1$ and $\mathcal{R}_2$ cannot be separated by a finite vertex set, i.e., for every finite subset $X \subset \mathcal{V}$ the remaining tails of $\mathcal{R}_1$ and $\mathcal{R}_2$ in $\mathcal{V} \setminus X$ belong to the same connected component of $\mathcal{V} \setminus X$.

Definition 2.4. An end ω of a graph $\mathcal{G}_d$ is called *free* if there is a finite set X of vertices such that X separates ω from all other ends of the graph.

Remark 2.5. Let us mention several examples.

(i) $\mathbb{Z}$ has two ends both of which are free.
(ii) $\mathbb{Z}^N$ has one end for all $N \geq 2$.
(iii) A k-regular tree, $k \geq 3$, has uncountably many ends, none of which is free.
(iv) If $\mathcal{G}_d$ is a Cayley graph of a finitely generated (countable) group G, then the number of ends of $\mathcal{G}_d$ is independent of the generating set and it has either one, two, or infinitely many ends. Moreover, $\mathcal{G}_d$ has exactly two ends only if G is virtually infinite cyclic (it has a finite normal subgroup N such that the quotient group G/N is isomorphic either to $\mathbb{Z}$ or $\mathbb{Z}_2 * \mathbb{Z}_2$). These results are due to Freudenthal [28] and Hopf [40] (see also [72]). The classification of finitely generated groups with infinitely many ends is due to Stallings [70]. Let us mention that if G has infinitely many ends, then the result of Stallings implies that it contains a non-abelian free subgroup and hence is non-amenable. For further details we refer to, e.g., [30, Chapter 13].
(v) Let us also mention that by Halin's theorem [36] every locally finite graph $\mathcal{G}_d$ with infinitely many ends contains at least one end which is not free.

One of the main features of graph ends is that they provide a rather refined way of compactifying graphs (see [27] and [21, §8.6], [73]). Namely, we introduce a topology on $\widehat{\mathcal{G}} := \mathcal{G} \cup \mathfrak{C}(\mathcal{G})$ as follows. For an open subset $U \subseteq \mathcal{G}$, denote its extension $\widehat{U}$ to $\widehat{\mathcal{G}}$ by

$$\widehat{U} = U \cup \{\gamma \in \mathfrak{C}(\mathcal{G}) |\, \exists \mathcal{U} = (U_n) \in \gamma \text{ such that } U_0 \subset U\}. \tag{2.2}$$

Now we can introduce a neighborhood basis of $\gamma \in \mathfrak{C}(\mathcal{G})$ as follows

$$\{\widehat{U} |\, U \subseteq \mathcal{G} \text{ is open}, \gamma \in \widehat{U}\}. \tag{2.3}$$

This turns $\widehat{\mathcal{G}}$ into a compact topological space, called the *end (or Freudenthal) compactification* of $\mathcal{G}$.

Remark 2.6. Notice that an end $\gamma \in \mathfrak{C}(\mathcal{G})$ is free exactly when $\{\gamma\}$ is open as a subset of $\mathfrak{C}(\mathcal{G})$. This is further equivalent to the existence of a connected subgraph $\widetilde{\mathcal{G}}$ with compact boundary $\partial\widetilde{\mathcal{G}}$[2] such that $U_n \subseteq \widetilde{\mathcal{G}}$ eventually for any sequence $\mathcal{U} = (U_n)$ representing γ and $U_n' \cap \widetilde{\mathcal{G}} = \varnothing$ eventually for all sequences $\mathcal{U}' = (U_n')$ representing an end $\gamma' \neq \gamma$.

Let us mention that ends $\gamma \in \mathfrak{C}(\mathcal{G})$ can be obtained in a constructive way by means of compact exhaustions. Namely, a sequence of connected subgraphs $(\mathcal{G}_n)$ of $\mathcal{G}$ such that each $\mathcal{G}_n$ has finitely many vertices and edges, $\mathcal{G}_n \subseteq \mathcal{G}_{n+1}$ for all $n \geq 0$ and $\bigcup_n \mathcal{G}_n = \mathcal{G}$ is called a *compact exhaustion* of $\mathcal{G}$. Clearly, each $\mathcal{G}_n$ may be identified with a compact subset of $\mathcal{G}$. Now iteratively construct a sequence (U_n) by choosing in each step a non-compact, connected component U_n of $\mathcal{G} \setminus \mathcal{G}_n$ satisfying $U_n \subseteq U_{n-1}$. It is easy to check that each such sequence (U_n) defines a topological end $\gamma \in \mathfrak{C}(\mathcal{G})$ and in fact all ends $\gamma \in \mathfrak{C}(\mathcal{G})$ are obtained by this construction. Notice also that the open subsets U_n of such representations $\gamma \sim (U_n)$ (actually, their topological closures, since we need to add endpoints of edges which also belong

[2] Notice that for a subgraph $\widetilde{\mathcal{G}}$ of $\mathcal{G}$ its boundary is $\partial\widetilde{\mathcal{G}} = \{v \in \mathcal{V}(\widetilde{\mathcal{G}}) |\, \deg_{\widetilde{\mathcal{G}}}(v) < \deg(v)\}$ and hence $\partial\widetilde{\mathcal{G}}$ is compact only if $\#\partial\widetilde{\mathcal{G}} < \infty$.

to $\mathcal{V}(\mathcal{G}_n)$) can again be identified with connected subgraphs $\mathcal{G}_n(\gamma) := \overline{U_n}$ and we will frequently use this fact.

Let us finish this section with a few more notations. Suppose $\mathcal{R}$ is a finite path without self-intersections or ray in $\mathcal{G}_d$. We may identify $\mathcal{R}$ with a subgraph of $\mathcal{G}_d$ and hence with the subset of $\mathcal{G}$, i.e., we can consider it as the union of all edges of $\mathcal{R}$. The latter can further be identified with the interval $I_{\mathcal{R}} = [0, |\mathcal{R}|)$ of length $|\mathcal{R}|$, where

$$|\mathcal{R}| := \sum_{e\in\mathcal{R}} |e|.$$

Also, we need to consider paths – and in particular rays – in $\mathcal{G}$ starting and ending at a non-vertex point. In particular, given a path $(v_0, v_1, \ldots, v_N)$ and a point x on an edge $e \in \mathcal{E}_{v_0}$, $e \neq e_{v_0,v_1}$, we add the interval $[x, v_0] \subseteq e$ to $(v_0, v_1, \ldots, v_N)$. For the resulting set, we shall write $(x, v_0, v_1, \ldots, v_N)$ and call it a *non-vertex path*; and likewise for rays. The set of all non-vertex rays will be denoted by $\mathfrak{R}(\mathcal{G})$.

2.3. **Kirchhoff Laplacian.** Let $\mathcal{G}$ be a metric graph satisfying Hypothesis 2.1. Upon identifying every $e \in \mathcal{E}$ with a copy of the interval $\mathcal{I}_e = [0, |e|]$, let us introduce the Hilbert space $L^2(\mathcal{G})$ of functions $f\colon \mathcal{G} \to \mathbb{C}$ such that

$$L^2(\mathcal{G}) = \bigoplus_{e\in\mathcal{E}} L^2(e) = \Big\{ f = \{f_e\}_{e\in\mathcal{E}} \big|\, f_e \in L^2(e),\ \sum_{e\in\mathcal{E}} \|f_e\|^2_{L^2(e)} < \infty \Big\}.$$

The subspace of compactly supported $L^2(\mathcal{G})$ functions will be denoted by

$$L^2_c(\mathcal{G}) = \big\{ f \in L^2(\mathcal{G}) |\ f \neq 0 \text{ only on finitely many edges } e \in \mathcal{E} \big\}.$$

For every $e \in \mathcal{E}$ consider the maximal operator $\mathrm{H}_{e,\max}$ acting on functions $f \in H^2(e)$ as a negative second derivative. Here and below $H^s(e)$ for $s \geq 0$ denotes the usual Sobolev space on e. In particular, $H^0(e) = L^2(e)$ and

$$H^1(e) = \{ f \in AC(e) |\, f' \in L^2(e) \}, \quad H^2(e) = \{ f \in H^1(e) |\, f' \in H^1(e) \}.$$

This defines the maximal operator on $L^2(\mathcal{G})$ by

$$\mathbf{H}_{\max} = \bigoplus_{e\in\mathcal{E}} \mathrm{H}_{e,\max}, \qquad \mathrm{H}_{e,\max} = -\frac{\mathrm{d}^2}{\mathrm{d}x_e^2}, \quad \mathrm{dom}(\mathrm{H}_{e,\max}) = H^2(e). \tag{2.4}$$

If v is a vertex of the edge $e \in \mathcal{E}$, then for every $f \in H^2(e)$ the following quantities

$$f_e(v) := \lim_{x_e\to v} f(x_e), \qquad\qquad f'_e(v) := \lim_{x_e\to v} \frac{f(x_e) - f(v)}{|x_e - v|}, \tag{2.5}$$

are well defined. Considering $\mathcal{G}$ as the union of all edges glued together at certain endpoints, let us equip a metric graph with the Laplace operator. The Kirchhoff (also called *standard* or *Kirchhoff–Neumann*) boundary conditions at every vertex $v \in \mathcal{V}$ are then given by

$$\begin{cases} f \text{ is continuous at } v, \\ \sum_{e\in\mathcal{E}_v} f'_e(v) = 0. \end{cases} \tag{2.6}$$

Imposing these boundary conditions on the maximal domain $\mathrm{dom}(\mathbf{H}_{\max})$ yields the *maximal Kirchhoff Laplacian*

$$\begin{aligned} \mathbf{H} &= \mathbf{H}_{\max} \restriction \mathrm{dom}(\mathbf{H}), \\ \mathrm{dom}(\mathbf{H}) &= \{ f \in \mathrm{dom}(\mathbf{H}_{\max}) \cap L^2(\mathcal{G}) |\, f \text{ satisfies (2.6)},\ v \in \mathcal{V} \}. \end{aligned} \tag{2.7}$$

Restricting further to compactly supported functions we end up with the pre-minimal operator

$$\begin{aligned} \mathbf{H}_0^0 &= \mathbf{H}_{\max} \restriction \operatorname{dom}(\mathbf{H}_0^0), \\ \operatorname{dom}(\mathbf{H}_0^0) &= \{f \in \operatorname{dom}(\mathbf{H}_{\max}) \cap L^2_c(\mathcal{G}) |\, f \text{ satisfies (2.6)},\ v \in \mathcal{V}\}. \end{aligned} \tag{2.8}$$

Integrating by parts one obtains

$$\langle \mathbf{H}_0^0 f, f\rangle_{L^2(\mathcal{G})} = \int_{\mathcal{G}} |f'(x)|^2\, dx, \qquad f \in \operatorname{dom}(\mathbf{H}_0^0), \tag{2.9}$$

and hence $\mathbf{H}_0^0$ is a non-negative symmetric operator. We call its closure $\mathbf{H}_0 := \overline{\mathbf{H}_0^0}$ in $L^2(\mathcal{G})$ *the minimal Kirchhoff Laplacian*. The following result is well-known (see, e.g., [14, Lemma 3.9]).

Lemma 2.7. *Let $\mathcal{G}$ be a metric graph. Then*

$$\mathbf{H}_0^* = \mathbf{H}. \tag{2.10}$$

2.4. **Deficiency indices.** In the following we are interested in the question whether $\mathbf{H}_0$ is self-adjoint, or equivalently whether the equality $\mathbf{H}_0 = \mathbf{H}$ holds true. Let us recall one sufficient condition. Define the *star weight* $m(v)$ of a vertex $v \in \mathcal{V}$ by

$$m(v) := \sum_{e \in \mathcal{E}_v} |e| = \operatorname{vol}(\mathcal{E}_v), \tag{2.11}$$

and also introduce the *star path metric* on $\mathcal{V}$ by

$$\varrho_m(u,v) := \inf_{\substack{\mathcal{P}=(v_0,\dots,v_n)\\ u=v_0,\ v=v_n}} \sum_{v_k \in \mathcal{P}} m(v_k). \tag{2.12}$$

Theorem 2.8 ([25]). *If $(\mathcal{V}, \varrho_m)$ is complete as a metric space, then $\mathbf{H}_0^0$ is essentially self-adjoint and $\overline{\mathbf{H}_0^0} = \mathbf{H}_0 = \mathbf{H}$.*

If a symmetric operator is not (essentially) self-adjoint, then the degree of its non-self-adjointness is determined by its *deficiency indices*. Recall that the *deficiency subspace* $\mathcal{N}_z(\mathbf{H}_0)$ of $\mathbf{H}_0$ is defined by

$$\mathcal{N}_z(\mathbf{H}_0) := \ker(\mathbf{H}_0^* - z) = \ker(\mathbf{H} - z), \quad z \in \mathbb{C}. \tag{2.13}$$

The numbers

$$\mathrm{n}_\pm(\mathbf{H}_0) := \dim \mathcal{N}_{\pm \mathrm{i}}(\mathbf{H}_0) = \dim\ker(\mathbf{H} \mp \mathrm{i}) \tag{2.14}$$

are called the deficiency indices of $\mathbf{H}_0$. Notice that $\mathrm{n}_+(\mathbf{H}_0) = \mathrm{n}_-(\mathbf{H}_0)$ since $\mathbf{H}_0$ is non-negative.

Lemma 2.9. *If 0 is a point of regular type for $\mathbf{H}_0$, then*[3]

$$\mathrm{n}_\pm(\mathbf{H}_0) = \dim\ker(\mathbf{H}). \tag{2.15}$$

Proof. It suffices to take into account (2.10) and use, e.g., [1, §78]. □

Using the Rayleigh quotient, define

$$\lambda_0(\mathcal{G}) := \inf_{\substack{f\in\operatorname{dom}(\mathbf{H}_0)\\ \|f\|=1}} \big\langle \mathbf{H}_0 f, f\big\rangle_{L^2(\mathcal{G})} = \inf_{\substack{f\in\operatorname{dom}(\mathbf{H}_0)\\ \|f\|=1}} \int_{\mathcal{G}} |f'|^2 dx. \tag{2.16}$$

[3] For an operator T with dense domain in a Hilbert space $\mathcal{H}$, $\lambda \in \mathbb{C}$ is called a *point of regular type* of T if there exists $c = c_\lambda > 0$ such that $\|(T-\lambda)f\| \ge c\|f\|$ for all $f \in \operatorname{dom}(T)$.

Noting that the operator $\mathbf{H}_0$ is non-negative, 0 is a point of regular type for $\mathbf{H}_0$ exactly when $\lambda_0(\mathcal{G}) > 0$. Thus, we arrive at the following result.

Corollary 2.10. *If $\lambda_0(\mathcal{G}) > 0$, then* (2.15) *holds true.*

The positivity of $\lambda_0(\mathcal{G})$ is known in the following simple situation.

Corollary 2.11. *If $\mathcal{G}$ has finite total volume,*

$$\mathrm{vol}(\mathcal{G}) := \sum_{e\in\mathcal{E}} |e| < \infty, \tag{2.17}$$

then $\mathbf{H}_0$ is not self-adjoint and (2.15) *holds true.*

Proof. Indeed, by the Cheeger-type estimate [53, Corollary 3.5(iv)], we have

$$\lambda_0(\mathcal{G}) \geq \frac{1}{4\,\mathrm{vol}(\mathcal{G})^2}, \tag{2.18}$$

and hence (2.15) holds true by Corollary 2.10. Moreover, $\mathbb{1}_{\mathcal{G}} \in \ker(\mathbf{H})$, where $\mathbb{1}_{\mathcal{G}}$ denotes the constant function on $\mathcal{G}$, and hence

$$\mathrm{n}_\pm(\mathbf{H}_0) = \dim(\ker \mathbf{H}) \geq 1. \qquad \square$$

Remark 2.12. By [53, Corollary 4.5], $\lambda_0(\mathcal{G}) > 0$ holds true if the combinatorial isoperimetric constant of $\mathcal{G}_d$ is positive and $\ell^*(\mathcal{G}) = \sup_{e\in\mathcal{E}} |e| < \infty$. For example, this holds true if $\mathcal{G}_d$ is an infinite tree without leaves [53, Lemma 8.1] or $\mathcal{G}_d$ is a Cayley graph of a non-amenable finitely generated group [53, Lemma 8.12(i)]. For antitrees, the positivity of a combinatorial isoperimetric constant is tightly related to the structure of its combinatorial spheres (see [54, Theorem 7.1]).

Finally, let us remark that $\ker(\mathbf{H}) = \mathbb{H}(\mathcal{G}) \cap L^2(\mathcal{G})$, where $\mathbb{H}(\mathcal{G})$ denotes the space of *harmonic functions* on $\mathcal{G}$, that is, the set of all "edgewise" affine functions satisfying Kirchhoff conditions (2.6) at each vertex $v \in \mathcal{V}$. Notice that every function $f \in \mathbb{H}(\mathcal{G})$ is uniquely determined by its vertex values $\mathbf{f} := f|_{\mathcal{V}} = (f(v))_{v\in\mathcal{V}}$. Recall also the following result (see, e.g., [53, eq. (2.32)]).

Lemma 2.13. *Let $\mathcal{G}$ be a metric graph satisfying the assumptions in Hypothesis 2.1. If $f \in \mathbb{H}(\mathcal{G})$, then $f \in L^2(\mathcal{G})$ if and only if $\mathbf{f} \in \ell^2(\mathcal{V}; m)$, that is,*

$$\sum_{v\in\mathcal{V}} |f(v)|^2 m(v) < \infty. \tag{2.19}$$

Remark 2.14. The above considerations indicate that in order to understand the deficiency indices of the Kirchhoff Laplacian one needs to find the dimension of the space of L^2 harmonic (or, more carefully, λ-harmonic) functions. Moreover, in order to describe self-adjoint extensions one has to understand the behavior of L^2 harmonic functions at "infinity", that is, near a "boundary" of a given metric graph. However, graphs admit a lot of different notions of boundary (ends, Poisson and Martin boundaries, Royden and Kuramochi boundary etc.) and search for a suitable notion in this context (namely, L^2 harmonic functions) is a highly non-trivial problem, which seems to be not very well studied neither in the context of incomplete manifolds nor in the case of weighted graphs.

Let us also mention that recently there has been a tremendous amount of work devoted to the study of harmonic functions and self-adjoint extensions of Laplacians on weighted graph (we only refer to a brief selection of articles [17, 33, 37, 41, 42, 43, 44, 49]).

3. Graph ends and $H^1(\mathcal{G})$

This section deals with the Sobolev space H^1 on metric graphs. Its importance stems, in particular, from the fact that it serves as a form domain for a large class of self-adjoint extensions of $\mathbf{H}_0$.

3.1. $H^1(\mathcal{G})$ and boundary values.

First recall that

$$H^1(\mathcal{G}) = \big\{f \in L^2(\mathcal{G}) \cap C(\mathcal{G}) |\ f_e \in H^1(e) \text{ for all } e \in \mathcal{E},\ \|f'\|^2_{L^2(\mathcal{G})} < \infty\big\}, \tag{3.1}$$

where $C(\mathcal{G})$ is the space of continuous complex-valued functions on $\mathcal{G}$ and

$$\|f'\|^2_{L^2(\mathcal{G})} := \sum_{e\in\mathcal{E}} \|f'_e\|^2_{L^2(e)}.$$

Notice that $(H^1(\mathcal{G}), \|\cdot\|_{H^1})$ is a Hilbert space when equipped with the standard norm

$$\|f\|^2_{H^1(\mathcal{G})} := \|f\|^2_{L^2(\mathcal{G})} + \|f'\|^2_{L^2(\mathcal{G})} = \sum_{e\in\mathcal{E}} \|f_e\|^2_{H^1(e)}, \quad f \in H^1(\mathcal{G}).$$

Moreover, $\mathrm{dom}(\mathbf{H}^0_0) \subset H^1(\mathcal{G})$ and we define $H^1_0(\mathcal{G})$ as the closure of $\mathrm{dom}(\mathbf{H}^0_0)$ with respect to $\|\cdot\|_{H^1(\mathcal{G})}$.

Remark 3.1. If $\mathbf{H}^0_0$ is essentially self-adjoint, then $H^1(\mathcal{G}) = H^1_0(\mathcal{G})$. However, the converse is not true in general. In fact this equality is tightly connected to the uniqueness of Markovian extensions of $\mathbf{H}_0$ and, as we shall see, it is possible to characterize it in terms of topological ends of $\mathcal{G}$ (see Corollary 5.5 below).

Notice also that $H^1_0(\mathcal{G})$ is the form domain of the Friedrichs extension $\mathbf{H}_F$ of $\mathbf{H}^0_0$ and $\lambda_0(\mathcal{G})$ defined by (2.16) is the bottom of the spectrum of $\mathbf{H}_F$.

By definition, $H^1(\mathcal{G})$ is densely and continuously embedded in $L^2(\mathcal{G})$.

Lemma 3.2. *$H^1(\mathcal{G})$ is continuously embedded in $C_b(\mathcal{G}) = C(\mathcal{G}) \cap L^\infty(\mathcal{G})$ and*

$$\|f\|_\infty := \sup_{x\in\mathcal{G}} |f(x)| \le C_{\mathcal{G}} \|f\|_{H^1(\mathcal{G})} \tag{3.2}$$

holds for all $f \in H^1(\mathcal{G})$ with $C_{\mathcal{G}} = \sqrt{\coth\left(\tfrac{1}{2}\,\mathrm{diam}(\mathcal{G})\right)}$. Here $\mathrm{diam}(\mathcal{G})$ denotes the diameter of $\mathcal{G}$, that is,

$$\mathrm{diam}(\mathcal{G}) = \sup_{\mathcal{R}} |\mathcal{R}|, \tag{3.3}$$

where the supremum is taken over all paths without self-intersections $\mathcal{R}$.

Proof. For every interval $\mathcal{I} \subseteq \mathbb{R}$ the embedding of $H^1(\mathcal{I})$ into $L^\infty(\mathcal{I})$ is bounded and

$$\sup_{x\in\mathcal{I}} |f(x)| \le C_{|\mathcal{I}|} \|f\|_{H^1(\mathcal{I})} \tag{3.4}$$

holds for all $f \in H^1(\mathcal{I})$ with $C_{|\mathcal{I}|} = \sqrt{\coth(|\mathcal{I}|)}$ (for optimal Sobolev constants see, e.g., [65]). Notice that we may identify the restriction $f|_{\mathcal{R}}$ of $f \in H^1(\mathcal{G})$ to a path without self-intersections $\mathcal{R}$ with a function on $\mathcal{I}_{\mathcal{R}} = [0, |\mathcal{R}|)$. It is easy to check that upon this identification $f|_{\mathcal{R}} \in H^1(\mathcal{I}_{\mathcal{R}})$ and $(f|_{\mathcal{R}})' = f'|_{\mathcal{R}}$.

Let $\mathcal{R} = (v_0, \dots, v_N)$ be a fixed finite path without self-intersections and let $x \in \mathcal{G}$. If $x \in \mathcal{R}$, then considering $\mathcal{R}$ as an interval $I_{\mathcal{R}} = [0, |\mathcal{R}|)$ of length $|\mathcal{R}|$, we immediately get

$$|f(x)| \le C_{|\mathcal{R}|/2} \|f\|_{H^1(\mathcal{R})} \le C_{|\mathcal{R}|/2} \|f\|_{H^1(\mathcal{G})} \tag{3.5}$$

for all $f \in H^1(\mathcal{G})$. If $x \notin \mathcal{R}$, then connecting x and v_0 by some finite non-vertex path $\mathcal{R}_0$, we conclude that there is a path without self-intersections $\mathcal{R}_x$ such that $x \in \mathcal{R}_x$ and $|\mathcal{R}_x| \geq |\mathcal{R}|/2$. Applying the same argument, we conclude that (3.5) holds for all $x \in \mathcal{G}$. $\square$

The above considerations, in particular, imply the following crucial property of H^1-functions: if $\mathcal{R} = (v_n)$ is a ray, then

$$f(\gamma_{\mathcal{R}}) := \lim_{n\to\infty} f(v_n)$$

exists. Moreover, this limit is independent of the choice of $\mathcal{R} \in \omega_\gamma$ (indeed, for any two equivalent rays $\mathcal{R}$ and $\mathcal{R}'$ there exists a third ray $\mathcal{R}''$ containing infinitely many vertices of both $\mathcal{R}$ and $\mathcal{R}'$, which immediately implies that $f(\gamma_{\mathcal{R}}) = f(\gamma_{\mathcal{R}''}) = f(\gamma_{\mathcal{R}'})$). This enables us to introduce the following notion.

Definition 3.3. For every $f \in H^1(\mathcal{G})$ and a (topological) end $\gamma \in \mathfrak{C}(\mathcal{G})$, we define

$$f(\gamma) := f(\gamma_{\mathcal{R}}), \tag{3.6}$$

where $\mathcal{R} \in \omega_\gamma$ is any ray belonging to the corresponding graph end ω_γ (see Theorem 2.3). Sometimes we shall also write $f(\omega_\gamma) := f(\gamma)$.

It turns out that (3.6) enables us to obtain an extension by continuity of every function $f \in H^1(\mathcal{G})$ to the end compactification $\widehat{\mathcal{G}}$ of $\mathcal{G}$ (see Section 2.2).

Lemma 3.4. *Let $\mathcal{G}$ be a metric graph and $\gamma \in \mathfrak{C}(\mathcal{G})$. If $f \in H^1(\mathcal{G})$, then*

$$\lim_{n\to\infty} \sup_{x\in U_n} |f(x) - f(\gamma)| = 0 \tag{3.7}$$

for every sequence $\mathcal{U} = (U_n)$ representing γ.

Proof. Let $\gamma \in \mathfrak{C}(\mathcal{G})$ and let $\mathcal{U} = (U_n)$ be a sequence representing γ. Let also

$$\mathfrak{R}_n(\gamma) := \{\mathcal{R} \in \mathfrak{R}(\mathcal{G}) |\ \mathcal{R} \subseteq U_n\}$$

be the set of all non-vertex rays contained in U_n, $n \geq 0$.

We proceed by case distinction. First, assume that for n sufficiently large, all rays in $\mathfrak{R}_n(\gamma)$ have length at most one. If $x \in U_n$, then there exists a (non-vertex) ray $\mathcal{R}_x \in \mathfrak{R}_n(\gamma)$ such that $\mathcal{R}_x = (x, v_0, \dots)$ and its tail $\mathcal{R} := (v_0, v_1, \dots)$ belongs to ω_γ.

By our assumption, $|\mathcal{R}_x| \leq 1$ and hence

$$|f(\gamma) - f(x)| = |f(\gamma_{\mathcal{R}_x}) - f(x)| = \Big|\int_{\mathcal{R}_x} f'(y)\, dy\Big| \leq \|f'\|_{L^2(\mathcal{R}_x)} \leq \|f'\|_{L^2(U_n)}.$$

Since $x \in U_n$ is arbitrary, this implies

$$\sup_{x\in U_n} |f(\gamma) - f(x)| \leq \|f'\|_{L^2(U_n)}.$$

Since $\mathcal{U} = (U_n)$ represents γ, $\bigcap_n \overline{U_n} = \varnothing$ and hence $\lim_{n\to\infty} \|f'\|_{L^2(U_n)} = 0$. This implies (3.7).

Assume now that for every $n \in \mathbb{Z}_{\geq 0}$ there is a ray $\mathcal{R} \in \mathfrak{R}_n(\gamma)$ with $|\mathcal{R}| > 1$. Take $n \geq 0$ and choose an $x \in U_n$. We can find a finite (non-vertex) path without self-intersections $\mathcal{R}_x \subseteq U_n$ such that $x \in \mathcal{R}_x$ and $|\mathcal{R}_x| = 1/2$ (take into account that U_n contains at least one ray of length greater than 1). Hence we get

$$|f(x)| \leq \sup_{y\in\mathcal{R}_x} |f(y)| \leq C_{1/2}\|f\|_{H^1(\mathcal{R}_x)} \leq C_{1/2}\|f\|_{H^1(U_n)},$$

where $C_{1/2} = \sqrt{\coth(1/2)}$ is the constant from (3.4). Since $x \in U_n$ is arbitrary,

$$\sup_{x\in U_n} |f(x)| \le C_{1/2}\|f\|_{H^1(U_n)}.$$

However, $\bigcap_n \overline{U_n} = \varnothing$ and hence $\sup_{x\in U_n} |f(x)| = o(1)$ as $n \to \infty$. It remains to notice that $f(\gamma) = 0$. Indeed, by Theorem 2.3, for every $n \ge 0$ there is a ray $\widetilde{\mathcal{R}}_n \in \omega_\gamma$ such that $\widetilde{\mathcal{R}}_n \subseteq U_n$ and hence

$$|f(\gamma)| = |f(\gamma_{\widetilde{\mathcal{R}}_n})| \le \sup_{x\in U_n} |f(x)| = o(1)$$

as $n \to \infty$. This finishes the proof. $\square$

Taking into account the topology on $\widehat{\mathcal{G}} = \mathcal{G} \cup \mathfrak{C}(\mathcal{G})$, the next result is a direct consequence of Lemma 3.2 and Lemma 3.4.

Proposition 3.5. *Each $f \in H^1(\mathcal{G})$ has a unique continuous extension to the end compactification $\widehat{\mathcal{G}}$ of $\mathcal{G}$ and this extension is given by* (3.6)*. Moreover,*

$$\|f\|_\infty = \sup_{x\in\widehat{\mathcal{G}}} |f(x)| \le C_{\mathcal{G}}\|f\|_{H^1(\mathcal{G})}.$$

3.2. **Nontrivial and finite volume ends.** Observe that some ends lead to trivial boundary values for H^1 functions. For example, $f(\gamma) = 0$ for all $f \in H^1(\mathcal{G})$ if $\omega_\gamma \in \Omega(\mathcal{G}_d)$ contains a ray $\mathcal{R}$ with infinite length $|\mathcal{R}| = \infty$. On the other hand, it might happen that all rays have finite length, however, $f(\gamma) = 0$ for all $f \in H^1(\mathcal{G})$ (see, e.g., the second step in the proof of Lemma 3.4).

Definition 3.6. A topological end $\gamma \in \mathfrak{C}(\mathcal{G})$ is called *nontrivial* if $f(\gamma) \ne 0$ for some $f \in H^1(\mathcal{G})$.

We also need the following notion.

Definition 3.7. A topological end $\gamma \in \mathfrak{C}(\mathcal{G})$ has *finite volume* (or, more precisely, *finite volume neighborhood)* if there is a sequence $\mathcal{U} = (U_n)$ representing γ such that $\mathrm{vol}(U_n) < \infty$[4] for some n. Otherwise γ has *infinite volume.* The set of all finite volume ends is denoted by $\mathfrak{C}_0(\mathcal{G})$.

Remark 3.8. If $\mathfrak{C}(\mathcal{G})$ contains only one end, then this end has finite volume exactly when $\mathrm{vol}(\mathcal{G}) < \infty$. Analogously, if $\gamma \in \mathfrak{C}(\mathcal{G})$ is a free end, then there is a finite set of vertices X separating ω_γ from all other ends and hence this end has finite volume exactly when the corresponding connected component $\mathcal{G}_\gamma$ has finite total volume.

If γ is not free, then the situation is more complicated. For example, for a rooted tree $\mathcal{G} = \mathcal{T}_o$ the ends are in one-to-one correspondence with the rays from the root o and hence one may possibly confuse the notion of a finite/infinite volume of an end with the finite/infinite length of the corresponding ray. More specifically, let γ be an end of $\mathcal{T}_o$ and let $\mathcal{R}_\gamma = (o, v_1, v_2, \dots)$ be the corresponding ray. For each $n \ge 1$, let $\mathcal{T}_n$ be the subtree of $\mathcal{T}_o$ having its root at v_n and containing all the "descendant" vertices of v_n. Then by definition γ has finite volume (neighborhood) if and only if there is $n \ge 1$ such that the corresponding subtree $\mathcal{T}_n$ has finite total volume. In particular, this implies that $\mathcal{G}$ would have uncountably many finite volume ends in this case (here we assume for simplicity that all vertices are essential, that is, $\deg(v_n) > 2$ for all n). In particular, $|\mathcal{R}_\gamma| < \infty$ is a necessary but not sufficient condition for γ to have finite volume.

[4]As usual, $\mathrm{vol}(A)$ denotes the Lebesgue measure of a measurable set $A \subseteq \mathcal{G}$.

It turns out that nontrivial and finite volume ends are closely connected.

Theorem 3.9. *Let $\mathcal{G}$ be a metric graph. Then $\gamma \in \mathfrak{C}(\mathcal{G})$ is nontrivial if and only if γ has finite volume. Moreover, for any finite collection of distinct nontrivial ends $\{\gamma_j\}_{j=1}^N$ there exists $f \in H^1(\mathcal{G}) \cap \mathrm{dom}(\mathbf{H})$ such that $f(\gamma_1) = 1$ and $f(\gamma_2) = \cdots = f(\gamma_N) = 0$.*

Proof. It is not difficult to see that $f(\gamma) = 0$ for all $f \in H^1(\mathcal{G})$ if γ has infinite volume. Indeed, assuming that there is $f \in H^1(\mathcal{G})$ such that $f(\gamma) \neq 0$, Lemma 3.4 would imply that there exists $\mathcal{U} = (U_n)$ representing γ such that

$$|f(x)| \geq |f(\gamma)|/2 > 0$$

for all $x \in U_n$. However, then $\mathrm{vol}(U_n) = \infty$ contradicts the fact that $f \in L^2(\mathcal{G})$.

Suppose now that $\gamma \in \mathfrak{C}(\mathcal{G})$ has finite volume. Take a sequence $\mathcal{U} = (U_n)$ representing γ with $\mathrm{vol}(U_0) < \infty$. Pick a function $\phi \in H^2(0,1)$ such that $\phi(0) = \phi'(0) = \phi'(1) = 0$ and $\phi(1) = 1$ and then define $f\colon \mathcal{G} \to \mathbb{C}$ by

$$f(x_e) = \begin{cases} 1, & x_e \in e \text{ and both vertices of } e \text{ are in } U_0, \\ 0, & x_e \in e \text{ and both vertices of } e \text{ are not in } U_0, \\ \phi\Big(\frac{|x_e - u|}{|e|}\Big), & x_e \in e = e_{u,v} \text{ and } u \in \mathcal{V} \setminus U_0, v \in U_0. \end{cases}$$

Clearly, $f \in H^2(e)$ for every $e \in \mathcal{E}$. Moreover, it is straightforward to check that f satisfies Kirchhoff conditions (2.6) at every $v \in \mathcal{V}$. By assumption, ∂U_0 is compact and hence it is contained in finitely many edges. Thus there are only finitely many edges $e \in \mathcal{E}$ such that one of its vertices belongs to U_0 and another one does not belong to U_0. This implies that $f \in L^2(\mathcal{G})$ and, moreover, $f' \not\equiv 0$ only on finitely many edges, which proves the inclusion $f \in \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$. Taking into account that $f \equiv 1$ on U_n for large enough n, we conclude that $f(\gamma) = 1$ and hence γ is nontrivial.

It remains to prove the second claim. Suppose that $\gamma_1, \ldots, \gamma_N \in \mathfrak{C}(\mathcal{G})$ are distinct nontrivial ends. Then we can find $\mathcal{U}^j = (U_n^j)$, sequences representing γ_j, $j \in \{1, \ldots, N\}$ such that $\mathrm{vol}(U_0^1) < \infty$ and $U_0^1 \cap U_0^j = \emptyset$ for all $j = 2, \ldots, N$ (see [27, Satz 3] or [22, Lemma 3.1]). Using the above procedure, we can construct a function $f \in \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$ such that $\mathrm{supp}(f) \subseteq U_0$ and $f(\gamma) = 1$. The latter also implies that $f(\gamma_2) = \cdots = f(\gamma_N) = 0$. $\square$

Remark 3.10. If $\mathrm{vol}(\mathcal{G}) = \sum_{e \in \mathcal{E}} |e| < \infty$, then all ends have finite volume and the end compactification $\widehat{\mathcal{G}}$ of $\mathcal{G}$ coincides with several other spaces, among them the *metric completion* of $\mathcal{G}$ and the *Royden compactification* of a related discrete graph (see [33, Corollary 4.22] and also [32, p. 1526]). Notice that the natural path metric ϱ can be extended to $\widehat{\mathcal{G}} = \mathcal{G} \cup \mathfrak{C}(\mathcal{G})$ (see [32]). That is, the distance $\varrho(x, \gamma)$ between a point $x \in \mathcal{G}$ and an end $\gamma \in \mathfrak{C}(\mathcal{G})$ is the infimum over all lengths of rays starting at x and belonging to γ. Similarly, the distance $\varrho(\gamma, \gamma')$ between two ends is the infimum over the lengths of all double rays with one tail part in γ and the other one in γ'. Then $(\widehat{\mathcal{G}}, \varrho)$ is a metric completion of $\mathcal{G}$ and $\widehat{\mathcal{G}}$ is compact and homeomorphic to the end compactification of $\mathcal{G}$ (see [32] for further details).

The metric completion was considered in connection with quantum graphs in [14, 15]; however, it can have a rather complicated structure if $\mathrm{vol}(\mathcal{G}) = \infty$ and a further analysis usually requires additional assumptions. Moreover, there are clear indications that metric completion is not a good candidate for these purposes.

3.3. **Description of $H^1_0(\mathcal{G})$.** Recall that the space $H^1_0(\mathcal{G})$ is defined as the closure of $\mathrm{dom}(\mathbf{H}^0_0) \subset H^1(\mathcal{G})$ with respect to $\|\cdot\|_{H^1(\mathcal{G})}$. One can naturally conjecture that $H^1_0(\mathcal{G})$ consists of those H^1-functions which vanish on $\mathfrak{C}(\mathcal{G})$. In fact, the results of the previous two sections enable us to show that this is indeed the case.

Theorem 3.11. *Let $\mathcal{G}$ be a metric graph and $\mathfrak{C}(\mathcal{G})$ be its ends. Then*

$$H^1_0(\mathcal{G}) = \{f \in H^1(\mathcal{G}) |\ f(\gamma) = 0 \text{ for all } \gamma \in \mathfrak{C}(\mathcal{G})\}. \tag{3.8}$$

Proof. First of all, it immediately follows from Proposition 3.5 that $f \in H^1_0(\mathcal{G})$ vanishes at every end $\gamma \in \mathfrak{C}(\mathcal{G})$ (since this holds for each $f \in \mathrm{dom}(\mathbf{H}^0_0)$).

To prove the converse inclusion, we will follow the arguments of the proof of [33, Theorem 4.14]. Namely, suppose that $f \in H^1(\mathcal{G})$ and $f(\gamma) = 0$ for all $\gamma \in \mathfrak{C}(\mathcal{G})$. Without loss of generality, we may assume that f is real-valued and $f \geq 0$. To prove that $f \in H^1_0(\mathcal{G})$, it suffices to construct a sequence of compactly supported functions $f_n \in H^1(\mathcal{G})$ which converges to f in $H^1(\mathcal{G})$. Define $\phi_n \colon \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ by

$$\phi_n(s) = \begin{cases} s - \frac{1}{n}, & \text{if } s \geq \frac{1}{n} \\ 0, & \text{if } s < \frac{1}{n}, \end{cases} \tag{3.9}$$

and then let $f_n \colon \mathcal{G} \to \mathbb{R}_{\geq 0}$ be the composition $f_n := \phi_n \circ f$, $n \geq 0$. Since $\phi_n(s) \leq s$ for all $s \geq 0$ and $|\phi_n(s) - \phi_n(t)| \leq |s - t|$ for all $s, t \geq 0$, $|f_n(x)| \leq |f(x)|$ and $|f_n'(x)| \leq |f'(x)|$ for almost every $x \in \mathcal{G}$. Hence $f_n \in H^1(\mathcal{G})$ and

$$\|f_n\|_{H^1(\mathcal{G})} \leq \|f\|_{H^1(\mathcal{G})} \tag{3.10}$$

for all n. Let us now show that f_n has compact support. Indeed, assuming the converse, there exist infinitely many distinct edges e_k in $\mathcal{E}$ such that f_n is non-zero on each e_k. Taking into account (3.9), for each k we can find a non-vertex point x_k on e_k such that $f_n(x_k) > \frac{1}{n}$. Since $\widehat{\mathcal{G}}$ is compact, the sequence (x_k) has an accumulation point $x \in \widehat{\mathcal{G}}$. By construction each edge $e \in \mathcal{E}$ contains at most one of the x_k's. It follows that $x \notin \mathcal{G}$ and hence $x \in \widehat{\mathcal{G}}$ is an end. On the other hand, f is continuous on $\widehat{\mathcal{G}}$ by Proposition 3.5 and thus $f(x) \geq \frac{1}{n}$, which contradicts our assumptions on f.

It remains to show that f_n converges to f in $H^1(\mathcal{G})$ as $n \to \infty$. Taking into account the above properties of f_n, we get

$$\|f - f_n\|^2_{L^2} + \|f' - f_n'\|^2_{L^2} \leq 2(\|f\|^2_{L^2} + \|f_n\|^2_{L^2} + \|f'\|^2_{L^2} + \|f_n'\|^2_{L^2}) \leq 4\|f\|^2_{H^1},$$

and hence by dominated convergence it is enough to show that $f_n \to f$ and $f_n' \to f'$ pointwise a.e. on $\mathcal{G}$. The first claim is clearly true since $\lim_{n\to\infty} \phi_n(s) = s$ for all $s \in \mathbb{R}_{\geq 0}$. To prove the second claim, suppose that f is differentiable at a non-vertex point $x \in \mathcal{G}$. If $f(x) > 0$, then by continuity of f, there is a neighborhood U of x such that $f_n = f - \frac{1}{n}$ holds on U for all sufficiently large $n > 0$. Hence f_n is differentiable at x with $f_n'(x) = f'(x)$ for all large enough n. Finally, if $f(x) = 0$, then for each n there is a neighborhood U_n of x such that $f \leq \frac{1}{n}$ on U_n. Hence $f_n \equiv 0$ on U_n and, in particular, f_n is differentiable at x with $f_n'(x) = 0$. However, since $f \geq 0$ on $\mathcal{G}$ and f is differentiable at x, it follows that $f'(x) = 0$ as well. This finishes the proof. ☐

Combining Theorem 3.11 with Theorem 3.9, we arrive at the following fact.

Corollary 3.12. *The equality $H^1(\mathcal{G}) = H^1_0(\mathcal{G})$ holds true if and only if all topological ends of $\mathcal{G}$ have infinite volume.*

Remark 3.13. In the related setting of (weighted) discrete graphs, an important concept is the construction of boundaries by employing C^*-algebra techniques (this includes both *Royden* and *Kuramochi boundaries*, see [33, 46, 51, 59, 68] for further details and references). Finite volume graph ends can also be constructed by using this method. Indeed, $\mathcal{A} := H^1(\mathcal{G}) \subset C_b(\mathcal{G})$ is a subalgebra by Lemma 3.2 and hence its $\|\cdot\|_\infty$-closure $\widetilde{\mathcal{A}} := \overline{\mathcal{A}}^{\|\cdot\|_\infty}$ is isomorphic to $C_0(\widetilde{X})$, where $\widetilde{X}$ is the space of characters equipped with the weak*-topology with respect to $\widetilde{\mathcal{A}}$. In general, finding $\widetilde{X}$ for some concrete C^*-algebra is a rather complicated task. However, it turns out that in our situation $\widetilde{X}$ coincides with $\widetilde{\mathcal{G}} := \mathcal{G} \cup \mathfrak{C}_0(\mathcal{G})$. Indeed, $\widetilde{\mathcal{G}} = \mathcal{G} \cup \mathfrak{C}_0(\mathcal{G})$ equipped with the induced topology of the end compactification $\widehat{\mathcal{G}}$ is a locally compact Hausdorff space. Proposition 3.5 together with Theorem 3.9 shows that each function $f \in H^1(\mathcal{G})$ has a unique continuous extension to $\widetilde{\mathcal{G}}$ and this extension belongs to $C_0(\widetilde{\mathcal{G}})$. Moreover, by Theorem 3.9, $H^1(\mathcal{G})$ is point-separating and nowhere vanishing on $\widetilde{\mathcal{G}}$ and hence $\widetilde{\mathcal{A}} = C_0(\widetilde{\mathcal{G}})$ by the Stone–Weierstrass theorem. Thus the resulting boundary notion is precisely the space of finite volume graph ends.

Let us also mention that $\widetilde{\mathcal{G}}$ is compact only if $\mathrm{vol}(\mathcal{G}) < \infty$ and in this case one can show that the Royden compactification of $\mathcal{G}$ as well as its Kuramochi compactification coincide with the end compactification $\widehat{\mathcal{G}}$ (see [33], [46, Theorem 7.11], [47, p.215] and also [39, p.2] for the discrete case).

4. Deficiency indices

Intuitively, deficiency indices should be linked to *boundary notions* for underlying combinatorial graphs. However, spectral properties of the operator $\mathbf{H}_0$ also depend on the edge lengths and this suggests that it is difficult to expect a purely combinatorial formula for the deficiency indices $\mathrm{n}_\pm(\mathbf{H}_0)$ of $\mathbf{H}_0$. Recall that throughout the paper we always assume that $\mathcal{G}$ satisfies Hypothesis 2.1.

4.1. Deficiency indices and graph ends.

The main result of this section provides criteria which allow to connect $\mathrm{n}_\pm(\mathbf{H}_0)$ with the number of graph ends.

Theorem 4.1. *Let $\mathcal{G}$ be a metric graph and let $\mathbf{H}_0$ be the corresponding minimal Kirchhoff Laplacian. Then*

$$\mathrm{n}_\pm(\mathbf{H}_0) \geq \#\mathfrak{C}_0(\mathcal{G}). \tag{4.1}$$

Moreover, the equality

$$\mathrm{n}_\pm(\mathbf{H}_0) = \#\mathfrak{C}_0(\mathcal{G}) \tag{4.2}$$

holds true if and only if either $\#\mathfrak{C}_0(\mathcal{G}) = \infty$ or $\mathrm{dom}(\mathbf{H}) \subset H^1(\mathcal{G})$.

Remark 4.2. Since the map

$$\begin{array}{cccc} D\colon & H^1(\mathcal{G}) & \to & L^2(\mathcal{G}) \\ & f & \mapsto & f' \end{array}$$

is bounded, the inclusion $\mathrm{dom}(\mathbf{H}) \subset H^1(\mathcal{G})$ holds true if and only if there is a positive constant $C > 0$ such that

$$\|f'\|^2_{L^2(\mathcal{G})} \leq C(\|f\|^2_{L^2(\mathcal{G})} + \|f''\|^2_{L^2(\mathcal{G})}) \tag{4.3}$$

holds for all $f \in \mathrm{dom}(\mathbf{H})$. It can be shown by examples that (4.3) may fail.

Before proving Theorem 4.1, let us first comment on some of its immediate consequences.

Corollary 4.3. *If $\mathcal{G}$ is a metric graph with finite total volume* $\operatorname{vol}(\mathcal{G}) < \infty$*, then*

$$\mathrm{n}_{\pm}(\mathbf{H}_0) \geq \#\Omega(\mathcal{G}_d). \tag{4.4}$$

Moreover,

$$\mathrm{n}_{\pm}(\mathbf{H}_0) = \#\Omega(\mathcal{G}_d) \tag{4.5}$$

if and only if either $\mathcal{G}$ contains a non-free end (and hence $\#\Omega(\mathcal{G}_d) = \infty$ in this case) or $\ker(\mathbf{H}) \subset H^1(\mathcal{G})$*.*

In fact, we only need to mention that by Halin's theorem [36] (see Remark 2.5(v)) and the finite total volume of $\mathcal{G}$, $\#\mathfrak{C}_0(\mathcal{G}) = \infty$ only if $\mathcal{G}$ contains a non-free end.

Recall that for a finitely generated group G, the number of graph ends of a Cayley graph is independent of the generating set (see, e.g., [30]). Combining this fact with the above statement, we obtain the following result.

Corollary 4.4. *Let $\mathcal{G}_d$ be a Cayley graph of a finitely generated countable group G with infinitely many ends.*[5] *If* $\operatorname{vol}(\mathcal{G}) < \infty$*, then* $\mathrm{n}_{\pm}(\mathbf{H}_0) = \infty$*.*

4.2. **Proof of Theorem 4.1.** The proof of Theorem 4.1 is based on the following observation. Let $\mathbf{H}_F$ be the Friedrichs extension of $\mathbf{H}_0$. Then $\operatorname{dom}(\mathbf{H})$ admits the following decomposition

$$\operatorname{dom}(\mathbf{H}) = \operatorname{dom}(\mathbf{H}_F) \dotplus \ker(\mathbf{H} - z) = \operatorname{dom}(\mathbf{H}_F) \dotplus \mathcal{N}_z(\mathbf{H}_0), \tag{4.6}$$

for every z in the resolvent set $\rho(\mathbf{H}_F)$ of $\mathbf{H}_F$ (see, e.g., [66, Proposition 14.11]). In particular, (4.6) holds for all $z \in (-\infty, \lambda_0(\mathcal{G}))$, where $\lambda_0(\mathcal{G}) \geq 0$ is defined by (2.16). Moreover, $\operatorname{dom}(\mathbf{H}_F) \subset H^1_0(\mathcal{G})$ and hence the inclusion $\operatorname{dom}(\mathbf{H}) \subset H^1(\mathcal{G})$ depends only on the inclusion $\ker(\mathbf{H} - z) \subset H^1(\mathcal{G})$ for some (and hence for all) $z \in \rho(\mathbf{H}_F)$. Let us stress that $\mathcal{N}_0(\mathbf{H}_0) = \ker(\mathbf{H}) = \mathbb{H}(\mathcal{G}) \cap L^2(\mathcal{G})$ and hence in the case $\lambda_0(\mathcal{G}) > 0$, one is interested in whether all L^2 harmonic functions belong to $H^1(\mathcal{G})$ or not, which is known to depend on the geometry of the underlying metric graph.

We also need the following fact stating that functions in $\mathcal{N}_\lambda(\mathbf{H}_0)$ with $\lambda \in (-\infty, 0)$ can be considered as subharmonic functions and hence they should satisfy a maximum principle.

Lemma 4.5. *Suppose $\mathcal{G}$ is a metric graph and let $\lambda \in (-\infty, 0)$.*

(i) *If $f \in \mathcal{N}_\lambda(\mathbf{H}_0) = \ker(\mathbf{H} - \lambda)$ is real-valued and $f(x_0) > 0$ for some $x_0 \in \mathcal{G}$, then*

$$\sup_{x\in\mathcal{G}} f(x) = \sup_{v\in\mathcal{V}} f(v). \tag{4.7}$$

(ii) *If additionally $f \in H^1(\mathcal{G})$, then*

$$\sup_{x\in\mathcal{G}} f(x) = \sup_{\gamma\in\mathfrak{C}(\mathcal{G})} f(\gamma). \tag{4.8}$$

(iii) *If (not necessarily real-valued) $f \in \mathcal{N}_\lambda(\mathbf{H}_0) \cap H^1(\mathcal{G})$ satisfies*

$$f(\gamma) = 0 \tag{4.9}$$

for all $\gamma \in \mathfrak{C}(\mathcal{G})$, then $f \equiv 0$.

[5] A classification of groups having infinitely many ends is given in Stallings's ends theorem [70] (see also [30, Theorem 13.5.10] and Remark 2.5(iv)).

Proof. (i) Let $f \in \mathcal{N}_\lambda(\mathbf{H}_0)$ be real-valued. If $x \in \mathcal{G}$ is such that $f(x) > 0$ and $e \in \mathcal{E}$ is an edge with $x \in e$, then upon identifying e with the interval $\mathcal{I}_e = [0, |e|]$ and taking into account that $-f'' = \lambda f$ on e, we get

$$f(y) = f(x)\cosh\left(\sqrt{-\lambda}(y-x)\right) + \frac{f'(x)}{\sqrt{-\lambda}}\sinh\left(\sqrt{-\lambda}(y-x)\right) \tag{4.10}$$

for all $y \in e$. If $f'(x) \geq 0$, then obviously $f(e_i) \geq f(x)$, where e_i is the vertex of e identified with the right endpoint of $\mathcal{I}_e$. Similarly, $f(e_o) \geq f(x)$ for the other vertex e_o of e if $f'(x) < 0$. Hence f attains its maximum on e at the vertices of e, which clearly implies (4.7).

(ii) Now let $v \in \mathcal{V}$ be a vertex with $f(v) > 0$. By (2.6), there is an edge $e \in \mathcal{E}_v$ such that $f_e'(v) \geq 0$. If $u \in \mathcal{V}$ is the other vertex of e, then by (4.10) we get

$$f(u) = f(v)\cosh\left(\sqrt{-\lambda}|e|\right) + \frac{f_e'(v)}{\sqrt{-\lambda}}\sinh\left(\sqrt{-\lambda}|e|\right) > f(v).$$

Observe that $f_e'(u) < 0$. Hence, setting $v_0 = v$ and $v_1 = u$ and using induction, we can construct a ray $\mathcal{R} = (v_n)$ such that $f(v_{n+1}) > f(v_n)$ for all $n \geq 0$. Since $f \in H^1(\mathcal{G})$, we get

$$0 < f(v) < \lim_{n\to\infty} f(v_n) = f(\gamma_{\mathcal{R}}) \leq \sup_{\gamma\in\mathfrak{C}(\mathcal{G})} f(\gamma),$$

which proves (4.8).

(iii) By considering $\pm f$ (and splitting into real and imaginary part, if necessary), (4.9) clearly follows from (4.8). $\square$

Remark 4.6. Notice that the arguments used in the proof of Lemma 4.5(ii) in fact show that functions in $\mathcal{N}_\lambda(\mathbf{H}_0)$ with $\lambda \in (-\infty, 0)$ admitting positive values on $\mathcal{G}$ cannot attain global maxima in $\mathcal{G}$, that is, if f attains a positive value at some $x \in \mathcal{G}$, then for every compact subgraph $\widetilde{\mathcal{G}} \subset \mathcal{G}$ the following holds

$$\sup_{x\in\mathcal{G}} f(x) = \sup_{x\in\mathcal{G}\setminus\widetilde{\mathcal{G}}} f(x).$$

Clearly, analogous statements hold true for functions admitting negative values, however, then sup must be replaced with inf.

Lemma 4.7. *Suppose $\mathcal{G}$ is a metric graph and let $\lambda \in (-\infty, 0)$. Then*

$$\dim(\mathcal{N}_\lambda \cap H^1(\mathcal{G})) = \#\mathfrak{C}_0(\mathcal{G}). \tag{4.11}$$

Proof. Using (4.6) with $z = \lambda \in (-\infty, 0)$ and noting that $\operatorname{dom}(\mathbf{H}_F) \subset H_0^1(\mathcal{G})$, Theorem 3.9 and Theorem 3.11 imply that $\dim(\mathcal{N}_\lambda \cap H^1(\mathcal{G})) \geq \#\mathfrak{C}_0(\mathcal{G})$. The converse inequality follows from Lemma 4.5(iii), which shows that the mapping $f \mapsto (f(\gamma))_{\gamma\in\mathfrak{C}_0(\mathcal{G})}$ is injective on $\mathcal{N}_\lambda \cap H^1(\mathcal{G})$. $\square$

After all these preparations, we are now in position to complete the proof of Theorem 4.1.

Proof of Theorem 4.1. Observe that the inequality (4.1) immediately follows from (4.6) and (4.11) since $\mathrm{n}_\pm(\mathbf{H}) = \dim(\mathcal{N}_\lambda)$.

Clearly, the second claim is trivial if $\#\mathfrak{C}_0(\mathcal{G}) = \infty$. Hence it remains to show that in the case $\#\mathfrak{C}_0(\mathcal{G}) < \infty$ equality (4.2) holds exactly when $\operatorname{dom}(\mathbf{H}) \subset H^1(\mathcal{G})$. Applying (4.6) once again, the inclusion $\operatorname{dom}(\mathbf{H}) \subset H^1(\mathcal{G})$ holds true exactly when $\mathcal{N}_\lambda \subset H^1(\mathcal{G})$. Taking into account once again that $\mathrm{n}_\pm(\mathbf{H}) = \dim(\mathcal{N}_\lambda)$ and using (4.11), we arrive at the conclusion. $\square$

Remark 4.8. Let us mention that one can prove the second claim of Theorem 4.1 in a different way. Namely, if $\#\mathfrak{C}_0(\mathcal{G}) < \infty$, then it is possible to reduce the problem to the study of a finite volume graph with a single end.

Let us stress that in the proof of Theorem 4.1 the inclusion $\mathrm{dom}(\mathbf{H}) \subset H^1(\mathcal{G})$ was proved in the case when all finite volume ends are free. The next result shows that it never holds if there is a finite volume end which is not free.

Proposition 4.9. *Let $\mathcal{G}$ be a metric graph having a finite volume end which is not free. Then there exists a function $f \in \mathrm{dom}(\mathbf{H})$ which does not belong to $H^1(\mathcal{G})$.*

Proof. To simplify considerations we restrict to the case of a metric graph $\mathcal{G}$ having finite total volume (the general case can easily be shown by similar methods upon restricting to a finite volume subgraph with compact boundary).

Let $\widetilde{\mathcal{G}} \subset \mathcal{G}$ be a connected, compact subgraph and consider the finitely many connected components of $\mathcal{G}\backslash\widetilde{\mathcal{G}}$. Since $\mathcal{G}$ has infinitely many ends, there is a connected component U which contains at least two distinct graph ends $\gamma, \gamma' \in \mathfrak{C}(\mathcal{G})$. Following the proof of Theorem 3.9, we readily construct a real-valued function $f = f_U \in \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$ with $f(\gamma) = 0$, $f(\gamma') = 1$ and $0 \le f \le 1$ on $\mathfrak{C}(\mathcal{G})$ (in fact, it suffices to choose the corresponding function ϕ with $0 \le \phi \le 1$). Taking into account Theorem 3.11 and decomposition (4.6), we can assume that f belongs to $H^1(\mathcal{G}) \cap \mathcal{N}_\lambda$ for some (fixed) $\lambda \in (-\infty, 0)$. However, Lemma 4.5 (iii) implies that

$$\|f\|_\infty = \sup_{x\in\mathcal{G}} |f(x)| = \sup_{x\in\mathcal{G}} f(x) = 1.$$

On the other hand, there exist two rays $\mathcal{R}$, $\mathcal{R}' \in \mathfrak{R}(\mathcal{G}_d)$ representing the ends γ and, respectively, γ' such that both $\mathcal{R}$, $\mathcal{R}'$ are contained in U and have the same initial vertex v_0. This leads to another estimate

$$\begin{aligned} 1 &= \big|f(\gamma) - f(\gamma')\big| = \big|f(\gamma) - f(v_0) + f(v_0) - f(\gamma')\big| \\ &= \Big| \int_{\mathcal{R}} f'(x)dx - \int_{\mathcal{R}'} f'(x)dx \Big| \le 2\sqrt{\mathrm{vol}(U)}\, \|f'\|_{L^2(U)} \le 2\sqrt{\mathrm{vol}(\mathcal{G})}\, \|f'\|_{L^2(\mathcal{G})}. \end{aligned}$$

Assume now that (4.3) holds for all functions $g \in \mathcal{N}_\lambda$. Then $\|\cdot\|_\infty$ and $\|\cdot\|_{H^1}$ are in fact equivalent norms on $\mathcal{N}_\lambda$. Indeed, combining (4.3) and the finite volume property,

$$\|g\|^2_{H^1} \le C(\|g\|^2_{L^2} + \|\mathbf{H}g\|^2_{L^2}) = C(1+\lambda^2)\|g\|^2_{L^2} \le C(1+\lambda^2)\mathrm{vol}(\mathcal{G})\|g\|^2_\infty$$

for all $g \in \mathcal{N}_\lambda$, whereas $\|g\|_\infty \le C_{\mathcal{G}}\|g\|_{H^1}$ by Lemma 3.2. Choosing compact subgraphs $\widetilde{\mathcal{G}}_\varepsilon$ with $\mathrm{vol}(\mathcal{G} \setminus \widetilde{\mathcal{G}}_\varepsilon) \le \varepsilon^2$ (which is possible since $\mathcal{G}$ has finite volume), we clearly get $\mathrm{vol}(U_\varepsilon) \le \varepsilon^2$ and hence the above constructed function $f_\varepsilon = f_{U_\varepsilon} \in H^1(\mathcal{G}) \cap \mathcal{N}_\lambda$ satisfies

$$\|f'_\varepsilon\|_{L^2(\mathcal{G})} \ge \|f'_\varepsilon\|_{L^2(U_\varepsilon)} \ge \frac{1}{2\sqrt{\mathrm{vol}(U_\varepsilon)}} \ge \frac{1}{2\varepsilon}.$$

However, by construction, $\|f_\varepsilon\|_\infty = 1$, which obviously contradicts to the equivalence of norms $\|\cdot\|_\infty$ and $\|\cdot\|_{H^1}$ on $\mathcal{N}_\lambda$ since $\varepsilon > 0$ is arbitrary. □

We conclude this section by mentioning some explicit examples.

Example 4.10 (Radially symmetric trees)**.** Let $\mathcal{G} = \mathcal{T}$ be a *radially symmetric (metric) tree*: that is, a rooted tree $\mathcal{T}$ such that for each $n \ge 0$, all vertices in the combinatorial sphere S_n have the same number of descendants and all edges between the combinatorial spheres S_n and S_{n+1} have the same length. It is well-known that in this case $\mathbf{H}$ is self-adjoint if and only if $\mathrm{vol}(\mathcal{T}) = \infty$ and deficiency indices are infinite, $\mathrm{n}_\pm(\mathbf{H}_0) = \infty$, otherwise (see, e.g., [13, 69]). Moreover, due to the symmetry assumptions, all graph ends are of finite volume simultaneously. Hence we arrive at the equality

$$\mathrm{n}_\pm(\mathbf{H}_0) = \#\mathfrak{C}_0(\mathcal{G}) = \begin{cases} \infty, & \text{if } \mathrm{vol}(\mathcal{T}) < \infty, \\ 0, & \text{if } \mathrm{vol}(\mathcal{T}) = \infty \end{cases}.$$

Moreover, by Theorem 4.1 and Proposition 4.9, the inclusion $\mathrm{dom}(\mathbf{H}) \subset H^1(\mathcal{G})$ holds true if and only if $\mathrm{vol}(\mathcal{T}) = \infty$.

Example 4.11 (Radially symmetric antitrees)**.** Consider a metric antitree $\mathcal{G} = \mathcal{A}$ (see Section 7.1 for definitions) and additionally suppose that $\mathcal{A}$ is *radially symmetric*, that is, for each $n \geq 0$, all edges between the combinatorial spheres S_n and S_{n+1} have the same length. Combining [54, Theorem 4.1] (see also Corollary 7.3 below) with the fact that antitrees have exactly one graph end, $\#\mathfrak{C}(\mathcal{A}) = 1$, we conclude that

$$\mathrm{n}_\pm(\mathbf{H}_0) = \#\mathfrak{C}_0(\mathcal{G}) = \begin{cases} 1, & \text{if } \mathrm{vol}(\mathcal{A}) < \infty, \\ 0, & \text{if } \mathrm{vol}(\mathcal{A}) = \infty \end{cases}.$$

In particular, $\mathbf{H}$ is self-adjoint if and only if $\mathrm{vol}(\mathcal{A}) = \infty$. Moreover, the inclusion $\mathrm{dom}(\mathbf{H}) \subset H^1(\mathcal{G})$ holds true for all radially symmetric antitrees by Theorem 4.1.

Remark 4.12. Both radially symmetric trees and antitrees are particular examples of the so-called *family preserving metric graphs* (see [11] and also [10]) . Employing the results from [11], it is in fact possible to extend the conclusions in Example 4.10 and Example 4.11 to this general setting. More precisely, for each *family preserving metric graph $\mathcal{G}$ without horizontal edges*, the Kirchhoff Laplacian $\mathbf{H}$ is self-adjoint if and only if $\mathrm{vol}(\mathcal{G}) = \infty$ and moreover

$$\mathrm{n}_\pm(\mathbf{H}_0) = \#\mathfrak{C}_0(\mathcal{G}) = \begin{cases} \#\mathfrak{C}(\mathcal{G}), & \text{if } \mathrm{vol}(\mathcal{G}) < \infty \\ 0, & \text{if } \mathrm{vol}(\mathcal{G}) = \infty \end{cases}.$$

If in addition $\mathcal{G}$ has finitely many ends, then the inclusion $\mathrm{dom}(\mathbf{H}) \subset H^1(\mathcal{G})$ holds true. On the other hand, if $\mathcal{G}$ has infinitely many ends, then $\mathrm{dom}(\mathbf{H}) \subset H^1(\mathcal{G})$ holds true if and only if $\mathrm{vol}(\mathcal{G}) = \infty$. The last two statements are again immediate consequences of Theorem 4.1 and Proposition 4.9.

In conclusion, let us also emphasize that the example of the rope ladder graph in Appendix B shows that the assumption on horizontal edges cannot be omitted. More precisely, the rope ladder graph is a *family preserving graph* in the sense of [10] with exactly one graph end. However, it possesses infinitely many horizontal edges (i.e., edges connecting vertices in the same combinatorial sphere) and Example B.5 shows that in general $\mathrm{n}_\pm(\mathbf{H}_0) > \#\mathfrak{C}_0(\mathcal{G})$, even if the edge lengths are chosen symmetrically to the root, $|e_n^+| = |e_n^-|$ for all $n \in \mathbb{Z}_{\geq 0}$.

5. Properties of self-adjoint extensions

The Sobolev space $H^1(\mathcal{G})$ plays a distinctive role in the study of self-adjoint extensions of the minimal operator $\mathbf{H}_0$. A self-adjoint extension $\widetilde{\mathbf{H}}$ of $\mathbf{H}_0$ is called a *finite energy extension* if its domain is contained in $H^1(\mathcal{G})$, that is, every function $f \in \mathrm{dom}(\widetilde{\mathbf{H}})$ has finite energy, $\|f'\|_{L^2(\mathcal{G})} < \infty$. The main result of this section already indicates that finite energy self-adjoint extensions of the minimal operator (notice that among those are the Friedrichs extension and, as we will see later in this section, all Markovian extensions) possess a number of important properties.

Theorem 5.1. *Let $\widetilde{\mathbf{H}}$ be a self-adjoint lower semibounded extension of $\mathbf{H}_0$. Assume that z belongs to its resolvent set $\rho(\widetilde{\mathbf{H}})$. Then the following assertions hold.*

(i) If the form domain of $\widetilde{\mathbf{H}}$ is contained in $H^1(\mathcal{G})$, then the resolvent $\mathcal{R}(z, \widetilde{\mathbf{H}})$ of $\widetilde{\mathbf{H}}$ is an integral operator whose kernel $\mathcal{K}_z$ is both of class $L^\infty(\mathcal{G}\times\mathcal{G})$ and jointly Hölder continuous of exponent $\beta = 1/2$.

(ii) If additionally $\mathcal{G}$ has finite total volume, then $\mathcal{R}(z, \widetilde{\mathbf{H}})$ is of trace class.

Proof. (i) Let $\widetilde{\mathbf{H}}$ be a self-adjoint lower semibounded extension of $\mathbf{H}_0$, $\widetilde{\mathbf{H}} \geq c$ for some $c \in \mathbb{R}$. Without loss of generality we may assume $c = 0$. Then we can consider its positive semi-definite square root $\widetilde{\mathbf{H}}^{1/2}$, which is again self-adjoint and whose domain agrees with the form domain of $\widetilde{\mathbf{H}}$. Accordingly, for all $z \in \mathbb{C} \setminus [0, \infty)$ and $\lambda = \sqrt{z}$ we get

$$\big(\widetilde{\mathbf{H}}^{1/2} - \lambda\big)\big(\widetilde{\mathbf{H}}^{1/2} + \lambda\big) = \widetilde{\mathbf{H}} - z,$$

and hence

$$\mathcal{R}(z, \widetilde{\mathbf{H}}) = \mathcal{R}(\lambda, \widetilde{\mathbf{H}}^{1/2})\mathcal{R}(-\lambda, \widetilde{\mathbf{H}}^{1/2}). \tag{5.1}$$

If the form domain of $\widetilde{\mathbf{H}}$ is contained in $H^1(\mathcal{G})$, and hence by Lemma 3.2 in $C_b(\mathcal{G})$, then $\mathcal{R}(\pm\lambda, \widetilde{\mathbf{H}}^{1/2})$ maps $L^2(\mathcal{G})$ into $L^\infty(\mathcal{G})$, and hence by duality also maps $L^1(\mathcal{G})$ into $L^2(\mathcal{G})$. Thus (5.1) implies that $\mathcal{R}(z, \widetilde{\mathbf{H}})$ maps $L^1(\mathcal{G})$ into $L^\infty(\mathcal{G})$ and hence, by the Kantorovich–Vulikh theorem (see, e.g., [4, Theorem 1.3] or [58, Theorem 1.1]), $\mathcal{R}(z, \widetilde{\mathbf{H}})$ is an integral operator with the L^∞-kernel $\mathcal{K}(z; \cdot, \cdot)$.

In order to prove the assertion about joint Hölder continuity, we need to take a closer look at the kernel $\mathcal{K}$ by adapting the proof of [3, Prop. 2.1]: as noticed before, the resolvent $\mathcal{R}(\lambda, \widetilde{\mathbf{H}}^{1/2})$ is bounded from $L^2(\mathcal{G})$ to $L^\infty(\mathcal{G})$ by Lemma 3.2 for any λ in the resolvent set of $\widetilde{\mathbf{H}}^{1/2}$. Applying the Kantorovich–Vulikh theorem (see, e.g., [4, page 113]) once again, we see that

$$\mathcal{R}(\lambda, \widetilde{\mathbf{H}}^{1/2})u(x) = \int_{\mathcal{G}} u(y)\kappa(\lambda, x; y)dy = \langle u, \kappa(\lambda, x; \cdot)^*\rangle_{L^2(\mathcal{G})}$$

for all $x \in \mathcal{G}$ and some $\kappa(\lambda, x; \cdot) \in L^2(\mathcal{G})$ such that $\sup_{x\in\mathcal{G}} \|\kappa(\lambda, x; \cdot)\|_{L^2(\mathcal{G})} < \infty$. Moreover, observe that there exists $C = C(\lambda) > 0$ such that

$$\|\kappa(\lambda, x; \cdot) - \kappa(\lambda, x'; \cdot)\|_{L^2(\mathcal{G})} \leq C\sqrt{\varrho(x, x')} \tag{5.2}$$

for all $x, x' \in \mathcal{G}$, where $\varrho(x, x')$ denotes the distance in the natural path metric on $\mathcal{G}$. Indeed, for any function $u \in L^2(\mathcal{G})$,

$$\begin{aligned}\Big|\int_{\mathcal{G}} u(y)(\kappa(\lambda, x; y) - \kappa(\lambda, x'; y))dy\Big| &= \big|\mathcal{R}(\lambda, \widetilde{\mathbf{H}}^{1/2})u(x) - \mathcal{R}(\lambda, \widetilde{\mathbf{H}}^{1/2})u(x')\big| \\ &\leq \sqrt{\varrho(x, x')}\|\mathcal{R}(\lambda, \widetilde{\mathbf{H}}^{1/2})u\|_{H^1} \\ &\leq C\sqrt{\varrho(x, x')}\|u\|_{L^2},\end{aligned} \tag{5.3}$$

where we have used the Cauchy–Schwarz inequality and the fact that the resolvent $\mathcal{R}(\lambda, \widetilde{\mathbf{H}}^{1/2})$ is a bounded operator from L^2 to the domain of $\widetilde{\mathbf{H}}^{1/2}$ equipped with the graph norm, and (5.2) immediately follows. Now, taking into account the equalities (5.1) and $\mathcal{R}(\lambda,\widetilde{\mathbf{H}}^{1/2})^* = \mathcal{R}(\lambda^*,\widetilde{\mathbf{H}}^{1/2})$, we conclude that

$$\begin{aligned}
\mathcal{R}(z,\widetilde{\mathbf{H}})u(x) &= \mathcal{R}(\lambda,\widetilde{\mathbf{H}}^{1/2})\big(\mathcal{R}(-\lambda,\widetilde{\mathbf{H}}^{1/2})u\big)(x)\\
&= \big\langle \mathcal{R}(-\lambda,\widetilde{\mathbf{H}}^{1/2})u, \kappa(\lambda,x;\cdot)^*\big\rangle_{L^2(\mathcal{G})}\\
&= \big\langle u, \mathcal{R}(-\lambda^*,\widetilde{\mathbf{H}}^{1/2})\kappa(\lambda,x;\cdot)^*\big\rangle_{L^2(\mathcal{G})}\\
&= \int_{\mathcal{G}} u(y)\int_{\mathcal{G}} \kappa(\lambda,x;s)\kappa(-\lambda^*,y;s)^* ds\, dy\\
&=: \int_{\mathcal{G}} u(y)\mathcal{K}(z;x,y)\, dy,
\end{aligned}$$

for all $u \in L^2(\mathcal{G})$. It remains to prove that the mapping

$$\mathcal{K} : \mathcal{G}\times\mathcal{G} \ni (x,y) \mapsto \int_{\mathcal{G}} \kappa(\lambda,x;s)\kappa(-\lambda^*,y;s)^* ds \in \mathbb{C}$$

is jointly Hölder continuous. However, recalling that $\sup_{x\in\mathcal{G}} \|\kappa(\lambda,x;\cdot)\|_{L^2(\mathcal{G})} < \infty$, this immediately follows from (5.2), since

$$\begin{aligned}
|\mathcal{K}(x,y) - \mathcal{K}(x',y')| \le{}& \|\kappa(\lambda,x;\cdot)(\kappa(-\lambda^*,y;\cdot)^* - \kappa(-\lambda^*,y';\cdot)^*)\|_{L^1}\\
&+ \|\kappa(-\lambda^*,y';\cdot)^*(\kappa(\lambda,x;\cdot) - \kappa(\lambda,x';\cdot))\|_{L^1}.
\end{aligned}$$

for all pairs $(x,y),(x',y') \in \mathcal{G}\times\mathcal{G}$.

(ii) If $\mathcal{G}$ has finite total volume, then $L^\infty(\mathcal{G}\times\mathcal{G}) \hookrightarrow L^2(\mathcal{G}\times\mathcal{G})$ and hence the resolvents $\mathcal{R}(\pm\lambda,\widetilde{\mathbf{H}}^{1/2})$ are Hilbert–Schmidt operators. Thus, by (5.1) we conclude that $\mathcal{R}(z,\widetilde{\mathbf{H}})$ is of trace class. □

Observe that the first step in the proof of Theorem 5.1 is the factorization (5.1), which has the natural counterpart for semigroups

$$\mathrm{e}^{-z\widetilde{\mathbf{H}}}\,\mathrm{e}^{-z\widetilde{\mathbf{H}}} = \mathrm{e}^{-2z\widetilde{\mathbf{H}}}, \qquad \operatorname{Re} z > 0.$$

Because the semigroup generated by a self-adjoint semibounded extension $\widetilde{\mathbf{H}}$ is analytic, it is a bounded operator from the Hilbert space into its generator's form domain whenever $\operatorname{Re} z > 0$. A careful look at the proof of Theorem 5.1 shows that this is sufficient to establish that $\mathrm{e}^{-z\widetilde{\mathbf{H}}}$ is an integral operator; all further steps in the proof of Theorem 5.1 carry over almost verbatim to the study of semigroups. We can hence easily deduce the following result.

Theorem 5.2. *Let $\widetilde{\mathbf{H}}$ be a self-adjoint lower semibounded extension of $\mathbf{H}_0$ and let $z \in \mathbb{C}$ with $\operatorname{Re} z > 0$. Then the following assertions hold.*

- *(i) If the domain of $\widetilde{\mathbf{H}}$ is contained in $H^1(\mathcal{G})$, then the semigroup $\mathrm{e}^{-z\widetilde{\mathbf{H}}}$ generated by $\widetilde{\mathbf{H}}$ is an integral operator whose kernel is both of class $L^\infty(\mathcal{G}\times\mathcal{G})$ and jointly Hölder continuous of exponent $\beta = 1/2$.*
- *(ii) If additionally $\mathcal{G}$ has finite total volume, then $\mathrm{e}^{-z\widetilde{\mathbf{H}}}$ is of trace class.*

Estimating as in (5.3) and using analyticity of $\mathrm{e}^{-z\widetilde{\mathbf{H}}}$ yields the inequality

$$|p_t(x,y) - p_t(x',y)| \le \frac{C}{\sqrt{t}}\sqrt{\varrho(x,x')}, \qquad t > 0,\ x,y,x' \in \mathcal{G}, \tag{5.4}$$

for the heat kernel $p_t(x,y)$ of a nonnegative extension $\widetilde{\mathbf{H}}$, where in contrast to (5.3) the constant $C > 0$ is independent of $t > 0$. Such Hölder estimates are known to be related to Sobolev-type inequalities and also important for upper and lower Gaussian bounds (cf., e.g., [18], [62, Chapter 6]). However, we do not pursue this line of study here and this will be done elsewhere.

Remark 5.3. A few remarks are in order.

(i) If $\mathcal{G}$ has finite diameter (see (3.3)), then the path metric ϱ has a natural extension to the end compactification and moreover $(\widehat{\mathcal{G}}, \varrho)$ is a metric completion of $\mathcal{G}$ (see Remark 3.10 and [32, p. 1526]). In this case, Theorem 5.1 and Theorem 5.2 imply that the corresponding resolvent and semigroup kernels have a bounded and uniformly continuous extension to $(\widehat{\mathcal{G}}, \varrho)$, however, we emphasize that if $\mathrm{vol}(\mathcal{G}) = \infty$, then in general $(\widehat{\mathcal{G}}, d)$ is not homeomorphic to the end compactification (cf., e.g., [32, p. 1526]).

(ii) Discreteness of the spectrum of the Friedrichs extension $\mathbf{H}_F$ is a standard fact in the case of finite total volume (see, e.g., [14, Prop. 3.11] or [54, Corollary 3.5(iv)]). However, Theorem 5.1(ii) implies the stronger assertion that the resolvent of $\mathbf{H}_F$ belongs to the trace class if $\mathrm{vol}(\mathcal{G}) < \infty$. Let us also stress that it is not true in general that every self-adjoint extension of $\mathbf{H}$ will have a discrete spectrum if $\mathrm{vol}(\mathcal{G}) < \infty$, since in case of infinite deficiency indices such a self-adjoint extension could have a domain large enough to make compactness of the embedding of $H^1(\mathcal{G})$ into $L^2(\mathcal{G})$ irrelevant.

Recall that a self-adjoint extension $\widetilde{\mathbf{H}}$ of $\mathbf{H}_0$ is called *Markovian* if $\widetilde{\mathbf{H}}$ is a non-negative self-adjoint extension and the corresponding quadratic form is a *Dirichlet form* (for definitions and further details we refer to [29, Chapter 1]). Hence the associated semigroup $\mathrm{e}^{-t\widetilde{\mathbf{H}}}$, $t > 0$ as well as resolvents $\mathcal{R}(-\lambda, \widetilde{\mathbf{H}})$, $\lambda > 0$ are Markovian: i.e., are both *positivity preserving* (map non-negative functions to non-negative functions) and L^∞*-contractive* (map the unit ball of $L^\infty(\mathcal{G})$, and then by duality of $L^p(\mathcal{G})$ for all $p \in [1, \infty]$, into itself). Let us stress that the Friedrichs extension $\mathbf{H}_F$ of $\mathbf{H}_0$ is a Markovian extension. Consider also the following quadratic form in $L^2(\mathcal{G})$

$$\mathfrak{t}_N[f] = \int_{\mathcal{G}} |f'(x)|^2 dx, \qquad \mathrm{dom}(\mathfrak{t}_N) = H^1(\mathcal{G}). \tag{5.5}$$

This form is non-negative and closed, hence we can associate in $L^2(\mathcal{G})$ a self-adjoint operator with it, let us denote it by $\mathbf{H}_N$. We will refer to it as the *Neumann extension*. It is straightforward to check that $\mathfrak{t}_N$ is a Dirichlet form and $\mathbf{H}_N$ is also a Markovian extension of $\mathbf{H}_0$.

It turns out that Theorems 5.1 and 5.2 apply to all Markovian extensions of $\mathbf{H}_0$. More specifically, the analog of the results for discrete Laplacians [37, Theorem 5.2] and Laplacians in Euclidean domains [29, Chapter 3] and Riemannian manifolds [35, Theorem 1.7] holds true for quantum graphs as well.

Theorem 5.4. *If $\widetilde{\mathbf{H}}$ is a Markovian extension of $\mathbf{H}_0$, then $\mathrm{dom}(\widetilde{\mathbf{H}}) \subset H^1(\mathcal{G})$ and, moreover,*

$$\mathbf{H}_N \le \widetilde{\mathbf{H}} \le \mathbf{H}_F, \tag{5.6}$$

where the inequalities are understood in the sense of forms.[6]

[6]We shall write $A \le B$ for two non-negative self-adjoint operators A and B if their quadratic forms $\mathfrak{t}_A$ and $\mathfrak{t}_B$ satisfy $\mathrm{dom}(\mathfrak{t}_B) \subseteq \mathrm{dom}(\mathfrak{t}_A)$ and $\mathfrak{t}_A[f] \le \mathfrak{t}_B[f]$ for every $f \in \mathrm{dom}(\mathfrak{t}_B)$.

We omit the proof of Theorem 5.4 since the proofs of either [37, Theorem 5.2] or [35, Lemma 3.6] carry over verbatim to our setting (see also the proof of [29, Theorem 3.3.1]).

Let us finish this section with the following observation.

Corollary 5.5. *The following are equivalent:*

(i) $\mathbf{H}_0$ *has a unique Markovian extension,*
(ii) $H^1_0(\mathcal{G}) = H^1(\mathcal{G})$,
(iii) *all topological ends of* $\mathcal{G}$ *have infinite volume,* $\mathfrak{C}_0(\mathcal{G}) = \emptyset$.

Proof. The claimed equivalences follow from Theorem 5.4 and Corollary 3.12. $\square$

Remark 5.6. Let us finish this section with a few comments.

(i) The equivalence $(i) \Leftrightarrow (ii)$ in Corollary 5.5 is known for Riemannian manifolds [35, Theorem 1.7] (see also [29, Chapter 3], [57, Theorem 1]) as well as for weighted Laplacians on graphs [37, Corollary 5.6]. However, to the best of our knowledge these settings do not admit any further geometric characterization.

(ii) The list of equivalences in Corollary 5.5 can be extended by adding a claim on the self-adjointness of the so-called *Gaffney Laplacian*. Namely, since $H^1_0(\mathcal{G})$ and $H^1(\mathcal{G})$ are Hilbert spaces, the operators denoted by ∇_D and ∇_N and defined in $L^2(\mathcal{G})$ on the domains, respectively, $H^1_0(\mathcal{G})$ and $H^1(\mathcal{G})$ by $f \mapsto f'$ are closed. Notice that with this notation at hand we have $\mathbf{H}_F = \nabla_D^*\nabla_D$ and $\mathbf{H}_N = \nabla_N^*\nabla_N$. Now we can introduce the Gaffney Laplacian $\mathbf{H}_G = \nabla_D^*\nabla_N$ as the restriction of the maximal operator $\mathbf{H}$ onto the domain
$$\operatorname{dom}(\mathbf{H}_G) := \{f \in H^1(\mathcal{G}) |\, \nabla_N f \in \operatorname{dom}(\nabla_D^*)\}. \tag{5.7}$$
Clearly, $\mathbf{H}_F \subseteq \mathbf{H}_G$, $\mathbf{H}_N \subseteq \mathbf{H}_G$, and $\mathbf{H}_G$ is not necessarily symmetric. It turns out that $\mathbf{H}_G$ is symmetric (and hence self-adjoint) if and only if the Kirchhoff Laplacian $\mathbf{H}_0$ has a unique Markovian extension. Moreover, in this case $\mathbf{H}_F = \mathbf{H}_N = \mathbf{H}_G$ (cf. [35, Theorem 1.7(ii)] in the manifold setting). Let us also mention that all Markovian/finite energy extensions of $\mathbf{H}_0$ are exactly the Markovian/self-adjoint restrictions of $\mathbf{H}_G$ and in particular the deficiency indices of $\mathbf{H}_G^* = \nabla_N^*\nabla_D$ are equal to $\#\mathfrak{C}_0(\mathcal{G})$.

6. Finite energy self-adjoint extensions

It turns out that finite volume (topological) ends provide the right notion of the boundary for metric graphs to deal with finite energy and also with Markovian extensions of the minimal Kirchhoff Laplacian $\mathbf{H}_0$. In particular, we are going to show that this end space is well-behaved as concerns the introduction of both traces and normal derivatives. More specifically, the goal of this section is to give a description of finite energy self-adjoint extensions of $\mathbf{H}_0$ in the case when the number of finite volume ends of $\mathcal{G}$ is finite, that is, $\#\mathfrak{C}_0(\mathcal{G}) < \infty$. Notice that in this case all finite volume ends are free.

6.1. **Normal derivatives at graph ends.** Let $\widetilde{\mathcal{G}} = (\widetilde{\mathcal{V}}, \widetilde{\mathcal{E}})$ be a (possibly infinite) connected subgraph of $\mathcal{G}$. Recall that its boundary $\partial\widetilde{\mathcal{G}}$ (w.r.t. the natural topology on $\mathcal{G}$, see Section 2.1) is given by
$$\partial\widetilde{\mathcal{G}} = \big\{v \in \widetilde{\mathcal{V}} |\ \deg_{\widetilde{\mathcal{G}}}(v) < \deg_{\mathcal{G}}(v)\big\}. \tag{6.1}$$

For a function $f \in \operatorname{dom}(\mathbf{H})$, we define its (inward) *normal derivative* at $v \in \partial\widetilde{\mathcal{G}}$ by

$$\frac{\partial f}{\partial n_{\widetilde{\mathcal{G}}}}(v) := \sum_{e \in \mathcal{E}_v \cap \widetilde{\mathcal{E}}} f_e'(v). \tag{6.2}$$

With this definition at hand, we end up with the following useful integration by parts formula.

Lemma 6.1. *Let $\widetilde{\mathcal{G}}$ be a compact (not necessarily connected) subgraph of the metric graph $\mathcal{G}$. Then*

$$-\int_{\widetilde{\mathcal{G}}} f''(x)g(x)dx = \int_{\widetilde{\mathcal{G}}} f'(x)g'(x)dx + \sum_{v \in \partial\widetilde{\mathcal{G}}} g(v)\frac{\partial f}{\partial n_{\widetilde{\mathcal{G}}}}(v) \tag{6.3}$$

for all $f \in \operatorname{dom}(\mathbf{H})$ and $g \in H^1(\widetilde{\mathcal{G}})$. In particular,

$$-\int_{\widetilde{\mathcal{G}}} f''(x)dx = \sum_{v \in \partial\widetilde{\mathcal{G}}} \frac{\partial f}{\partial n_{\widetilde{\mathcal{G}}}}(v). \tag{6.4}$$

Proof. The claim follows immediately from integrating by parts, taking into account that f satisfies (2.6). Setting $g \equiv 1$ in (6.3), we arrive at (6.4). □

In order to simplify our considerations, we need to introduce the following notion. Let $\gamma \in \mathfrak{C}(\mathcal{G})$ be a (topological) end of $\mathcal{G}$. Consider a sequence $(\mathcal{G}_n)$ of connected subgraphs of $\mathcal{G}$ such that $\mathcal{G}_n \supseteq \mathcal{G}_{n+1}$ and $\#\partial\mathcal{G}_n < \infty$ for all n. We say that the sequence $(\mathcal{G}_n)$ is a *graph representation of the end* $\gamma \in \mathfrak{C}(\mathcal{G})$ if there is a sequence of open sets $\mathcal{U} = (U_n)$ representing γ such that for each $n \geq 0$ there exist j and k such that $\mathcal{G}_n \supseteq U_j$ and $U_n \supseteq \mathcal{G}_k$. It is easily seen that all graphs $\mathcal{G}_n$ are infinite (they have infinitely many edges). Moreover, representing sequences $(\mathcal{G}_n)$ can be constructed with the help of compact exhaustions; in particular each graph end $\gamma \in \mathfrak{C}(\mathcal{G})$ has a representation by subgraphs (see Section 2.2).

Proposition 6.2. *Let $\mathcal{G}$ be a metric graph and let $\gamma \in \mathfrak{C}(\mathcal{G})$ be a free end of finite volume. Then for every function $f \in \operatorname{dom}(\mathbf{H})$ and any sequence $(\mathcal{G}_k)$ of subgraphs representing γ, the limit*

$$\lim_{k\to\infty} \sum_{v \in \partial\mathcal{G}_k} \frac{\partial f}{\partial n_{\mathcal{G}_k}}(v) \tag{6.5}$$

exists and is independent of the choice of $(\mathcal{G}_k)$.

Proof. First of all, notice that uniqueness of the limit follows from the inclusion property in the definition of the graph representations of γ. Hence we only need to show that the limit in (6.5) indeed exists.

Let $(\mathcal{G}_k)$ be a graph representation of a free finite volume end $\gamma \in \mathfrak{C}_0(\mathcal{G})$. Since γ is free, we can assume that $\operatorname{vol}(\mathcal{G}_0) < \infty$ and that $\mathcal{G}_0 \cap U_k = \varnothing$ eventually for every sequence $\mathcal{U} = (U_k)$ representing an end $\gamma' \neq \gamma$. First observe that $\widetilde{\mathcal{G}} = \mathcal{G}_k \setminus \mathcal{G}_j$ can again be identified with a compact subgraph of $\mathcal{G}$ whenever $k \leq j$. Indeed, if $\widetilde{\mathcal{G}}$ has infinitely many edges $\{e_n\} \subset \mathcal{E}$, choose for each n a point x_n in the interior of the edge e_n. Since $\widehat{\mathcal{G}} = \mathcal{G} \cup \mathfrak{C}(\mathcal{G})$ is compact, the set $\{x_n\}$ has an accumulation point $x \in \widehat{\mathcal{G}}$. By construction, $x \notin \mathcal{G}$ and hence $x \in \widehat{\mathcal{G}} \setminus \mathcal{G} = \mathfrak{C}(\mathcal{G})$ is an end. However, we have that $x_n \notin \mathcal{G}_j$ and recalling (2.2) and (2.3), this implies that $x = \gamma'$ for a topological end $\gamma' \neq \gamma$. On the other hand, $x_n \in \mathcal{G}_0$ for all n and using the properties of $\mathcal{G}_0$ and (2.2)–(2.3) once again, we arrive at a contradiction.

Now, using (6.1) it is straightforward to verify that

$$\sum_{v\in\partial\mathcal{G}_k}\frac{\partial f}{\partial n_{\mathcal{G}_k}}(v)-\sum_{v\in\partial\mathcal{G}_j}\frac{\partial f}{\partial n_{\mathcal{G}_j}}(v)=\sum_{v\in\partial\widetilde{\mathcal{G}}}\frac{\partial f}{\partial n_{\widetilde{\mathcal{G}}}}(v).$$

Hence by (6.4) and the Cauchy–Schwarz inequality, we get

$$\Big|\sum_{v\in\partial\mathcal{G}_k}\frac{\partial f}{\partial n_{\mathcal{G}_k}}(v)-\sum_{v\in\partial\mathcal{G}_j}\frac{\partial f}{\partial n_{\mathcal{G}_j}}(v)\Big|=\Big|\int_{\mathcal{G}_k\setminus\mathcal{G}_j}f''(x)dx\Big|\le\sqrt{\mathrm{vol}(\mathcal{G}_k)}\,\|\mathbf{H}f\|_{L^2(\mathcal{G})},\tag{6.6}$$

whenever $k\le j$. This implies the existence of the limit in (6.5) since $\mathrm{vol}(\mathcal{G}_k)=o(1)$ as $k\to\infty$. □

Proposition 6.2 now enables us to introduce a normal derivative at graph ends.

Definition 6.3. Let $\gamma\in\mathfrak{C}(\mathcal{G})$ be a free end of finite volume and let $(\mathcal{G}_k)$ be a graph representation of γ. Then for every $f\in\mathrm{dom}(\mathbf{H})$

$$\partial_n f(\gamma):=\frac{\partial f}{\partial n}(\gamma):=\lim_{k\to\infty}\sum_{v\in\partial\mathcal{G}_k}\frac{\partial f}{\partial n_{\mathcal{G}_k}}(v)\tag{6.7}$$

is called the *normal derivative* of f at γ.

Remark 6.4. In fact, it is not difficult to extend the definitions (6.2) and (6.7) to general sequences $\mathcal{U}=(U_n)$ of open sets representing the free end $\gamma\in\mathfrak{C}_0(\mathcal{G})$. However, while the idea of the proof of Proposition 6.2 naturally carries over, the analysis becomes more technical and we restrict to the case of subgraphs for the sake of a clear exposition.

Let us mention that the normal derivative can also be expressed in terms of compact exhaustions.

Lemma 6.5. *Let $\mathcal{G}$ be a metric graph having finite total volume and only one end γ, $\mathfrak{C}(\mathcal{G})=\{\gamma\}$. If $(\mathcal{G}_k)$ is a compact exhaustion of $\mathcal{G}$ and $f\in\mathrm{dom}(\mathbf{H})$, then*

$$\partial_n f(\gamma)=-\lim_{k\to\infty}\sum_{v\in\partial\mathcal{G}_k}\frac{\partial f}{\partial n_{\mathcal{G}_k}}(v).\tag{6.8}$$

The fact that we are not approximating γ by its neighborhoods, but rather by compact subgraphs, is responsible for the different sign in (6.7) and (6.8).

Proof. First of all, notice that $\mathcal{G}\setminus\mathcal{G}_k$ can be identified with a subgraph of $\mathcal{G}$ and

$$-\sum_{v\in\partial\mathcal{G}_k}\frac{\partial f}{\partial n_{\mathcal{G}_k}}(v)=\sum_{v\in\partial(\mathcal{G}\setminus\mathcal{G}_k)}\frac{\partial f}{\partial n_{\mathcal{G}\setminus\mathcal{G}_k}}(v)$$

for all $f\in\mathrm{dom}(\mathbf{H})$. If, moreover, $\mathcal{G}\setminus\mathcal{G}_k$ is a connected subgraph for all $k\ge 0$, then it is clear that $(\mathcal{G}_k')$ with $\mathcal{G}_k':=\mathcal{G}\setminus\mathcal{G}_k$ for all $k\ge 0$, is a graph representation of γ and this proves (6.8) in this case.

If $\mathcal{G}\setminus\mathcal{G}_k$ is not connected, then it has only one infinite connected component $\mathcal{G}_k^\gamma$ and finitely many compact components (since $\mathfrak{C}(\mathcal{G})=\{\gamma\}$). Adding these compact components to $\mathcal{G}_k$, we obtain a compact exhaustion $(\widetilde{\mathcal{G}}_k)$ with $\mathcal{G}\setminus\widetilde{\mathcal{G}}_k = \mathcal{G}_k^\gamma$. Arguing as in the proof of Proposition 6.2 (see (6.6)), we get

$$\Big|\sum_{v\in\partial\widetilde{\mathcal{G}}_k}\frac{\partial f}{\partial n_{\widetilde{\mathcal{G}}_k}}(v) - \sum_{v\in\partial\mathcal{G}_k}\frac{\partial f}{\partial n_{\mathcal{G}_k}}(v)\Big| = \Big|\int_{\widetilde{\mathcal{G}}_k\setminus\mathcal{G}_k} f''(x)dx\Big| = o(1)$$

as $k\to\infty$. Hence (6.8) holds true also in the general case. $\square$

6.2. **Properties of the trace and normal derivatives.** In this section, we collect some basic properties of the trace maps. We shall adopt the following notation. Since we shall always assume throughout this section that $\#\mathfrak{C}_0(\mathcal{G})<\infty$, we set $\mathcal{H} := \ell^2(\mathfrak{C}_0(\mathcal{G}))$, which can be further identified with $\mathbb{C}^{\#\mathfrak{C}_0(\mathcal{G})}$. Next, we introduce the maps $\Gamma_0\colon H^1(\mathcal{G})\to\mathcal{H}$ and $\Gamma_1\colon \operatorname{dom}(\mathbf{H})\cap H^1(\mathcal{G})\to\mathcal{H}$ by

$$\Gamma_0\colon f\mapsto \big(f(\gamma)\big)_{\gamma\in\mathfrak{C}_0(\mathcal{G})}, \qquad\qquad \Gamma_1\colon f\mapsto \big(\partial_n f(\gamma)\big)_{\gamma\in\mathfrak{C}_0(\mathcal{G})}, \tag{6.9}$$

where the boundary values and normal derivative of f are defined by (3.3) and (6.7), respectively.

Proposition 6.6. *Let $\mathcal{G}$ be a metric graph with $\#\mathfrak{C}_0(\mathcal{G})<\infty$. Then:*

(i) For every $\widehat{f}\in\mathcal{H}$, there exists $f\in\operatorname{dom}(\mathbf{H})\cap H^1(\mathcal{G})$ such that

$$\Gamma_0 f = \widehat{f}, \qquad\qquad \Gamma_1 f = 0.$$

(ii) Moreover, the Gauss–Green formula

$$\langle \mathbf{H}f, g\rangle_{L^2(\mathcal{G})} = \langle f', g'\rangle_{L^2(\mathcal{G})} - \langle\Gamma_1 f, \Gamma_0 g\rangle_{\mathcal{H}}, \tag{6.10}$$

holds true for every $f\in\operatorname{dom}(\mathbf{H})\cap H^1(\mathcal{G})$ and $g\in H^1(\mathcal{G})$.

Proof. (i) Since $\#\mathfrak{C}_0(\mathcal{G})<\infty$, each finite volume end $\gamma\in\mathfrak{C}_0(\mathcal{G})$ is free. For every $\gamma\in\mathfrak{C}_0(\mathcal{G})$, let $\mathcal{G}^\gamma$ be a subgraph with the properties as in Remark 2.6. We can also assume that $\operatorname{vol}(\mathcal{G}^\gamma)<\infty$. Following the proof of Theorem 3.9, we can construct for each end $\gamma\in\mathfrak{C}_0(\mathcal{G})$ a function $f_\gamma\in\operatorname{dom}(\mathbf{H})\cap H^1(\mathcal{G})$ such that f_γ is non-constant only on finitely many edges (since $\#\partial\mathcal{G}^\gamma<\infty$), $f_\gamma(\gamma)=1$ and $f_\gamma(\gamma')=0$ for all other ends $\gamma'\in\mathfrak{C}_0(\mathcal{G})\setminus\{\gamma\}$. Clearly, $\Gamma_1 f_\gamma = 0$ for every $\gamma\in\mathfrak{C}_0(\mathcal{G})$. Thus, setting

$$f = \sum_{\gamma\in\mathfrak{C}_0(\mathcal{G})}\widehat{f}(\gamma)f_\gamma$$

for a given $\widehat{f}\in\mathcal{H}$, we clearly have $\Gamma_0 f = \widehat{f}$ and $\Gamma_1 f = 0$.

(ii) Let us first show that (6.10) holds true for all $f\in\operatorname{dom}(\mathbf{H})\cap H^1(\mathcal{G})$ if $g = f_\gamma\in H^1(\mathcal{G})$. Take a compact exhaustion $(\mathcal{G}_k)$ of $\mathcal{G}$. Then by Lemma 6.1,

$$\begin{aligned}\langle\mathbf{H}f, f_\gamma\rangle_{L^2(\mathcal{G})} - \langle f', f_\gamma'\rangle_{L^2(\mathcal{G})} &= \lim_{k\to\infty}\langle\mathbf{H}f, f_\gamma\rangle_{L^2(\mathcal{G}_k)} - \langle f', f_\gamma'\rangle_{L^2(\mathcal{G}_k)}\\ &= \lim_{k\to\infty}\sum_{v\in\partial\mathcal{G}_k}\frac{\partial f}{\partial n_{\mathcal{G}_k}}(v)f_\gamma(v)^* = \lim_{k\to\infty}\sum_{v\in\partial\mathcal{G}_k\cap\mathcal{V}^\gamma}\frac{\partial f}{\partial n_{\mathcal{G}_k}}(v),\end{aligned}$$

where $\mathcal{V}^\gamma$ is the set of vertices of $\mathcal{G}^\gamma$. Notice that the subgraph $\mathcal{G}^\gamma$ itself is a connected infinite graph having finite total volume and exactly one end, which can be identified with γ in an obvious way. Moreover, setting $\mathcal{G}_k^\gamma := \mathcal{G}_k\cap\mathcal{G}^\gamma$ for all $k\geq 0$ and noting that $\mathcal{G}_k^\gamma$ is connected for all sufficiently large k, the sequence $(\mathcal{G}_k^\gamma)$ provides a compact exhaustion of $\mathcal{G}^\gamma$. Since $\partial_{\mathcal{G}^\gamma}\mathcal{G}_k^\gamma = \partial\mathcal{G}_k\cap\mathcal{V}^\gamma$ and

$$\frac{\partial f}{\partial n_{\mathcal{G}_k^\gamma}}(v) = \frac{\partial f}{\partial n_{\mathcal{G}_k}}(v), \qquad v\in\partial_{\mathcal{G}^\gamma}\mathcal{G}_k^\gamma,$$

for all large enough $k \geq 0$, we get by applying Lemma 6.5

$$\langle \mathbf{H}f, f_\gamma\rangle_{L^2(\mathcal{G})} - \langle f', f'_\gamma\rangle_{L^2(\mathcal{G})} = \lim_{k\to\infty} \sum_{v\in\mathcal{G}_k\cap\mathcal{V}^\gamma} \frac{\partial f}{\partial n_{\mathcal{G}_k^\gamma}}(v) = -\frac{\partial f}{\partial n}(\gamma).$$

Hence (6.10) holds true if $g = f_\gamma \in H^1(\mathcal{G})$.

Now observe that a simple integration by parts implies that (6.10) is valid for all compactly supported $g \in H^1(\mathcal{G})$. By continuity and Theorem 3.11 this extends further to all $g \in H^1_0(\mathcal{G})$. Finally, setting $\tilde{g} := g - \sum_{\gamma\in\mathfrak{C}_0(\mathcal{G})} g(\gamma) f_\gamma$ for $g \in H^1(\mathcal{G})$, it is immediate to check that, by Theorem 3.11, $\tilde{g} \in H^1_0(\mathcal{G})$. It remains to use the linearity of Γ_0. □

It turns out that the domain of the Neumann extension admits a simple description.

Corollary 6.7. *Let $\mathcal{G}$ be a metric graph with $\#\mathfrak{C}_0(\mathcal{G}) < \infty$. Then the Neumann extension $\mathbf{H}_N$ is given as the restriction $\mathbf{H}_N = \mathbf{H}|_{\mathrm{dom}(\mathbf{H}_N)}$ to the domain*

$$\mathrm{dom}(\mathbf{H}_N) = \big\{ f \in \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G}) |\, \Gamma_1 f = 0 \big\}. \tag{6.11}$$

Proof. By the first representation theorem [48, Chapter VI.2.1], $\mathrm{dom}(\mathbf{H}_N)$ consists of all functions $f \in H^1(\mathcal{G})$ such that there exists $h \in L^2(\mathcal{G})$ with

$$\langle f', g'\rangle_{L^2(\mathcal{G})} = \langle h, g\rangle_{L^2(\mathcal{G})}, \qquad \text{for all } g \in H^1(\mathcal{G}).$$

Moreover, in this case $\mathbf{H}_N f := h$. Taking into account Proposition 6.6 and the fact that $\mathbf{H}_N$ is a restriction of $\mathbf{H}$, we immediately arrive at (6.11). □

Our next goal is to prove surjectivity of the normal derivative map.

Proposition 6.8. *If $\mathcal{G}$ is a metric graph with $\#\mathfrak{C}_0(\mathcal{G}) < \infty$, then the mapping Γ_1 is surjective.*

In fact, Proposition 6.8 will follow from the following lemma.

Lemma 6.9. *Suppose $\mathcal{G}$ is a metric graph with $\mathrm{vol}(\mathcal{G}) < \infty$ and only one end, $\mathfrak{C}(\mathcal{G}) = \{\gamma\}$. Then there exists $f \in \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$ such that*

$$\partial_n f(\gamma) \neq 0.$$

Proof. We will proceed by contradiction. Suppose that $\partial_n g(\gamma) = 0$ for all $g \in \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$. Then, by Corollary 6.7, $\mathrm{dom}(\mathbf{H}_F) \subseteq \mathrm{dom}(\mathbf{H}_N) = \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$. However, both $\mathbf{H}_F$ and $\mathbf{H}_N$ are self-adjoint restrictions of $\mathbf{H}$ and hence $\mathrm{dom}(\mathbf{H}_F) = \mathrm{dom}(\mathbf{H}_N)$. Therefore, $\mathbf{H}_F = \mathbf{H}_N$ and their quadratic forms also coincide, which implies that $H^1_0(\mathcal{G}) = H^1(\mathcal{G})$. This contradicts Corollary 3.12 and hence completes the proof. □

Proof of Proposition 6.8. Let $\mathcal{G}^\gamma$, $\gamma \in \mathfrak{C}_0(\mathcal{G})$ be the subgraphs of $\mathcal{G}$ constructed in the proof of Proposition 6.6(i). Every $\mathcal{G}^\gamma$ is a connected graph with $\mathrm{vol}(\mathcal{G}^\gamma) < \infty$ and only one end, which can be identified with γ. Hence we can apply Lemma 6.9 to obtain a function $\tilde{g}_\gamma \in \mathrm{dom}(\mathbf{H}^\gamma) \cap H^1(\mathcal{G}^\gamma)$ such that $\partial_n \tilde{g}_\gamma(\gamma) = 1$. Here $\mathbf{H}^\gamma$ denotes the Kirchhoff Laplacian on $\mathcal{G}^\gamma$.

Since $\#\partial\mathcal{G}^\gamma < \infty$, we can obviously extend $\tilde{g}_\gamma$ to a function g_γ on $\mathcal{G}$ such that $g_\gamma \in \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$ and g_γ is identically zero on a neighborhood of each end $\gamma' \neq \gamma$ (see also the proof of Theorem 3.9). In particular, this implies that $\partial_n g_\gamma(\gamma') = 0$

for all $\gamma' \in \mathfrak{C}_0(\mathcal{G}) \setminus \{\gamma\}$. Upon identification of γ with the single end of $\mathcal{G}^\gamma$ we also have that

$$\partial_n g_\gamma(\gamma) = \partial_n \tilde{g}_\gamma(\gamma) = 1.$$

This immediately implies surjectivity. $\square$

6.3. **Description of self-adjoint extensions.** Our next goal is a description of all finite energy self-adjoint extensions of $\mathbf{H}_0$, that is, self-adjoint extensions $\widetilde{\mathbf{H}}$ satisfying the inclusion $\mathrm{dom}(\widetilde{\mathbf{H}}) \subset H^1(\mathcal{G})$. We would be able to do this under the additional assumption that $\mathcal{G}$ has finitely many finite volume ends. Recall that in this case $\mathcal{H} = \ell^2(\mathfrak{C}_0(\mathcal{G}))$ is a finite dimensional Hilbert space.

Let C, D be two linear operators on $\mathcal{H}$ satisfying *Rofe-Beketov conditions* [64]:

$$CD^* = DC^*, \qquad \mathrm{rank}(C|D) = \dim \mathcal{H} = \#\mathfrak{C}_0(\mathcal{G}). \tag{6.12}$$

Consider the quadratic form $\mathfrak{t}_{C,D}$ defined by

$$\mathfrak{t}_{C,D}[f] := \int_{\mathcal{G}} |f'(x)|^2 dx + \langle D^{-1} C \Gamma_0 f, \Gamma_0 f \rangle_{\mathcal{H}} \tag{6.13}$$

on the domain

$$\mathrm{dom}(\mathfrak{t}_{C,D}) := \{ f \in H^1(\mathcal{G}) |\, \Gamma_0 f \in \mathrm{ran}(D^*)\}. \tag{6.14}$$

Here and in the following the mappings Γ_0 and Γ_1 are given by (6.9) and $D^{-1} \colon \mathrm{ran}(D) \to \mathrm{ran}(D^*)$ denotes the inverse of the restriction $D|_{\ker(D)^\perp} \colon \mathrm{ran}(D^*) \to \mathrm{ran}(D)$. In particular, (6.12) implies that $\mathfrak{t}_{C,D}[f]$ is well-defined for all $f \in \mathrm{dom}(\mathfrak{t}_{C,D})$ (see also (A.4)).

Remark 6.10. It is straightforward to check that $\mathfrak{t}_{I,0} = \mathfrak{t}_F$ and $\mathfrak{t}_{0,I} = \mathfrak{t}_N$ are the quadratic forms corresponding to the Friedrichs extension $\mathbf{H}_F$ and, respectively, Neumann extension $\mathbf{H}_N$ (see Remark 3.1 and (5.5)).

Now we are in position to state the main result of this section.

Theorem 6.11. *Let $\mathcal{G}$ be a metric graph with finitely many finite volume ends, $\#\mathfrak{C}_0(\mathcal{G}) < \infty$. Let also C, D be linear operators on $\mathcal{H}$ satisfying Rofe-Beketov conditions* (6.12). *Then:*

(i) The form $\mathfrak{t}_{C,D}$ given by (6.13), (6.14) *is closed and lower semibounded in $L^2(\mathcal{G})$.*

(ii) The self-adjoint operator $\mathbf{H}_{C,D}$ associated with the form $\mathfrak{t}_{C,D}$ is a self-adjoint extension of $\mathbf{H}_0$ and its domain is explicitly given by

$$\mathrm{dom}(\mathbf{H}_{C,D}) = \{ f \in \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G}) |\ C\Gamma_0 f + D\Gamma_1 f = 0\}. \tag{6.15}$$

(iii) Conversely, if $\widetilde{\mathbf{H}}$ is a self-adjoint extension of $\mathbf{H}_0$ such that $\mathrm{dom}(\widetilde{\mathbf{H}}) \subset H^1(\mathcal{G})$, then there are C, D satisfying (6.12) *such that $\widetilde{\mathbf{H}} = \mathbf{H}_{C,D}$.*

(iv) Moreover, $\widetilde{\mathbf{H}} = \mathbf{H}_{C,D}$ is a Markovian extension if and only if the corresponding quadratic form $\widehat{\mathfrak{t}}_{C,D}[y] = \langle D^{-1} C y, y \rangle_{\mathcal{H}}$, $\mathrm{dom}(\widehat{\mathfrak{t}}) = \mathrm{ran}(D^*)$ is a Dirichlet form on $\mathcal{H}$ in the wide sense.[7]

[7] Here we do not assume that $\widehat{\mathfrak{t}}$ is densely defined, see [29, p.29]. We stress that in order for $\widehat{\mathfrak{t}}$ to be a Dirichlet form even merely in the wide sense, it is necessary that $\mathrm{dom}(\widehat{\mathfrak{t}})$ is a sublattice of $\mathcal{H}$, hence that the orthogonal projector onto $\mathrm{ran}(D^*)$ is a positivity preserving operator.

Proof. (i) Since $\mathcal{H}$ is finite dimensional, it is straightforward to see that the form $\mathfrak{t}_{C,D}$ is closed and lower semibounded in $L^2(\mathcal{G})$ whenever C and D satisfy (6.12).

(ii) By the first representation theorem [48, Chapter VI.2.1], $\mathrm{dom}(\mathbf{H}_{C,D})$ consists of all functions $f \in \mathrm{dom}(\mathfrak{t}_{C,D}) \subseteq H^1(\mathcal{G})$ for which there exists $h \in L^2(\mathcal{G})$ such that

$$\langle f', g'\rangle_{L^2(\mathcal{G})} + \langle D^{-1}C\Gamma_0 f, \Gamma_0 g\rangle_{\mathcal{H}} = \langle h, g\rangle_{L^2(\mathcal{G})} \tag{6.16}$$

for all $g \in \mathrm{dom}(\mathfrak{t}_{C,D})$. Moreover, in this case $\mathbf{H}_{C,D} f := h$.

The Gauss–Green identity (6.10) implies that for any $f \in \mathrm{dom}(\mathbf{H}_{C,D})$ and $g \in \mathrm{dom}(\mathfrak{t}_{C,D})$,

$$\langle D^{-1}C\Gamma_0 f, \Gamma_0 g\rangle_{\mathcal{H}} = -\langle \Gamma_1 f, \Gamma_0 g\rangle_{\mathcal{H}}.$$

Taking into account the surjectivity property in Proposition 6.6(i), the inclusion "$\subseteq$" in (6.15) follows. The converse inclusion is then an immediate consequence of the Gauss–Green identity (6.10).

(iii) To prove the claim, it suffices to show that

$$\Theta = \{(\Gamma_0 f, \Gamma_1 f) |\, f \in \mathrm{dom}(\widetilde{\mathbf{H}})\} \subseteq \mathcal{H} \times \mathcal{H}$$

is a self-adjoint linear relation (for further details we refer to Appendix A). By definition (see (A.2)), Θ^* is given by

$$\Theta^* = \{(g, h) \in \mathcal{H} \times \mathcal{H} |\, \langle \Gamma_1 f, g\rangle_{\mathcal{H}} = \langle \Gamma_0 f, h\rangle_{\mathcal{H}} \text{ for all } f \in \mathrm{dom}(\widetilde{\mathbf{H}})\}.$$

The inclusion $\Theta \subseteq \Theta^*$ follows immediately from the Gauss–Green identity (6.10) and the self-adjointness of $\widetilde{\mathbf{H}}$. Indeed, we clearly have

$$0 = \langle \widetilde{\mathbf{H}} f, \tilde{f}\rangle_{L^2(\mathcal{G})} - \langle f, \widetilde{\mathbf{H}}\tilde{f}\rangle_{L^2(\mathcal{G})} = -\langle \Gamma_1 f, \Gamma_0 \tilde{f}\rangle_{\mathcal{H}} + \langle \Gamma_0 f, \Gamma_1 \tilde{f}\rangle_{\mathcal{H}}$$

for all functions $f, \tilde{f} \in \mathrm{dom}(\widetilde{\mathbf{H}})$. On the other hand, by Proposition 6.8 and Proposition 6.6, for any $(g, h) \in \Theta^*$ there is a function $\tilde{f} \in \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$ such that $g = \Gamma_0 \tilde{f}$ and $h = \Gamma_1 \tilde{f}$. Employing the identity (6.10) once again, we see that

$$\begin{aligned}\langle \widetilde{\mathbf{H}} f, \tilde{f}\rangle_{L^2(\mathcal{G})} &= \langle f', \tilde{f}'\rangle_{L^2(\mathcal{G})} - \langle \Gamma_1 f, g\rangle_{\mathcal{H}} \\ &= \langle f', \tilde{f}'\rangle_{L^2(\mathcal{G})} - \langle \Gamma_0 f, h\rangle_{\mathcal{H}} = \langle f, \mathbf{H}\tilde{f}\rangle_{L^2(\mathcal{G})}\end{aligned}$$

for all $f \in \mathrm{dom}(\widetilde{\mathbf{H}})$. Hence, $\tilde{f} \in \mathrm{dom}(\widetilde{\mathbf{H}})$ and in particular $(g, h) \in \Theta$. Since Θ is self-adjoint, there are C and D in $\mathcal{H}$ satisfying Rofe-Beketov conditions (6.12) and such that $\Theta = \{(f, g) \in \mathcal{H} \times \mathcal{H} |\, Cf + Dg = 0\}$.

(iv) The first direction of the equivalence is clear: since the quadratic form $\mathfrak{t}_N$ associated with the Neumann extension $\mathbf{H}_N$ is Markovian and

$$\Gamma_0(\varphi \circ f) = \big((\varphi \circ f)(\gamma)\big)_{\gamma \in \mathfrak{C}_0(\mathcal{G})} =: \varphi \circ (\Gamma_0 f)$$

for all functions $f \in H^1(\mathcal{G})$ and every normal contraction φ,[8] the extension $\mathbf{H}_{C,D}$ is Markovian if $\widehat{\mathfrak{t}}_{C,D}$ is a Dirichlet form on $\mathcal{H}$ in the wide sense.

To prove the converse direction, let, for simplicity, $f \in \mathrm{dom}(\widehat{\mathfrak{t}}_{C,D})$ be real-valued and fix some real-valued $\tilde{f} \in H^1(\mathcal{G})$ with $\Gamma_0 \tilde{f} = f$ (the existence of such an $\tilde{f}$ follows from Proposition 6.6). For any (real-valued) normal contraction $\varphi\colon \mathbb{R} \to \mathbb{R}$, we can construct a continuous and piecewise affine function $\psi\colon \mathbb{R} \to \mathbb{R}$ (i.e., ψ is affine on every component of $\mathbb{R} \setminus \{x_1, \dots, x_M\}$ for finitely many points $x_1, \dots, x_M$) such that $\psi(0) = 0$, $\psi(f(\gamma)) = \varphi(f(\gamma))$ for all $\gamma \in \mathfrak{C}_0(\mathcal{G})$ and $|\psi'(x)| = 1$ for almost

[8]A *normal contraction* is a function $\varphi\colon \mathbb{C} \to \mathbb{C}$ such that $\varphi(0) = 0$ and $|\varphi(x) - \varphi(y)| \le |x - y|$ for all $x, y \in \mathbb{C}$.

every $x \in \mathbb{R}$.[9] Notice that every function ψ with the above properties is a normal contraction. Hence, if $\mathfrak{t}_{C,D}$ is Markovian, it follows that $\psi \circ \tilde{f} \in \mathrm{dom}(\mathfrak{t}_{C,D})$. However, its boundary values are precisely given by

$$\Gamma_0(\psi \circ \tilde{f}) = \psi \circ f = \varphi \circ f$$

and we conclude that $\varphi \circ f$ belongs to $\mathrm{dom}(\widehat{\mathfrak{t}}_{C,D})$. Finally, the Markovian property of $\mathfrak{t}_{C,D}$ implies that

$$\mathfrak{t}_{C,D}[\psi \circ \tilde{f}] = \int_{\mathcal{G}} |(\psi \circ \tilde{f})'|^2 dx + \widehat{\mathfrak{t}}_{C,D}[\varphi \circ f] \le \mathfrak{t}_{C,D}[\tilde{f}] = \int_{\mathcal{G}} |\tilde{f}'|^2 dx + \widehat{\mathfrak{t}}_{C,D}[f],$$

and noticing that $|(\psi \circ \tilde{f})'| = |\tilde{f}'|$ almost everywhere on $\mathcal{G}$, the proof is complete. $\square$

Let us demonstrate Theorem 6.11 by applying it to Cayley graphs of finitely generated groups.

Corollary 6.12. *Let $\mathcal{G}_d$ be a Cayley graph of a finitely generated countable group G with one end. Then the Kirchhoff Laplacian $\mathbf{H}_0$ admits a unique Markovian extension if and only if the underlying metric graph $\mathcal{G} = (\mathcal{G}_d, |\cdot|)$ has infinite total volume,* $\mathrm{vol}(\mathcal{G}) = \infty$. *Moreover, if $\mathcal{G}$ has finite total volume, then the set of all Markovian extensions of $\mathbf{H}_0$ forms a one-parameter family given explicitly by*

$$\mathrm{dom}(\mathbf{H}_\theta) = \{f \in \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G}) |\ \cos(\theta)\Gamma_0 f + \sin(\theta)\Gamma_1 f = 0\}, \qquad (6.17)$$

where $\theta \in [0, \pi/2]$.

Taking into account that amenable groups have finitely many ends, the above result applies to amenable finitely generated countable groups, which are not virtually infinite cyclic (see Remark 2.5(iv)). In a similar way one can obtain a complete description of Markovian extensions in the case of virtually infinite cyclic groups, however, they have two ends and the corresponding description looks a little bit more cumbersome and we leave it to the reader (cf. [29, p.147]). The case of groups with infinitely many ends remains an open highly nontrivial problem.

Remark 6.13. A few remarks are in order.

(i) Let us mention that in the case when the domain of the maximal operator $\mathbf{H}$ is contained in $H^1(\mathcal{G})$ and $\mathcal{G}$ has finitely many finite volume ends (notice that by Theorem 4.1 in this case $\mathrm{n}_\pm(\mathbf{H}_0) = \#\mathfrak{C}_0(\mathcal{G}) < \infty$), *Proposition 6.11 provides a complete description of all self-adjoint extensions of* $\mathbf{H}_0$. Let us also mention that Proposition 6.11 provides a complete description of all self-adjoint restrictions of the Gaffney Laplacian $\mathbf{H}_G$, see Remark 5.6(ii).

(ii) Some of the results of this section extend (to a certain extent) to the case of infinitely many ends. Let us stress that by Proposition 4.9 in the case when $\mathcal{G}$ has a finite volume end which is not free the above results would lead only to some (not all!) self-adjoint extensions of $\mathbf{H}_0$. In our opinion, even in the case of radially symmetric trees having finite total volume the description of all self-adjoint extensions of $\mathbf{H}_0$ is a difficult problem.

[9]For instance, for any $s, L > 0$ such that $s \le L$, the function $\psi_0(x) := \frac{L+s}{2} - \left|x - \frac{L+s}{2}\right|$ satisfies $\psi_0(0) = 0$, $\psi_0(L) = s$ and $|\psi_0'| \equiv 1$. The construction in the general case follows easily from this example.

(iii) Similar relations between Markovian realizations of elliptic operators on domains or finite metric graphs (with general couplings at the vertices) on one hand, and Dirichlet property of the corresponding quadratic form's boundary term on the other hand, are of course well known in the literature (see, e.g., [12, Proposition 5.1], [55, Theorem 6.1], [45, Theorem 3.5]). However, the setting of infinite metric graphs additionally requires much more advanced considerations of combinatorial and topological nature. In particular, it seems noteworthy to us that the results of the previous sections provide the right notion of the boundary for metric graphs, namely, the set of finite volume ends, to deal with finite energy and also with Markovian extensions of the minimal Kirchhoff Laplacian. In particular, this end space is well-behaved as concerns the introduction of traces and normal derivatives.

(iv) Taking into account certain close relationships between quantum graphs and discrete Laplacians (see [25, §4]), one can easily obtain the results analogous to Theorem 4.1 and Theorem 6.11 for a particular class of discrete Laplacians on $\mathcal{G}_d$ defined by the following expression

$$(\tau f)(v) = \frac{1}{m(v)} \sum_{u\sim v} \frac{f(v)-f(u)}{|e_{u,v}|}, \quad v \in \mathcal{V}, \tag{6.18}$$

where m is the star weight (2.11). Markovian extensions of weighted discrete Laplacians were considered also in [50]. On the other hand, [50] does not contain a finiteness assumption, however, the conclusion in our setting appears to be slightly stronger than in [50, Theorem 3.5], where the correspondence between Markovian extensions and Markovian forms on the boundary is in general not bijective.

7. Deficiency indices of antitrees

The main aim of this section is to construct for any $N \in \mathbb{Z}_{\geq 1} \cup \{\infty\}$ a metric antitree such that the corresponding minimal Kirchhoff Laplacian $\mathbf{H}_0$ has deficiency indices $\mathrm{n}_\pm(\mathbf{H}_0) = N$. Our motivation stems from the fact that every antitree has exactly one end and hence, according to considerations in the previous sections, $\mathbf{H}_0$ admits at most one-parameter family of Markovian extensions.

7.1. **Antitrees.** Let $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ be a connected, simple combinatorial graph. Fix a root vertex $o \in \mathcal{V}$ and then order the graph with respect to the combinatorial spheres S_n, $n \geq 0$ (notice that $S_0 = \{o\}$). $\mathcal{G}_d$ is called an *antitree* if every vertex in S_n, $n \geq 1$, is connected to all vertices in S_{n-1} and S_{n+1} and no vertices in S_k for all $|k-n| \neq 1$ (see Figure 1). Notice that each antitree is uniquely determined by its sequence of sphere numbers (s_n), $s_n := \#S_n$ for $n \geq 0$.

While antitrees first appeared in connection with random walks [23, 52, 74], they were actively studied from various different perspectives in the last years (see [11, 20, 54] for quantum graphs and [19, Section 2] for further references).

Let us enumerate the vertices in every combinatorial sphere S_n by $(v_i^n)_{i=1}^{s_n}$ and denote the edge connecting v_i^n with v_j^{n+1} by e_{ij}^n, $1 \leq i \leq s_n$, $1 \leq j \leq s_{n+1}$. We shall always use $\mathcal{A}$ to denote (metric) antitrees.

It is clear that every (infinite) antitree has exactly one end. By Theorem 4.1, the deficiency indices of the corresponding minimal Kirchhoff Laplacian are at least 1 if $\mathrm{vol}(\mathcal{A}) < \infty$. On the other hand, under the additional symmetry assumption that

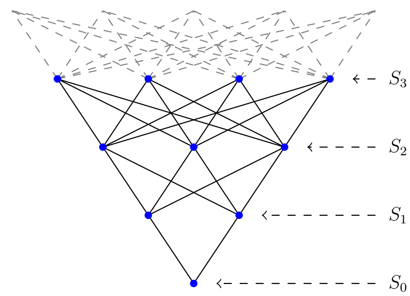

FIGURE 1. Antitree with sphere numbers $s_n = n + 1$.

$\mathcal{A}$ is radially symmetric (that is, for each $n \geq 0$, all edges connecting combinatorial spheres S_n and S_{n+1} have the same length), it is known that the deficiency indices are at most 1 (see [54, Theorem 4.1] and Example 4.11). It turns out that upon removing the symmetry assumption it is possible to construct antitrees such that the corresponding minimal Kirchhoff Laplacian has arbitrary finite or infinite deficiency indices. More precisely, the main aim of this section is to prove the following result.

Theorem 7.1. *Let $\mathcal{A}$ be the antitree with sphere numbers $s_n = n+1$, $n \geq 0$ (Figure 1). Then for each $N \in \mathbb{Z}_{\geq 1} \cup \{\infty\}$ there are lengths such that the corresponding minimal Kirchhoff Laplacian $\mathbf{H}_0$ has the deficiency indices $\mathrm{n}_\pm(\mathbf{H}_0) = N$.*

7.2. **Harmonic functions.** As it was mentioned already, every harmonic function is uniquely determined by its values at the vertices. On the other hand, $\mathbf{f} \in C(\mathcal{V})$ defines a function $f \in \mathbb{H}(\mathcal{A})$ with $f|_\mathcal{V} = \mathbf{f}$ if and only if the following conditions are satisfied:

$$\sum_{j=1}^{s_{n+1}} \frac{f(v_j^{n+1}) - f(v_k^n)}{|e_{kj}^n|} + \sum_{i=1}^{s_{n-1}} \frac{f(v_i^{n-1}) - f(v_k^n)}{|e_{ik}^{n-1}|} = 0, \tag{7.1}$$

at each v_k^n, $1 \leq k \leq s_n$ with $n \geq 0$. We set $s_{-1} := 0$ for notational simplicity and hence the second summand in (7.1) is absent when $n = 0$. We can put the above difference equations into the more convenient matrix form. Denote $\mathbf{f}_n = f|_{S_n} = (f(v_i^n))_{i=1}^{s_n}$ for all $n \in \mathbb{Z}_{\geq 0}$ and introduce matrices

$$M_{n+1} = \begin{pmatrix} \frac{1}{|e_{11}^n|} & \frac{1}{|e_{12}^n|} & \cdots & \frac{1}{|e_{1s_{n+1}}^n|} \\ \frac{1}{|e_{21}^n|} & \frac{1}{|e_{22}^n|} & \cdots & \frac{1}{|e_{2s_{n+1}}^n|} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{1}{|e_{s_n1}^n|} & \frac{1}{|e_{s_n2}^n|} & \cdots & \frac{1}{|e_{s_ns_{n+1}}^n|} \end{pmatrix} \in \mathbb{R}^{s_n \times s_{n+1}}, \tag{7.2}$$

and

$$D_n = \mathrm{diag}(d_k^n) \in \mathbb{R}^{s_n \times s_n}, \qquad d_k^n = \sum_{j=1}^{s_{n+1}} \frac{1}{|e_{kj}^n|} + \sum_{i=1}^{s_{n-1}} \frac{1}{|e_{ik}^{n-1}|}, \tag{7.3}$$

for all $n \in \mathbb{Z}_{\geq 0}$. Notice the following useful identity

$$d_1^0 = M_1 \mathbb{1}_{s_1}, \qquad \begin{pmatrix} d_1^n \\ \vdots \\ d_{s_n}^n \end{pmatrix} = D_n \mathbb{1}_{s_n} = (M_{n+1} \ M_n^*) \begin{pmatrix} \mathbb{1}_{s_{n+1}} \\ \mathbb{1}_{s_{n-1}} \end{pmatrix}, \quad n \geq 1, \tag{7.4}$$

where $\mathbb{1}_{s_n} := (1, \dots, 1)^\top \in \mathbb{C}^{s_n}$. Hence (7.1) can be written as follows

$$M_1 \mathbf{f}_1 = \sum_{j=1}^{s_1} \frac{1}{|e^0_{1j}|} \mathbf{f}_0 = d^0_1 \mathbf{f}_0, \tag{7.5}$$

$$M_{n+1} \mathbf{f}_{n+1} = D_n \mathbf{f}_n - M_n^* \mathbf{f}_{n-1}, \quad n \geq 1. \tag{7.6}$$

Since D_n is invertible, we get

$$\mathbf{f}_n = D_n^{-1} (M_{n+1}\ M_n^*) \begin{pmatrix} \mathbf{f}_{n+1} \\ \mathbf{f}_{n-1} \end{pmatrix} \tag{7.7}$$

for all $n \geq 1$. In particular, $\mathbf{f}_n \in \operatorname{ran}\left(D_n^{-1}(M_{n+1}\ M_n^*)\right)$ for all $n \geq 1$, which implies that the number of linearly independent solutions to the above difference equations (and hence the number of linearly independent harmonic functions) depends on the ranks of the matrices $(M_{n+1}\ M_n^*)$, $n \geq 1$. Let us demonstrate this by considering the following example.

Lemma 7.2. *Let $\mathcal{A}$ be a radially symmetric antitree. Then*

$$\mathbb{H}(\mathcal{A}) = \operatorname{span}\{\mathbb{1}_{\mathcal{G}}\}. \tag{7.8}$$

Proof. Let for each $n \geq 0$, all edges connecting combinatorial spheres S_n and S_{n+1} have the same length, say $\ell_n > 0$. Clearly, in this case

$$\operatorname{ran}(M_{n+1}) = \operatorname{ran}(M_n^*) = \operatorname{span}\{\mathbb{1}_{s_n}\},$$

for all $n \geq 1$. Moreover, each D_n is a scalar multiple of the identity matrix I_{s_n} and hence (7.7) implies that $\mathbf{f}_n = c_n \mathbb{1}_{s_n}$ with some $c_n \in \mathbb{C}$ for all $n \geq 0$. Plugging this into (7.5)–(7.6), we get

$$c_1 = c_0, \qquad\qquad c_{n+1} = c_n + \frac{s_{n-1}\ell_n}{s_{n+1}\ell_{n-1}}(c_n - c_{n-1}), \quad n \geq 1.$$

Hence $c_n = c_0 = f(o)$ for all $n \geq 0$, which proves the claim. □

The latter in particular implies the following statement (cf. [54, Theorem 4.1]).

Corollary 7.3. *If $\mathcal{A}$ is a radial antitree with finite total volume, then* $\mathrm{n}_\pm(\mathbf{H}_0) = 1$.

Proof. By Corollary 2.11, we only need to show that $\mathrm{n}_\pm(\mathbf{H}_0) \leq 1$. However, $\mathrm{n}_\pm(\mathbf{H}_0) = \dim(\ker(\mathbf{H})) \leq \dim(\mathbb{H}(\mathcal{A})) = 1$. □

7.3. **Finite deficiency indices.** We restrict our further considerations to a special case of polynomially growing antitrees. Namely, for every $N \in \mathbb{Z}_{\geq 1}$, the antitree $\mathcal{A}_N$ has sphere numbers $s_0 = 1$ and $s_n = n + N$ for all $n \in \mathbb{Z}_{\geq 1}$. To define its lengths, pick a sequence of positive numbers (ℓ_n) and set

$$|e^n_{ij}| = \begin{cases} 2\ell_n, & \text{if } 1 \leq i = j \leq N, \\ \ell_n, & \text{otherwise}, \end{cases} \tag{7.9}$$

for all $n \in \mathbb{Z}_{\geq 0}$.

Lemma 7.4. *If a metric antitree $\mathcal{A}_N$ has lengths given by* (7.9)*, then*

$$\dim \mathbb{H}(\mathcal{A}_N) = N + 1. \tag{7.10}$$

Proof. Denoting

$$B_{n,m} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & 1 & \dots & 1 \\ \dots & \dots & \dots & \dots \\ 1 & 1 & \dots & 1 \end{pmatrix} \in \mathbb{R}^{n\times m}, \qquad B_n := B_{n,n} \in \mathbb{C}^{n\times n}, \tag{7.11}$$

we get the following block-matrix form of the matrices M_{n+1}:

$$M_{n+1} = \frac{1}{\ell_n}\begin{pmatrix} B_N - \frac{1}{2}I_N & B_{N,n+1} \\ B_{n,N} & B_{n,n+1} \end{pmatrix} \tag{7.12}$$

for all $n \geq 1$. Taking into account (7.3) and denoting

$$d_n^1 = \frac{n+N-3/2}{\ell_{n-1}} + \frac{n+N+1/2}{\ell_n}, \quad d_n^2 = \frac{n+N-1}{\ell_{n-1}} + \frac{n+N+1}{\ell_n},$$

we get

$$D_n = \begin{pmatrix} d_n^1 I_N & \\ & d_n^2 I_n \end{pmatrix}, \tag{7.13}$$

for all $n \geq 2$. Since $M_1 \in \mathbb{C}^{1\times(N+1)}$ and

$$\operatorname{ran}(M_{n+1}) = \operatorname{ran}(M_n^*) = \operatorname{span}\left\{ \begin{pmatrix} \mathbf{f}_N \\ \mathbb{1}_n \end{pmatrix} \mid \mathbf{f}_N \in \mathbb{C}^N \right\}, \tag{7.14}$$

for all $n \geq 2$, (7.7) implies that every $\mathbf{f}$ solving (7.5)–(7.6) must be of the form

$$\mathbf{f}_n = \begin{pmatrix} \mathbf{f}_n^N \\ c_n \mathbb{1}_n \end{pmatrix} \in \mathbb{C}^{N+n}, \qquad \mathbf{f}_n^N \in \mathbb{C}^N, \quad c_n \in \mathbb{C}, \tag{7.15}$$

for all $n \geq 1$. Plugging (7.15) into (7.6) and taking into account that

$$B_N \mathbf{f}_n^N = \overline{\mathbf{f}}_n^N \mathbb{1}_N, \qquad \overline{\mathbf{f}}_n^N := \langle \mathbf{f}_n^N, \mathbb{1}_N \rangle = B_{1,N}\mathbf{f}_n^N,$$

we get after straightforward calculations

$$\frac{\overline{\mathbf{f}}_{n+1}^N + c_{n+1}(n+1)}{\ell_n}\mathbb{1}_N - \frac{1}{2\ell_n}\mathbf{f}_{n+1}^N = d_n^1\mathbf{f}_n^N - \frac{\overline{\mathbf{f}}_{n-1}^N + c_{n-1}(n-1)}{\ell_{n-1}}\mathbb{1}_N + \frac{1}{2\ell_{n-1}}\mathbf{f}_{n-1}^N, \tag{7.16}$$

$$\frac{\overline{\mathbf{f}}_{n+1}^N + c_{n+1}(n+1)}{\ell_n} = c_n d_n^2 - \frac{\overline{\mathbf{f}}_{n-1}^N + c_{n-1}(n-1)}{\ell_{n-1}}, \tag{7.17}$$

for all $n \geq 2$. Multiplying (7.17) with $\mathbb{1}_N$ and then subtracting (7.16), we end up with

$$\mathbf{f}_{n+1}^N = 2\ell_n(c_n d_n^2 \mathbb{1}_N - d_n^1 \mathbf{f}_n^N) - \frac{\ell_n}{\ell_{n-1}}\mathbf{f}_{n-1}^N, \quad n \geq 2. \tag{7.18}$$

Next taking the inner product in (7.16) with $\mathbb{1}_N$ and then subtracting (7.17) multiplied by $N - 1/2$, we finally get

$$c_{n+1} = \frac{\ell_n}{n+1}(2d_n^1\overline{\mathbf{f}}_n^N - (2N-1)d_n^2 c_n) - c_{n-1}\frac{(n-1)\ell_n}{(n+1)\ell_{n-1}}, \quad n \geq 2. \tag{7.19}$$

Taking into account that the value of f at the root o is determined by $\mathbf{f}_1$ via

$$f(o) = \mathbf{f}_0 = \frac{2\ell_0}{2N+1}M_1\mathbf{f}_1, \tag{7.20}$$

and noting that $\mathbf{f}_2^N$ and c_2 are also determined by $\mathbf{f}_1$, we conclude that (7.18)–(7.19) define $\mathbf{f}$ uniquely once $\mathbf{f}_1 \in \mathbb{C}^{N+1}$ is given. ☐

Lemma 7.4 immediately implies that $\mathrm{n}_\pm(\mathbf{H}_0) \le N+1$ if $\mathrm{vol}(\mathcal{A}_N) < \infty$, where $\mathbf{H}_0$ is the associated minimal operator. The next result shows that it can happen that $\mathrm{n}_\pm(\mathbf{H}_0) = N+1$ upon choosing lengths ℓ_n with a sufficiently fast decay.

Proposition 7.5. *Let $\mathcal{A}_N$ be the antitree as in Lemma 7.4. If (ℓ_n) is decreasing and*

$$\sqrt{\ell_n} = \mathcal{O}\left(\frac{1}{(6\sqrt{N})^n (n+N+3)!}\right) \tag{7.21}$$

as $n \to \infty$, then $\mathrm{n}_\pm(\mathbf{H}_0) = N+1$.

Proof. It is immediate to see that $\mathrm{vol}(\mathcal{A}_N) < \infty$ if (7.21) is satisfied. Next, taking into account (7.9), observe that

$$m(v) = \sum_{v\in\mathcal{E}_v} |e| \le (n+N)\ell_{n-1} + (n+N+2)\ell_n \lesssim n\ell_{n-1}, \quad v \in S_n,$$

as $n \to \infty$. Suppose $f \in \mathbb{H}(\mathcal{A})$ and set $\mathbf{f} = f|_{\mathcal{V}}$. Then $\mathbf{f}$ has the form (7.15) and hence

$$\|\mathbf{f}_n\|^2 = \sum_{v\in S_n} |f(v)|^2 = \|\mathbf{f}_n^N\|^2 + n|c_n|^2,$$

for all $n \ge 1$. This implies the following estimate

$$\sum_{v\in\mathcal{V}} |f(v)|^2 m(v) = \sum_{n\ge 0}\sum_{v\in S_n} |f(v)|^2 m(v) \lesssim \sum_{n\ge1} n^2 \ell_{n-1}(\|\mathbf{f}_n^N\|^2 + |c_n|^2). \tag{7.22}$$

Next, (7.18)–(7.19) can be written as follows

$$\begin{pmatrix} \mathbf{f}_{n+1}^N \\ c_{n+1}\end{pmatrix} = A_{1,n}\begin{pmatrix} \mathbf{f}_{n}^N \\ c_{n}\end{pmatrix} + A_{2,n}\begin{pmatrix} \mathbf{f}_{n-1}^N \\ c_{n-1}\end{pmatrix}, \tag{7.23}$$

where the matrices $A_{1,n}, A_{2,n} \in \mathbb{R}^{(N+1)\times(N+1)}$ are given explicitly by

$$A_{1,n} = \begin{pmatrix} -2\ell_n d_n^1 I_N & 2\ell_n d_n^2 B_{N,1} \\ \frac{2\ell_n d_n^1}{n+1} B_{1,N} & -\frac{(2N-1)\ell_n d_n^2}{n+1} I_1 \end{pmatrix}, \quad A_{2,n} = -\frac{\ell_n}{\ell_{n-1}}\begin{pmatrix} I_N & \\ & \frac{n-1}{n+1} I_1\end{pmatrix}, \tag{7.24}$$

for all $n \ge 2$. Since $\ell_{n-1} \le \ell_n$ and

$$d_n^1 < d_n^2 = \frac{n+N-1}{\ell_{n-1}} + \frac{n+N+1}{\ell_n} \le \frac{2(n+N)}{\ell_n} \tag{7.25}$$

for all $n \ge 2$, it is not difficult to get the following rough bounds [10]

$$\|A_{1,n}\| \le 6\sqrt{N}(n+N), \qquad \|A_{2,n}\| = \frac{\ell_n}{\ell_{n-1}} \le 1, \tag{7.26}$$

for all $n \ge 2N$. Denoting

$$F_n = \begin{pmatrix} \mathbf{f}_n^N \\ c_n \end{pmatrix}, \quad n \ge 1,$$

the recurrence relations (7.18)–(7.19) can be written in the following matrix form

$$\begin{pmatrix} F_{n+1} \\ F_n \end{pmatrix} = \begin{pmatrix} A_{1,n} & A_{2,n} \\ I_{N+1} & 0_{N+1}\end{pmatrix}\begin{pmatrix} F_n \\ F_{n-1}\end{pmatrix} = A_n \begin{pmatrix} F_n \\ F_{n-1}\end{pmatrix}. \tag{7.27}$$

[10] Here and below to estimate norms, we use the equality $\|A\| = \sqrt{\|A^*A\|}$ and the following simple estimate for non-negative 2×2 block-matrices $A = \begin{pmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22}\end{pmatrix}$: $\|A\| \le \|A_{11}\| + \|A_{22}\|$. There are other estimates (e.g., [34, ineq. (2.3.8)]), however, they do not seem to work as good as the above approach.

Taking into account (7.26), we get $\|A_n\| \le 6\sqrt{N}(n+N+1)$ for all $n \ge 2N$, which implies the estimate

$$\sqrt{\|\mathbf{f}_n^N\|^2 + |c_n|^2} = \|F_n\| \le C \prod_{k=1}^{n-1} \|A_k\| \lesssim (6\sqrt{N})^n (n+N)! \tag{7.28}$$

for all $n \ge 2$. Combining this bound with (7.21), it is easy to see that the series on the righthand side in (7.22) converges and hence by Lemma 2.13 we conclude that $\mathbb{H}(\mathcal{A}_N) \subset L^2(\mathcal{A})$. Thus $\ker(\mathbf{H}) = \mathbb{H}(\mathcal{A}_N)$ and the use of Corollary 2.11 finishes the proof. $\square$

7.4. **Infinite deficiency indices.** Consider the antitree $\mathcal{A}$ with sphere numbers $s_n = n+1$, $n \ge 0$. Next pick a sequence of positive numbers (ℓ_n) and define lengths as follows

$$|e_{ij}^n| = \begin{cases} 2\ell_n, & 1 \le i = j \le n+1, \\ \ell_n, & \text{otherwise}, \end{cases} \tag{7.29}$$

for all $n \in \mathbb{Z}_{\ge 0}$. Thus, the corresponding matrix M_{n+1} given by (7.2) has the form

$$M_{n+1} = \frac{1}{\ell_n} \begin{pmatrix} B_{n+1} - \frac{1}{2} I_{n+1} & B_{n+1,1} \end{pmatrix} \in \mathbb{R}^{(n+1)\times(n+2)} \tag{7.30}$$

for all $n \ge 0$. Let us denote this antitree by $\mathcal{A}_\infty$.

Lemma 7.6. $\dim(\mathbb{H}(\mathcal{A}_\infty)) = \infty$.

Proof. Consider the difference equations (7.5)–(7.6). Clearly, the matrix M_{n+1} has the maximal rank $n+1$ for every $n \ge 0$. Taking into account that

$$\Big(B_{n+1} - \frac{1}{2} I_{n+1}\Big)^{-1} = \frac{4}{2n+1} B_{n+1} - 2I_{n+1} =: C_n, \quad n \ge 0,$$

(7.6) then reads

$$\begin{pmatrix} I_{n+1} & \frac{2}{2n+1} B_{n+1,1} \end{pmatrix} \mathbf{f}_{n+1} = \ell_n C_n (D_n \mathbf{f}_n - M_n^* \mathbf{f}_{n-1}) \tag{7.31}$$

for all $n \ge 1$. Observe that

$$\begin{pmatrix} I_{n+1} & \frac{2}{2n+1} B_{n+1,1} \end{pmatrix} \begin{pmatrix} f_1 \\ \vdots \\ f_{n+1} \\ 0 \end{pmatrix} = \begin{pmatrix} f_1 \\ \vdots \\ f_{n+1} \end{pmatrix}$$

and hence for any $\mathbf{f}_n \in \mathbb{C}^{n+1}$ and $\mathbf{f}_{n-1} \in \mathbb{C}^n$ there always exists a unique $\mathbf{f}_{n+1} = (f_1, \dots, f_{n+1}, 0)^\top$ satisfying (7.31). Now pick a natural number N and define $\mathbf{f}^N \in C(\mathcal{A}_\infty)$ by setting $\mathbf{f}_n^N = (0, \dots, 0)^\top \in \mathbb{C}^{n+1}$ for all $n \in \{0, \dots, N\}$,

$$\mathbf{f}_{N+1}^N = (1, \dots, 1, -N - 1/2)^\top,$$

and

$$\mathbf{f}_{n+1}^N = \begin{pmatrix} \ell_n C_n (D_n \mathbf{f}_n^N - M_n^* \mathbf{f}_{n-1}^N) \\ 0 \end{pmatrix} \in \mathbb{C}^{n+2} \tag{7.32}$$

for all $n \ge N+1$. Clearly, $\mathbf{f}^N$ satisfies (7.5)–(7.6) and hence defines a harmonic function $f^N \in \mathbb{H}(\mathcal{A}_\infty)$. Moreover, it is easy to see that $\operatorname{span}\{\mathbf{f}^N\}_{N \ge 1}$ is infinite dimensional, which proves the claim. $\square$

Proposition 7.7. *Let $\mathbf{H}_0$ be the minimal Kirchhoff Laplacian associated with the antitree $\mathcal{A}_\infty$. If ℓ_n is decreasing and*

$$\sqrt{\ell_n} = \mathcal{O}\left(\frac{1}{6^n(n+3)!}\right) \tag{7.33}$$

as $n \to \infty$, then $\mathrm{n}_\pm(\mathbf{H}_0) = \infty$.

Proof. Clearly, it suffices to show that every f^N constructed in the proof of Lemma 7.6 belongs to $L^2(\mathcal{G})$ if ℓ_n decays as in (7.33). To prove this we shall proceed as in the proof of Proposition 7.5. First, taking into account (7.29), observe that

$$m(v) \lesssim n\ell_{n-1}, \quad v \in S_n,$$

as $n \to \infty$. Since $\|\mathbf{f}_n^N\|^2 = \sum_{v\in S_n} |f^N(v)|^2$ for all $n \geq 0$, we get the estimate

$$\sum_{v\in\mathcal{V}} |f^N(v)|^2 m(v) \lesssim \sum_{n\geq N+1}\sum_{v\in S_n} |f^N(v)|^2 m(v) \lesssim \sum_{n\geq N+1} n\ell_{n-1}\|\mathbf{f}_n^N\|^2. \tag{7.34}$$

Denoting $F_n = \mathbf{f}_n^N$ for all $n \geq 1$, we can put (7.31) into the matrix form

$$\begin{pmatrix} F_{n+1} \\ F_n \end{pmatrix} = \begin{pmatrix} A_{1,n} & A_{2,n} \\ I_{n+1} & 0_{n+1,n} \end{pmatrix}\begin{pmatrix} F_n \\ F_{n-1} \end{pmatrix} = A_n \begin{pmatrix} F_n \\ F_{n-1} \end{pmatrix} \tag{7.35}$$

for all $n \geq N+1$, where

$$A_{1,n} = \begin{pmatrix} \ell_n C_n D_n \\ 0_{1,n+1} \end{pmatrix} \in \mathbb{R}^{(n+2)\times(n+1)}, \quad A_{2,n} = \begin{pmatrix} -\ell_n C_n M_n^* \\ 0_{1,n} \end{pmatrix} \in \mathbb{R}^{(n+2)\times n}. \tag{7.36}$$

Now observe that $\|C_n\| = 2$ and $\|\ell_n D_n\| \leq 2(n+1)$ for all $n \geq 1$. Moreover, $\|\ell_n M_n^*\| \leq n+1$ for all $n \geq 1$, which immediately implies the following estimate

$$\|A_n\| \leq \sqrt{\|\ell_n C_n D_n\|^2 + 1 + \|\ell_n C_n M_n^*\|^2} \leq 6(n+1), \quad n \geq N+1. \tag{7.37}$$

Hence we get

$$\|\mathbf{f}_{n+1}^N\| \leq C\prod_{k=N+1}^{n} \|A_k\| \leq C6^{n-N}\frac{(n+1)!}{(N+1)!} \lesssim 6^n(n+1)!$$

for all $n \geq N+1$. Combining this estimate with (7.34) and (7.33) and using Lemma 2.13, we conclude that $f^N \in L^2(\mathcal{A}_\infty)$ for each $N \geq 1$. ☐

Remark 7.8. It is not difficult to show that f^N does not belong to $H^1(\mathcal{A}_\infty)$ for the above choices of edge lengths. In fact, it follows from the maximum principle for $\mathbb{H}(\mathcal{A})$ that if $\mathrm{vol}(\mathcal{A}) < \infty$, then $\mathbb{H}(\mathcal{A}) \cap H^1(\mathcal{A})$ consists only of constant functions.

7.5. **Proof of Theorem 7.1.** Clearly, the case of infinite deficiency indices follows from Proposition 7.7. On the other hand, since adding and/or removing finitely many edges and vertices to a graph does not change the deficiency indices of the minimal Kirchhoff Laplacian, Proposition 7.5 completes the proof of Theorem 7.1. Indeed, every antitree $\mathcal{A}_N$ can be obtained from $\mathcal{A}$ by first removing all the edges between combinatorial spheres S_0 and S_N and then adding $N+1$ edges connecting the root o with the vertices in S_N. ☐

Remark 7.9. Since every infinite antitree has exactly one end, Theorem 6.11(iv) implies that the Kirchhoff Laplacian $\mathbf{H}_0$ in Theorem 7.1 has a unique Markovian extension exactly when $\mathrm{vol}(\mathcal{A}) = \infty$. If $\mathrm{vol}(\mathcal{A}) < \infty$, then Markovian extensions of $\mathbf{H}_0$ form a one-parameter family explicitly given by (6.17). Notice that (6.17) looks similar to the description of self-adjoint extensions of the minimal Kirchhoff Laplacian on radially symmetric antitrees obtained recently in [54].

Let us also emphasize that the antitree constructed in Proposition 7.7 has finite total volume and $\mathbf{H}_0$ has infinite deficiency indices, however, the set of Markovian extensions of $\mathbf{H}_0$ forms a one-parameter family.

Let us finish this section with one more comment. As it was proved, the dimension of the space of Markovian extensions depends only on the space of graph ends and, moreover, it is equal to the number of finite volume ends. However, deficiency indices (dimension of the space of self-adjoint extensions) are in general independent of graph ends and we can only provide a lower bound. Moreover, the above example of a polynomially growing antitree shows that the space of harmonic functions heavily depends on the choice of edge lengths (in particular, its dimension may vary between zero and infinity). In this respect let us also emphasize that in the case of Cayley graphs of finitely generated countable groups the end space is independent of the choice of a generating set, however, simple examples show that the space of harmonic functions does depend on this choice.

Appendix A. Linear relations in Hilbert spaces

In this section we collect basic notions and facts on linear relations in Hilbert spaces, a very convenient concept of multivalued linear operators. For simplicity, we shall assume that $\mathcal{H}$ *is a finite dimensional Hilbert space*, $\dim(\mathcal{H}) = N < \infty$.

A *linear relation* Θ in $\mathcal{H}$ is a linear subspace in $\mathcal{H} \times \mathcal{H}$. Linear operators become special linear relations (single valued) after identifying them with their graphs in $\mathcal{H} \times \mathcal{H}$. Every linear relation in $\mathcal{H}$ has the form

$$\Theta_{C,D} = \{(f, g) \in \mathcal{H} \times \mathcal{H} |\, Cf + Dg = 0\}, \tag{A.1}$$

where C, D are linear operators on $\mathcal{H}$, however, different C and D may define the same linear relation. The *domain* and the *multi-valued part* of $\Theta_{C,D}$ are given by

$$\begin{aligned} \mathrm{dom}(\Theta_{C,D}) &= \{f \in \mathcal{H} |\, \exists g \in \mathcal{H}, Cf + Dg = 0\} = \{f \in \mathcal{H} |\, Cf \in \mathrm{ran}(D)\}, \\ \mathrm{mul}(\Theta_{C,D}) &= \{g \in \mathcal{H} |\, Dg = 0\} = \ker(D). \end{aligned}$$

In particular, $\Theta_{C,D}$ is a graph of a linear operator only if $\ker(D) = \{0\}$. A linear relation is called *self-adjoint* if $\Theta = \Theta^*$, where

$$\Theta^* = \{(f, g) \in \mathcal{H} \times \mathcal{H} |\, \langle \widetilde{g}, f\rangle_{\mathcal{H}} = \langle \widetilde{f}, g\rangle_{\mathcal{H}}\ \forall (\widetilde{f}, \widetilde{g}) \in \Theta\}. \tag{A.2}$$

A linear relation $\Theta_{C,D}$ is self-adjoint if and only if C and D satisfy the *Rofe-Beketov conditions* [64] (see also [66, Exercises 14.9.3-4]):

$$CD^* = DC^*, \qquad\qquad 0 \in \rho(C^*C + D^*D). \tag{A.3}$$

Notice that the second condition in (A.3) is equivalent to the fact that the matrix $(C|D) \in \mathbb{C}^{N\times 2N}$ has the maximal rank N.

Recall also that every self-adjoint linear relation admits the representation $\Theta = \Theta_{\mathrm{op}} \oplus \Theta_{\mathrm{mul}}$, where $\Theta_{\mathrm{mul}} = \{0\} \times \mathrm{mul}(\Theta)$ and Θ_{op}, called the operator part of Θ, is a graph of a linear operator. In particular, for a self-adjoint linear relation $\Theta_{C,D}$ one has

$$\mathrm{dom}(\Theta_{C,D}) = \mathrm{mul}(\Theta_{C,D})^{\perp} = \ker(D)^{\perp} = \mathrm{ran}(D^*). \tag{A.4}$$

For further details on linear relations we refer the reader to, e.g., [66, Chapter 14.1].

Appendix B. A rope ladder graph

Let us introduce a rope ladder graph depicted on Figure 2. Let $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ be a simple graph with the vertex set $\mathcal{V} := \{o\} \cup \mathcal{V}^+ \cup \mathcal{V}^-$, where $o = v_0$ is a root, $\mathcal{V}^+ = (v_n^+)_{n\geq 1}$ and $\mathcal{V}^- = (v_n^-)_{n\geq 1}$ are two disjoint countably infinite sets of vertices. The edge set $\mathcal{E}$ is defined as follows:

- o is connected to v_1^+ and v_1^- by the "diagonal" edges e_0^+ and e_0^-, respectively;
- for each $n \geq 1$, $v_n^\pm$ is connected to $v_{n+1}^\pm$ by the vertical edge $e_n^\pm$;
- for each $n \geq 1$, v_n^+ and v_n^- are connected by the horizontal edge e_n.

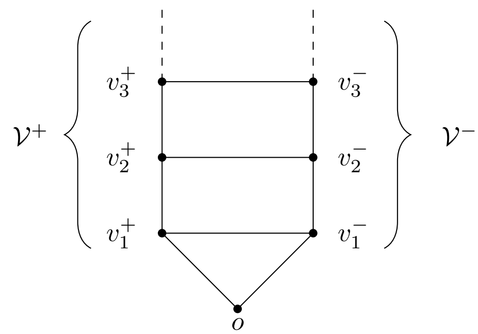

Figure 2. The rope ladder graph.

By construction, $\deg(o) = 2$ and $\deg(v_n^+) = \deg(v_n^-) = 3$ for all $n \geq 1$. Moreover, an infinite rope ladder graph has exactly one end. Notice also that a similar example was studied in [44, Section 7] (see also [31, §5]) in context with the construction of non-constant harmonic functions of finite energy.

Equip now $\mathcal{G}_d$ with edge lengths $|\cdot|\colon \mathcal{E} \to \mathbb{R}_{>0}$ and consider the corresponding minimal Kirchhoff Laplacian $\mathbf{H}_0$ on the metric graph $\mathcal{G} = (\mathcal{G}_d, |\cdot|)$. The next result immediately follows from Theorem 2.8 and Corollary 2.11.

Corollary B.1. *If*

$$\sum_{n\geq 1} |e_n^+| + |e_n| = \infty, \quad \textit{and} \quad \sum_{n\geq 1} |e_n^-| + |e_n| = \infty, \tag{B.1}$$

then the Kirchhoff Laplacian $\mathbf{H}_0$ *is self-adjoint. If*

$$\mathrm{vol}(\mathcal{G}) = \sum_{n\geq 1} |e_n^+| + |e_n^-| + |e_n| < \infty, \tag{B.2}$$

then $\mathrm{n}_\pm(\mathbf{H}_0) \geq 1$.

We omit the proof since it is easy to check that the first condition is equivalent to the geodesic completeness of $(\mathcal{V}, \varrho_m)$ (cf. Theorem 2.8). Due to the symmetry of the underlying combinatorial graph, the gap between the above two conditions is equivalent to the fact that the corresponding lengths satisfy

$$\sum_{n\geq 1} |e_n^+| = \infty, \qquad\qquad \sum_{n\geq 1} |e_n^-| + |e_n| < \infty. \tag{B.3}$$

Next, let us describe the space of harmonic functions $\mathbb{H}(\mathcal{G})$.

Lemma B.2. *Let $a, b \in \mathbb{C}$. Then there is exactly one $f \in \mathbb{H}(\mathcal{G})$ such that*

$$f(v_1^+) = a, \qquad\qquad f(v_1^-) = b. \tag{B.4}$$

Moreover, this function f is recursively given by

$$f(o) = \frac{b|e_0^+| + a|e_0^-|}{|e_0^+| + |e_0^-|} \tag{B.5}$$

and

$$f(v_{n+1}^\pm) = \left(1 + \frac{|e_n^\pm|}{|e_{n-1}^\pm|} + \frac{|e_n^\pm|}{|e_n|}\right) f(v_n^\pm) - \frac{|e_n^\pm|}{|e_{n-1}^\pm|} f(v_{n-1}^\pm) - \frac{|e_n^\pm|}{|e_n|} f(v_n^\mp), \tag{B.6}$$

for all $n \in \mathbb{Z}_{\geq 1}$, where we use the notation $v_0^+ := v_0^- := o$.

Proof. Suppose $a, b \in \mathbb{C}$ are given and $f \in \mathbb{H}(\mathcal{G})$ satisfies (B.4). Since f is linear on every edge and satisfies (2.6) at $v = o$, we get

$$0 = f'_{e_0^+}(o) + f'_{e_0^-}(o) = \frac{f(v_1^+) - f(o)}{|e_0^+|} + \frac{f(v_1^-) - f(o)}{|e_0^-|} = \frac{a - f(o)}{|e_0^+|} + \frac{b - f(o)}{|e_0^-|},$$

which implies (B.5). Moreover, Kirchhoff conditions (2.6) at $v = v_n^\pm$, $n \geq 1$ read

$$\frac{f(v_{n+1}^\pm) - f(v_n^\pm)}{|e_n^\pm|} + \frac{f(v_{n-1}^\pm) - f(v_n^\pm)}{|e_{n-1}^\pm|} + \frac{f(v_n^\mp) - f(v_n^\pm)}{|e_n|} = 0.$$

This implies that f is given by (B.6). Hence there is at most one $f \in \mathbb{H}(\mathcal{G})$ satisfying (B.4) for given $a, b \in \mathbb{C}$. However, the same calculation shows that f defined by (B.5) and (B.6) has this property. Thus, existence follows as well. $\square$

From Lemma B.2, it is clear that $\dim(\mathbb{H}(\mathcal{G})) = 2$, and, moreover,

$$\mathbb{H}(\mathcal{G}) = \operatorname{span}\{\mathbb{1}_{\mathcal{G}}, g_0\},$$

where $\mathbb{1}_{\mathcal{G}}$ denotes the constant function on $\mathcal{G}$ and $g_0 \in \mathbb{H}(\mathcal{G})$ is the function defined, for example, by the following normalization

$$g_0(0) = 0, \qquad g_0(v_1^+) = |e_0^+|, \qquad g_0(v_1^-) = -|e_0^-|. \tag{B.7}$$

Notice that $g_0(v_n^\pm)$, $n \geq 1$ are then given recursively by (B.6).

Lemma B.3. *If* $\operatorname{vol}(\mathcal{G}) < \infty$, *then*

$$\mathbb{H}(\mathcal{G}) \cap H^1(\mathcal{G}) = \operatorname{span}\{\mathbb{1}_{\mathcal{G}}\}. \tag{B.8}$$

The claim immediately follows from the fact that a rope ladder graph has exactly one end. However, let us present a direct proof based on the analysis of harmonic functions.

Proof. Taking into account (B.8), we only need to show that $g_0 \notin H^1(\mathcal{G})$. First, observe that $(g_0(v_n^+))_{n\geq 1}$ and $(g_0(v_n^-))_{n\geq 1}$ are strictly increasing positive, respectively, strictly decreasing negative sequences. Indeed,

$$-|e_0^-| = g_0(v_1^-) < 0 = g_0(o) < g_0(v_1^+) = |e_0^+|$$

by the very definition of g_0. Let $n \geq 1$ and assume now that we have already shown that $(g_0(v_k^+))_{k=1}^n$ is strictly increasing and $(g_0(v_k^-))_{k=1}^n$ is strictly decreasing. Since $g_0(o) = 0$, (B.6) implies

$$\begin{aligned} g_0(v_{n+1}^+) &= \Big(1 + \frac{|e_n^+|}{|e_{n-1}^+|} + \frac{|e_n^+|}{|e_n|}\Big) g_0(v_n^+) - \frac{|e_n^+|}{|e_{n-1}^+|} g_0(v_{n-1}^+) - \frac{|e_n^+|}{|e_n|} g_0(v_n^-) \\ &> \left(1 + \frac{|e_n^+|}{|e_n|}\right) g_0(v_n^+) + \frac{|e_n^+|}{|e_{n-1}^+|}(g_0(v_n^+) - g_0(v_{n-1}^+)) > g_0(v_n^+). \end{aligned}$$

A similar argument shows that $g_0(v_{n+1}^-) < g_0(v_n^-)$ and hence the claim follows by induction. Now monotonicity immediately implies

$$\begin{aligned} \|g_0'\|_{L^2(\mathcal{G})}^2 &= \sum_{e \in \mathcal{E}} \int_e |g_0'(x_e)|^2 \, dx_e \geq \sum_{n \geq 0} \int_{e_n} |g_0'(x_e)|^2 \, dx_e \\ &= \sum_{n=0}^{\infty} \frac{|g_0(v_n^+) - g_0(v_n^-)|^2}{|e_n|} \geq |g_0(v_1^+) - g_0(v_1^-)|^2 \sum_{n=0}^{\infty} \frac{1}{|e_n|} = \infty, \end{aligned}$$

since $\operatorname{vol}(\mathcal{G}) < \infty$. Thus $g_0 \notin H^1(\mathcal{G})$. $\square$

In particular, this also leads to the following result:

Corollary B.4. *If* $\operatorname{vol}(\mathcal{G}) < \infty$*, then* $\mathrm{n}_\pm(\mathbf{H}_0) \in \{1, 2\}$*. Moreover,* $\mathrm{n}_\pm(\mathbf{H}_0) = 1$ *if and only if* $g_0 \notin L^2(\mathcal{G})$*.*

Proof. The claim about the deficiency indices follows from Corollary 2.11 and the fact that $\mathbb{1}_{\mathcal{G}} \in L^2(\mathcal{G})$. The equivalences then follow from Lemma B.3. $\square$

As the next example shows, the inclusion $g_0 \in L^2(\mathcal{G})$ heavily depends on the choice of edge lengths.

Example B.5. Fix $s > 3$ and equip the rope ladder graph with edge lengths

$$|e_n^+| = |e_n^-| := \frac{1}{(n+1)^s}, \qquad |e_n| := \frac{2n}{(n+1)^s - n^s}, \quad n \in \mathbb{Z}_{\geq 0},$$

where is fixed. Then $|e_n| \sim n^{2-s}$ for large n and hence $\operatorname{vol}(\mathcal{G}) < \infty$. Moreover, for this particular choice of edge lengths we have $g_0(v_n^\pm) = \pm n$ for all $n \geq 1$. Indeed, $g_0(v_1^\pm) = \pm 1$ by (B.7). Assuming we have already proven that $g_0(v_k^\pm) = \pm k$ for $k \leq n$ with some $n \geq 1$, we have by (B.6):

$$\begin{aligned} g_0(v_{n+1}^+) &= \Big(1 + \frac{n^s}{(n+1)^s} + \frac{1}{(n+1)^s |e_n|}\Big) n - \frac{n^s(n-1)}{(n+1)^s} + \frac{n}{(n+1)^s |e_n|} \\ &= n + \frac{n^s}{(n+1)^s} + \frac{2n}{(n+1)^s |e_n|} = n + \frac{n^s}{(n+1)^s} + \frac{(n+1)^s - n^s}{(n+1)^s} = n + 1. \end{aligned}$$

Analogously, $g_0(v_{n+1}^-) = -(n+1)$ and hence the claim follows by induction.

Applying Lemma B.3 and using again that $|e_n| \sim n^{2-s}$ as $n \to \infty$, we conclude that $g_0 \in L^2(\mathcal{G})$ exactly (see Lemma 2.13) when

$$\sum_{n \geq 1} |g_0(v_n^\pm)|^2 (|e_{n-1}^\pm| + |e_n^\pm|) = \sum_{n \geq 1} n^2((n+1)^{-s} + n^{-s}) < \infty$$

and

$$\sum_{n \geq 1} |g_0(v_n^\pm)|^2 |e_{n-1}| = \sum_{n \geq 1} \frac{2n^3}{(n+1)^s - n^s} < \infty.$$

Clearly, the latter holds only if $s > 5$. Hence, by Lemma B.4, $\mathrm{n}_\pm(\mathbf{H}_0) = 2$ for all $s > 5$. In particular, $\ker(\mathbf{H}) \subset H^1(\mathcal{G}) \Leftrightarrow s \le 5$.

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A NOTE ON THE GAFFNEY LAPLACIAN ON INFINITE METRIC GRAPHS

ALEKSEY KOSTENKO AND NOEMA NICOLUSSI

ABSTRACT. We show that the deficiency indices of the minimal Gaffney Laplacian on an infinite locally finite metric graph are equal to the number of finite volume graph ends. Moreover, we provide criteria, formulated in terms of finite volume graph ends, for the Gaffney Laplacian to be closed.

1. INTRODUCTION

The standard way to associate an operator with the Laplacian in a domain in $\mathbb{R}^n$ or on a Riemannian manifold is to consider it either on smooth compactly supported functions (the so-called *pre-minimal operator*) or on the largest possible domain, that is, on all L^2 functions such that the distributional Laplacian applied to these functions can be identified with an L^2 function (the *maximal operator*). Then the pre-minimal Laplacian is essentially self-adjoint if and only if its L^2 closure, the *minimal operator*, coincides with the maximal operator. For geodesically complete manifolds the essential self-adjointness was proved by W. Roelcke [23] (see also [5, 27]). It is impossible to give even a brief account on the subject and we only refer to [1, 7, 25], some recent work in the case of non-complete manifolds [20, 21] and also for weighted graph Laplacians [14, 16]. Let us also mention the work of M. P. Gaffney [10], where the maximal operator was further restricted to functions having finite energy. It turns out that the self-adjointness of this operator (sometimes called the *Gaffney Laplacian* [12]) is equivalent to the uniqueness of a Markovian extension. Clearly, essential self-adjointness implies the uniqueness of Markovian extensions, but the converse is not necessarily true. We refer to [7, Chapter I] for an excellent account on importance and applications of self-adjoint and Markovian uniqueness.

The main object of our paper is a *quantum graph*, i.e., a Laplacian on a metric graph. From the perspective of Dirichlet forms, quantum graphs play an important role as an intermediate setting between Laplacians on Riemannian manifolds and discrete Laplacians on weighted graphs. The most studied quantum graph operator is the *Kirchhoff Laplacian*, which provides the analog of the Laplace–Beltrami operator in the setting of metric graphs. Whereas on finite metric graphs the Kirchhoff Laplacian is always self-adjoint, the question is more subtle for *graphs with infinitely many edges*. Geodesic completeness (w.r.t. the natural path metric) guarantees self-adjointness of the (minimal) Kirchhoff Laplacian, however, this result is far from

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being optimal [8, §4]. The present paper is a complement to the recent work [18], where a relationship between one of the classical notions of boundaries for infinite graphs, *graph ends*, and self-adjoint extensions of the minimal Kirchhoff Laplacian on a metric graph was established. More precisely, the notion of *finite volume* for ends of a metric graph introduced in [18] turns out to be a proper notion of a boundary for Markovian extensions of the Kirchhoff Laplacian. Our main goal is to elaborate on the relationship between finite volume graph ends and the Gaffney Laplacian, which is defined as the restriction of the maximal Kirchhoff Laplacian to functions having finite energy (i.e., H^1 functions). First of all, one of the main results of [18] provides a transparent geometric characterization of the self-adjointness of the Gaffney Laplacian: *the underlying metric graph has no finite volume ends* (see Lemma 3.4 below). Our first main result shows that the deficiency indices of the (minimal) Gaffney Laplacian (i.e., the dimension of the space of its self-adjoint extensions) are in fact equal to the number of finite volume graph ends (Theorem 3.8). The Gaffney Laplacian has several advantages comparing to the maximal Kirchhoff Laplacian, although one of the main disadvantages is the fact that it is not necessarily closed. Our second main result, Theorem 3.9 provides necessary and sufficient conditions for the Gaffney Laplacian to be closed. These conditions are stated in terms of finite volume graphs ends and in certain cases of interest (graphs of finite total volume or Cayley graphs of countable finitely generated groups) they give rise to a transparent geometrical criterion: *the Gaffney Laplacian is closed if and only if the underlying metric graph has finitely many finite volume ends*, which is further equivalent to the fact that the deficiency indices of the minimal Gaffney Laplacian are finite. If the Gaffney Laplacian is not closed, then the most important question is how to describe its L^2 closure. It does not seem realistic to us to obtain a complete answer to this question and we demonstrate by examples that under certain symmetry assumptions the closure of the Gaffney Laplacian may coincide with the maximal Kirchhoff Laplacian.

Let us now briefly describe the structure of the article. Section 2 is of preliminary character where we collect basic notions and facts about graphs and metric graphs (Section 2.1); graph ends (Section 2.2); Sobolev spaces on metric graphs (Section 2.3); Kirchhoff, Dirichlet and Neumann Laplacians on metric graphs (Section 2.4). The main results of the present paper are collected in Section 3. First we introduce the minimal Gaffney Laplacian and the Gaffney Laplacian, study their properties and also investigate their relationship with the Kirchhoff, Dirichlet and Neumann Laplacians. In the final section we discuss several explicit examples.

Notation. $\mathbb{Z}$, $\mathbb{R}$, $\mathbb{C}$ have their usual meaning; $\mathbb{Z}_{\geq a} := \mathbb{Z} \cap [a, \infty)$.
z^* denotes the complex conjugate of $z \in \mathbb{C}$.
For a given set S, $\#S$ denotes its cardinality if S is finite; otherwise we set $\#S = \infty$.
If it is not explicitly stated otherwise, we shall denote by (x_n) a sequence $(x_n)_{n=0}^{\infty}$.

2. Quantum graphs and graph ends

2.1. **Combinatorial and metric graphs.** In what follows, $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ will be an unoriented graph with countably infinite sets of vertices $\mathcal{V}$ and edges $\mathcal{E}$. For two vertices u, $v \in \mathcal{V}$ we shall write $u \sim v$ if there is an edge $e_{u,v} \in \mathcal{E}$ connecting u with v. For every $v \in \mathcal{V}$, we denote the set of edges incident to the vertex v by $\mathcal{E}_v$ and

$$\deg(v) := \#\{e |\, e \in \mathcal{E}_v\} \tag{2.1}$$

is called *the degree* of a vertex $v \in \mathcal{V}$. *A path* $\mathcal{P}$ of length $n \in \mathbb{Z}_{\geq 0} \cup \{\infty\}$ is a sequence of vertices $(v_0, v_1, \dots, v_n)$ such that $v_{k-1} \sim v_k$ for all $k \in \{1, \dots, n\}$.

The following assumption is imposed throughout the paper.

Hypothesis 2.1. $\mathcal{G}_d$ *is* locally finite *(*$\deg(v) < \infty$ *for every* $v \in \mathcal{V}$*) and* connected *(for any two vertices* $u, v \in \mathcal{V}$ *there is a path connecting* u *and* v*).*

Assigning to each edge $e \in \mathcal{E}$ a finite length $|e| \in (0, \infty)$ turns $\mathcal{G}_d$ into a *metric graph* $\mathcal{G} := (\mathcal{V}, \mathcal{E}, |\cdot|) = (\mathcal{G}_d, |\cdot|)$. The latter equips $\mathcal{G}$ with a (natural) topology and metric. More specifically (see, e.g., [15, Chapter 1.1]), a metric graph $\mathcal{G}$ is a Hausdorff topological space with countable base such that each point $x \in \mathcal{G}$ has a neighbourhood $\mathcal{E}_x(r)$ homeomorphic to a star-shaped set $\mathcal{E}(\deg(x), r_x)$ of degree $\deg(x) \geq 1$,

$$\mathcal{E}(\deg(x), r_x) := \{z = r\mathrm{e}^{2\pi \mathrm{i}k/\deg(x)} |\, r \in [0, r_x),\ k = 1, \dots, \deg(x)\} \subset \mathbb{C}.$$

Identifying every edge $e \in \mathcal{E}$ with a copy of an interval of length $|e|$ and also identifying the ends of the edges that correspond to the same vertex v, $\mathcal{G}$ can be equipped with *the natural path metric* ϱ — the distance between two points $x, y \in \mathcal{G}$ is defined as the length of the "shortest" path connecting x and y.

2.2. **Graph ends.** A sequence of distinct vertices (v_n) such that $v_n \sim v_{n+1}$ for all $n \in \mathbb{Z}_{\geq 0}$ is called a *ray*. Two rays $\mathcal{R}_1, \mathcal{R}_2$ are called *equivalent* – and we write $\mathcal{R}_1 \sim \mathcal{R}_2$ – if there is a third ray containing infinitely many vertices of both $\mathcal{R}_1$ and $\mathcal{R}_2$. An equivalence class of rays is called a *graph end of* $\mathcal{G}_d$.

Considering a metric graph $\mathcal{G}$ as a topological space, one can introduce topological ends. Consider sequences $\mathcal{U} = (U_n)$ of non-empty open connected subsets of $\mathcal{G}$ with compact boundaries and such that $U_{n+1} \subseteq U_n$ for all $n \geq 0$ and $\bigcap_{n \geq 0} \overline{U_n} = \emptyset$. Two such sequences $\mathcal{U}$ and $\mathcal{U}'$ are called *equivalent* if for all $n \geq 0$ there exist j and k such that $U_n \supseteq U'_j$ and $U'_n \supseteq U_k$. An equivalence class γ of sequences is called a *topological end* of $\mathcal{G}$ and $\mathfrak{C}(\mathcal{G})$ denotes the set of topological ends of $\mathcal{G}$. There is a natural bijection between topological ends of a locally finite metric graph $\mathcal{G}$ and graph ends of the underlying combinatorial graph $\mathcal{G}_d$: for every topological end $\gamma \in \mathfrak{C}(\mathcal{G})$ of $\mathcal{G}$ there exists a unique graph end ω_γ of $\mathcal{G}_d$ such that for every sequence $\mathcal{U}$ representing γ, each U_n contains a ray from ω_γ (see [28, §21], [6, §8.6 and also p.277–278] for further details).

One of the main features of graph ends is that they provide a rather refined way of compactifying graphs, called the *end (or Freudenthal) compactification* of $\mathcal{G}$ (see [6, §8.6], [28] and also [18, §2.2]).

Definition 2.1. An end ω of a graph $\mathcal{G}_d$ is called *free* if there is a finite set X of vertices such that X separates ω from all other ends of the graph.

Remark 2.2. Notice that an end $\gamma \in \mathfrak{C}(\mathcal{G})$ is free exactly when there exists a connected subgraph $\widetilde{\mathcal{G}}$ with compact boundary $\partial\widetilde{\mathcal{G}}$[1] such that $U_n \subseteq \widetilde{\mathcal{G}}$ eventually for any sequence $\mathcal{U} = (U_n)$ representing γ and $U'_n \cap \widetilde{\mathcal{G}} = \varnothing$ eventually for all sequences $\mathcal{U}' = (U'_n)$ representing an end $\gamma' \neq \gamma$.

We also need the following notion introduced in [18].

[1]Notice that for a subgraph $\widetilde{\mathcal{G}}$ of $\mathcal{G}$ its boundary is $\partial\widetilde{\mathcal{G}} = \{v \in \mathcal{V}(\widetilde{\mathcal{G}}) |\, \deg_{\widetilde{\mathcal{G}}}(v) < \deg(v)\}$ and hence $\partial\widetilde{\mathcal{G}}$ is compact exactly when $\#\partial\widetilde{\mathcal{G}} < \infty$.

Definition 2.3. A topological end $\gamma \in \mathfrak{C}(\mathcal{G})$ has *finite volume* if there is a sequence $\mathcal{U} = (U_n)$ representing γ such that $\mathrm{vol}(U_n) < \infty$[2] for some n. Otherwise γ has *infinite volume*. The set of all finite volume ends is denoted by $\mathfrak{C}_0(\mathcal{G})$.

2.3. **Function spaces on metric graphs.** Identifying every edge $e \in \mathcal{E}$ with the copy of $\mathcal{I}_e = [0, |e|]$ (and hence assigning an orientation on $\mathcal{G}$), we can introduce Sobolev spaces on edges and on $\mathcal{G}$. First of all, the Hilbert space $L^2(\mathcal{G})$ of functions $f\colon \mathcal{G} \to \mathbb{C}$ is defined by

$$L^2(\mathcal{G}) = \bigoplus_{e\in\mathcal{E}} L^2(e) = \Big\{ f = \{f_e\}_{e\in\mathcal{E}} \big|\, f_e \in L^2(e),\ \sum_{e\in\mathcal{E}} \|f_e\|^2_{L^2(e)} < \infty \Big\}.$$

The subspace of compactly supported $L^2(\mathcal{G})$ functions will be denoted by

$$L^2_c(\mathcal{G}) = \big\{ f \in L^2(\mathcal{G}) |\ f \neq 0 \text{ only on finitely many edges } e \in \mathcal{E} \big\}.$$

For edgewise locally absolutely continuous functions on $\mathcal{G}$ let us denote by ∇ the edgewise first derivative,

$$\nabla f := f'. \tag{2.2}$$

Then for every edge $e \in \mathcal{E}$,

$$H^1(e) = \{ f \in AC(e) |\, \nabla f \in L^2(e)\}, \quad H^2(e) = \{ f \in H^1(e) |\, \nabla f \in H^1(e)\},$$

Next $H^n(\mathcal{G} \setminus \mathcal{V})$, $n \in \{1, 2\}$ is defined as a space of functions $f\colon \mathcal{G} \to \mathbb{C}$ such that

$$H^n(\mathcal{G} \setminus \mathcal{V}) = \bigoplus_{e\in\mathcal{E}} H^n(e) = \Big\{ f = \{f_e\}_{e\in\mathcal{E}} \big|\, f_e \in H^n(e),\ \sum_{e\in\mathcal{E}} \|f_e\|^2_{H^n(e)} < \infty \Big\}.$$

It becomes a Hilbert space when equipped with the norm $\|f\|^2_{H^n} := \sum_{e\in\mathcal{E}} \|f_e\|^2_{H^n(e)}$.

The first Sobolev space on $\mathcal{G}$ is defined by

$$H^1(\mathcal{G}) = H^1(\mathcal{G} \setminus \mathcal{V}) \cap C(\mathcal{G}),$$

which is also a Hilbert space when equipped with the above norm. We also define $H^1_0(\mathcal{G})$ as the closure in $H^1(\mathcal{G})$ of $H^1_c(\mathcal{G}) = H^1(\mathcal{G}) \cap L^2_c(\mathcal{G})$.

The Sobolev space $H^1(\mathcal{G})$ is continuously embedded in $C_b(\mathcal{G}) = C(\mathcal{G}) \cap L^\infty(\mathcal{G})$ (see, e.g., [18, Lemma 3.2]) and, moreover, every function $f \in H^1(\mathcal{G})$ admits a unique continuous extension to the end compactification $\widehat{\mathcal{G}}$ of $\mathcal{G}$ ([18, Proposition 3.5]): for every $f \in H^1(\mathcal{G})$ and a (topological) end $\gamma \in \mathfrak{C}(\mathcal{G})$, we define

$$f(\gamma) := \lim_{n\to\infty} f(v_n), \tag{2.3}$$

where $\mathcal{R} = (v_n) \in \omega_\gamma$ is any ray belonging to the corresponding graph end ω_γ.

It turns out that finite volume graph ends serve as a proper boundary for the Sobolev space $H^1(\mathcal{G})$. Namely, considering $H^1(\mathcal{G})$ as a subalgebra of $C_b(\mathcal{G})$, it was proved in [18, §3] that its closure is isomorphic to $C_0(\mathcal{G} \cup \mathfrak{C}_0(\mathcal{G}))$. In particular, ends having infinite volume lead to trivial values, that is,

$$f(\gamma) = 0$$

for every $f \in H^1(\mathcal{G})$ if and only if $\gamma \notin \mathfrak{C}_0(\mathcal{G})$. Moreover, by Theorem 3.10 from [18],

$$H^1_0(\mathcal{G}) = \{ f \in H^1(\mathcal{G}) |\ f(\gamma) = 0 \text{ for all } \gamma \in \mathfrak{C}(\mathcal{G})\}, \tag{2.4}$$

and hence $H^1(\mathcal{G}) = H^1_0(\mathcal{G})$ exactly when $\mathcal{G}$ has no finite volume ends, $\mathfrak{C}_0(\mathcal{G}) = \emptyset$.

[2] As usual, $\mathrm{vol}(A)$ denotes the Lebesgue measure of a measurable set $A \subseteq \mathcal{G}$.

2.4. **Kirchhoff, Dirichlet and Neumann Laplacians.** Let $\mathcal{G}$ be a metric graph satisfying Hypothesis 2.1. If v is a vertex of the edge $e \in \mathcal{E}$, then for every $f \in H^2(e)$ the following quantities

$$f_e(v) := \lim_{x_e \to v} f(x_e), \qquad \partial_e f(v) := \lim_{x_e \to v} \frac{f(x_e) - f(v)}{|x_e - v|}, \tag{2.5}$$

are well defined. The Kirchhoff (also called *standard* or *Kirchhoff–Neumann*) boundary conditions at every vertex $v \in \mathcal{V}$ are then given by

$$\begin{cases} f \text{ is continuous at } v, \\ \sum\limits_{e \in \mathcal{E}_v} \partial_e f(v) = 0. \end{cases} \tag{2.6}$$

Imposing these boundary conditions on the maximal domain yields the *maximal Kirchhoff Laplacian*

$$\mathbf{H} = -\Delta \restriction \mathrm{dom}(\mathbf{H}), \quad \mathrm{dom}(\mathbf{H}) = \{f \in H^2(\mathcal{G} \setminus \mathcal{V}) |\, f \text{ satisfies (2.6)},\ v \in \mathcal{V}\}. \tag{2.7}$$

Restricting further to compactly supported functions we end up with the pre-minimal operator

$$\mathbf{H}_0^0 = -\Delta \restriction \mathrm{dom}(\mathbf{H}_0^0), \qquad \mathrm{dom}(\mathbf{H}_0^0) = \mathrm{dom}(\mathbf{H}) \cap L^2_c(\mathcal{G}). \tag{2.8}$$

We call its closure $\mathbf{H}_0 := \overline{\mathbf{H}_0^0}$ in $L^2(\mathcal{G})$ *the minimal Kirchhoff Laplacian*. Integrating by parts one obtains

$$\langle \mathbf{H}_0^0 f, f\rangle_{L^2(\mathcal{G})} = \int_{\mathcal{G}} |\nabla f(x)|^2\, dx =: \mathfrak{t}[f], \qquad f \in \mathrm{dom}(\mathbf{H}_0^0), \tag{2.9}$$

and hence both $\mathbf{H}_0^0$ and $\mathbf{H}_0$ are non-negative symmetric operators. It is known that

$$\mathbf{H}_0^* = \mathbf{H}. \tag{2.10}$$

The equality $\mathbf{H}_0 = \mathbf{H}$ holds if and only if $\mathbf{H}_0$ is self-adjoint (or, equivalently, $\mathbf{H}_0^0$ is essentially self-adjoint). To the best of our knowledge, the strongest sufficient condition which guaranties self-adjointness is provided by the next result.

Theorem 2.4 ([8]). *Let ϱ_m be the* star path metric *on $\mathcal{V}$,*

$$\varrho_m(u, v) := \inf_{\substack{\mathcal{P}=(v_0,\dots,v_n) \\ u=v_0,\ v=v_n}} \sum_{v_k \in \mathcal{P}} m(v_k), \tag{2.11}$$

where $m\colon \mathcal{V} \to (0,\infty)$ is the star weight

$$m(v) := \sum_{e \in \mathcal{E}_v} |e| = \mathrm{vol}(\mathcal{E}_v). \tag{2.12}$$

If $(\mathcal{V}, \varrho_m)$ is complete as a metric space, then $\mathbf{H}_0^0$ is essentially self-adjoint.

The degree of non-self-adjointness of $\mathbf{H}_0$ is determined by its *deficiency indices* $\mathrm{n}_\pm(\mathbf{H}_0) = \dim \mathcal{N}_{\pm\mathrm{i}}(\mathbf{H}_0)$, where

$$\mathcal{N}_z(\mathbf{H}_0) := \ker(\mathbf{H}_0^* - z) = \ker(\mathbf{H} - z), \quad z \in \mathbb{C}, \tag{2.13}$$

are called the *deficiency subspaces* of $\mathbf{H}_0$. Notice that $\mathrm{n}_+(\mathbf{H}_0) = \mathrm{n}_-(\mathbf{H}_0)$ since $\mathbf{H}_0$ is non-negative and hence $\mathrm{n}_\pm(\mathbf{H}_0)$ is equal to the dimension of the space of self-adjoint extensions of $\mathbf{H}_0$.

There is a standard procedure to construct at least one self-adjoint extension of $\mathbf{H}_0$, the so-called *Friedrichs extension*, let us denote it by $\mathbf{H}_D$. Namely, $\mathbf{H}_D$ is defined as the operator associated with the closure in $L^2(\mathcal{G})$ of the quadratic form (2.9). Clearly, the domain of the closure coincides with $H_0^1(\mathcal{G})$ and hence $\mathbf{H}_D$ is given as a restriction of $\mathbf{H}$ to the domain $\mathrm{dom}(\mathbf{H}_D) := \mathrm{dom}(\mathbf{H}) \cap H_0^1(\mathcal{G})$ (see, e.g., [24, Theorem 10.17]). Taking into account (2.4), $\mathbf{H}_D$ is often called the *Dirichlet Laplacian* (which also explains the subscript). On the other hand, the form $\mathfrak{t}$ is well defined on $H^1(\mathcal{G})$ and, moreover,

$$\mathfrak{t}_N[f] := \mathfrak{t}[f], \qquad f \in \mathrm{dom}(\mathfrak{t}_N) = H^1(\mathcal{G})$$

is closed (since $H^1(\mathcal{G})$ is a Hilbert space). The self-adjoint operator $\mathbf{H}_N$ associated with this form is usually called the *Neumann extension* of $\mathbf{H}_0$ or *Neumann Laplacian*.

Remark 2.5. Following the analogy with the Dirichlet Laplacian, it might be tempting to take $\mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$ as the domain of the Neumann Laplacian. However, the operator defined on this domain has a different name — the Gaffney Laplacian – and it is not even symmetric in general. The main focus of the following two sections will be on the study of this operator.

3. The Gaffney Laplacian

Let us fix an orientation on $\mathcal{G}$. In the Hilbert space $L^2(\mathcal{G})$, we can associate (at least) two operators with ∇ defined by (2.2). Namely, set

$$\nabla_D := \nabla \restriction \mathrm{dom}(\nabla_D), \qquad\qquad \nabla_N := \nabla \restriction \mathrm{dom}(\nabla_N), \tag{3.1}$$

where

$$\mathrm{dom}(\nabla_D) = H_0^1(\mathcal{G}), \qquad\qquad \mathrm{dom}(\nabla_N) = H^1(\mathcal{G}). \tag{3.2}$$

The importance of ∇_D and ∇_N stems from the following fact.

Lemma 3.1. *Let $\mathbf{H}_D$ and $\mathbf{H}_N$ be the Friedrichs and the Neumann extensions of $\mathbf{H}_0$, respectively. Then*

$$\mathbf{H}_D = \nabla_D^* \nabla_D, \qquad\qquad \mathbf{H}_N = \nabla_N^* \nabla_N, \tag{3.3}$$

where $*$ denotes the adjoint operator.

Proof. Since $H_0^1(\mathcal{G})$ and $H^1(\mathcal{G})$ are Hilbert spaces, both ∇_D and ∇_N are closed operators in $L^2(\mathcal{G})$ and hence $\nabla_D^*\nabla_D$ and $\nabla_N^*\nabla_N$ are self-adjoint non-negative operators in $L^2(\mathcal{G})$. The quadratic forms associated with $\nabla_D^*\nabla_D$ and $\nabla_N^*\nabla_N$ coincide with, respectively, the quadratic forms of $\mathbf{H}_D$ and $\mathbf{H}_N$ and the claim now follows from the representation theorem (see, e.g., [17, Chapter VI.2.1]). $\square$

Remark 3.2. Clearly, ∇ and hence both ∇_D and ∇_N do depend on the choice of an orientation on $\mathcal{G}$. However, it is straightforward to see that the second order operators $\mathbf{H}_D$ and $\mathbf{H}_N$ do not depend on it.

Now we are in position to introduce the main object. In the Hilbert space $L^2(\mathcal{G})$, define the following operators

$$\mathbf{H}_{G,\min} = \nabla_N^* \nabla_D, \qquad\qquad \mathbf{H}_G = \nabla_D^* \nabla_N. \tag{3.4}$$

Both operators are understood as a product of (unbounded) operators in a Hilbert space: they act edgewise as the negative second derivative and their domains are

$$\begin{aligned} \mathrm{dom}(\mathbf{H}_{G,\min}) &= \{f \in H_0^1(\mathcal{G}) |\, \nabla f \in \mathrm{dom}(\nabla_N^*)\}, \\ \mathrm{dom}(\mathbf{H}_G) &= \{f \in H^1(\mathcal{G}) |\, \nabla f \in \mathrm{dom}(\nabla_D^*)\}. \end{aligned}$$

The operator $\mathbf{H}_G$ is called the *Gaffney Laplacian*. We shall call $\mathbf{H}_{G,\min}$ the *minimal Gaffney Laplacian*.

Lemma 3.3. *Both operators* $\mathbf{H}_G$ *and* $\mathbf{H}_{G,\min}$ *are restrictions of the maximal Kirchhoff Laplacian* $\mathbf{H}$*/extensions of the minimal Kirchhoff Laplacian* $\mathbf{H}_0$*,*

$$\mathbf{H}_0 \subseteq \mathbf{H}_{G,\min} \subseteq \mathbf{H}_G \subseteq \mathbf{H}. \tag{3.5}$$

Proof. It is straightforward to verify both claims, however, we would like to show that

$$\mathrm{dom}(\nabla_D^*) = \Big\{ f \in H^1(\mathcal{G}\setminus\mathcal{V}) \Big| \sum_{e\in\mathcal{E}_v} \vec{f}_e(v) = 0 \text{ for all } v \in \mathcal{V} \Big\}, \tag{3.6}$$

which then makes the inclusions in (3.5) obvious. Here we employ the following notation

$$\vec{f}_e(v) = \begin{cases} f_e(v), & v \text{ is terminal,} \\ -f_e(v), & v \text{ is initial.} \end{cases}$$

If f belongs to the RHS in (3.6), then an integration by parts gives

$$\ell_f(g) := \langle \nabla_D g, f\rangle_{L^2} = -\langle g, \nabla f\rangle_{L^2} \tag{3.7}$$

for all $g \in H^1(\mathcal{G}) \cap L^2_c(\mathcal{G})$. Clearly, ℓ_f extends to a bounded linear functional on L^2, which implies that $f \in \mathrm{dom}(\nabla_D^*)$ and hence this proves the inclusion "$\supseteq$".

Suppose now that $f \in \mathrm{dom}(\nabla_D^*)$. Fixing an edge $e \in \mathcal{E}$ and taking a test function $g \in H^1_0(\mathcal{G})$ such that g equals zero everywhere except e, we immediately conclude that f belongs to H^1 on e. Next pick a vertex $v \in \mathcal{V}$. Choose $g \in H^1_0(\mathcal{G})$ such that $g \equiv 0$ on $\mathcal{E}\setminus\mathcal{E}_v$. Moreover, for every $e \in \mathcal{E}_v$ we assume that $g(x_e) = 1$ if $x_e \in e$ and $|x_e - v| < |e|/4$ and $g(x_e) = 0$ if $|x_e - v| > |e|/2$. Thus we get

$$\begin{aligned} 0 = \langle f, \nabla_D g\rangle - \langle \nabla_D^* f, g\rangle &= \sum_{e\in\mathcal{E}_v} \int_e f(\nabla g)^* + \nabla f\, g^* dx_e \\ &= \sum_{e\in\mathcal{E}_v} \vec{f}_e(v) g_e(v)^* = \sum_{e\in\mathcal{E}_v} \vec{f}_e(v). \end{aligned}$$

This also implies that we can perform the integration by parts in (3.7) for every $g \in H^1(\mathcal{G}) \cap L^2_c(\mathcal{G})$. Since ℓ_f extends to a bounded linear functional on $L^2(\mathcal{G})$, we conclude that $\nabla f \in L^2(\mathcal{G})$, which completes the proof. □

Clearly, all four operators in (3.5) coincide exactly when $\mathbf{H}_0$ is self-adjoint (and hence all four operators are self-adjoint). Moreover, by the very definition we have

$$\mathbf{H}_{G,\min} \subseteq \mathbf{H}_D \subseteq \mathbf{H}_G, \qquad \mathbf{H}_{G,\min} \subseteq \mathbf{H}_N \subseteq \mathbf{H}_G. \tag{3.8}$$

In particular, $\mathbf{H}_{G,\min}$ is symmetric, however, $\mathbf{H}_G$ may not be symmetric (and hence self-adjoint). The next result provides several self-adjointness criteria for $\mathbf{H}_G$ including a transparent geometric characterization.

Lemma 3.4. *The following statements are equivalent:*

(i) *The Gaffney Laplacian* $\mathbf{H}_G$ *is self-adjoint,*
(ii) $\mathbf{H}_{G,\min} = \mathbf{H}_G$*,*
(iii) $H^1_0(\mathcal{G}) = H^1(\mathcal{G})$*,*
(iv) $\mathbf{H}_0$ *has a unique Markovian extension,*
(v) $\mathcal{G}$ *has no finite volume ends,* $\mathfrak{C}_0(\mathcal{G}) = \emptyset$*.*

Proof. The equivalence $(iii) \Leftrightarrow (iv)$ is well known; $(iii) \Leftrightarrow (v)$ was established in [18, Corollary 3.12]. The remaining equivalences follow upon noting that $\nabla_D = \nabla_N$ if and only if $H^1_0(\mathcal{G}) = H^1(\mathcal{G})$. □

Recall that an extension $\widetilde{\mathbf{H}}$ of the minimal Kirchhoff Laplacian $\mathbf{H}_0$ is called *Markovian* if $\widetilde{\mathbf{H}}$ is a non-negative self-adjoint extension and the corresponding quadratic form is a *Dirichlet form* (for further details we refer to [9, Chapter 1]). Hence the associated semigroup $\mathrm{e}^{-t\widetilde{\mathbf{H}}}$, $t > 0$ as well as resolvents $(\widetilde{\mathbf{H}} + \lambda)^{-1}$, $\lambda > 0$ are Markovian: i.e., are both *positivity preserving* (map non-negative functions to non-negative functions) and L^∞*-contractive* (map the unit ball of $L^\infty(\mathcal{G})$ into itself). Notice that both the Dirichlet and Neumann Laplacians are Markovian extensions. A self-adjoint extension $\widetilde{\mathbf{H}}$ of $\mathbf{H}_0$ is called a *finite energy extension* if its domain is contained in $H^1(\mathcal{G})$. In particular, every Markovian extension is a finite energy extension (for further details we refer to [18, §5]).

The importance of the Gaffney Laplacian in the study of Markovian and, more generally, finite energy extensions of $\mathbf{H}_0$ stems from the following fact.

Lemma 3.5. *The domain of the Gaffney Laplacian is given by*

$$\mathrm{dom}(\mathbf{H}_G) = \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G}). \tag{3.9}$$

In particular, $\widetilde{\mathbf{H}}$ *is a Markovian/finite energy self-adjoint extension of* $\mathbf{H}_0$ *if and only if* $\widetilde{\mathbf{H}}$ *is a Markovian/self-adjoint restriction of* $\mathbf{H}_G$*.*

Proof. The inclusion $\mathrm{dom}(\mathbf{H}_G) \subseteq \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$ follows from the definition of $\mathbf{H}_G$. The converse inclusion is immediate from (3.6). □

As in the case of the maximal and minimal Kirchhoff Laplacians, there is a close connection between the Gaffney Laplacians.

Lemma 3.6. *The minimal Gaffney Laplacian is closed in* $L^2(\mathcal{G})$ *and*

$$\mathbf{H}_{G,\min} = \mathbf{H}_G^*. \tag{3.10}$$

Proof. By the very definition of $\mathbf{H}_G$, we get

$$\nabla_N^* \nabla_D \subseteq \mathbf{H}_G^*$$

and hence $\mathbf{H}_{G,\min} \subseteq \mathbf{H}_G^*$. To prove the converse inclusion, observe that $\mathbf{H}_G^* \subseteq \mathbf{H}_D$ and $\mathbf{H}_G^* \subseteq \mathbf{H}_N$. Taking into account Lemma 3.1, we thus get

$$\begin{aligned}
\mathrm{dom}(\mathbf{H}_G^*) &\subseteq \mathrm{dom}(\mathbf{H}_D) \cap \mathrm{dom}(\mathbf{H}_N) \\
&= \{f \in H^1_0(\mathcal{G}) |\, \nabla_D f \in \mathrm{dom}(\nabla_D^*)\} \cap \{f \in H^1(\mathcal{G}) |\, \nabla_N f \in \mathrm{dom}(\nabla_N^*)\} \\
&= \{f \in H^1_0(\mathcal{G}) |\, \nabla_D f \in \mathrm{dom}(\nabla_N^*)\} \\
&= \mathrm{dom}(\mathbf{H}_{G,\min}),
\end{aligned}$$

which implies (3.10). Since the adjoint is always closed, the first claim follows. □

Remark 3.7. The fact that $\mathbf{H}_{G,\min}$ is a closed operator can be seen by noting that its domain is the intersection of domains of the Friedrichs and Neumann extensions,

$$\mathrm{dom}(\mathbf{H}_{G,\min}) = \mathrm{dom}(\mathbf{H}_D) \cap \mathrm{dom}(\mathbf{H}_N). \tag{3.11}$$

Indeed, one simply needs to compare the definition of $\mathbf{H}_{G,\min}$ with (3.3) and take into account that $\nabla_N^* \subseteq \nabla_D^*$. Since both $\mathbf{H}_D$ and $\mathbf{H}_N$ are closed, one concludes that so is $\mathbf{H}_{G,\min}$.

Our first main result is the following connection between deficiency indices of $\mathbf{H}_{G,\min}$ and graph ends.

Theorem 3.8. *The deficiency indices of the minimal Gaffney Laplacian* $\mathbf{H}_{G,\min}$ *coincide with the number of finite volume ends of* $\mathcal{G}$*,*

$$\mathrm{n}_\pm(\mathbf{H}_{G,\min}) = \#\mathfrak{C}_0(\mathcal{G}). \tag{3.12}$$

Proof. If $\#\mathfrak{C}_0(\mathcal{G}) < \infty$, then using the results of [18, §6] one can easily see that $\dim(\mathrm{dom}(\mathbf{H}_N)/\,\mathrm{dom}(\mathbf{H}_{G,\min})) = \#\mathfrak{C}_0(\mathcal{G})$ (indeed, combine Prop. 6.6(i) and Corollary 6.7 with Theorem 3.11 from [18]). This immediately implies (3.12) since $\mathbf{H}_N$ is a self-adjoint extension of $\mathbf{H}_{G,\min}$ (cf. [24, Theorem 13.10]).

It remains to consider the case $\#\mathfrak{C}_0(\mathcal{G}) = \infty$. By (3.9) and [18, Lemma 4.7],

$$\dim(\ker(\mathbf{H}_G - \lambda)) = \dim(\ker(\mathbf{H} - \lambda) \cap H^1(\mathcal{G})) = \#\mathfrak{C}_0(\mathcal{G}) \tag{3.13}$$

for all negative real λ. It remains to notice that $\mathbf{H}_G \subseteq \mathbf{H}^*_{G,\min}$ and hence the claim follows from the positivity of $\mathbf{H}_{G,\min}$. □

In contrast to the minimal Gaffney Laplacian, $\mathbf{H}_G$ is not automatically closed, that is, $\mathbf{H}^*_{G,\min} = \overline{\mathbf{H}_G}$, although it is not necessarily true that

$$\mathbf{H}^*_{G,\min} = \mathbf{H}_G. \tag{3.14}$$

Our second main result provides necessary and sufficient conditions for the Gaffney Laplacian to be closed.

Theorem 3.9. *Let* $\mathcal{G}$ *be a metric graph satisfying Hypothesis 2.1 and let* $\mathbf{H}_G$ *be the corresponding Gaffney Laplacian.*

(i) *If* $\#\mathfrak{C}_0(\mathcal{G}) < \infty$*, then* $\mathbf{H}_G$ *is closed and* (3.14) *holds true.*
(ii) *If* $\mathcal{G}$ *contains a non-free finite volume end, then* $n_\pm(\mathbf{H}_{G,\min}) = \infty$ *and* $\mathbf{H}_G$ *is not closed.*

Proof. (i) It suffices to employ the following decomposition

$$\mathrm{dom}(\mathbf{H}^*_{G,\min}) = \mathrm{dom}(\mathbf{H}_D) \dotplus \ker(\mathbf{H}^*_{G,\min} - z) = \mathrm{dom}(\mathbf{H}_D) \dotplus \mathcal{N}_z(\mathbf{H}_{G,\min}), \tag{3.15}$$

which holds for every z in the resolvent set of $\mathbf{H}_D$ (see, e.g., [24, Prop. 14.11]). By Theorem 3.8, $\dim(\ker(\mathbf{H}^*_{G,\min} - z)) = \#\mathfrak{C}_0(\mathcal{G}) < \infty$. Combining (3.13) with $\mathrm{dom}(\mathbf{H}_G) \subseteq \mathrm{dom}(\mathbf{H}^*_{G,\min})$, we conclude that $\mathrm{dom}(\mathbf{H}_G) = \mathrm{dom}(\mathbf{H}^*_{G,\min})$.

(ii) Since the mapping $\nabla\colon H^1(\mathcal{G}) \to L^2(\mathcal{G})$ is bounded, (3.14) holds if and only if there exists a positive constant $C > 0$ such that

$$\|\nabla f\|^2_{L^2(\mathcal{G})} \le C(\|f\|^2_{L^2(\mathcal{G})} + \|\mathbf{H}f\|^2_{L^2(\mathcal{G})}), \tag{3.16}$$

for all $f \in \mathrm{dom}(\mathbf{H}_G) = \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$.

Let $\gamma \in \mathfrak{C}_0(\mathcal{G})$ be a non-free finite volume end of $\mathcal{G}$. For a sequence of open sets $\mathcal{U} = (U_n)$ representing γ, we can choose a sequence $(\mathcal{G}_n)$ of connected subgraphs of $\mathcal{G}$ such that $\#\partial\mathcal{G}_n < \infty$, $\mathcal{G}_n \supseteq \mathcal{G}_{n+1}$ and $\mathcal{G}_n \subset U_n$ for all n. Notice that $\#\mathfrak{C}_0(\mathcal{G}_n) = \infty$ for every $n \ge 0$ and $\bigcap_{n\ge 0} \mathcal{G}_n = \emptyset$ and hence $\mathrm{vol}(\mathcal{G}_n) \to 0$ as $n \to \infty$.

Fix $\lambda < 0$ and denote by $\mathbf{H}_n$ the Gaffney Laplacian on the subgraph $\mathcal{G}_n$, $n \ge 0$. Taking into account (3.13), there exists a real-valued function $f_n \in \ker(\mathbf{H}_n - \lambda)$ with $f_n(v) = 0$ for all $v \in \partial\mathcal{G}_n$ and such that $\|f_n\|_\infty = 1$ Moreover, extending f_n by zero on $\mathcal{G} \setminus \mathcal{G}_n$ gives a function (also denoted by f_n) belonging to the domain of the Gaffney Laplacian $\mathbf{H}_G$ on $\mathcal{G}$.

Assuming that $\mathbf{H}_G$ is closed, (3.16) would imply that

$$\|\nabla f_n\|_{L^2(\mathcal{G})} \lesssim \|f_n\|^2_{L^2(\mathcal{G})} + \|\mathbf{H}f_n\|^2_{L^2(\mathcal{G})} = (1+\lambda^2)\|f_n\|^2_{L^2(\mathcal{G}_n)} \le (1+\lambda^2)\mathrm{vol}(\mathcal{G}_n)$$

for all $n \ge 0$. Next, for each n there is $x_n \in \mathcal{G}_n$ with $|f_n(x_n)| \ge 1/2$. Choosing $y_n \in \partial\mathcal{G}_n$ and a path $\mathcal{P}_n$ in $\mathcal{G}_n$ connecting x_n and y_n, we get

$$\frac{1}{2} = |f_n(x_n) - f_n(y_n)| \le \int_{\mathcal{P}_n} |\nabla f_n(x)|dx \le \mathrm{vol}(\mathcal{P}_n)\|\nabla f_n\|_{L^2(\mathcal{G})} \lesssim \mathrm{vol}(\mathcal{G}_n)^2$$

for all $n \ge 0$. However, the right-hand side tends to zero when $n \to \infty$. This contradiction completes the proof. □

Let us now present two particular cases of interest when Theorem 3.9 provides necessary and sufficient condition for $\mathbf{H}_G$ to be closed.

Corollary 3.10. *Suppose $\mathcal{G}$ has finite total volume. The following are equivalent:*

(i) *The Gaffney Laplacian $\mathbf{H}_G$ is closed,*
(ii) (3.14) *holds true,*
(iii) *$\mathcal{G}$ has finitely many ends, $\#\mathfrak{C}(\mathcal{G}) < \infty$.*

Proof. We only need to notice that $\mathfrak{C}(\mathcal{G}) = \mathfrak{C}_0(\mathcal{G})$ in the case when $\mathrm{vol}(\mathcal{G}) < \infty$. By Halin's theorem [13], a locally finite graph $\mathcal{G}$ has at least one end which is not free if $\mathfrak{C}(\mathcal{G}) = \infty$. Thus, it remains to apply Theorem 3.9. □

Theorem 3.9 also gives rise to a criterion in the case of Cayley graphs.

Corollary 3.11. *Suppose $\mathcal{G}_d$ is a Cayley graph of a countable finitely generated group G. Then $\mathbf{H}_G$ is not closed if and only if $\#\mathfrak{C}(\mathcal{G}) = \infty$ and $\mathcal{G}$ has at least one finite volume end.*

Proof. If there are infinitely many ends, then the end space is known to be homeomorphic to the Cantor set and hence there are no free graph ends. Theorem 3.9 completes the proof. □

Remark 3.12. By the Freudenthal–Hopf theorem, a Cayley graph of a countable finitely generated group has 1, 2 or infinitely many ends. Moreover, the number of ends is independent of the choice of the finite generating set. By Hopf's theorem, $\mathcal{G}_d$ has exactly two ends if and only if G is virtually infinite cyclic. The classification of finitely generated groups with infinitely many ends is due to J. R. Stallings (see, e.g., [11, Chapter 13]). In particular, if G is amenable, then it has finitely many ends (actually, either 1 or 2) and hence the Gaffney Laplacian is always closed for Cayley graphs of amenable groups.

Remark 3.13. The above considerations shed more light on the results obtained in [18].

(i) First of all, combining (3.5) with (3.9) and Theorem 3.9(i) we obtain one of the main results in [18], Theorem 4.1, on the deficiency indices of the Kirchhoff Laplacian:

$$\mathrm{n}_\pm(\mathbf{H}_0) \ge \#\mathfrak{C}_0(\mathcal{G}), \tag{3.17}$$

with equality if and only if either $\#\mathfrak{C}_0(\mathcal{G}) = \infty$ or $\mathrm{dom}(\mathbf{H}) \subset H^1(\mathcal{G})$.

(ii) It is straightforward to see that in the case when $\mathcal{G}$ has finitely many finite volume ends, $\#\mathfrak{C}_0(\mathcal{G}) < \infty$, the triplet $\Pi = \{\mathbb{C}^{\#\mathfrak{C}_0(\mathcal{G})}, \Gamma_0, \Gamma_1\}$, where the mappings $\Gamma_0, \Gamma_1 \colon \operatorname{dom}(\mathbf{H}) \cap H^1(\mathcal{G}) \to \mathbb{C}^{\#\mathfrak{C}_0(\mathcal{G})}$ are defined by

$$\Gamma_0 \colon f \mapsto \big(f(\gamma)\big)_{\gamma\in\mathfrak{C}_0(\mathcal{G})}, \qquad \Gamma_1 \colon f \mapsto \big(\partial_n f(\gamma)\big)_{\gamma\in\mathfrak{C}_0(\mathcal{G})}, \tag{3.18}$$

(see Prop. 6.6 and Lemma 6.9 in [18, §6]) is a *boundary triplet*[3] for the Gaffney Laplacian $\mathbf{H}_G$. This also implies the description of Markovian and finite energy extensions of $\mathbf{H}_0$ obtained in [18, Theorem 6.11].

4. Examples

The case not covered by Theorem 3.9 is when $\mathcal{G}$ has infinitely many finite volume free ends, however, all non-free ends have infinite volume. Moreover, there is one more problem: it is not clear what is the closure of $\mathbf{H}_G$ if it is not closed. We begin with the following result.

Proposition 4.1. *Let $\mathcal{G}$ contain a sequence of connected subgraphs $(\mathcal{G}_n)$ such that*

(a) $\lim_{n\to\infty} \operatorname{vol}(\mathcal{G}_n) = 0$, *and*

(b) $\#\partial\mathcal{G}_n < \#\mathfrak{C}(\mathcal{G}_n)$ *for all* $n \ge 0$.

Then $\mathbf{H}_G$ is not closed.

Proof. It is easy to see that properties (a) and (b) are exactly the ones used in the proof of Theorem 3.9(ii) (in the case of a free finite volume end $\#\partial\mathcal{G}_n < \infty$ and $\#\mathfrak{C}(\mathcal{G}_n) = \#\mathfrak{C}_0(\mathcal{G}_n) = \infty$ for all $n \ge 0$) and hence the proof of Proposition 4.1 is literally the same and we leave it to the reader. □

Remark 4.2. In fact, one can replace (a) in Proposition 4.1 by the weaker assumption:

(a') $\sup_n \operatorname{vol}(\mathcal{G}_n) < \infty$ and $\lim_n \operatorname{diam}(\mathcal{G}_n) = 0$,

where $\operatorname{diam}(\mathcal{G}_n)$ is the diameter of $\mathcal{G}_n$, i.e., the length of the "longest" path in $\mathcal{G}_n$.

Proposition 4.1 enables us to construct graphs without finite volume non-free ends, however with the corresponding Gaffney Laplacian $\mathbf{H}_G$ being not closed.

Example 4.3. Take a path graph $\mathcal{P}_0 = (\mathbb{Z}_{\ge 0}, |\cdot|)$ equipped with some positive lengths and attach to each vertex $v_n \in \mathbb{Z}_{\ge 0}$ an infinite rooted graph $\mathcal{G}_n$. If each $\mathcal{G}_n$ has at least two ends (e.g., each $\mathcal{G}_n$ consists of two rooted antitrees joined at the root vertices) and $\liminf_n \operatorname{vol}(\mathcal{G}_n) = 0$, then $\mathbf{H}_G$ is not closed (see Figure 1).

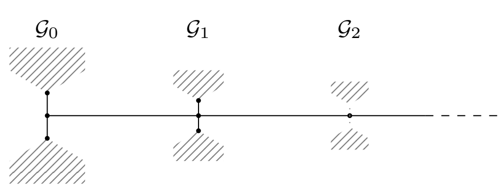

Figure 1. $\mathbb{Z}_{\ge 0}$ with attached graphs $\mathcal{G}_n$.

[3] For definitions and basic properties we refer to, e.g., [24, Chapter 14] or [8, Appeendix A].

Remark 4.4. If one of the conditions (a), (a'), or (b) fails to hold, then the corresponding Gaffney Laplacian may or may not be closed. Indeed, consider the graph depicted on Figure 1. Assuming that each $\mathcal{G}_n$ has finitely many graph ends and finite total volume, the Gaffney Laplacian $\mathbf{H}_n$ on $\mathcal{G}_n$ is closed, which is further equivalent to the validity of Sobolev-type inequality (3.16) with some constant $C_n > 0$, $n \geq 0$. Also one has similar inequalities on every edge of a path graph, however, the corresponding constants do depend on the edges lengths (see, e.g., [17, Chapter IV.2]). When we "glue" the graphs $(\mathcal{G}_n)$ and edges of a path graph, the space $H^1(\mathcal{G})$ is a subspace of the direct sum of H^1 spaces and hence if all the constants admit a uniform upper bound, then (3.16) would trivially hold true on $\mathcal{G}$ (e.g., take all $\mathcal{G}_n$ being identical and assume that the path graph is equilateral).

Obtaining a complete answer in the case of a metric graph depicted on Figure 1 seems to be an interesting and nontrivial problem.

In conclusion we would like to show that for a large class of metric graphs the closure of the Gaffney Laplacian may coincide with the maximal Kirchhoff Laplacian (which is also equivalent to the fact that $\mathbf{H}_0 = \mathbf{H}_{G,\min}$).

Example 4.5 (Radially symmetric trees)**.** Let $\mathcal{G} = \mathcal{T}$ be a *radially symmetric metric tree*: that is, a tree $\mathcal{T}$ with a root o such that for each $n \geq 0$, all vertices in the combinatorial sphere S_n have the same number of descendants $b_n \in \mathbb{Z}_{\geq 2}$ and all edges between S_n and S_{n+1} have the same length $\ell_n \in (0, \infty)$. Clearly, a radially symmetric tree $\mathcal{T}$ is uniquely determined by the sequences (b_n) and (ℓ_n). The assumptions imply that $\mathcal{T}$ has uncountably many ends. Define

$$\mu_n = \prod_{k=0}^{n} b_k, \qquad\qquad t_n = \sum_{k=0}^{n-1} \ell_k,$$

for all $n \geq 0$. Notice that $(\mathcal{T}, \varrho)$ is complete exactly when $\mathcal{L} := \lim_{n\to\infty} t_n = \infty$.

Lemma 4.6. *Let $\mathcal{G} = \mathcal{T}$ be a radially symmetric tree. The corresponding Gaffney Laplacian $\mathbf{H}_G$ is closed if and only if*

$$\operatorname{vol}(\mathcal{T}) = \sum_{n\geq 0} \mu_n \ell_n = \infty. \tag{4.1}$$

If $\operatorname{vol}(\mathcal{T}) < \infty$*, then the closure of* $\mathbf{H}_G$ *coincides with the maximal Kirchhoff Laplacian* $\mathbf{H}$*,* $\mathbf{H}_G \neq \overline{\mathbf{H}}_G = \mathbf{H}$.

Proof. It is well-known (see, e.g., [4, 26]) that in the radially symmetric case $\mathbf{H}$ is self-adjoint if and only if $\operatorname{vol}(\mathcal{T}) = +\infty$. In particular, in this case all four operators in (3.5) coincide and hence $\mathbf{H}_G = \mathbf{H}_G^*$ is closed. If $\mathcal{T}$ has finite volume, then by Corollary 3.10 the Gaffney Laplacian $\mathbf{H}_G$ is not closed. Thus we only need to prove the second claim.

Since $\operatorname{vol}(\mathcal{T}) < \infty$, the Friedrichs extensions $\mathbf{H}_D$ has strictly positive spectrum (e.g. [19, Corollary 3.5]) and hence

$$\operatorname{dom}(\mathbf{H}) = \operatorname{dom}(\mathbf{H}_D) \dot{+} \ker(\mathbf{H}).$$

However, $\operatorname{dom}(\mathbf{H}_D) \subseteq \operatorname{dom}(\mathbf{H}_G)$ and it suffices to show that $\ker(\mathbf{H}) \subseteq \operatorname{dom}(\overline{\mathbf{H}_G})$. According to [4, 22] (see also [26, Section 7] and [3]), the Kirchhoff Laplacian on a radially symmetric trees $\mathbf{H}$ is unitarily equivalent to

$$\widetilde{\mathbf{H}} = \mathrm{H}_{\mathrm{sym}} \bigoplus_{n\geq 0} \mathrm{H}_n \otimes \mathbb{I}_{\mu_n - \mu_{n-1}}, \tag{4.2}$$

where the operators $\mathrm{H}_{\mathrm{sym}}$ and H_n in (4.2) are Sturm–Liouville operators defined by the differential expression

$$\tau = -\frac{1}{\mu(t)}\frac{d}{dt}\mu(t)\frac{d}{dt}, \tag{4.3}$$

however, in different L^2 spaces: $\mathrm{H}_{\mathrm{sym}}$ acts in $L^2([0,\mathcal{L});\mu)$ on the domain

$$\mathrm{dom}(\mathrm{H}_{\mathrm{sym}}) = \big\{f \in L^2([0,\mathcal{L});\mu) |\, f,\, \mu f' \in AC([0,\mathcal{L}]),\ \tau f \in L^2([0,\mathcal{L});\mu);\ f'(0) = 0\big\},$$

and H_n, $n \geq 0$ are defined in $L^2([t_n,\mathcal{L});\mu)$ on the domain

$$\mathrm{dom}(\mathrm{H}_n) = \big\{f \in L^2([t_n,\mathcal{L});\mu) |\, f,\, \mu f' \in AC([t_n,\mathcal{L}]),\ \tau f \in L^2([t_n,\mathcal{L});\mu);\ f(t_n) = 0\big\}.$$

The weight function $\mu\colon [0,\mathcal{L}) \to [0,\infty)$ is explicitly given by

$$\mu(s) = \sum_{n\geq 0} \mu_n \mathbb{1}_{[t_n,t_{n+1})}(s), \quad s \in [0,\mathcal{L}). \tag{4.4}$$

By (4.2), $\ker(\mathbf{H})$ can be decomposed via the kernels of $\mathrm{H}_{\mathrm{sym}}$ and H_n. Notice that $\ker(\mathrm{H}_{\mathrm{sym}}) = \mathrm{span}\{\mathbb{1}_{[0,\mathcal{L})}\}$ and $\ker(\mathrm{H}_n) = \mathrm{span}\{g_n\}$, where g_n is given by

$$g_n(x) = \int_{t_n}^{x} \frac{1}{\mu(s)} ds, \qquad x \in [t_n,\mathcal{L}).$$

With respect to the decomposition (4.2), every g_n as well as $\mathbb{1}_{(0,\mathcal{L})}$ define a function in $\ker(\mathbf{H})$. In particular, $\mathbb{1}_{(0,\mathcal{L})}$ gives rise to $\mathbb{1}_{\mathcal{T}}$, which is clearly in $H^1(\mathcal{T})$. Since

$$\int_{t_n}^{\infty} |g_n'(x)|^2 \mu(x) dx = \int_{t_n}^{\infty} \frac{dx}{\mu(x)} = \sum_{k=n}^{\infty} \frac{\ell_k}{\mu_n} < \infty,$$

according to [22, Theorem 3.1] (see also [26, equation (3.12)]), the other functions are also in $H^1(\mathcal{T})$. Thus $\ker(\mathbf{H}_G)$ is dense in $\ker(\mathbf{H})$, which completes the proof. □

Remark 4.7. Radially symmetric trees are a particular example of the so-called *family preserving metric graphs* (see [3] and also [2]). Employing the results from [3] (and also assuming no horizontal edges), it is in fact possible to show that for family preserving metric graphs $\mathbf{H}_0 = \mathbf{H}_{G,\min}$ and hence either $\mathbf{H}_G$ is closed (which holds exactly when the corresponding metric graph either has infinite volume, and hence $\mathbf{H}_0$ is self-adjoint [18, Remark 4.12], or it has finite volume and finitely many ends) or its closure coincides with the maximal Kirchhoff Laplacian.

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