Laplacians on Infinite Graphs

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Contents

Abstract

The main focus in this memoir is on Laplacians on both weighted graphs and weighted metric graphs. Let us emphasize that we consider infinite locally finite graphs and do not make any further geometric assumptions. Whereas the existing literature usually treats these two types of Laplacian operators separately, we approach them in a uniform manner in the present work and put particular emphasis on the relationship between them. One of our main conceptual messages is that these two settings should be regarded as complementary (rather than opposite) and exactly their interplay leads to important further insight on both sides.

Our central goal is twofold. First of all, we explore the relationships between these two objects by comparing their basic spectral (self-adjointness, spectral gap, etc.), parabolic (Markovian uniqueness, recurrence, stochastic completeness, etc.), and metric (quasi-isometries, intrinsic metrics, etc.) properties. In turn, we exploit these connections either to prove new results for Laplacians on metric graphs or to provide new proofs and perspective on the recent progress in weighted graph Laplacians. We also demonstrate our findings by considering several important classes of graphs (Cayley graphs, tessellations, and antitrees).

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CHAPTER 1

1.1. Introduction

The central object of this study is a Laplace-type operator either on a weighted graph or on a metric graph. Both objects have a venerable history and enjoy deep connections to several diverse branches of mathematics and mathematical physics, placing them at the intersection of many subjects in mathematics and engineering. It is impossible to give even a very brief account on these matters. The key features of Laplacians on metric graphs, which are also widely known as *quantum graphs*, include their use as simplified models of complicated quantum systems and the appearance of metric graphs in tropical and algebraic geometry, where they can be seen as non-Archimedean analogues of Riemann surfaces (we only refer to a very brief selection of recent monographs and collected works [**11**], [**23**], [**24**], [**61**], [**66**], [**68**], [**179**]). The subject of *discrete Laplacians on graphs* is even wider and has been intensively studied from several perspectives (a partial overview of the immense literature can be found in [**12**], [**42**], [**43**], [**89**], [**134**], [**209**]).

Whereas the existing literature usually treats these two Laplacian-type operators separately, we approach them in a uniform manner in the present work and put particular emphasis on the relationship between them. One of our main conceptual messages is that these two settings should be regarded as complementary (rather than opposite) and exactly their interplay leads to important further insight on both sides. In fact, the idea of using metric graphs in context with studying random walks on graphs can be traced back at least to the 1980's. Namely, there is a close relationship between random walks on graphs and Brownian motion on metric graphs and, for example, N.Th. Varopoulos used this in [**202**] to prove long-range estimates for discrete time random walks by first establishing similar estimates for heat kernels on specifically designed metric graphs (see also the recent works [**13**], [**15**], [**20**], [**70**], [**71**], [**152**] for further manifestations of this point of view). In more structural terms, difficulties in analyzing random walks on graphs often stem from the fact that the Dirichlet form associated with a weighted discrete Laplacian is non-local (e.g., no Leibniz rule), whereas the corresponding quadratic form for metric graphs is, in general, a strongly local Dirichlet form and hence many familiar tools from analysis are available. On the other hand, having in mind a metric graph, it is rather natural to think of weighted discrete Laplacians as discretizations and hence simplified models of quantum graphs (replacing differential equations by difference equations, which is similar to triangulations of surfaces, see, e.g., [**43**, § 3.2]).

Our main focus is on infinite graphs (with countably many vertices and edges), however, we always restrict to locally finite graphs (for definitions we refer to the next chapter). The study of Laplacians on weighted graphs, i.e., difference expressions of the form

$$(L\mathbf{f})(v) = \frac{1}{m(v)} \sum_{u \in \mathcal{V}} b(v,u)(\mathbf{f}(v) - \mathbf{f}(u)), \quad v \in \mathcal{V}, \tag{1.1.1}$$

has seen a tremendous progress during the last decade (see [**134**]). Whereas this setting is rather general, most works on metric graph Laplacians impose strong restrictions on edge lengths (e.g., a strictly positive lower bound on edge lengths [**24**], [**179**]), which excludes a number of interesting models and phenomena. On a conceptual level, removing these assumptions can be considered as similar to the case when the difference expression (1.1.1) gives rise to an unbounded operator (i.e., the *weighted degree function* (2.2.8) is unbounded on the vertex set). In fact, the arising difficulties in both cases are of the same nature and, since we are considering unbounded operators, one of the crucial issues is the correct choice of the domain of definition. Namely, the first mathematical problem arising in any quantum mechanical model is **self-adjointness** (see, e.g., [**181**, Chap. VIII.11]), that is, usually a formal symmetric expression for the Hamiltonian has some natural domain of definition in a given Hilbert space (e.g., pre-minimally or maximally defined Laplacians) and then one has to verify that it gives rise to an (essentially) self-adjoint operator. Otherwise[†], there are infinitely many self-adjoint extensions (or restrictions in the maximally defined case) and one has to determine the right one which is the observable.

Let us put all that in a slightly different context. For a given metric measure space (X, μ), denote the formal expression in question by Δ. Moreover, we shall assume that Δ is formally symmetric and non-positive, that is, the corresponding quadratic form $\mathfrak{Q}[f] = \langle -\Delta f, f\rangle_{L^2(X;\mu)}$ is non-negative (one may think of X as either a manifold or a graph/metric graph and then Δ is the corresponding Laplacian). Suppose the evolution of a system is governed by one of the three most common equations — heat, wave or Schrödinger equation — and one is lead to investigate the corresponding Cauchy problem. For instance, in quantum mechanics, one is interested in the solvability in L^2 of the Cauchy problem for the Schrödinger equation

$$\mathrm{i}\partial_t u = -\Delta u, \qquad u|_{t=0} = u_0 \in L^2(X;\mu). \tag{1.1.2}$$

It is exactly the self-adjointness of Δ defined on the maximal domain of definition in $L^2(X;\mu)$ which ensures the existence and uniqueness of solutions to (1.1.2). If the maximally defined Laplacian is not a self-adjoint operator in $L^2(X;\mu)$, then one needs to impose additional boundary conditions on X. Similarly, the self-adjointness of the maximally defined Δ ensures the solvability of the Cauchy problem in L^2 for both the heat and the wave equations. However, under the above assumptions on Δ, the solvability of those two equations is in fact equivalent to the self-adjointness (see, e.g., [**189**, §1.1]).

When considering the Cauchy problem for the heat equation

$$\partial_t u = \Delta u, \qquad u|_{t=0} = u_0 \in L^2(X;\mu), \tag{1.1.3}$$

[†]Of course, one needs to check whether the corresponding symmetric operator has equal deficiency indices, which is always the case for Laplacians or, more generally, for symmetric operators which are bounded from below or from above.

and having in mind, for instance, either a Brownian motion on a manifold or a random walk on a graph, one can be a bit more specific: the corresponding semigroup $(e^{-\Delta t})_{t>0}$ should be positivity preserving and L^∞ contractive, that is, the semigroup possesses properties reflecting heat diffusion. Thus, one is interested in very specific self-adjoint extensions — extensions enjoying the *Markov property.* According to the Beurling–Deny criteria (see, e.g., [**50**]), the latter is equivalent to the fact that the corresponding quadratic form is a *Dirichlet form.* Clearly, the self-adjoint uniqueness implies Markovian uniqueness (i.e., the uniqueness of extensions enjoying the Markov property), however, the converse is not true in general. Furthermore, if there are several different Markovian extensions, one is led to the analogous question of their description via additional boundary conditions on X.

On the other hand, both problems (self-adjoint and Markovian uniqueness) can be restated in a more transparent way via solutions to the Helmholz equation

$$\Delta u = \lambda u, \qquad \lambda \in \mathbb{R}. \tag{1.1.4}$$

Since Δ is assumed non-positive, the maximally defined operator is self-adjoint if and only if for some (and hence for all) $\lambda > 0$ equation (1.1.4) admits a unique solution $u \in L^2(X;\mu)$ (which is clearly identically zero in this case). Moreover, Markovian uniqueness can be expressed in these terms as well: the Helmholz equation (1.1.4) for $\lambda > 0$ admits a unique solution $u \in L^2(X;\mu)$ having *finite energy*, that is, u has finite Dirichlet integral $\mathfrak{Q}[u] < \infty$. Recalling that in the context of both manifolds and graphs functions satisfying (1.1.4) are called λ-harmonic, the self-adjoint and Markovian uniqueness can be seen as some kind of a Liouville-type property of X (e.g., L^2 Liouville-type property [**123**], [**151**], [**214**])† and this indicates their close connections with the geometry of the underlying metric space (e.g., Gaffney-type theorems connecting completeness with Markovian and self-adjoint uniqueness [**78**]).

As it was mentioned already, one of the main objects under consideration in this text is a Laplacian on an infinite metric graph. A metric graph $\mathcal{G}$ is a graph $\mathcal{G}_d = (\mathcal{V},\mathcal{E})$ whose edges $e \in \mathcal{E}$ are assigned some lengths $|e|$ and hence can be considered as intervals (for the sake of a clear exposition, $\mathcal{G}_d$ is assumed simple throughout the present chapter; strict definitions of all objects can be found in Chapter 2). Let also $\mu,\nu\colon \mathcal{G} \to (0,\infty)$ be edgewise constant weights. The corresponding Laplacian Δ‡ acts edgewise in $L^2(\mathcal{G};\mu)$ as a Sturm–Liouville operator

$$\frac{1}{\mu(e)}\frac{\mathrm{d}}{\mathrm{d}x_e}\nu(e)\frac{\mathrm{d}}{\mathrm{d}x_e}, \qquad e \in \mathcal{E}. \tag{1.1.5}$$

In order to reflect the underlying combinatorial structure, we impose the Kirchhoff conditions (see (2.4.6) for details)

$$\begin{cases} f \text{ is continuous at } v \\ \sum_{e\sim v} \nu(e)\partial_e f(v) = 0 \end{cases} \tag{1.1.6}$$

at all vertices. The second condition means that the sum of the slopes over all edges emanating from a given vertex is zero and can be interpreted as a zero total

†Under the positivity of the spectral gap one can in fact replace $\lambda > 0$ by $\lambda = 0$ and hence in this case one is led to harmonic functions on X.

‡Here and in the following sections, Δ shall always denote the Laplacian on a weighted metric graph.

flow condition in vertices.† The corresponding energy form in $L^2(X;\mu)$ is given by

$$\mathfrak{Q}[f] = \langle -\Delta f, f\rangle_{L^2(X;\mu)} = \int_{\mathcal{G}} |\nabla f(x)|^2 \nu(\mathrm{d}x). \tag{1.1.7}$$

Our second object of interest is the weighted graph Laplacian L given by (1.1.1) and acting in $\ell^2(\mathcal{V};m)$, where $m\colon \mathcal{V}\to(0,\infty)$ is a positive weight on $\mathcal{V}$. The function $b\colon \mathcal{V}\times\mathcal{V}\to[0,\infty)$ is symmetric, has vanishing diagonal and also satisfies certain natural restrictions (e.g., local summability, see Section 2.2). The corresponding energy form in $\ell^2(\mathcal{V};m)$ is given by

$$\mathfrak{q}[\mathbf{f}] = \langle L\mathbf{f},\mathbf{f}\rangle_{\ell^2(\mathcal{V};m)} = \frac{1}{2}\sum_{u,v} b(u,v)|\mathbf{f}(v)-\mathbf{f}(u)|^2. \tag{1.1.8}$$

One of the immediate ways to relate Laplacians on weighted metric and discrete graphs is by noticing a connection between their harmonic functions. Despite being elementary, this observation lies at the core of many of our considerations and hence we briefly sketch it here. By (1.1.5), every harmonic function f on a weighted metric graph $\mathcal{G}$ (i.e., f satisfies $\Delta f = 0$), must be edgewise affine. The Kirchhoff conditions (1.1.6) imply that f is continuous and, moreover, satisfies

$$\sum_{e\sim v}\nu(e)\partial_e f(v) = \sum_{u\sim v}\frac{\nu(e_{u,v})}{|e_{u,v}|}\big(f(u)-f(v)\big) = 0$$

at each vertex $v\in\mathcal{V}$. This suggests to consider a discrete Laplacian (1.1.1) with edge weights given by

$$b(u,v) = \begin{cases} \frac{\nu(e_{u,v})}{|e_{u,v}|}, & u\sim v\\ 0, & u\not\sim v\end{cases}, \qquad (u,v)\in\mathcal{V}\times\mathcal{V}. \tag{1.1.9}$$

Indeed, then for every Δ-harmonic function f on the weighted metric graph $\mathcal{G}$, its restriction to vertices $\mathbf{f} := f|_{\mathcal{V}}$ is an L-harmonic function, that is, it satisfies $L\mathbf{f} = 0$. Moreover, the converse is also true. Phrased in a more formal way, the map

$$\imath_{\mathcal{V}}\colon \begin{array}{ccc} C(\mathcal{G}) & \to & C(\mathcal{V}) \\ f & \mapsto & f|_{\mathcal{V}} \end{array}, \tag{1.1.10}$$

when restricted further to the space of continuous, edgewise affine functions on $\mathcal{G}$ becomes bijective and establishes a bijective correspondence between Δ-harmonic and L-harmonic functions (this immediately connects, for instance, the corresponding Poisson and Martin boundaries). Taking into account what we have said above regarding the self-adjointness problem, this also indicates a possible connection between the self-adjoint uniqueness for the corresponding Laplacians on $\mathcal{G}$ and $\mathcal{G}_d$, however, one also has to take into account the measures μ and m, that is, we need to connect the corresponding Hilbert spaces $L^2(\mathcal{G};\mu)$ and $\ell^2(\mathcal{V};m)$. It turns out

†On the one hand, (1.1.6) is just a conservation of the flow generated by the vector field $\nu f'$ upon considering $\nabla\colon f\mapsto f'$ as the exterior derivative and hence interpreting f' as a 1-form, that is, as a vector field with orientation (see also Remark 2.19). From this perspective (1.1.6) is also reminiscent of the Kirchhoff laws for electric networks. On the other hand, if one speaks about the quantum mechanical probability flow, its conservation at a given vertex is equivalent to the self-adjointness of the corresponding vertex conditions, and Kirchhoff conditions (1.1.6) is a particular case of this large family of boundary conditions.

that the desired connection (under the additional assumption that $(\mathcal{G}, \mu, \nu)$ has *finite intrinsic size*, see Definition 3.16) is given by

$$m \colon v \mapsto \sum_{u \sim v} |e_{u,v}| \mu(e_{u,v}), \qquad v \in \mathcal{V}. \tag{1.1.11}$$

This correspondence has been widely known for a quite long time in at least two particular cases. First of all, in the case of so-called unweighted *equilateral metric graphs* (i.e., $\mu = \nu = \mathbb{1}$ on $\mathcal{G}$ and $|e| = 1$ for all edges e), (1.1.1) with the weights (1.1.9),(1.1.11) turns into the *normalized (or physical) Laplacian*:

$$(L_{\mathrm{norm}}\mathbf{f})(v) = \frac{1}{\deg(v)} \sum_{u \sim v} \mathbf{f}(v) - \mathbf{f}(u), \quad v \in \mathcal{V}. \tag{1.1.12}$$

Connections between their spectral properties have been established in [**169**], [**204**] for finite metric graphs and then extended in [**40**], [**65**], [**34**] to infinite metric graphs, and in fact one can even prove some sort of local unitary equivalence [**176**]. These results allow to reduce the study of Laplacians on equilateral metric graphs to a widely studied object — the normalized Laplacian L_{norm}, the generator of the simple random walk on $\mathcal{G}_d$ (see [**12**], [**43**], [**192**], [**209**]). The second well-studied case is a slight generalization of the above setting: again, $|e| = 1$ for all edges e, however, $\mu = \nu$ on $\mathcal{G}$ (these are named *cable systems* in the work of Varopoulos [**202**]). The corresponding Laplacian L with the coefficients (1.1.9),(1.1.11) is the generator of a discrete time random walk on $\mathcal{G}_d$ with the probability of jumping from v to u given by

$$p(u, v) = \frac{\mu(e_{u,v})}{\sum_{w \sim v} \mu(e_{u,w})} \quad \text{when} \quad u \sim v,$$

and 0 otherwise. There is a close connection between this random walk and the Brownian motion on the cable system and exactly this link has been exploited several times in the literature (see [**20**], [**202**] as well as the recent works [**13**], [**15**], [**63**], [**70**], [**71**], [**152**]).

In fact, the idea to relate the properties of Δ and L by taking into account the relationship between their kernels has its roots in the fundamental works of M.G. Krein, M.I. Vishik and M.Sh. Birman in the 1950s. Indeed, it turns out that L serves as a "boundary operator" for Δ (for the precise meaning see Prop. 3.11) and exactly this fact allows to connect basic spectral properties of these two operators. However, in order to make all that precise one needs to use the machinery of boundary triplets and the corresponding Weyl functions, a modern language of extension theory of symmetric operators in Hilbert spaces, which can be seen as far-reaching development of the Birman–Krein–Vishik theory (see [**54**], [**55**], [**188**]). First applications of this approach to finite and infinite metric graphs can be traced back to the 2000s (see, e.g., [**34**], [**66**], [**179**]). One of its advantages is the fact that the boundary triplets approach allows to treat metric graphs avoiding the standard assumptions on the edge lengths [**67**], [**141**].

In order to make the above more precise, one of our main observations is the following connection between self-adjoint restrictions of the maximal Kirchhoff Laplacian $\mathbf{H}$ (the maximal operator associated with Δ in $L^2(\mathcal{G}; \mu)$) and self-adjoint restrictions of the maximal graph Laplacian $\mathbf{h}$ (the maximal operator associated with

L in $\ell^2(\mathcal{V};\mu)$, where b and m are defined by (1.1.9) and (1.1.11)):

$$\begin{aligned} \mathrm{Ext}_S(\widetilde{\mathbf{h}}) \ni \widetilde{\mathbf{h}} \quad &\mapsto \quad \widetilde{\mathbf{H}} \in \mathrm{Ext}_S(\widetilde{\mathbf{H}}), \\ &\mathrm{dom}(\widetilde{\mathbf{H}}) := \{f \in \mathrm{dom}(\mathbf{H}) \,|\, \imath_{\mathcal{V}}(f) \in \mathrm{dom}(\widetilde{\mathbf{h}})\} \end{aligned} \tag{1.1.13}$$

where $\imath_{\mathcal{V}}$ is the restriction map (1.1.10). It turns out that this map establishes a bijective correspondence between the sets $\mathrm{Ext}_S(\mathbf{H})$ of self-adjoint restrictions of $\mathbf{H}$ and $\mathrm{Ext}_S(\mathbf{h})$ of self-adjoint restrictions of $\mathbf{h}$ (Lemma 4.7). Moreover, it remains bijective upon further restricting it to certain classes of self-adjoint extensions (e.g., non-negative, Markovian) and connects their basic spectral and parabolic properties (e.g. positive spectral gap, discreteness, recurrence, stochastic completeness, and on-diagonal heat kernel bounds). It should be mentioned that some of these connections are only valid after a suitable subdivison of edges, which can intuitively be understood as choosing a fine enough discretization of a weighted metric graph.

In our opinion, a tremendous part of the progress during the last decade in the study of non-local Dirichlet forms (1.1.8) (notice that (1.1.13) enables us to use these results to investigate metric graph Laplacians) is connected with the successful introduction and systematic use of the notion of an *intrinsic metric* in the discrete setting (see [**73**], [**127**]). As it was underlined in the work of K.-T. Sturm in the 1990s [**195**]–[**197**], it is exactly this instrument which allows to transfer many important results from the manifold setting to the abstract setting of strongly local Dirichlet forms (which of course includes metric graphs). Taking all this into account, one may look at the restriction map (1.1.10) from a different perspective. First of all, every path metric ϱ on $\mathcal{G}$ induces a path metric on $\mathcal{V}$ in an obvious way:

$$\varrho_{\mathcal{V}}(u,v) := \varrho(u,v), \qquad u,v \in \mathcal{V}, \tag{1.1.14}$$

The crucial observation is that $\varrho_{\mathcal{V}}$ is intrinsic (in the sense of [**73**], [**127**]) for $(\mathcal{V},m;b)$ with b and m defined by (1.1.9) and (1.1.11) if ϱ is intrinsic for $(\mathcal{G},\mu,\nu)$ (the precise meaning of all these notions can be found in Section 6.4). What is more important, it turns out that under certain natural assumptions every path metric, which is intrinsic w.r.t. $(\mathcal{V},m;b)$, can be obtained in this way (see Theorem 6.34). Recall also that every regular Dirichlet form (no killing term) in $\ell^2(\mathcal{V};m)$, where $\mathcal{V}$ is at most countable and m is a measure of full support, arises as a closure of (1.1.8) restricted to $C_c(\mathcal{V})$ (see [**130**, §2]). These facts, in combination with the results for strongly local Dirichlet forms as well as with the correspondence (1.1.13), indicate that many of the important principles extend from the manifold setting to the setting of weighted graph Laplacians. The latter is by no means surprising, however, in our opinion this point of view provides another natural motivation for the striking analogies between results as in, e.g., [**18, 73, 127**] and the setting of manifolds.

A detailed description of the content of this memoir as well as of our main results can be found in the next section. Let us emphasize that the main thrust of our investigations is conceptual in nature and for this reason we would like to conclude this lengthy introduction with one more comment. Let us look at the maps (1.1.10) and (1.1.14) from the perspective of *quasi-isometries* (quite often going by the name of *rough isometries*) [**36**], [**173**], [**184**]. It is straightforward to check that the metric spaces $(\mathcal{G},\varrho)$ and $(\mathcal{V},\varrho_{\mathcal{V}})$ are quasi-isometric (again, under the finite intrinsic size assumption, which guarantees the net property) and this fact connects their large scale properties. The notion of a quasi-isometry has its roots in the Švarc–Milnor Lemma [**53**], [**173**], [**184**], one of the most fundamental observations in geometric group theory. It is a standard practice to investigate a finitely generated group by turning its Cayley graph into a length space, which is nothing but an equilateral metric graph (see, e.g., [**184**, Rem. 1.16]). Our results in Chapter 6 show that with any locally finite weighted graph b over $(\mathcal{V}, m)$ equipped with an intrinsic path metric ϱ one can associate a weighted metric graph $(\mathcal{G}, \mu, \nu)$, a cable system, whose intrinsic path metric ϱ_η is such that $\varrho = \varrho_\eta|_{\mathcal{V}}$ and the metric spaces $(\mathcal{V}, \varrho)$ and $(\mathcal{G}, \varrho_\eta)$ are quasi-isometric. One immediate advantage is the fact that $(\mathcal{G}, \varrho_\eta)$ is a length space. Moreover, exactly this correspondence provides, in our opinion, a transparent perspective on many results for graph Laplacians obtained during the last decade. Let us stress that, although quasi-isometric spaces are known to share many important properties (e.g., geometric properties such as volume growth and isoperimetric inequalities; Liouville-type theorems for harmonic functions etc.), most of these connections require additional conditions on the local geometry of the spaces in question. On the other hand, in our particular setting, the local structures of the spaces $(\mathcal{G}, \varrho_\eta)$ and $(\mathcal{V}, \varrho)$ are connected by (1.1.10) an (1.1.14) (at least they enjoy the same combinatorial structure), and exactly this fact, in our opinion, enables us to prove a number of correspondences which are not true in the general setting of quasi-isometric spaces.

1.2. Overview of the results

Let us now outline the content of this memoir as well as our main results.

Chapter 2 is of a preliminary character, where we introduce basic objects, notions and facts. We begin with graph theoretic notions, metric graphs and graph ends (Section 2.1). In the next section, following [**130**], [**134**] we present basic definitions and facts about Laplacians on weighted graphs. Sections 2.3–2.4 are dedicated to Laplacians on metric graphs. First, we recall the definitions of the most important function spaces on metric graphs (Section 2.3). The minimal and maximal Kirchhoff Laplacians are then defined in Section 2.4.1. Using the form approach, which can be considered as a variational definition of a Laplacian on a metric graph, we introduce Dirichlet and Neumann Laplacians, and also we define the so-called Gaffney Laplacian (Section 2.4.2), which plays a crucial role in the study of Markovian extensions of the minimal Kirchhoff Laplacian and also can be seen as the Hodge Laplacian on a metric graph (Remark 2.19).

Chapter 3 provides the first major step towards establishing connections between Kirchhoff Laplacians on metric graphs and graph Laplacians on locally finite graphs. The main results of this chapter are Theorem 3.1 and also Theorem 3.22, which relate basic spectral properties of Laplacians with δ-couplings at the vertices with those of certain Schrödinger-type operators on the underlying combinatorial graph. Section 3.1 states the central result, Theorem 3.1, and then Section 3.2 is dedicated to its proof. Let us stress that the main tool is the concept of boundary triplets and the corresponding Weyl functions [**54**], [**55**], [**85**], [**188**]. The concluding Section 3.3 elaborates further on the consequences of Theorem 3.1 in the case of Kirchhoff Laplacians. First of all, every metric graph has infinitely many models and each such model gives rise to a graph Laplacian. Thus we begin by discussing Theorem 3.1 from this perspective. On the other hand, if the minimal Kirchhoff Laplacian is not self-adjoint, then it admits infinitely many self-adjoint extensions. It is not at all surprising that these extensions can be parameterized by means of self-adjoint extensions of the corresponding minimal graph Laplacian (see Lemma 3.20). The latter allows us to extend Theorem 3.1 to the case of non-trivial deficiency indices (see Theorem 3.22). Let us also stress that this bijective correspondence between self-adjoint extensions, according to Theorem 3.22, remains bijective upon restriction to certain classes of self-adjoint extensions (e.g., semibounded or non-negative extensions), however, some of these relations require a careful choice of the underlying model for a given metric graph (e.g., for uniformly positive extensions the corresponding model should have *finite intrinsic size*).

The main focus in **Chapter** 4 is on connections between parabolic properties of Laplacians on weighted graphs and metric graphs. We begin by recalling the definition of Markovian extensions and by underlining the role of the Dirichlet and Neumann Laplacians (Section 4.1). Section 4.2 is of conceptual importance and gives a good motivation for subsequent considerations. Namely, following [**70**], we review some connections between transfer probabilities of a Brownian motion on a metric graph and of a continuous time random walk on a weighted graph. Sections 4.3 and 4.4 form the core of this chapter. We begin with the study of the map $\imath_{\mathcal{V}}$ defined by (1.1.10). First of all, $\imath_{\mathcal{V}}$ becomes injective when further restricted to the space of continuous, edgewise affine functions $\mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ on a metric graph $\mathcal{G}$. It turns out that this map connects the corresponding energy forms as well, and even more, it allows to describe the bijective correspondence (1.1.13) from Lemma 3.20 between self-adjoint extensions of the minimal Kirchhoff and graph Laplacians in a much more transparent and concrete way (see Lemma 4.7). Moreover, the map (1.1.13) induces a bijection between the sets of Markovian extensions $\mathrm{Ext}_M(\mathbf{H}^0)$ and $\mathrm{Ext}_M(\mathbf{h}^0)$ (Section 4.4). These results enable us to relate basic parabolic properties of Laplacians on metric and weighted graphs. More precisely, Section 4.5 and Section 4.6 deal with transience/recurrence and stochastic completeness, respectively. To a certain extent these connections are not new and under some additional restrictions they have been discussed earlier in [**70**], [**112**] (stochastic completeness) and [**95**, Chap. 4] (transience/recurrence). In Section 4.7, we elaborate further on the relationship between spectral gaps of Laplacians on metric and weighted graphs. We conclude this chapter by looking at ultracontractivity estimates for heat semigroups on weighted graphs and metric graphs (Section 4.8).

Chapter 5 is dedicated to the simplest possible example – an infinite path graph. Since this case can be thoroughly analyzed, it is a suitable toy model to demonstrate our findings from the previous two chapters. Indeed, in this case the corresponding Laplacian (with δ-couplings at the vertices) is nothing but the Sturm–Liouville operator defined by the differential expression

$$\tau = \frac{1}{\mu(x)}\Big(-\frac{\mathrm{d}}{\mathrm{d}x}\nu(x)\frac{\mathrm{d}}{\mathrm{d}x} + \sum_{k\geq 1}\alpha_k\delta(x-x_k)\Big), \tag{1.2.1}$$

on the interval $\mathcal{I} := [0, L)$ with $L \in (0,\infty]$, where $(x_k)_{k\geq 0} \subset \mathcal{I}$ is a strictly increasing sequence such that $x_0 = 0$, $x_k \uparrow \mathcal{L}$ and the weights $\mu, \nu \colon \mathcal{I} \to \mathbb{R}_{>0}$ are given by

$$\mu(x) = \sum_{k\geq 0}\mu_k \mathbb{1}_{[x_k,x_{k+1})}(x), \qquad \nu(x) = \sum_{k\geq 0}\nu_k \mathbb{1}_{[x_k,x_{k+1})}(x). \tag{1.2.2}$$

If $\alpha = (\alpha_k) \equiv 0$, then (1.2.1) is a Sturm–Liouville operator in the divergence form and its basic spectral properties are rather well studied (let us only mention the contributions of H. Weyl [**206**], M.G. Krein and I.S. Kac [**117**], [**118**], [**119**]). The study of its parabolic properties (recurrence, stochastic completeness) was initiated in the work of W. Feller [**69**]. It is not at all surprising that, in this particular situation, one can obtain a complete answer to most basic questions and we collect some of these results in Section 5.1. In the next Section 5.2 we look at the corresponding difference expression associated with (1.2.1) by means of Theorem 3.1. Looking at this difference operator in the unweighted Hilbert space $\ell^2(\mathbb{Z}_{\geq 0})$, we end up with the usual semi-infinite Jacobi (tri-diagonal) matrix (5.2.8). If $\alpha \not\equiv 0$, then we briefly demonstrate that the self-adjointness problem for (1.2.1) is a rather complicated issue. Actually, in the unweighted case $\mu = \nu \equiv 1$, the corresponding results were obtained in [**141**] and even for this operator, known as the 1d Schrödinger operator with δ-interactions [**3**], a complete answer to the self-adjointness problem is not yet known. In Section 5.3 we are interested in the following problem: *How large is the set of Jacobi matrices* (5.2.8) *arising as boundary operators for* (1.2.1)*?*[†] Proposition 5.18 shows that even when restricting to the case of operators with $\mu \equiv 1$, every Jacobi matrix can be realized as a boundary operator for (1.2.1). The latter in particular implies that the self-adjointness problem for the particular class of operators (1.2.1)–(1.2.2), which are Laplacians on weighted path graphs, is equivalent to the self-adjointness problem for Jacobi matrices, which is the classical problem in spectral theory and of vital importance in the classical moment problem [**2**]. However, when considering the boundary operator in the weighted space $\ell^2(\mathbb{Z}_{\geq 0}; m)$, that is, a weighted graph Laplacians (1.1.1) on a path graph (which is known in the literature as a *Krein–Stieltjes string* [**2**, Appendix], [**118**, §13]),

$$(\tau f)(k) := \frac{1}{m(k)} \sum_{|n-k|=1} b(\min\{n,k\})(f(k) - f(n)), \quad k \in \mathbb{Z}_{\geq 0}, \tag{1.2.3}$$

the situation changes drastically. It turns out that the answer to the above question depends on the weight m in a rather non-trivial way. Namely, (1.2.3) arises as a boundary operator for some Sturm–Liouville operator (1.2.1) with the weights (1.2.2) if and only if a positive sequence $m = (m_k)_{k\geq 0}$ satisfies

$$\sum_{k=0}^{n} (-1)^{n-k} m(k) > 0 \tag{1.2.4}$$

for all $n \geq 0$ (see Proposition 5.20).

In **Chapter** 6 we study the problems raised in Section 5.3, however, for Laplacians on arbitrary locally finite graphs. Surprisingly enough, the answers obtained for a path graph extend to the general setting. Namely, if one looks at symmetric Jacobi matrices on graphs (i.e., second order symmetric difference expressions on graphs) acting in the unweighted space $\ell^2(\mathcal{V})$, then every such operator can be realized as a boundary operator (in the sense of Theorem 3.1) for a metric graph Laplacian with δ-couplings. For graph Laplacians (1.1.1) the situation is more involved. There are two different cases. First of all, one may look only at simple graphs and then the answer is very much similar to (1.2.4). Let us stress that M. Folz faced precisely the same problem in [**70**]. The way to overcome this difficulty is to allow loops. Namely, it is immediate to notice that the difference

[†]A possibility to exploit spectral properties of (1.2.1) in order to study the corresponding properties of Jacobi matrices has already been emphasized in [**4**, §7]. Moreover, in 2010 during the OTAMP Conference in Bedlewo, Sergei Naboko (1950-2020) posed to one of us (A.K.) exactly this question.

expression (1.1.1) does not "see" loops in the coefficient b, however, loops enter the weight m in (1.1.11) and exactly this observation allows to realize every locally finite graph $(\mathcal{V}, m; b)$ as a boundary operator for some metric graph Laplacian.

We begin Chapter 6 by introducing the notion of a *cable system* and a *minimal cable system* (Definition 6.1) and then explicitly state the problems (see Problems 6.1–6.4). In Section 6.1, we provide several illustrative examples showing that some important classes of graph Laplacians admit minimal cable systems (e.g., generators of discrete time random walks on graphs) and some of them do not (e.g., combinatorial Laplacians). The next section is dedicated to Problem 6.1, where we demonstrate that the answer is very much similar to the case of a path graph. We also recall here one interesting result due to H. Zaimi providing a combinatorial answer to Problem 6.1 in the particular case of the combinatorial Laplacian (Lemma 6.13). Section 6.3 answers Problem 6.2 in the affirmative (see also [**70**]). A solution to Problem 6.4 is contained Section 6.6.

Sections 6.4-6.5 attempt to deepen the connections established in Chapters 3–4. More specifically, Section 6.4 provides a quasi-isometric perspective on the obtained results. First, in Subsection 6.4.1 we recall the notion of the intrinsic metric ϱ_η on a weighted metric graph $(\mathcal{G}, \mu, \nu)$. In the next Subsection 6.4.2, we briefly recall following [**73**], [**127**] the notion of an intrinsic metric on a weighted graph. The intrinsic path metric ϱ_η on $\mathcal{G}$ induces a path metric $\varrho_\mathcal{V}$ on $\mathcal{V}$ in an obvious way (see (1.1.14)). It then turns out that the metric $\varrho_\mathcal{V}$ is intrinsic with respect to $(\mathcal{V}, m; b)$ if the graph b over $(\mathcal{V}, m)$ is related to $(\mathcal{G}, \mu, \nu)$ in the sense of Chapter 3 (see Lemma 6.25). Moreover, we show that for a locally finite weighted graph every intrinsic path metric of finite jump size arises in this way (Lemma 6.31). In particular, imposing some natural restrictions on cable systems (the so-called *canonical cable systems*), this correspondence between continuous and discrete intrinsic path metrics becomes bijective (Theorem 6.34). Notice that $(\mathcal{G}, \varrho_\eta)$ and $(\mathcal{V}, \varrho_\mathcal{V})$ are quasi-isometric metric spaces (Lemma 6.28) and hence these results allow to associate to a discrete locally compact metric space a quasi-isometric length space, which also respects its local combinatorial structure. For example, in Section 6.4.5 we demonstrate these findings by looking at Hopf–Rinow-type theorems, which connect completeness with bounded compactness and geodesic completeness. Originally established for manifolds, the Hopf–Rinow theorem was extended to length spaces by M. Gromov and the above connections enable us to immediately extend it to the discrete setting. Of course, the discrete version of the Hopf–Rinow theorem is by no means new [**165**], [**113**, Theorem A.1] (see also [**127**]). The next Section 6.5 is dedicated to harmonic and sub-/superharmonic functions on graphs. As it was mentioned already, there is a 1-to-1 correspondence between harmonic functions. Moreover, this correspondence extends to sub- and superharmonic functions on $(\mathcal{G}, \mu, \nu)$ which are assumed edgewise affine. The results of Section 4.3 and Section 6.4 enable us to connect Liouville-type properties in discrete and continuous settings (e.g., Yau's L^p-Liouville-type theorems, see Subsection 6.5.3). Let us emphasize once again that results of this type usually do not extend to the whole equivalence class of quasi-isometric spaces (see, e.g., [**46**], [**149**], [**158**], [**191**]).

The aim of **Chapter** 7 is to employ the established connections in order to prove new results for Laplacians on metric graphs, as well as to provide another perspective on recent results for weighted graph Laplacians.

Section 7.1 deals with the self-adjointness problem. We start by proving the Gaffney-type theorem for Kirchhoff Laplacians. On the one hand, this result seems to be a folklore, however, it is hard to find its proof in the existing literature (actually, we are aware of only two such sources [**95**, Theorem 3.49] and [**67**]) and, moreover, we provide a very short proof using the L^2-Liouville theorem for metric graphs from [**195**]). As an immediate corollary, we obtain a Gaffney-type theorem for weighted graph Laplacians proved by a different approach than in [**113**, Theorem 2]. On the other hand, one can use the results from [**113**] and [**130**] to prove sufficient self-adjointness conditions for Kirchhoff Laplacians. Let us stress that Theorem 7.7, first established in [**67**] for unweighted metric graphs, has an obvious analog in the case of Sturm–Liouville operators, however, we are unaware of its analogs in the manifold setting (Remark 7.8). Then we consider the self-adjointness problem for Laplacians with δ-couplings. First, following [**143**] we present the Glazman–Povzner–Wienholtz theorem for metric graphs (Theorem 7.9), which also provides another proof of Theorem 7.1, and then immediately obtain its analog for graph Laplacians (Theorem 7.11). Moreover, we discuss semiboundedness and also relate it with the notion of criticality on graphs [**138**].

Section 7.2 is dedicated to Markovian uniqueness. Here we extend the results from [**144**] to the setting of weighted metric graphs. More specifically, using the notion of *finite volume graph ends* introduced in [**144**], we are interested in conditions on the edge weights μ and ν under which finite volume graph ends serve as the proper boundary for Markovian extensions. Let us also mention that these results can be seen at the study of self-adjointness for the Gaffney Laplacian [**147**].

We investigate spectral gap estimates in Section 7.3. Motivated by [**146**], we introduce an isoperimetric constant for weighted metric graphs (Definition 7.31). First, we prove the analogs of Cheeger and Buser estimates (Theorem 7.33). Taking into account that the isoperimetric constant has a combinatorial flavour (which is in sharp contrast with the case of finite metric graphs [**170**]), we are able to connect it with the combinatorial isoperimetric constant (a classical widely studied object [**209**]) as well as with isoperimetric constants for weighted graph Laplacians, recently introduced in [**18**]. The section is concluded with a quick discussion of volume growth estimates.

The remaining two sections briefly touch the most important parabolic properties – recurrence and stochastic completeness (a.k.a. conservativeness). On the one hand, we follow the road indicated in earlier work of M. Folz [**70**], [**71**]. Namely, by combining volume growth criteria for strongly local Dirichlet forms with the results from Chapter 4, one can obtain volume growth criteria for weighted graph Laplacians. On the other hand, let us mention one result, which seems to be new. Theorem 7.49 relates recurrence of the Brownian motion on a weighted metric graph to that of a particular discrete time random walk (reversible Markov chain) on a graph $(\mathcal{V}, b)$. Notice that this fact can be seen as a significant improvement of the results in Section 4.5.

Chapter 8 continues along the lines of Chapter 7, however, here we restrict ourselves to three particular classes of graphs.

Section 8.1 deals with *antitrees*. Imposing an additional radial symmetry assumption, one can perform a very detailed analysis in this case since the Sturm–Liouville operator (or weighted Laplacian on a path graph) studied in Section 5.1 plays a crucial role in this analysis (see Theorem 8.2). Thus for this class of graphs we can obtain complete answers to most basic questions (self-adjointness, Markovian uniqueness, positive spectral gap, recurrence, stochastic completeness etc.). However, we should stress that removing the radial symmetry assumption makes the analysis much more complicated and, for instance, the self-adjointness problem is widely open in this case (Subsection 8.1.2). In Subsection 8.1.3 we collect some historical remarks and further references to the existing literature.

Section 8.2 is dedicated to *Cayley graphs*. Taking into account that random walks on groups is a classical subject, the results obtained in the previous chapters enable us to prove many new results for Laplacians on weighted metric Cayley graphs. First of all, the classical theorems of H. Freudenthal, H. Hopf and J.R. Stallings about ends of groups enable us to make a rather thorough study of the Markovian uniqueness on metric Cayley graphs (Section 8.2.1). In sharp contrast to the Markovian uniqueness, the self-adjointness depends on the choice of a generating set. In particular, the self-adjointness problem remains widely open for metric Cayley graphs (see Remark 8.25). In Subsection 8.2.2, employing connections between isoperimetric constants and amenability we, among other results, prove a metric graph analog of Kesten's amenability criterion (Corollary 8.31). Similarly, taking into account the classification of recurrent groups, we prove a number of results regarding transience/recurrence on metric Cayley graphs (see Subsection 8.2.4). In Subsection 8.2.5, we study ultracontractivity estimates by employing the classical results of N.Th. Varopoulos, which relate growth in groups with the decay rate of simple random walks. Moreover, we use these results to establish Cwiekel–Lieb–Rozenblum-type estimates (Theorem 8.42). Again, we conclude this part with some historical remarks and further references to the existing literature (Subsection 8.2.6).

The aim of Section 8.3 is to discuss graphs arising in context with *tessellations* (or tilings) of the Euclidian plane $\mathbb{R}^2$. In Section 8.3.1, we first observe that our criteria for Markovian uniqueness become particularly transparent in this case (see Corollary 8.47). Moreover, in the past several discrete curvature-like notions have been introduced for plane graphs to study their geometric and spectral properties (see [**128**] for an overview). In Section 8.3.2, we develop this approach in context with weighted metric graphs and spectral gap estimates. We introduce a characteristic value on edges of a weighted metric graph, which takes over the role of the classical discrete curvature. Theorem 8.50 then provides a lower estimate on the isoperimetric constant (and the spectrum of the Dirichlet Laplacian) in terms of the characteristic values. Finally, Section 8.3.3 contains further historical remarks, references and a discussion of the relation to other discrete curvature notions for plane graphs.

Finally, in order to make the exposition (reasonably) self-contained we provide three appendices. **Appendix** A collects basic notions and facts on linear relations, boundary triplets and the corresponding Weyl functions. **Appendix** B is dedicated to Dirichlet forms. In **Appendix** C, we recall results relating ultracontractivity estimates with Sobolev and Nash-type inequalities.

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CHAPTER 2

Laplacians on Graphs

2.1. Combinatorial and metric graphs

2.1.1. Graphs. Let $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ be a (undirected) *graph*, that is, $\mathcal{V}$ is a finite or countably infinite set of vertices and $\mathcal{E}$ is a finite or countably infinite set of edges. Two vertices u, $v \in \mathcal{V}$ are called *neighbors* and we shall write $u \sim v$ if there is an edge $e_{u,v} \in \mathcal{E}$ connecting u and v. For every $v \in \mathcal{V}$, we define $\mathcal{E}_v$ as the set of edges incident to v. We stress that we allow *multigraphs*, that is, we allow *multiple edges* (two vertices can be joined by several edges) and *loops* (edges from one vertex to itself). Graphs without loops and multiple edges are called *simple*. Sometimes it is convenient to assign an *orientation* on $\mathcal{G}_d$: to each edge $e \in \mathcal{E}$ one assigns the pair $(e_\imath, e_\tau)$ of its *initial* $e_\imath$ and *terminal* e_τ vertices. We shall denote the corresponding oriented graph by $\vec{\mathcal{G}}_d = (\mathcal{V}, \vec{\mathcal{E}})$, where $\vec{\mathcal{E}}$ denotes the set of oriented edges. Notice that for an oriented loop we do distinguish between its initial and terminal vertices. Next, for every vertex $v \in \mathcal{V}$, set

$$\mathcal{E}_v^+ = \big\{(e_\imath, e_\tau) \in \vec{\mathcal{E}} \,|\, e_\imath = v\big\}, \qquad \mathcal{E}_v^- = \big\{(e_\imath, e_\tau) \in \vec{\mathcal{E}} \,|\, e_\tau = v\big\}, \tag{2.1.1}$$

and let $\vec{\mathcal{E}}_v$ be the disjoint union of outgoing $\mathcal{E}_v^+$ and incoming $\mathcal{E}_v^-$ edges,

$$\vec{\mathcal{E}}_v := \mathcal{E}_v^+ \sqcup \mathcal{E}_v^- = \vec{\mathcal{E}}_v^+ \cup \vec{\mathcal{E}}_v^-, \qquad \vec{\mathcal{E}}_v^\pm := \big\{(\pm, e) \,|\, e \in \mathcal{E}_v^\pm\big\}. \tag{2.1.2}$$

We shall denote the elements of $\vec{\mathcal{E}}_v$ by $\vec{e}$. The *(combinatorial) degree* or *valency* of $v \in \mathcal{V}$ is defined by

$$\deg(v) := \#(\vec{\mathcal{E}}_v) = \#(\vec{\mathcal{E}}_v^+) + \#(\vec{\mathcal{E}}_v^-) = \#(\mathcal{E}_v) + \#\{e \in \mathcal{E}_v | \, e \text{ is a loop}\}. \tag{2.1.3}$$

Notice that if $\mathcal{E}_v$ has no loops, then $\deg(v) = \#(\mathcal{E}_v)$. The graph $\mathcal{G}_d$ is called *locally finite* if $\deg(v) < \infty$ for all $v \in \mathcal{V}$. If furthermore $\sup_{v\in\mathcal{V}} \deg(v) < \infty$, then $\mathcal{G}_d$ has *bounded geometry*.

A sequence of (unoriented) edges $\mathcal{P} = (e_{v_0,v_1}, e_{v_1,v_2}, \dots, e_{v_{n-1},v_n})$ is called a *path* of (combinatorial) length $n \in \mathbb{Z}_{\geq 0} \cup \{\infty\}$. If $v_0 = v_n$ and all other vertices as well as all edges are distinct, then such a path is called a *cycle*[‡]. Notice that for simple graphs each path $\mathcal{P}$ can be identified with its sequence of vertices, i.e., $\mathcal{P} = (v_k)_{k=0}^n$. A graph $\mathcal{G}_d$ is called *connected* if for any two vertices there is a path connecting them.

We shall always make the following assumptions on the geometry of $\mathcal{G}_d$:

HYPOTHESIS 2.1. *$\mathcal{G}_d$ is connected and locally finite.*

[‡]Sometimes in the literature cycles are called loops and in such a case what we call a "loop" is called a *self-loop*. On the other hand, in our terminology each loop is a cycle of length 1.

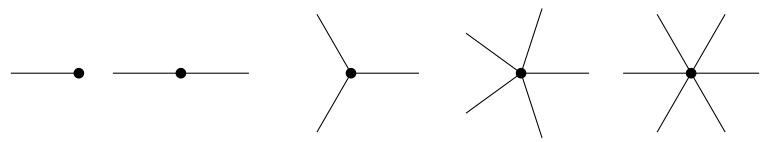

FIGURE 2.1. Star shaped sets for $\deg(x) = 1$, 2, 3, 5 and 6.

2.1.2. Metric graphs. Next, let us assign each edge $e \in \mathcal{E}$ a finite length $|e| \in (0, \infty)$. We can then naturally associate with $(\mathcal{G}_d, |\cdot|) = (\mathcal{V}, \mathcal{E}, |\cdot|)$ a metric space $\mathcal{G}$: first, we identify each edge $e \in \mathcal{E}$ with a copy of the interval $\mathcal{I}_e = [0, |e|]$, which also assigns an orientation on $\mathcal{E}$ upon identification of $e_\imath$ and e_τ with the left, respectively, right endpoint of $\mathcal{I}_e$. The topological space $\mathcal{G}$ is then obtained by "glueing together" the ends of edges corresponding to the same vertex v (in the sense of a topological quotient, see, e.g., [**36**, Chapter 3.2.2]). The topology on $\mathcal{G}$ is metrizable by the *length metric* ϱ_0 — the distance between two points $x, y \in \mathcal{G}$ is defined as the arc length of the "shortest path" connecting them (notice that $\mathcal{G}$ may not be a geodesic space, that is, such a path does not necessarily exist and one needs to take the infimum over all paths connecting x and y). Moreover, each point $x \in \mathcal{G}$ has a neighborhood isometric to a star-shaped set $\mathcal{E}(\deg(x), r_x)$ of degree $\deg(x) \in \mathbb{Z}_{\geq 1}$ (see Figure 2.1),

$$\mathcal{E}(\deg(x), r_x) := \big\{z = r\mathrm{e}^{2\pi \mathrm{i} k/\deg(x)} | \, r \in [0, r_x),\ k = 1, \dots, \deg(x)\big\} \subset \mathbb{C}. \tag{2.1.4}$$

Notice that $\deg(x)$ in (2.1.4) coincides with the combinatorial degree if x belongs to the vertex set, and $\deg(x) = 2$ for every non-vertex point x of $\mathcal{G}$.

A *metric graph* is a metric space $\mathcal{G}$ arising from the above construction for some collection $(\mathcal{G}_d, |\cdot|) = (\mathcal{V}, \mathcal{E}, |\cdot|)$. More specifically, $\mathcal{G}$ is then called the *metric realisation* of $(\mathcal{G}_d, |\cdot|)$. On the other hand, we will call a pair $(\mathcal{G}_d, |\cdot|)$ whose metric realization coincides with $\mathcal{G}$ a *model* of $\mathcal{G}$.

REMARK 2.1 (Metric graph as a length space). A metric graph $\mathcal{G}$ equipped with its length metric ϱ_0 is a *length space* (see [**36**, Chapter 2.1] for definitions and further details). Concerning terminology, let us only stress that the metric ϱ_0 is *intrinsic* in the sense of [**36**, Definition 2.1.6], however, we are going to use the notion of an *intrinsic metric* in a different context — intrinsic w.r.t. to a Dirichlet form — and in certain situations of interest ϱ_0 turns out to be intrinsic in both senses (see Section 6.4 for further details).

REMARK 2.2 (Paths in metric graphs). Let us make one more convention. Usually, for length spaces one introduces the class of admissible paths (e.g., rectifiable curves, see [**36**]), however, taking into account the one-dimensional local structure of metric graphs, we shall define a *path* $\mathcal{P}$ in $\mathcal{G}$ as a continuous map $\gamma \colon I \to \mathcal{G}$, which is piecewise injective. Here $I \subset \mathbb{R}$ is an interval, that is, a connected subset of $\mathbb{R}$, and piecewise injectivity means that for any $[a, b] \subseteq I$ there is a finite partition $a = t_0 < t_1 < \cdots < t_n = b$ such that γ is injective on each open interval (t_{k-1}, t_k), $k \in \{1, \dots, n\}$. Notice that this definition of paths in $\mathcal{G}$ allows self-intersections and backtracking.

Clearly, different models may give rise to the same metric graph. Moreover, any metric graph has infinitely many models (e.g., they can be constructed by subdividing edges using vertices of degree 2). On this set we can introduce a partial order by saying that a model $(\mathcal{V}', \mathcal{E}', |\cdot|')$ of $\mathcal{G}$ is a *refinement* of $(\mathcal{V}, \mathcal{E}, |\cdot|)$ if $\mathcal{V} \subseteq \mathcal{V}'$. A model $(\mathcal{V}, \mathcal{E}, |\cdot|)$ is called *simple* if the corresponding graph $(\mathcal{V}, \mathcal{E})$ is simple. In particular, every locally finite metric graph has a simple model and hence this indicates that restricting to simple graphs, that is, assuming in addition to Hypothesis 2.1 that $\mathcal{G}_d$ has no loops or multiple edges, would not be a restriction at all when dealing with metric graphs.

Let us emphasize that one can introduce metric graphs without the use of models. From topological point of view, a locally finite metric graph is precisely a connected (second countable and locally compact) Hausdorff space $\mathcal{G}$ such that each point $x \in \mathcal{G}$ has a neighborhood U_x homeomorphic to a star-shaped set $\mathcal{E}_x$ of the form (2.1.4). As metric spaces, they are characterized by requiring additionally that the homeomorphism between U_x and the star $\mathcal{E}_x$ is an isometry and the metric on $\mathcal{G}$ coincides with the associated path metric. Given a metric graph $\mathcal{G}$, one can construct a model $(\mathcal{V}, \mathcal{E}, |\cdot|)$ of $\mathcal{G}$ as follows: fix a discrete set $\mathcal{V} \subset \mathcal{G}$ containing all the points $x \in \mathcal{G}$ with $\deg(x) \neq 2$ and such that each connected component of $\mathcal{G} \setminus \mathcal{V}$ is isometric to a bounded, open interval. The edge set $\mathcal{E}$ then consists of all connected components of $\mathcal{G} \setminus \mathcal{V}$ and the edge length $|e|$ of $e \in \mathcal{E}$ is chosen as the distance between the respective endpoints. For a thorough discussion of metric graphs as topological and metric spaces we refer to [**95**, Chapter I].

REMARK 2.3. In most parts of our manuscript, we will consider a metric graph together with a fixed choice of its model. In this situation, we will usually be slightly imprecise and do not distinguish between these two objects. In particular, we will denote both objects by the same letter $\mathcal{G}$ and also write $\mathcal{G} = (\mathcal{V}, \mathcal{E}, |\cdot|)$ or $\mathcal{G} = (\mathcal{G}_d, |\cdot|)$. However, for certain questions it is crucial to consider different models of the same metric graph or even the whole set of its models. Whenever this is the case, we will specifically indicate it in order to avoid a possible confusion.

REMARK 2.4 (Metric graph as a 1d manifold with singularities). Let us mention that one may also consider metric graphs as one-dimensional manifolds with singularities. Since every point $x \in \mathcal{G}$ has a neighborhood isomorphic to a star-shaped set (2.1.4), one may introduce the set of *tangential directions* $T_x(\mathcal{G})$ at x as the set of unit vectors $\mathrm{e}^{2\pi \mathrm{i} k/\deg(x)}$, $k = 1, \dots, \deg(x)$. Then all vertices $v \in \mathcal{V}$ with $\deg(v) \geq 3$ are considered as *branching points/singularities* and vertices $v \in \mathcal{V}$ with $\deg(v) = 1$ as a *boundary.* Notice that for every vertex $v \in \mathcal{V}$ the set of tangential directions $T_v(\mathcal{G})$ can be identified with $\vec{\mathcal{E}}_v$. If there are no loop edges at the vertex $v \in \mathcal{V}$, then $T_v(\mathcal{G})$ is identified with $\mathcal{E}_v$ in this way.

2.1.3. Graph ends. There are many different notions of graph boundaries. In this subsection we recall basic facts about, perhaps, the simplest graph boundary – graph ends. The notion of graph ends was introduced independently by H. Freudenthal [**75**] and R. Halin [**100**] and its origins are closely related to the study of finitely generated groups [**75**], [**76**], [**107**] (see Remark 8.19 for further information).

An infinite path $\mathcal{P} = (e_{v_n, v_{n+1}})_{n \geq 0}$ without self-intersections (i.e., all vertices $(v_n)_{n \geq 0}$ are distinct) is called a *ray*. Two rays $\mathcal{R}_1, \mathcal{R}_2$ are called *equivalent* 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 $\mathcal{U} = (U_n)$ representing γ, each U_n contains a ray from ω_γ (see [**209**, § 21], [**57**, § 8.6 and also p.277–278] for further details).

One of the main features of graph ends is that they provide a rather convenient way of compactifying graphs (see [**57**, § 8.6], [**209**]). 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

$$\widehat{U} = U \cup \{\gamma \in \mathfrak{C}(\mathcal{G}) \,|\, \exists \mathcal{U} = (U_n) \in \gamma \text{ such that } U_0 \subset U\}. \tag{2.1.5}$$

Now we can introduce a neighborhood basis of $\gamma \in \mathfrak{C}(\mathcal{G})$ as follows

$$\{\widehat{U} \,|\, U \subseteq \mathcal{G} \text{ is open}, \gamma \in \widehat{U}\}. \tag{2.1.6}$$

This turns $\widehat{\mathcal{G}}$ into a compact topological space, called the *end (or Freudenthal) compactification* of $\mathcal{G}$.

Definition 2.5. 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. Otherwise, ω is called *non-free*.

Remark 2.6. Let us mention that by Halin's theorem [**100**] every locally finite graph $\mathcal{G}_d$ with infinitely many ends has at least one end which is not free.

2.2. Discrete Laplacians on graphs

There are several ways to introduce Laplacians on (combinatorial) graphs and here we follow the approach from [**130**], [**134**]. Let $\mathcal{V}$ be a finite or countable set (one may think of $\mathcal{V}$ as the set of vertices from the previous section). A function $m\colon \mathcal{V} \to (0,\infty)$ defines a measure of full support on $\mathcal{V}$ in an obvious way. A pair $(\mathcal{V}, m)$ is called a *discrete measure space*. The set of square summable functions

$$\ell^2(\mathcal{V}; m) = \Big\{ f \in C(\mathcal{V}) \,|\, \|f\|^2_{\ell^2(\mathcal{V};m)} := \sum_{v\in\mathcal{V}} |f(v)|^2 m(v) < \infty \Big\}$$

has a natural Hilbert space structure. Here $C(\mathcal{V})$ denotes the space of all complex-valued functions on $\mathcal{V}$. Next, let $c\colon \mathcal{V} \to [0,\infty)$ and suppose $b\colon \mathcal{V}\times\mathcal{V} \to [0,\infty)$ satisfies the following conditions:

(i) *symmetry*: $b(u,v) = b(v,u)$ for each pair $(u,v) \in \mathcal{V}\times\mathcal{V}$,
(ii) *vanishing diagonal*: $b(v,v) = 0$ for all $v \in \mathcal{V}$,
(iii) *local summability*: $\sum_{v\in\mathcal{V}} b(u,v) < \infty$ for all $u \in \mathcal{V}$.

Following [**130**], [**134**], such a pair (b,c) is called a *(weighted) graph* over $\mathcal{V}$ (or over $(\mathcal{V}, m)$ if in addition a measure m of full support on $\mathcal{V}$ is given); b is called an *edge weight* and c is a *killing term*. If $c \equiv 0$, then we would say a *graph b over $\mathcal{V}$*. To simplify notation, we shall denote a graph b or (b,c) over $(\mathcal{V}, m)$ by $(\mathcal{V}, m; b)$ or, respectively, $(\mathcal{V}, m; b, c)$.

REMARK 2.7. Let us quickly explain how the above notion is related to the previous section. To any graph b over $\mathcal{V}$, we can naturally associate a simple combinatorial graph $\mathcal{G}_b$. Namely, $\mathcal{V}$ is the vertex set of $\mathcal{G}_b$ and its edge set $\mathcal{E}_b$ is defined by calling two vertices $u, v \in \mathcal{V}$ neighbors, $u \sim v$, exactly when $b(u,v) > 0$. Clearly, $\mathcal{G}_b = (\mathcal{V}, \mathcal{E}_b)$ is an undirected graph in the sense of Section 2.1. Let us stress, however, that the constructed graph $\mathcal{G}_b$ is always simple. Moreover, for a given metric graph $\mathcal{G}$, each model $(\mathcal{V}, \mathcal{E}, |\cdot|)$ can be seen as a weighted graph over $\mathcal{V}$ with the edge weight $1/|\cdot|$, which further connects it with *electrical networks* when lengths are thought of as resistances (see, e.g., [**192**]).

With each graph (b,c) one can associate the *energy form* $\mathfrak{q}\colon C(\mathcal{V}) \to [0,\infty]$ defined by

$$\mathfrak{q}[f] = \mathfrak{q}_{b,c}[f] := \frac{1}{2}\sum_{u,v\in\mathcal{V}} b(v,u)|f(v)-f(u)|^2 + \sum_{v\in\mathcal{V}} c(v)|f(v)|^2. \tag{2.2.1}$$

Functions $f \in C(\mathcal{V})$ such that $\mathfrak{q}[f] < \infty$ are called *finite energy functions.* The local summability condition ensures that the set of compactly supported functions $C_c(\mathcal{V})$, i.e., functions which vanish everywhere on $\mathcal{V}$ except finitely many vertices, is contained in the set $\mathcal{D}(\mathfrak{q})$ of finite energy functions. If (b,c) is a graph over $(\mathcal{V}, m)$, introduce the graph norm

$$\|f\|^2_{\mathfrak{q}} := \mathfrak{q}[f] + \|f\|^2_{\ell^2(\mathcal{V};m)} \tag{2.2.2}$$

for all $f \in \mathcal{D} \cap \ell^2(\mathcal{V};m) =: \mathrm{dom}(\mathfrak{q})$. Clearly, $\mathrm{dom}(\mathfrak{q})$ is the maximal domain of definition of the form $\mathfrak{q}$ in the Hilbert space $\ell^2(\mathcal{V};m)$; let us denote this form by $\mathfrak{q}_N$. Restricting further to compactly supported functions and then taking the graph norm closure, we get another form:

$$\mathfrak{q}_D := \mathfrak{q} \restriction \mathrm{dom}(\mathfrak{q}_D), \qquad \mathrm{dom}(\mathfrak{q}_D) := \overline{C_c(\mathcal{V})}^{\|\cdot\|_{\mathfrak{q}}}.$$

It turns out that both $\mathfrak{q}_D$ and $\mathfrak{q}_N$ are *Dirichlet forms* (for definitions see Appendix B). Moreover, $\mathfrak{q}_D$ is a *regular Dirichlet form.* The converse is also true (see [**130**, Theorem 7]): *every regular Dirichlet form over* $(\mathcal{V}, m)$ *arises as the energy form* $\mathfrak{q}_D$ *for some graph* (b,c) *over* $(\mathcal{V}, m)$.

REMARK 2.8. The notion of *irreducibility* for Dirichlet forms on graphs correlates with the notion of *connectivity.* Recall that a graph (b,c) is called *connected* if the corresponding graph $\mathcal{G}_b$ is connected, i.e., for any $u, v \in \mathcal{V}$ there is a finite set $\{v_0, v_1, \dots, v_n\} \subset \mathcal{V}$ such that $u = v_0$, $v = v_n$ and $b(v_{k-1}, v_k) > 0$ for all $k \in \{1, \dots, n\}$. Then the regular Dirichlet form $\mathfrak{q}_D$ is irreducible exactly when the underlying graph (b,c) is connected (see, e.g., [**134**, Chapter 1.4]).

Now using the representation theorems for quadratic forms (see, e.g., [**125**]) one can associate in $\ell^2(\mathcal{V};m)$ the self-adjoint operators $\mathbf{h}_D$ and $\mathbf{h}_N$, the so-called *Dirichlet* and *Neumann Laplacians* over $(\mathcal{V}, m)$, with, respectively, $\mathfrak{q}_D$ and $\mathfrak{q}_N$. Usually, it is a rather nontrivial task to provide an explicit description of the operators $\mathbf{h}_D$ and, especially, $\mathbf{h}_N$†. Let us first introduce the *formal Laplacian* $L = L_{c,b,m}$

†In fact, to decide whether $\mathbf{h}_N$ and $\mathbf{h}_D$ coincide, or equivalently that $\mathfrak{q}_N = \mathfrak{q}_D$, is already a nontrivial and still open problem. This property is related to the uniqueness of a *Markovian extension* (Section 4.1) and we shall return to this issue in Chapter 7.

associated to a graph (b,c) over the measure space $(\mathcal{V},m)$:

$$(Lf)(v) := \frac{1}{m(v)}\Big(\sum_{u\in\mathcal{V}} b(v,u)(f(v)-f(u)) + c(v)f(v)\Big). \tag{2.2.3}$$

It acts on functions $f\in\mathcal{F}_b(\mathcal{V})$, where

$$\mathcal{F}_b(\mathcal{V}) = \Big\{f\in C(\mathcal{V})\,\Big|\,\sum_{u\in\mathcal{V}} b(v,u)|f(u)|<\infty \text{ for all } v\in\mathcal{V}\Big\}. \tag{2.2.4}$$

This naturally leads to the *maximal* Laplacian $\mathbf{h}$ in $\ell^2(\mathcal{V};m)$ defined by

$$\mathbf{h} := L\restriction \mathrm{dom}(\mathbf{h}),\qquad \mathrm{dom}(\mathbf{h}) := \{f\in\mathcal{F}_b(\mathcal{V})\cap\ell^2(\mathcal{V};m)\,|\,Lf\in\ell^2(\mathcal{V};m)\}. \tag{2.2.5}$$

This operator is closed, however, if $\mathcal{V}$ is infinite, it is not symmetric in general (cf. [**130**, Theorem 6]). On the other hand, one gets

$$\mathbf{h}_D = \mathbf{h}\restriction \mathrm{dom}(\mathbf{h}_D),\qquad \mathrm{dom}(\mathbf{h}_D) = \mathrm{dom}(\mathbf{h})\cap\mathrm{dom}(\mathfrak{q}_D), \tag{2.2.6}$$

which also implies that $\mathbf{h}_D$ is the Friedrichs extension of the adjoint $\mathbf{h}^*$ to $\mathbf{h}$.

In order to proceed further we need to make some additional assumptions on the edge weight b. Namely, in contrast to the energy form $\mathfrak{q}$, compactly supported functions are not necessarily in the domain of $\mathbf{h}$, which does not allow us to define the minimal operator in the standard way (i.e., to describe the adjoint $\mathbf{h}^*$ to $\mathbf{h}$). In many situations of interest, in particular, it would be sufficient for the purposes of the present text, it makes sense to assume that b is

(iv) *locally finite*: $\#\{u\in\mathcal{V}\,|\,b(u,v)\neq 0\}<\infty$ for all $v\in\mathcal{V}$.

It is straightforward to verify that $C_c(\mathcal{V})\subseteq\mathcal{F}_b(\mathcal{V})$ for locally finite graphs. In this case, the *minimal* Laplacian $\mathbf{h}^0$ is defined in $\ell^2(\mathcal{V};m)$ as the closure of the *pre-minimal* Laplacian

$$\mathbf{h}' := L\restriction\mathrm{dom}(\mathbf{h}'),\qquad \mathrm{dom}(\mathbf{h}') := C_c(\mathcal{V}). \tag{2.2.7}$$

Then $\mathbf{h}'\subseteq\mathbf{h}^0\subseteq\mathbf{h}$ and $(\mathbf{h}')^*=(\mathbf{h}^0)^*=\mathbf{h}$.

Let us provide one transparent sufficient condition which ensures that all graph Laplacians coincide (see, e.g., [**51**, Lemma 1], [**129**, Theorem 11], [**198**, Rem. 1]).

Lemma 2.9. *The Laplacian $L=L_{0,b,m}$ (with $c\equiv 0$) is bounded on $\ell^2(\mathcal{V},m)$ if and only if the weighted degree function* $\mathrm{Deg}\colon\mathcal{V}\to[0,\infty)$ *given by*

$$\mathrm{Deg}\colon v\mapsto\frac{1}{m(v)}\sum_{u\in\mathcal{V}} b(u,v) \tag{2.2.8}$$

is bounded on $\mathcal{V}$. In this case, $\mathbf{h}^0=\mathbf{h}_D=\mathbf{h}_N=\mathbf{h}$ for any $c\colon\mathcal{V}\to[0,+\infty)$.

A few remarks are in order.

Remark 2.10 (Schrödinger-type operators on graphs). The positivity restriction on the killing term c comes from the theory of Dirichlet forms (or, equivalently, from its probabilistic interpretation), however, it of course makes sense to consider the case when c takes values of both signs. Then L is usually called a *Schrödinger-type operator* on a graph. To distinguish between the nonnegative and sign indefinite cases, we shall denote c in the latter case with α, that is, $\alpha\colon\mathcal{V}\to\mathbb{R}$, and call it a *potential*. In the locally finite case, the definitions of the pre-minimal, minimal and maximal operators remain the same in the case of potentials. However, one very important difference between these cases is that the quadratic form approach applies only if the negative part of α is not “too negative”. Let us mention that this also allows to keep the positivity preserving property for the corresponding resolvent and the semigroup, however, L^p-contractivity is lost once the potential is sign indefinite.

REMARK 2.11 (Random walks on graphs). If the weighted degree function is bounded by 1 on $\mathcal{V}$,

$$\sup_{v\in\mathcal{V}} \mathrm{Deg}(v) \le 1, \tag{2.2.9}$$

then the graph Laplacian $\mathbf{h}$ is a generator of a discrete time random walk on a weighted graph: for a vertex $v \in \mathcal{V}$, the jump probabilities are defined by (see, e.g., [**12**, Chapter 1.2])

$$p(u,v) = \begin{cases} \frac{b(u,v)}{m(v)}, & u \neq v, \\ 1 - \mathrm{Deg}(v), & u = v. \end{cases}$$

In particular, the probability $p(v,v)$ to stay at v equals $1 - \mathrm{Deg}(v)$ and hence, if $\mathrm{Deg}(v) < 1$ for some vertex $v \in \mathcal{V}$, then $p(v,v) > 0$, which can be interpreted as a loop at v. The matrix $\mathrm{P} = \big(p(u,v)\big)_{u,v\in\mathcal{V}}$ is called the *transition matrix* of the associated discrete time (reversible) Markov chain.

REMARK 2.12 (Laplacians on multi-graphs). The above remark indicates that (2.2.3)–(2.2.7) allow to treat weighted discrete Laplacians on multigraphs. Namely, for a multigraph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ and a given edge weight $b_{\mathcal{E}} : \mathcal{E} \to (0,\infty)$, vertex weight $m \colon \mathcal{V} \to (0,\infty)$ and killing term $c \colon \mathcal{V} \to [0,\infty)$, the corresponding (minimal and maximal) Laplacians are associated with the formal expression

$$(L_{\mathcal{G}} f)(v) := \frac{1}{m(v)} \Big(\sum_{u\sim v} \sum_{e\in\mathcal{E}_{u,v}} b_{\mathcal{E}}(e)(f(v) - f(u)) + c(v) f(v) \Big), \quad v \in \mathcal{V},$$

where $\mathcal{E}_{u,v}$ denotes the set of edges between the vertices $u, v \in \mathcal{V}$. Defining the function $b \colon \mathcal{V} \times \mathcal{V} \to [0,\infty)$ as

$$b(u,v) = \begin{cases} \sum_{e\in\mathcal{E}_{u,v}} b_{\mathcal{E}}(e), & u \neq v, \\ 0, & u = v, \end{cases}$$

it is clear that $L_{\mathcal{G}} = L$ (see (2.2.3)). However, notice that in general $\mathcal{G}_d \neq \mathcal{G}_b$ for the simple graph $\mathcal{G}_b = (\mathcal{V}, \mathcal{E}_b)$ associated with b in Remark 2.7.

2.3. Function spaces on metric graphs

Let $\mathcal{G}$ be a metric graph together with a fixed model $(\mathcal{V}, \mathcal{E}, |\cdot|)$. Let also $\mu \colon \mathcal{E} \to (0,\infty)$ be a weight function assigning a positive weight $\mu(e)$ to each edge $e \in \mathcal{E}$. We shall assume that edge weights are orientation independent and we set

$$\mu(\vec{e}) = \mu(e)$$

for all $\vec{e} \in \vec{\mathcal{E}}_v$, $v \in \mathcal{V}$. Identifying every edge $e \in \mathcal{E}$ with a copy of $\mathcal{I}_e = [0, |e|]$, we can introduce Lebesgue and Sobolev spaces on edges and also on $\mathcal{G}$. First of all, with the weight μ we associate the measure μ on $\mathcal{G}$ defined as the edgewise scaled Lebesgue measure such that $\mu(\mathrm{d}x) = \mu(e)\mathrm{d}x_e$ on every edge $e \in \mathcal{E}$. Thus, we can define the Hilbert space $L^2(\mathcal{G};\mu)$ of measurable functions $f \colon \mathcal{G} \to \mathbb{C}$ which are square integrable w.r.t. the measure μ on $\mathcal{G}$. Similarly, one defines the Banach spaces $L^p(\mathcal{G};\mu)$ for any $p\in[1,\infty]$. In fact, if $p\in[1,\infty)$, then $L^p(\mathcal{G};\mu)$ can be seen as the edgewise direct sum of L^p spaces

$$L^p(\mathcal{G};\mu)\cong\Big\{f=(f_e)_{e\in\mathcal{E}}\,\big|\,f_e\in L^p(e;\mu),\ \sum_{e\in\mathcal{E}}\|f_e\|^p_{L^p(e;\mu)}<\infty\Big\},$$

where

$$\|f_e\|^p_{L^p(e;\mu)}=\int_e|f_e(x_e)|^p\mu(\mathrm{d}x_e)=\mu(e)\int_e|f_e(x_e)|^p\,\mathrm{d}x_e,$$

that is, $L^p(e;\mu)$ stands for the usual L^p space upon identifying e with $\mathcal{I}_e$ and μ with the scaled Lebesgue measure $\mu(e)\mathrm{d}x_e$ on $\mathcal{I}_e$. If $\mu(e)=1$, then we shall simply write $L^p(e)$. The subspace of compactly supported L^p functions will be denoted by $L^p_c(\mathcal{G};\mu)$. The space $L^p_{\mathrm{loc}}(\mathcal{G};\mu)$ of locally L^p functions consists of all measurable functions f such that $fg\in L^p_c(\mathcal{G};\mu)$ for all $g\in C_c(\mathcal{G})$. Notice that both L^p_{loc} and L^p_c are independent of the weight μ.

For edgewise locally absolutely continuous functions on $\mathcal{G}$, let us denote by ∇ the edgewise first derivative,

$$\nabla\colon f\mapsto f'. \tag{2.3.1}$$

Then for every edge $e\in\mathcal{E}$,

$$H^1(e)=\{f\in AC(e)\,|\,\nabla f\in L^2(e)\},\qquad H^2(e)=\{f\in H^1(e)\,|\,\nabla f\in H^1(e)\},$$

are the usual Sobolev spaces (upon the identification of e with $\mathcal{I}_e=[0,|e|]$), and $AC(e)$ is the space of absolutely continuous functions on e. Let us denote by $H^1_{\mathrm{loc}}(\mathcal{G}\setminus\mathcal{V})$ and $H^2_{\mathrm{loc}}(\mathcal{G}\setminus\mathcal{V})$ the spaces of measurable functions f on $\mathcal{G}$ such that their edgewise restrictions belong to H^1, respectively, H^2, that is,

$$H^j_{\mathrm{loc}}(\mathcal{G}\setminus\mathcal{V})=\{f\in L^2_{\mathrm{loc}}(\mathcal{G})\,|\,f|_e\in H^j(e)\text{ for all }e\in\mathcal{E}\}$$

for $j\in\{1,2\}$. Clearly, for each measurable $f\in H^2_{\mathrm{loc}}(\mathcal{G}\setminus\mathcal{V})$ the following quantities

$$f(e_\imath):=\lim_{x_e\to e_\imath}f(x_e),\qquad\qquad f(e_\tau):=\lim_{x_e\to e_\tau}f(x_e), \tag{2.3.2}$$

and the normal derivatives

$$\partial f(e_\imath):=\lim_{x_e\to e_\imath}\frac{f(x_e)-f(e_\imath)}{|x_e-e_\imath|},\qquad \partial f(e_\tau):=\lim_{x_e\to e_\tau}\frac{f(x_e)-f(e_\tau)}{|x_e-e_\tau|}, \tag{2.3.3}$$

are well defined for all edges $e\in\mathcal{E}$. We also need the following notation

$$f_{\vec e}(v):=\begin{cases}f(e_\imath), & \vec e\in\vec{\mathcal{E}}^+_v,\\ f(e_\tau), & \vec e\in\vec{\mathcal{E}}^-_v,\end{cases}\qquad \partial_{\vec e}f(v):=\begin{cases}\partial f(e_\imath), & \vec e\in\vec{\mathcal{E}}^+_v,\\ \partial f(e_\tau), & \vec e\in\vec{\mathcal{E}}^-_v,\end{cases} \tag{2.3.4}$$

for every $v\in\mathcal{V}$ and $\vec e\in\vec{\mathcal{E}}_v$. In the case of a loopless graph, the above notation simplifies since we can identify $\vec{\mathcal{E}}_v$ with $\mathcal{E}_v$ for all $v\in\mathcal{V}$.

2.4. Laplacians on weighted metric graphs

Again, let $\mathcal{G}$ be a metric graph together with a fixed model $(\mathcal{V},\mathcal{E},|\cdot|)$. Suppose we are also given two edge weights

$$\mu\colon\mathcal{E}\to(0,\infty),\qquad\qquad \nu\colon\mathcal{E}\to(0,\infty). \tag{2.4.1}$$

To motivate our definitions, let us look at ∇ given by (2.3.1) as a differentiation operator on $\mathcal{G}$ acting on functions which are edgewise locally absolutely continuous and also continuous at the vertices. Notice that when considering ∇ as an operator acting from $L^2(\mathcal{G};\mu)$ to $L^2(\mathcal{G};\nu)$, its formal adjoint $\nabla^\dagger$ acting from $L^2(\mathcal{G};\nu)$ to $L^2(\mathcal{G};\mu)$ acts edgewise as

$$\nabla^\dagger\colon f\mapsto -\frac{1}{\mu}(\nu f)'. \tag{2.4.2}$$

Thus, the weighted Laplacian Δ acting in $L^2(\mathcal{G};\mu)$, written in the divergence form

$$\Delta\colon f\mapsto -\nabla^\dagger(\nabla f), \tag{2.4.3}$$

acts edgewise as the following divergence form Sturm–Liouville operator

$$\Delta\colon f\mapsto \frac{1}{\mu}(\nu f')'. \tag{2.4.4}$$

The continuity assumption imposed on f results for Δ in a one-parameter family of symmetric boundary conditions at each vertex $v\in\mathcal{V}$

$$\begin{cases} f \text{ is continuous at } v,\\ \sum\limits_{\vec{e}\in\vec{\mathcal{E}}_v}\nu(e)\partial_{\vec{e}}f(v)=\alpha(v)f(v), \end{cases} \tag{2.4.5}$$

where $\alpha(v)\in\mathbb{R}\cup\{\infty\}$, and $\alpha(v)=\infty$ should be understood as the Dirichlet boundary condition at v. With the Laplacian Δ acting on $\mathcal{G}$ we shall shall always associate the *Kirchhoff* vertex conditions†

$$\begin{cases} f \text{ is continuous at } v,\\ \sum\limits_{\vec{e}\in\vec{\mathcal{E}}_v}\nu(e)\partial_{\vec{e}}f(v)=0, \end{cases}\qquad v\in\mathcal{V}, \tag{2.4.6}$$

that is, conditions (2.4.5) with $\alpha(v)=0$ for all $v\in\mathcal{V}$. Notice that for non-zero $\alpha\colon\mathcal{V}\to\mathbb{R}\cup\{\infty\}$, the Laplacian with boundary conditions (2.4.5) can be written as

$$-\Delta+\sum_{v\in\mathcal{V}}\alpha(v)\delta_v, \tag{2.4.7}$$

(at least when $\mu\equiv 1$), where δ_v is the Dirac delta centred at v.

Remark 2.13. Of course, since both weights are edgewise constant, on every edge $e\in\mathcal{E}$ the corresponding differential expression for Δ simplifies to

$$-\frac{\nu(e)}{\mu(e)}\frac{\mathrm{d}^2}{\mathrm{d}x_e^2}$$

and then the definition of Δ looks simpler, especially if $\mu=\nu$. However, the form (2.4.4) is important for us since it reflects, on the one hand, the choice of the Hilbert space $L^2(\mathcal{G};\mu)$ and, on the other hand, the proper choice of boundary conditions at the vertices, see (2.4.6).

There are several standard ways to associate an operator with Δ in the Hilbert space $L^2(\mathcal{G};\mu)$ and this will be our main goal in the following subsections. Notice that different definitions may lead to different operators (the choice of a domain of definition is very important when dealing with unbounded operators) and each definition has its advantages and disadvantages.

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†Seems, there is no agreement in the literature regarding the name of the boundary conditions (2.4.6). Sometimes they are called *standard* or *Kirchhoff–Neumann* boundary conditions. The last name can be explained by looking at vertices with $\deg(v)=1$, in which case (2.4.6) is nothing but the usual Neumann condition $\partial f(v)=0$.

2.4.1. (Weighted) Kirchhoff Laplacian. For every $e \in \mathcal{E}$ consider the maximal operator $\mathrm{H}_{e,\max}$ defined in $L^2(e;\mu)$ by

$$\mathrm{H}_{e,\max} = -\frac{1}{\mu(e)}\frac{\mathrm{d}}{\mathrm{d}x_e}\nu(e)\frac{\mathrm{d}}{\mathrm{d}x_e}, \qquad \mathrm{dom}(\mathrm{H}_{e,\max}) = H^2(e). \tag{2.4.8}$$

Then one can define the maximal operator in $L^2(\mathcal{G};\mu)$ as the edgewise direct sum

$$\mathbf{H}_{\max} = \bigoplus_{e\in\mathcal{E}} \mathrm{H}_{e,\max}. \tag{2.4.9}$$

However, the definition of $\mathbf{H}_{\max}$ does not reflect the underlying graph structure. Moreover, to make the maximal operator symmetric, one needs to impose appropriate boundary conditions at the vertices. Imposing Kirchhoff boundary conditions on the maximal domain yields the *(maximal) Kirchhoff Laplacian*:

$$\mathbf{H} = -\Delta \restriction \mathrm{dom}(\mathbf{H}), \quad \mathrm{dom}(\mathbf{H}) = \{f \in \mathrm{dom}(\mathbf{H}_{\max}) \,|\, f \text{ satisfies (2.4.6) on } \mathcal{V}\}. \tag{2.4.10}$$

Restricting further to compactly supported functions we end up with the pre-minimal operator

$$\mathbf{H}' = -\Delta \restriction \mathrm{dom}(\mathbf{H}'), \qquad \mathrm{dom}(\mathbf{H}') = \mathrm{dom}(\mathbf{H}) \cap C_c(\mathcal{G}). \tag{2.4.11}$$

We shall call its closure $\mathbf{H}^0 := \overline{\mathbf{H}'}$ in $L^2(\mathcal{G};\mu)$ the *minimal Kirchhoff Laplacian*.

Integrating by parts one obtains

$$\langle \mathbf{H}'f, f\rangle_{L^2} = \int_{\mathcal{G}} |\nabla f(x)|^2\,\nu(\mathrm{d}x) = \|\nabla f\|^2_{L^2(\mathcal{G};\nu)} =: \mathfrak{Q}[f] \tag{2.4.12}$$

for each $f \in \mathrm{dom}(\mathbf{H}')$, and hence both $\mathbf{H}'$ and $\mathbf{H}^0$ are nonnegative symmetric operators. It is known that

$$\mathbf{H}^* = \mathbf{H}^0. \tag{2.4.13}$$

The equality $\mathbf{H}^0 = \mathbf{H}$ holds if and only if $\mathbf{H}^0$ is self-adjoint (or, equivalently, $\mathbf{H}'$ is essentially self-adjoint).

Alongside Kirchhoff boundary conditions (2.4.6) we are going to consider a slightly more general class of boundary conditions (2.4.5). These vertex conditions are interpreted as *δ-couplings (or δ-interactions) of strength* α (see (2.4.7)).[†] Indeed, define the maximal operator

$$\begin{aligned}\mathbf{H}_\alpha &= -\Delta \restriction \mathrm{dom}(\mathbf{H}_\alpha),\\ &\qquad \mathrm{dom}(\mathbf{H}_\alpha) = \{f \in \mathrm{dom}(\mathbf{H}_{\max}) \,|\, f \text{ satisfies (2.4.5) on } \mathcal{V}\}\end{aligned} \tag{2.4.14}$$

and the pre-minimal operator

$$\mathbf{H}'_\alpha = -\Delta \restriction \mathrm{dom}(\mathbf{H}'_\alpha), \qquad \mathrm{dom}(\mathbf{H}'_\alpha) = \mathrm{dom}(\mathbf{H}_\alpha) \cap C_c(\mathcal{G}). \tag{2.4.15}$$

Integrating by parts one obtains

$$\langle \mathbf{H}'_\alpha f, f\rangle_{L^2} = \int_{\mathcal{G}} |\nabla f(x)|^2\,\nu(\mathrm{d}x) + \sum_{v\in\mathcal{V}} \alpha(v)|f(v)|^2 =: \mathfrak{Q}_\alpha[f] \tag{2.4.16}$$

[†]In fact, one can interpret these boundary conditions as a perturbation of the Kirchhoff Laplacian by δ-potentials, see [**143**, Remark 4.5].

for all $f \in \mathrm{dom}(\mathbf{H}'_\alpha)$, which implies that $\mathbf{H}'_\alpha$ is a symmetric operator in $L^2(\mathcal{G};\mu)$. We define $\mathbf{H}^0_\alpha$ as the closure of $\mathbf{H}'_\alpha$. It is standard to show that

$$(\mathbf{H}'_\alpha)^* = \mathbf{H}_\alpha. \tag{2.4.17}$$

In particular, the equality $\mathbf{H}^0_\alpha = \mathbf{H}_\alpha$ holds if and only if $\mathbf{H}_\alpha$ is self-adjoint (or, equivalently, $\mathbf{H}'_\alpha$ is essentially self-adjoint).

2.4.2. Gaffney Laplacian. One can also associate self-adjoint operators with the Laplacian Δ in a different way, which to a certain extent can be interpreted as the quadratic form approach. Setting

$$H^1_{\mathrm{loc}}(\mathcal{G}) := H^1_{\mathrm{loc}}(\mathcal{G}\setminus\mathcal{V}) \cap C(\mathcal{G}), \qquad H^1_c(\mathcal{G}) := H^1_{\mathrm{loc}}(\mathcal{G}\setminus\mathcal{V}) \cap C_c(\mathcal{G}), \tag{2.4.18}$$

let us introduce two (weighted) Sobolev spaces on $\mathcal{G}$. First define

$$H^1(\mathcal{G}) = H^1(\mathcal{G};\mu,\nu) := \big\{ f \in H^1_{\mathrm{loc}}(\mathcal{G}) \,\big|\, f \in L^2(\mathcal{G};\mu),\ \nabla f \in L^2(\mathcal{G};\nu)\big\}. \tag{2.4.19}$$

Equipping $H^1(\mathcal{G})$ with the graph norm

$$\|f\|^2_{H^1(\mathcal{G})} := \|f\|^2_{L^2(\mathcal{G};\mu)} + \|\nabla f\|^2_{L^2(\mathcal{G};\nu)} \tag{2.4.20}$$

turns it into a Hilbert space. Next, we set

$$H^1_0(\mathcal{G}) = \overline{H^1_c(\mathcal{G})}^{\|\cdot\|_{H^1}}. \tag{2.4.21}$$

Notice that in contrast to $H^1_c(\mathcal{G})$ and $H^1_{\mathrm{loc}}(\mathcal{G})$, the Sobolev spaces $H^1(\mathcal{G})$ and $H^1_0(\mathcal{G})$ do depend on the weights μ and ν.

The *Friedrichs extension* of $\mathbf{H}'$, let us denote it by $\mathbf{H}_D$, is defined as the operator associated with the closure in $L^2(\mathcal{G};\mu)$ of the quadratic form (2.4.12). Clearly, the domain of the closure coincides with $H^1_0(\mathcal{G})$ and hence $\mathbf{H}_D$ is given as the restriction of $\mathbf{H}$ to the domain $\mathrm{dom}(\mathbf{H}_D) := \mathrm{dom}(\mathbf{H}) \cap H^1_0(\mathcal{G})$ (see, e.g., [**188**, Theorem 10.17]). On the other hand, the form $\mathfrak{Q}$ is well defined on $H^1(\mathcal{G})$ and, moreover, the form

$$\mathfrak{Q}_N[f] := \mathfrak{Q}[f], \qquad f \in \mathrm{dom}(\mathfrak{Q}_N) = H^1(\mathcal{G})$$

is closed (since $H^1(\mathcal{G})$ is a Hilbert space). The self-adjoint operator $\mathbf{H}_N$ associated with $\mathfrak{Q}_N$ is usually called the *Neumann extension* of $\mathbf{H}^0$ or *Neumann Laplacian.*

Remark 2.14. Following the analogy with the Friedrichs extension, it might be tempting to think that the domain of the Neumann Laplacian $\mathbf{H}_N$ is given by $\mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$. However, the operator defined on this domain has a different name — the *Gaffney Laplacian* — and it is not symmetric in general. Moreover, this operator is not always closed (see [**147**]).

In the Hilbert space $L^2(\mathcal{G};\mu)$, we can associate (at least) two gradient operators with ∇ defined by (2.3.1). Namely, we define ∇_D and ∇_N as the operators

$$\nabla_D, \nabla_N : \quad \begin{array}{ccc} L^2(\mathcal{G};\mu) & \to & L^2(\mathcal{G};\nu) \\ f & \mapsto & \nabla f \end{array} \tag{2.4.22}$$

acting on the domains

$$\mathrm{dom}(\nabla_D) = H^1_0(\mathcal{G}), \qquad\qquad \mathrm{dom}(\nabla_N) = H^1(\mathcal{G}). \tag{2.4.23}$$

Both operators are closed and their importance stems from the following fact.

LEMMA 2.15. *Let $\mathbf{H}_D$ and $\mathbf{H}_N$ be the Friedrichs and the Neumann extensions of $\mathbf{H}_0$, respectively. Then*

$$\mathbf{H}_D = \nabla_D^*\nabla_D, \qquad \mathbf{H}_N = \nabla_N^*\nabla_N, \tag{2.4.24}$$

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 and hence, by von Neumann's theorem (see [**125**, Chapter V.3.7] or [**182**, Theorem X.25]), $\nabla_D^*\nabla_D$ and $\nabla_N^*\nabla_N$ are self-adjoint nonnegative operators in $L^2(\mathcal{G};\mu)$. 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., [**125**, Chapter VI.2.1]). □

REMARK 2.16. A few remarks are in order.

(i) $\mathbf{H}_D$ is often called the *Dirichlet Laplacian*, which explains the subscript.
(ii) 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 $\mathbf{H}_N$ are orientation independent.

In the Hilbert space $L^2(\mathcal{G};\mu)$, define the following operators

$$\mathbf{H}_{G,\min} = \nabla_N^*\nabla_D, \qquad \mathbf{H}_G = \nabla_D^*\nabla_N. \tag{2.4.25}$$

Both operators act edgewise as the Laplacian $-\Delta$ and their domains are

$$\operatorname{dom}(\mathbf{H}_{G,\min}) = \{f \in H_0^1(\mathcal{G}) \mid \nabla f \in \operatorname{dom}(\nabla_N^*)\},$$
$$\operatorname{dom}(\mathbf{H}_G) = \{f \in H^1(\mathcal{G}) \mid \nabla f \in \operatorname{dom}(\nabla_D^*)\}.$$

The operator $\mathbf{H}_G$ is called the *Gaffney Laplacian*. We shall refer to $\mathbf{H}_{G,\min}$ as the *minimal Gaffney Laplacian*.

REMARK 2.17. Notice that the above definition is not precisely the original definition of M.P. Gaffney [**78**] (roughly speaking H^1 was replaced by $C^1\cap H^1$ in [**78**], [**79**]). The obvious drawback is that the corresponding Laplacian in [**78**] is always non-closed. Let us also stress that we are unaware of $\mathbf{H}_{G,\min}$ in the manifold context and this natural, in our opinion, object seems to be new.

The following transparent description of $\mathbf{H}_G$ will be useful.

LEMMA 2.18. *The domain of the maximal Gaffney Laplacian is given by*

$$\operatorname{dom}(\mathbf{H}_G) = \operatorname{dom}(\mathbf{H}) \cap H^1(\mathcal{G}) = \{f \in \operatorname{dom}(\mathbf{H}) \,|\, \nabla f \in L^2(\mathcal{G};\nu)\}. \tag{2.4.26}$$

Moreover, the minimal Gaffney Laplacian is closed in $L^2(\mathcal{G})$ and

$$\mathbf{H}_{G,\min} = \mathbf{H}_G^*. \tag{2.4.27}$$

PROOF. The inclusion $\operatorname{dom}(\mathbf{H}_G) \subseteq \operatorname{dom}(\mathbf{H})\cap H^1(\mathcal{G})$ follows from the definition of $\mathbf{H}_G$. The converse inclusion is immediate from the following description of the adjoint ∇_D^* to ∇_D (see [**147**, Lemma 3.5]):

$$\operatorname{dom}(\nabla_D^*) = \Big\{f \in H^1(\mathcal{G}\setminus\mathcal{V};\mu,\nu) \,\Big|\, \sum_{\vec{e}\in\vec{\mathcal{E}}_v} \nu(\vec{e})\vec{f}_{\vec{e}}(v) = 0 \text{ for all } v\in\mathcal{V}\Big\}, \tag{2.4.28}$$

[†]The product AB of two unbounded operators A, B in a Hilbert space $\mathfrak{H}$ is understood as their composition: $(AB)(f) := A(Bf)$ for all $f \in \operatorname{dom}(AB) := \{f \in \operatorname{dom}(B) \,|\, Bf \in \operatorname{dom}(A)\}$.

which then makes the converse inclusion in (2.4.26) obvious. Here we employ the following notation

$$\vec{f}_{\vec{e}}(v) = \begin{cases} f_{\vec{e}}(v), & e \in \vec{\mathcal{E}}_v^+, \\ -f_{\vec{e}}(v), & e \in \vec{\mathcal{E}}_v^- \end{cases}$$

and

$$H^1(\mathcal{G} \setminus \mathcal{V}; \mu, \nu) := \{f \in H^1_{\mathrm{loc}}(\mathcal{G} \setminus \mathcal{V}) \,|\, f \in L^2(\mathcal{G}; \mu),\ \nabla f \in L^2(\mathcal{G}; \nu)\}. \qquad \square$$

It is immediate from the above description that

$$\mathbf{H}_0 \subseteq \mathbf{H}_{G,\min} \subseteq \mathbf{H}_G \subseteq \mathbf{H} \tag{2.4.29}$$

and

$$\mathbf{H}_{G,\min} \subseteq \mathbf{H}_D \subseteq \mathbf{H}_G, \qquad \mathbf{H}_{G,\min} \subseteq \mathbf{H}_N \subseteq \mathbf{H}_G. \tag{2.4.30}$$

Remark 2.19 (Hodge Laplacians). One can introduce 0-forms and 1-forms on $\mathcal{G}$ (due to the local 1d nature of metric graphs, the space of 2-forms on $\mathcal{G}$ is trivial) and, upon assigning an orientation, both can be further identified with functions. From this perspective the operator

$$\vec{\Delta} = \nabla_N \nabla_D^*$$

is a metric graph analogue of the Hodge Laplacian on 1-forms (see [**17**, § 5.1], [**80**], [**178**]). Indeed, the Hodge Laplacian on smooth k-forms on a Riemannian manifold is given by

$$\Delta_k = \delta^{k+1}\mathrm{d}^k + \mathrm{d}^{k-1}\delta^k,$$

where d^k is the exterior derivative (mapping k-forms to $(k+1)$-forms) and the codifferential δ^{k+1} is its formal adjoint (mapping $(k+1)$-forms to k-forms). Working in the L^2-framework and replacing smooth by H^1 for metric graphs, one can identify $\mathrm{d}^0 = \nabla_N$ and $\delta^1 = \nabla_D^*$. In particular, the Gaffney Laplacian (2.4.25) can be viewed as the Hodge Laplacian on 0-forms. Let us also stress that due to the supersymmetry, the properties of $\mathbf{H}_G$ and $\vec{\Delta}$ are closely connected.

2.4.3. Inessential vertices and models. So far we have defined (weighted) Laplacian operators by viewing a given metric graph $\mathcal{G}$ as a metric realization of a fixed model $(\mathcal{G}_d, |\cdot|)$. Of course, one can introduce these operators also by starting with a given metric graph $\mathcal{G}$, however, from the metric space perspective. Moreover, as it was already mentioned, sometimes it is important to consider different models of the same metric graph and hence we need to introduce the following notions. Let $\mathcal{G}$ be a metric graph. A positive function $\mu\colon \mathcal{G} \to (0,\infty)$ is called an *edge weight* if there is a discrete subset $\mathcal{V}_\mu \subset \mathcal{G}$ such that $\mathcal{V}_\mu$ contains all the points of $\mathcal{G}$ having degree not equal to 2 and, moreover, μ is constant on each connected component of $\mathcal{G}\setminus\mathcal{V}_\mu$. Clearly, for each model $(\mathcal{G}_d, |\cdot|)$ of $\mathcal{G}$, we can lift any function $\mu_{\mathcal{E}}\colon \mathcal{E} \to (0,\infty)$ to an edge weight $\mu\colon \mathcal{G} \to (0,\infty)$ in an obvious way. Conversely, each edge weight $\mu\colon \mathcal{G} \to (0,\infty)$ arises in this way.

Definition 2.20. A triple $(\mathcal{G}, \mu, \nu)$, where $\mathcal{G}$ is a metric graph and μ, ν are edge weights, is called a *weighted metric graph*.

A collection $(\mathcal{G}_d, |\cdot|, \mu_{\mathcal{E}}, \nu_{\mathcal{E}}) = (\mathcal{V}, \mathcal{E}, |\cdot|, \mu_{\mathcal{E}}, \nu_{\mathcal{E}})$ is called a *model of a weighted graph* $(\mathcal{G}, \mu, \nu)$ if $(\mathcal{G}_d, |\cdot|)$ is a model of $\mathcal{G}$ and the weights $\mu_{\mathcal{E}}$, $\nu_{\mathcal{E}}$ lifted to $\mathcal{G}$ coincide with μ and ν, respectively.

For a given model $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu_{\mathcal{E}}, \nu_{\mathcal{E}})$ of $(\mathcal{G}, \mu, \nu)$, a vertex $v \in \mathcal{V}$ is called *inessential* if $\deg(v) = 2$ and both μ and ν are constant in some neighborhood of v.

Notice that we can introduce a partial order on the set of models of $(\mathcal{G},\mu,\nu)$ in exactly the same way as for metric graphs: a model $(\mathcal{V}',\mathcal{E}',|\cdot|',\mu_{\mathcal{E}'},\nu_{\mathcal{E}'})$ is a *refinement* of $(\mathcal{V},\mathcal{E},|\cdot|,\mu_{\mathcal{E}},\nu_{\mathcal{E}})$ if $\mathcal{V}\subseteq\mathcal{V}'$.

Having introduced these notions, it is clear that the spaces $H^1(\mathcal{G})$ and $H^1_0(\mathcal{G})$ together with the Laplacian operators introduced in Section 2.4.1–2.4.2 only depend on the weighted metric graph $(\mathcal{G},\mu,\nu)$ (and not the concrete choice of a model). For instance, if $v\in\mathcal{V}$ is an inessential vertex, then the differential expression remains the same on its two adjacent edges and the corresponding Kirchhoff conditions (2.4.6) turn into the usual continuity condition at v for f and its gradient. Therefore, replacing these two edges by a single edge whose length equals the sum of lengths and also taking the same edge weights would not change the corresponding Kirchhoff Laplacian.

Remark 2.21. A few remarks are in order.

(i) By construction, μ enters the differential expression and ν appears in (2.4.6) (one can notice this also by looking at the graph norm (2.4.20), where μ and ν enter the first and the second summand, respectively, on the RHS (2.4.20)).

(ii) If both edge weights μ and ν are constant on $\mathcal{G}$, then each vertex of degree 2 is inessential.

(iii) We often abuse the notation and denote both a weighted metric graph and its model by $(\mathcal{G},\mu,\nu)$. However, when different models of the same weighted metric graph or the whole set of its models are considered, we will specifically indicate it in order to avoid a possible confusion. Moreover, sometimes we will call a model $(\mathcal{V},\mathcal{E},|\cdot|,\mu_{\mathcal{E}},\nu_{\mathcal{E}})$ of $(\mathcal{G},\mu,\nu)$ a *(weighted) metric graph over* $(\mathcal{V},\mathcal{E})$.

2.4.4. More general operators on graphs. As one may easily notice, our setting is rather restrictive from the perspective of differential operators involved. Indeed, (2.4.8) is nothing but a divergence form Sturm–Liouville differential expression with constant coefficients and, of course, one can consider more general differential expressions on edges. The use of more general operators can be justified from the quantum mechanical perspective (in particular, this leads to the consideration of magnetic Schrödinger operators) as well as from the Brownian motion perspective (which leads to the study of Sturm–Liouville expressions with distributional coefficients, e.g., Krein strings which are also widely known as Krein–Feller operators). Moreover, the one-parameter family of vertex conditions (2.4.5) obviously does not cover all self-adjoint vertex conditions if the degree of a vertex is greater than 1. However, some of our results (especially those in Chapter 3) allow to treat both more general differential expressions (clearly, not all) and arbitrary self-adjoint vertex conditions, although this requires separate considerations. One may even attempt to establish the analogs of some results regarding connections between magnetic Schrödinger operators on graphs and metric graphs. We refer for further details to [**34**, § 3.5], [**178**] as well as to the case of 1d Schrödinger operators with point interactions [**65**], [**141**] (see also Remark 3.14).

CHAPTER 3

Connections via boundary triplets

To simplify the exposition we begin by looking at a weighted metric graph $(\mathcal{G}, \mu, \nu)$ as a metric realization of one of its models, that is, we start with a given combinatorial graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ equipped with edge lengths $|\cdot|\colon \mathcal{E} \to (0,\infty)$ and weights $\mu, \nu\colon \mathcal{E} \to (0,\infty)$. Let also $\alpha\colon \mathcal{V} \to \mathbb{R}$, that is, we are going to consider Laplacians with δ-couplings (2.4.5) at vertices. The main results of this chapter (see Theorem 3.1 and also Theorem 3.22 below) relate basic spectral properties of the Laplacian with δ-couplings $\mathbf{H}_\alpha$ with those of a certain Schrödinger-type operator on the corresponding combinatorial graph $\mathcal{G}_d$. At the very end of this chapter, in Section 3.3, we shall look at a weighted metric graph from the metric space perspective, which allows to understand the whole family of graph Laplacians associated with the models of a given weighted metric graph.

Let us stress once again that we always assume Hypothesis 2.1.

3.1. Spectral properties: graph Laplacians vs Kirchhoff Laplacians

To state the result, we first define the *intrinsic edge length*

$$\eta(e) := |e|\sqrt{\frac{\mu(e)}{\nu(e)}}, \qquad e \in \mathcal{E}, \tag{3.1.1}$$

together with the following quantity[‡]

$$\eta^*(\mathcal{E}) := \sup_{e\in\mathcal{E}} \eta(e). \tag{3.1.2}$$

Now introduce the edge weight $r\colon \mathcal{E} \to (0,\infty)$ by distinguishing two cases:

- if the underlying model of a weighted metric graph satisfies $\eta^*(\mathcal{E}) < \infty$, then we set

$$r(e) = |e|\mu(e), \qquad e \in \mathcal{E}, \tag{3.1.3}$$

- if $\eta^*(\mathcal{E}) = \infty$, we define the weight r by

$$r(e) = \begin{cases} |e|\mu(e), & \eta(e) \le 1, \\ \sqrt{\mu(e)\nu(e)}, & \eta(e) > 1. \end{cases} \tag{3.1.4}$$

Next, with a given metric graph $\mathcal{G}$ and weights μ, ν we associate:

- the *vertex weight* $m\colon \mathcal{V} \to (0,\infty)$

$$m(v) = \sum_{\vec{e}\in\vec{\mathcal{E}}_v} r(e), \qquad v \in \mathcal{V}, \tag{3.1.5}$$

[‡]In Section 3.3, we shall call it *the intrinsic size of a model* and its meaning will be clarified in Chapter 6 (see Remark 6.19).

- the *edge weight* $b\colon \mathcal{V}\times\mathcal{V}\to[0,\infty)$,

$$b(u,v) = \begin{cases} \sum_{\vec{e}\in\vec{\mathcal{E}}_u\colon e\in\mathcal{E}_v} \frac{\nu(e)}{|e|}, & u\neq v,\\ 0, & u=v,\end{cases} \qquad (u,v)\in\mathcal{V}\times\mathcal{V}. \tag{3.1.6}$$

It is straightforward to verify that b satisfies all the properties (i)-(iv) of Section 2.2. Since $\mathcal{G}_d$ is connected, so is the edge weight b. Moreover, the vertex weight m is strictly positive on $\mathcal{V}$ and hence defines a measure of full support on $\mathcal{V}$. Therefore, following considerations in Section 2.2, with the discrete Schrödinger expression

$$(\tau f)(v) := \frac{1}{m(v)}\Big(\sum_{u\in\mathcal{V}} b(v,u)(f(v)-f(u)) + \alpha(v)f(v)\Big), \quad v\in\mathcal{V}, \tag{3.1.7}$$

we can associate in the weighted Hilbert space $\ell^2(\mathcal{V};m)$ the minimal operator $\mathbf{h}_\alpha^0$ and the maximal operator $\mathbf{h}_\alpha$.

The main aim of this section is to prove the following result:

Theorem 3.1. *Let $\mathbf{H}_\alpha^0$ be the minimal Laplacian on $(\mathcal{G},\mu,\nu)$ equipped with the δ-coupling conditions (2.4.5) at the vertices and let also $\mathbf{h}_\alpha^0$ be the corresponding minimal discrete Schrödinger operator defined in $\ell^2(\mathcal{V};m)$ by (3.1.7). Then:*

(i) *The deficiency indices of $\mathbf{H}_\alpha^0$ and $\mathbf{h}_\alpha^0$ are equal and*

$$\mathrm{n}_+(\mathbf{H}_\alpha^0) = \mathrm{n}_-(\mathbf{H}_\alpha^0) = \mathrm{n}_\pm(\mathbf{h}_\alpha^0) \le \infty. \tag{3.1.8}$$

In particular, $\mathbf{H}_\alpha$ is self-adjoint if and only if $\mathbf{h}_\alpha$ is self-adjoint.

Assume in addition that $\mathbf{H}_\alpha$ (and hence also $\mathbf{h}_\alpha$) is self-adjoint. Then:

(ii) *The operator $\mathbf{H}_\alpha$ is lower semibounded if and only if the operator $\mathbf{h}_\alpha$ is lower semibounded.*

(iii) *The operator $\mathbf{H}_\alpha$ is nonnegative if and only if $\mathbf{h}_\alpha$ is nonnegative.*

(iv) *The total multiplicities of negative spectra of $\mathbf{H}_\alpha$ and $\mathbf{h}_\alpha$ coincide,*

$$\kappa_-(\mathbf{H}_\alpha) = \kappa_-(\mathbf{h}_\alpha).$$

(v) *The spectrum of $\mathbf{H}_\alpha$ is purely discrete if and only if $\#\{e\in\mathcal{E}\,|\,\eta(e)>\varepsilon\}$ is finite for every $\varepsilon>0$ and the spectrum of $\mathbf{h}_\alpha$ is purely discrete.*

Assume also that $\eta^*(\mathcal{E}) = \sup_{e\in\mathcal{E}}\eta(e) < \infty$. Then:

(vi) *The operator $\mathbf{H}_\alpha$ is positive definite if and only if $\mathbf{h}_\alpha$ is positive definite.*

(vii) *If, in addition, the operator $\mathbf{h}_\alpha$ is lower semibounded, then $\lambda_0^{\mathrm{ess}}(\mathbf{H}_\alpha)>0$ ($\lambda_0^{\mathrm{ess}}(\mathbf{H}_\alpha)=0$) exactly when $\lambda_0^{\mathrm{ess}}(\mathbf{h}_\alpha)>0$ (respectively, $\lambda_0^{\mathrm{ess}}(\mathbf{h}_\alpha)=0$).*

(viii) *Moreover, the following equivalence*

$$\mathbf{H}_\alpha^- \in \mathfrak{S}_p(L^2) \quad\Longleftrightarrow\quad \mathbf{h}_\alpha^- \in \mathfrak{S}_p(\ell^2),$$

holds for all $p\in(0,\infty]$. In particular, the negative spectrum of $\mathbf{H}_\alpha$ is discrete if and only if so is the negative spectrum of $\mathbf{h}_\alpha$.

Here and below for a self-adjoint operator T in a Hilbert space $\mathfrak{H}$, $\lambda_0(T)$ and $\lambda_0^{\mathrm{ess}}(T)$ denote the bottoms of its spectrum, respectively, of its essential spectrum,

$$\lambda_0(T) = \inf\sigma(T), \qquad \lambda_0^{\mathrm{ess}}(T) = \inf\sigma_{\mathrm{ess}}(T).$$

Moreover, $T^- := T\mathbb{1}_{(-\infty,0)}(T)$, where $\mathbb{1}_{(-\infty,0)}(T)$ is the spectral projection on the negative subspace of T.

As an immediate corollary we obtain the following result for the Kirchhoff Laplacian.

COROLLARY 3.2. *Let* $\mathbf{H}^0$ *be the minimal Kirchhoff Laplacian on* $(\mathcal{G}, \mu, \nu)$ *and let also* $\mathbf{h}^0$ *be the corresponding minimal weighted graph Laplacian defined in* $\ell^2(\mathcal{V}; m)$ *by* (3.1.7) *with* $\alpha \equiv 0$. *Then:*

(i) *The deficiency indices of* $\mathbf{H}^0$ *and* $\mathbf{h}^0$ *are equal and*

$$\mathrm{n}_+(\mathbf{H}^0) = \mathrm{n}_-(\mathbf{H}^0) = \mathrm{n}_\pm(\mathbf{h}^0) \le \infty. \tag{3.1.9}$$

In particular, $\mathbf{H}^0$ *is self-adjoint if and only if* $\mathbf{h}^0$ *is self-adjoint.*

Assume in addition that $\mathbf{H}^0$ *is self-adjoint (and hence coincides with the maximal Kirchhoff Laplacian* $\mathbf{H}$*). Then:*

(ii) *The spectrum of* $\mathbf{H}$ *is purely discrete if and only if* $\#\{e \in \mathcal{E} \,|\, \eta(e) > \varepsilon\}$ *is finite for every* $\varepsilon > 0$ *and the spectrum of the operator* $\mathbf{h}$ *is purely discrete.*

Assume also that $\sup_{e\in\mathcal{E}} \eta(e) < \infty$. *Then:*

(iii) *The operator* $\mathbf{H}$ *is positive definite,* $\lambda_0(\mathbf{H}) > 0$ *if and only if the operator* $\mathbf{h}$ *is positive definite,* $\lambda_0(\mathbf{h}) > 0$.

(iv) $\lambda_0^{\mathrm{ess}}(\mathbf{H}_\alpha) > 0$ *exactly when* $\lambda_0^{\mathrm{ess}}(\mathbf{h}_\alpha) > 0$.

PROOF. The proof is a straightforward application of Theorem 3.1 to the case $\alpha \equiv 0$. One only needs to take into account that both the minimal Kirchhoff Laplacian $\mathbf{H}^0$ and the minimal graph Laplacian $\mathbf{h}^0$ are nonnegative operators. □

REMARK 3.3. A few remarks are in order.

(i) In the case $\eta^*(\mathcal{E}) = \infty$ the weight r can be chosen in many different ways by changing the threshold 1 in (3.1.4) to any positive number.

(ii) In the following specific case

$$\inf_{e\in\mathcal{E}} \eta(e) > 0,$$

the choice of r can be further simplified to

$$r(e) := \sqrt{\mu(e)\nu(e)}, \qquad e \in \mathcal{E}. \tag{3.1.10}$$

Notice that if $\mu = \nu \equiv \mathbb{1}$, the assumption $\inf_{e\in\mathcal{E}} \eta(e) > 0$ is equivalent to $\inf_{e\in\mathcal{E}} |e| > 0$, which is the most common restriction in the spectral theory of quantum graphs [**24**], [**179**]. In this case $r(e) \equiv 1$ for all $e \in \mathcal{E}$ and hence the vertex weight m given by (3.1.5) is nothing but the combinatorial degree (2.1.3).

(iii) In the papers [**141**], [**67**] it is assumed that $\mu = \nu \equiv \mathbb{1}$ and $\sup_{e\in\mathcal{E}} \eta(e) = \sup_{e\in\mathcal{E}} |e| < \infty$. Usually, the latter is not a restriction since this condition can always be achieved by adding inessential vertices, that is by choosing an appropriate model of a metric graph since this choice does not have any impact on spectral properties of the corresponding Kirchhoff Laplacian (see Section 2.4.3). However, this changes the combinatorial structure of the underlying graph $\mathcal{G}_d$, which is important for our future purposes. This will be discussed in greater details in Section 3.3

(iv) Let us also mention that the list of equivalences in Theorem 3.1 is not complete and we refer to, e.g., [**67**] for further details.

3.2. Graph Laplacians as boundary operators

This section is devoted to the proof of Theorem 3.1, which is based on the boundary triplets approach (see Appendix A) and essentially follows the lines of [**67**].

3.2.1. Edge-based boundary triplet. We begin with constructing a suitable boundary triplet for the operator $\mathbf{H}_{\max}$. First of all, the following simple fact holds true (cf. [**67**, Lemma 2.1]).

LEMMA 3.4. *Let* $\mathrm{H}_{e,\max}$, $e \in \mathcal{E}$ *be the maximal operator* (2.4.8). *The triplet* $\widetilde{\Pi}_e = \{\mathbb{C}^2, \widetilde{\Gamma}_{0,e}, \widetilde{\Gamma}_{1,e}\}$, *where the mappings* $\widetilde{\Gamma}_{0,e}$, $\widetilde{\Gamma}_{1,e} \colon H^2(e) \to \mathbb{C}^2$ *are defined by*

$$\widetilde{\Gamma}_{0,e} \colon f \mapsto \begin{pmatrix} f(e_\imath) \\ f(e_\tau) \end{pmatrix}, \qquad \widetilde{\Gamma}_{1,e} \colon f \mapsto \begin{pmatrix} \nu(e)\partial f(e_\imath) \\ \nu(e)\partial f(e_\tau) \end{pmatrix}, \tag{3.2.1}$$

is a boundary triplet for $\mathrm{H}_{e,\max}$. *The corresponding Weyl function is*

$$\widetilde{M}_e \colon z \mapsto \sqrt{\mu(e)\nu(e)z} \begin{pmatrix} -\cot\big(\eta(e)\sqrt{z}\big) & \csc\big(\eta(e)\sqrt{z}\big) \\ \csc\big(\eta(e)\sqrt{z}\big) & -\cot\big(\eta(e)\sqrt{z}\big) \end{pmatrix}, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

Next we proceed as follows (see, e.g., [**141**, § 4] and also [**67**, § 2]): set

$$\mathrm{R}_e := r(e)\,\mathrm{I}_2, \qquad \mathrm{Q}_e := \lim_{z\to 0} \widetilde{M}_e(z) = \frac{\nu(e)}{|e|}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{3.2.2}$$

where $r \colon \mathcal{E} \to (0,\infty)$ is given by (3.1.3), (3.1.4). Define the mappings

$$\Gamma_{0,e} := \mathrm{R}_e^{1/2}\widetilde{\Gamma}_{0,e}, \qquad \Gamma_{1,e} := \mathrm{R}_e^{-1/2}(\widetilde{\Gamma}_{1,e} - \mathrm{Q}_e\widetilde{\Gamma}_{0,e}), \tag{3.2.3}$$

that is, $\Gamma_{0,e}$, $\Gamma_{1,e} \colon H^2(e) \to \mathbb{C}^2$ are given by

$$\Gamma_{0,e} \colon f \mapsto \sqrt{r(e)}\begin{pmatrix} f(e_\imath) \\ f(e_\tau) \end{pmatrix}, \quad \Gamma_{1,e} \colon f \mapsto \frac{\nu(e)}{\sqrt{r(e)}}\begin{pmatrix} \partial f(e_\imath) - \frac{f(e_\tau)-f(e_\imath)}{|e|} \\ \partial f(e_\tau) + \frac{f(e_\tau)-f(e_\imath)}{|e|} \end{pmatrix}. \tag{3.2.4}$$

Clearly, $\Pi_e = \{\mathbb{C}^2, \Gamma_{0,e}, \Gamma_{1,e}\}$ is also a boundary triplet for $\mathrm{H}_{e,\max}$. In addition, the following claim holds (cf. [**141**, Theorem 4.1] and [**67**, Theorem 2.2]).

PROPOSITION 3.5. *The direct sum of boundary triplets*

$$\Pi_{\mathcal{E}} = \bigoplus_{e\in\mathcal{E}} \Pi_e = \big\{\mathcal{H}_{\mathcal{E}}, \Gamma_0^{\mathcal{E}}, \Gamma_1^{\mathcal{E}}\big\}, \tag{3.2.5}$$

where

$$\mathcal{H}_{\mathcal{E}} = \bigoplus_{e\in\mathcal{E}} \mathbb{C}^2, \qquad \Gamma_0^{\mathcal{E}} := \bigoplus_{e\in\mathcal{E}} \Gamma_{0,e}, \qquad \Gamma_1^{\mathcal{E}} := \bigoplus_{e\in\mathcal{E}} \Gamma_{1,e}, \tag{3.2.6}$$

is a boundary triplet for the operator $\mathbf{H}_{\max} = \oplus_{e\in\mathcal{E}}\mathbf{H}_{e,\max}$.

PROOF. Since $\mathrm{H}_{e,\max}^*$ is a positive symmetric operator for every $e \in \mathcal{E}$, so is $\mathbf{H}_{\max}^*$. Therefore, we need to apply Theorem A.11 and to verify conditions (A.4.3). Notice that for each $e \in \mathcal{E}$, the corresponding Weyl function is given by

$$M_e(z) = \mathrm{R}_e^{-1/2}(\widetilde{M}_e(z) - \mathrm{Q}_e)\mathrm{R}_e^{-1/2} = \frac{1}{r(e)}\widetilde{M}_e(z) - \frac{1}{r(e)}\mathrm{Q}_e.$$

(i) First of all, straightforward calculations yield that for all $e \in \mathcal{E}$

$$M_e(-1) = \frac{\sqrt{\mu(e)\nu(e)}}{r(e)}\begin{pmatrix} \frac{1}{\eta(e)} - \coth\eta(e) & \frac{1}{\sinh\eta(e)} - \frac{1}{\eta(e)} \\ \frac{1}{\sinh\eta(e)} - \frac{1}{\eta(e)} & \frac{1}{\eta(e)} - \coth\eta(e) \end{pmatrix},$$

$$M_e'(-1) = \frac{\sqrt{\mu(e)\nu(e)}}{r(e)} \begin{pmatrix} \coth\eta(e) - \frac{\eta(e)}{\sinh^2\eta(e)} & \frac{\eta(e)\cosh\eta(e)}{\sinh^2\eta(e)} - \frac{1}{\sinh\eta(e)} \\ \frac{\eta(e)\cosh\eta(e)}{\sinh^2\eta(e)} - \frac{1}{\sinh\eta(e)} & \coth\eta(e) - \frac{\eta(e)}{\sinh^2\eta(e)} \end{pmatrix},$$

where $r(e)$ is given by (3.1.4). Clearly, $\|M_e(-1)\| = \max(|\lambda_+(M_e)|, |\lambda_-(M_e)|)$, where $\lambda_+(M_e)$ and $\lambda_-(M_e)$ are the eigenvalues of $M_e(-1)$ given explicitly by

$$\lambda_\pm(M_e) = \frac{\sqrt{\mu(e)\nu(e)}}{r(e)} \left(\frac{1}{\eta(e)} - \coth\eta(e) \pm \left(\frac{1}{\sinh\eta(e)} - \frac{1}{\eta(e)}\right)\right).$$

Since $|\lambda_+(M_e)| > |\lambda_-(M_e)|$, we get

$$\|M_e(-1)\| = |\lambda_+(M_e)| = \frac{\sqrt{\mu(e)\nu(e)}}{r(e)} \frac{\cosh\eta(e) - 1}{\sinh\eta(e)} = \frac{\sqrt{\mu(e)\nu(e)}}{r(e)} \tanh\left(\frac{\eta(e)}{2}\right).$$

Similarly, one obtains that

$$\|M_e'(-1)\| = \lambda_+(M_e') = \frac{\sqrt{\mu(e)\nu(e)}}{r(e)} \frac{(\sinh\eta(e) + \eta(e))(\cosh\eta(e) - 1)}{2\sinh^2\eta(e)},$$

$$\|(M_e'(-1))^{-1}\| = \frac{1}{\lambda_-(M_e')} = \frac{r(e)}{\sqrt{\mu(e)\nu(e)}} \frac{2\sinh^2\eta(e)}{(\sinh\eta(e) - \eta(e))(\cosh\eta(e) + 1)},$$

where $\lambda_+(M_e')$ and $\lambda_-(M_e')$ are the eigenvalues of $M_e'(-1)$.

(ii) Assume first that $\eta^*(\mathcal{E}) < \infty$. Then $r(e) = \mu(e)|e|$, $e \in \mathcal{E}$ and in particular,

$$\|M_e(-1)\| \le \sup_{0<s\le\eta^*(\mathcal{E})} \frac{1}{s} \tanh\left(\frac{s}{2}\right) = \sup_{0<s\le\eta^*(\mathcal{E})} f(s).$$

Since the function $f(s)$ defined by the RHS admits an analytic continuation at 0, we conclude that $\sup_e M_e(-1) < \infty$. Similar considerations imply that

$$\sup_e (\|M_e'(-1)\| + \|(M_e'(-1))^{-1}\|) < \infty \tag{3.2.7}$$

and hence (A.4.3) holds true in this case.

(iii) Suppose now that $\eta^*(\mathcal{E}) = \infty$. If $e \in \mathcal{E}$ is an edge with $\eta(e) > 1$, then $r(e) = \sqrt{\mu(e)\nu(e)}$ and hence

$$\|M_e(-1)\| \le \sup_{s>1} \tanh\left(\frac{s}{2}\right) = 1, \tag{3.2.8}$$

and

$$\|M_e'(-1)\| \le \sup_{s>1} \frac{(\sinh s + s)(\cosh s - 1)}{2\sinh^2 s} < \infty, \tag{3.2.9}$$

$$\|(M_e'(-1))^{-1}\| \le \sup_{s>1} \frac{2\sinh^2 s}{(\sinh s - s)(\cosh s + 1)} < \infty. \tag{3.2.10}$$

On the other hand, if $\eta(e) \le 1$, then $r(e) = \mu(e)|e|$ as in (ii), and the same steps as there give uniform bounds on $\|M_e(-1)\|$, $\|M_e'(-1)\|$ and$\|(M_e'(-1))^{-1}\|$. Altogether, we conclude that the condition (A.4.3) holds true and this completes the proof. □

REMARK 3.6. It is easy to see that Proposition 3.5 holds true if instead of (3.1.4) the weight r is defined as in Remark 3.3(i).

Clearly, the Weyl function corresponding to the boundary triplet constructed in Proposition 3.5 has a very transparent form and enjoys some important properties.

LEMMA 3.7. *The Weyl function corresponding to the boundary triplet $\Pi_{\mathcal{E}}$ is given by*

$$M_{\mathcal{E}}(z) = \bigoplus_{e\in\mathcal{E}} M_e(z), \qquad M_e(z) = \mathrm{R}_e^{-1/2}(\widetilde{M}_e(z) - \mathrm{Q}_e)\mathrm{R}_e^{-1/2}. \tag{3.2.11}$$

Moreover,

(i) $M_{\mathcal{E}}(0) = \mathbb{O}_{\mathcal{H}_{\mathcal{E}}}$, *where*

$$M_{\mathcal{E}}(0) := s - R - \lim_{x\uparrow 0} M_{\mathcal{E}}(x). \tag{3.2.12}$$

(ii) $M_{\mathcal{E}}(x)$ *uniformly tends to* $-\infty$ *as* $x\to-\infty$, *that is, for every* $N>0$ *there is* $x_N<0$ *such that for all* $x<x_N$, $M_{\mathcal{E}}$ *satisfies*

$$M_{\mathcal{E}}(x) < -N\cdot \mathrm{I}_{\mathcal{H}}.$$

PROOF. First of all, (3.2.11) is immediate from Proposition 3.5. To prove (i), it suffices to mention that $M_e(0) = \mathbb{O}_2$ for all $e\in\mathcal{E}$.

(ii) Denote by $\lambda_e^+(x)$ and $\lambda_e^-(x)$ the eigenvalues of $M_e(-x^2)$. Straightforward calculations yield

$$\lambda_e^{\pm}(x) = -x\frac{\sqrt{\mu(e)\nu(e)}}{r(e)}\cdot\frac{\cosh(\eta(e)x)\mp 1}{\sinh(\eta(e)x)} + \frac{\nu(e)}{|e|r(e)}(1\mp 1),$$

and noting that $\lambda_e^+(x) < \lambda_e^-(x) < 0$ for all $x>0$, we get

$$M_e(-x^2) \le \lambda_e^-(x)\mathrm{I}_2 = \mathrm{I}_2\times\begin{cases}\frac{2}{\eta(e)^2} - \frac{x}{\eta(e)}\coth(\frac{\eta(e)x}{2}), & \text{if } r(e) = |e|\mu(e),\\ \frac{2}{\eta(e)} - x\coth(\frac{\eta(e)x}{2}), & \text{if } r(e) = \sqrt{\mu(e)\nu(e)}.\end{cases}$$

For an $e\in\mathcal{E}$ with $r(e) = \sqrt{\mu(e)\nu(e)}$, we have $\eta(e)>1$ and one easily verifies

$$M_e(-x^2) \le (2-x)\mathrm{I}_2.$$

If $r(e) = |e|\mu(e)$, then $\eta(e)\le C$ for all such edges e and some uniform constant $C>0$ (e.g., take $C=\eta^*(\mathcal{E})$ if $\eta^*(\mathcal{E})<\infty$ and $C=1$ otherwise). Let us now proceed as in the proof of [**141**, Prop. 4.10] and consider the function

$$F(s) = \frac{\coth(s)}{s} - \frac{1}{s^2}, \qquad s>0.$$

Clearly, F is strictly positive and continuous on $(0,\infty)$. Moreover, $F(s) = \frac{1}{3}+\mathcal{O}(s^2)$ as $s\to 0$ and $F'(s) = -\frac{1}{s^2}+\mathcal{O}(s^{-3})$ as $s\to+\infty$ and hence

$$\inf_{s\in(0,a)} F(s) = F(a) = \frac{1}{a}\coth(a) - \frac{1}{a^2}$$

for all sufficiently large $a>1$. It remains to notice that

$$\lambda_e^-(x) = -\frac{x^2}{2}F\Big(\frac{\eta(e)x}{2}\Big)$$

and hence

$$\lambda_e^-(x) \le -\frac{x^2}{2}\inf_{s\in(0,Cx/2)} F(s) = -\frac{x^2}{2}F\Big(\frac{Cx}{2}\Big) = \frac{2}{C^2} - \frac{x}{C}\coth\Big(\frac{Cx}{2}\Big) \le -\frac{x}{2C}$$

for all sufficiently large $x>1$. Taking into account (3.2.11), we get

$$M_{\mathcal{E}}(-x^2) \le \mathrm{I}_{\mathcal{H}}\inf_{e\in\mathcal{E}}\lambda_e^-(x) \le -\frac{x}{2\max\{1,C\}}\mathrm{I}_{\mathcal{H}}$$

for all sufficiently large $x>1$. $\square$

3.2.2. Vertex-based boundary triplet. It will be convenient for us to work with another boundary triplet for $\mathbf{H}_{\max}$, which can be obtained from the triplet $\Pi_{\mathcal{E}}$ by regrouping all its components with respect to the vertices. Define

$$\mathcal{H}_{\mathcal{V}} = \bigoplus_{v\in\mathcal{V}} \mathbb{C}^{\deg(v)}, \qquad \Gamma_0^{\mathcal{V}} = \bigoplus_{v\in\mathcal{V}} \Gamma_{0,v}, \qquad \Gamma_1^{\mathcal{V}} = \bigoplus_{v\in\mathcal{V}} \Gamma_{1,v}, \tag{3.2.13}$$

where

$$\Gamma_{0,v} f = \Big(\sqrt{r(e)} f_{\vec{e}}(v)\Big)_{\vec{e}\in\vec{\mathcal{E}}_v}, \tag{3.2.14}$$

$$\Gamma_{1,v} f = \left(\frac{\nu(e)}{\sqrt{r(e)}}\Big(\partial_{\vec{e}} f(v) - \pi_v(\vec{e})\frac{f(e_\tau) - f(e_\imath)}{|e|}\Big)\right)_{\vec{e}\in\vec{\mathcal{E}}_v}, \tag{3.2.15}$$

with $\pi_v\colon \vec{\mathcal{E}}_v \to \{-1, 1\}$ denoting the orientation function

$$\pi_v(\vec{e}) := \begin{cases} 1, & \vec{e}\in\vec{\mathcal{E}}_v^+, \\ -1, & \vec{e}\in\vec{\mathcal{E}}_v^-. \end{cases} \tag{3.2.16}$$

COROLLARY 3.8. *The triplet $\Pi_{\mathcal{V}} = \{\mathcal{H}_{\mathcal{V}}, \Gamma_0^{\mathcal{V}}, \Gamma_1^{\mathcal{V}}\}$ given by* (3.2.13)–(3.2.15) *is a boundary triplet for $\mathbf{H}_{\max}$.*

PROOF. For $f_{\mathcal{E}} = \big((f_{e_\imath}, f_{e_\tau})\big)_{e\in\vec{\mathcal{E}}} \in \mathcal{H}_{\mathcal{E}}$ define the operator $U_{\mathcal{G}} : \mathcal{H}_{\mathcal{E}} \to \mathcal{H}_{\mathcal{V}}$ by

$$U_{\mathcal{G}}\colon f_{\mathcal{E}} \mapsto \big((f_{v,\vec{e}})_{\vec{e}\in\vec{\mathcal{E}}_v}\big)_{v\in\mathcal{V}}, \quad f_{v,\vec{e}} := \begin{cases} f_{e_\imath}, & \vec{e}\in\vec{\mathcal{E}}_v^+, \\ f_{e_\tau}, & \vec{e}\in\vec{\mathcal{E}}_v^-, \end{cases} \quad \vec{e}\in\vec{\mathcal{E}}_v,\ v\in\mathcal{V}. \tag{3.2.17}$$

Clearly, $U_{\mathcal{G}}$ is an isometric isomorphism. Moreover, it is straightforward to check that

$$\Gamma_0^{\mathcal{V}} = U_{\mathcal{G}}\Gamma_0^{\mathcal{E}}, \qquad \Gamma_1^{\mathcal{V}} = U_{\mathcal{G}}\Gamma_1^{\mathcal{E}}, \tag{3.2.18}$$

which completes the proof. □

Let us also mention other important relations.

COROLLARY 3.9. *The Weyl function $M_{\mathcal{V}}$ corresponding to the boundary triplet* (3.2.13)–(3.2.15) *is given by*

$$M_{\mathcal{V}}(z) = U_{\mathcal{G}} M_{\mathcal{E}}(z) U_{\mathcal{G}}^{-1}, \tag{3.2.19}$$

where $M_{\mathcal{E}}$ is given by (3.2.11) *and $U_{\mathcal{G}}$ is the operator defined by* (3.2.17). *In particular, $s - R - \lim_{x\uparrow 0} M_{\mathcal{V}}(x) = \mathbb{O}_{\mathcal{H}_{\mathcal{V}}}$ and, moreover, $M_{\mathcal{V}}(x)$ uniformly tends to $-\infty$ as $x\to-\infty$.*

PROOF. The proof is straightforward and the last claim is an immediate consequence of Lemma 3.7 and equality (3.2.19). □

REMARK 3.10. Consider the mappings $\widetilde{\Gamma}_0^{\mathcal{E}} = \bigoplus_{e\in\mathcal{E}} \widetilde{\Gamma}_{0,e}$ and $\widetilde{\Gamma}_1^{\mathcal{E}} = \bigoplus_{e\in\mathcal{E}} \widetilde{\Gamma}_{1,e}$ given by (3.2.1). If $f\in\operatorname{dom}(\mathbf{H}_{\max})\cap C_c(\mathcal{G})$, then

$$\widetilde{\Gamma}_0^{\mathcal{V}} f := U_{\mathcal{G}}\widetilde{\Gamma}_0^{\mathcal{E}} f, \qquad \widetilde{\Gamma}_1^{\mathcal{V}} f := U_{\mathcal{G}}\widetilde{\Gamma}_0^{\mathcal{E}} f, \tag{3.2.20}$$

have the following form $\widetilde{\Gamma}_0^{\mathcal{V}} = \bigoplus_{v\in\mathcal{V}} \widetilde{\Gamma}_{0,v}$ and $\widetilde{\Gamma}_1^{\mathcal{V}} = \bigoplus_{v\in\mathcal{V}} \widetilde{\Gamma}_{1,v}$, where

$$\widetilde{\Gamma}_{0,v} f = \big(f_{\vec{e}}(v)\big)_{\vec{e}\in\vec{\mathcal{E}}_v}, \qquad \widetilde{\Gamma}_{1,v} f = \big(\nu(e)\partial_{\vec{e}} f(v)\big)_{\vec{e}\in\vec{\mathcal{E}}_v}. \tag{3.2.21}$$

3.2.3. Boundary operators for Laplacians on metric graphs. Let Θ be a linear relation in $\mathcal{H}_{\mathcal{V}}$ and define the following operator

$$\begin{aligned} &\mathbf{H}_{\Theta} := \mathbf{H}_{\max} \upharpoonright \mathrm{dom}(\mathbf{H}_{\Theta}), \\ &\qquad\qquad \mathrm{dom}(\mathbf{H}_{\Theta}) := \big\{ f \in \mathrm{dom}(\mathbf{H}_{\max}) \,|\, (\Gamma_0^{\mathcal{V}} f, \Gamma_1^{\mathcal{V}} f) \in \Theta \big\}, \end{aligned} \tag{3.2.22}$$

where the mappings $\Gamma_0^{\mathcal{V}}$ and $\Gamma_1^{\mathcal{V}}$ are defined by (3.2.13)–(3.2.15). Since $\Pi_{\mathcal{V}}$ is a boundary triplet for $\mathbf{H}_{\max}$, every proper extension of the operator $\mathbf{H}_{\min}$ has the form (3.2.22) (see Theorem A.4) and hence so does $\mathbf{H}_{\alpha}^0$. The next result provides the explicit form of the linear relation parameterizing $\mathbf{H}_{\alpha}^0$.

Proposition 3.11. *Assume Hypotheses 2.1 and let $\Pi_{\mathcal{V}}$ be the boundary triplet* (3.2.13)–(3.2.15)*. Suppose Θ_{α}^0 is the boundary relation for the operator $\mathbf{H}_{\alpha}^0$,*

$$\mathrm{dom}(\mathbf{H}_{\alpha}^0) = \big\{ f \in \mathrm{dom}(\mathbf{H}_{\max}) \,|\, (\Gamma_0^{\mathcal{V}} f, \Gamma_1^{\mathcal{V}} f) \in \Theta_{\alpha}^0 \big\}. \tag{3.2.23}$$

Then the operator part $\Theta_{\alpha}^{\mathrm{op}}$ of Θ_{α}^0 is unitarily equivalent to the operator $\mathbf{h}_{\alpha}^0 = \overline{\mathbf{h}_{\alpha}'}$ acting in $\ell^2(\mathcal{V};m)$ and defined by (3.1.7) *with* (3.1.4)*,* (3.1.5) *and* (3.1.6)*.*

Proof. We divide its proof in several steps.

(i) For each vertex $v \in \mathcal{V}$, the boundary conditions (2.4.5) can be written as

$$\widetilde{D}_v \widetilde{\Gamma}_{1,v} f = \widetilde{C}_v \widetilde{\Gamma}_{0,v} f,$$

where we recall that (see (3.2.21))

$$\widetilde{\Gamma}_{0,v} f = \big(f_{\vec{e}}(v)\big)_{\vec{e} \in \vec{\mathcal{E}}_v}, \qquad \widetilde{\Gamma}_{1,v} f = \big(\nu(e) \partial_{\vec{e}} f(v)\big)_{\vec{e} \in \vec{\mathcal{E}}_v},$$

and the matrices $\widetilde{C}_v$, $\widetilde{D}_v \in \mathbb{C}^{\deg(v) \times \deg(v)}$ are given by

$$\widetilde{C}_v = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 \\ 0 & 1 & -1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & -1 \\ \alpha(v) & 0 & 0 & \dots & 0 \end{pmatrix}, \qquad \widetilde{D}_v = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 0 \\ 1 & 1 & 1 & \dots & 1 \end{pmatrix}.$$

It is straightforward to verify the Rofe–Beketov conditions (A.1.4), that is,

$$\widetilde{C}_v \widetilde{D}_v^* = \widetilde{D}_v \widetilde{C}_v^*, \qquad \mathrm{rank}(\widetilde{C}_v | \widetilde{D}_v) = \deg(v),$$

holds for all $v \in \mathcal{V}$, and hence

$$\widetilde{\Theta}_v := \big\{ (f,g) \in \mathbb{C}^{\deg(v)} \times \mathbb{C}^{\deg(v)} \,|\, \widetilde{C}_v f = \widetilde{D}_v g \big\} \tag{3.2.24}$$

is a self-adjoint linear relation in $\mathbb{C}^{\deg(v)}$. Now set

$$\widetilde{C} := \bigoplus_{v \in \mathcal{V}} \widetilde{C}_v, \qquad \widetilde{D} := \bigoplus_{v \in \mathcal{V}} \widetilde{D}_v.$$

Both $\widetilde{C}$ and $\widetilde{D}$ are closed operators in $\mathcal{H}_{\mathcal{V}}$. Clearly, $f \in \mathrm{dom}(\mathbf{H}_{\max}) \cap C_c(\mathcal{G})$ satisfies

$$\widetilde{D} \widetilde{\Gamma}_1^{\mathcal{V}} f = \widetilde{C} \widetilde{\Gamma}_0^{\mathcal{V}} f$$

if and only if $f \in \mathrm{dom}(\mathbf{H}_{\alpha}') = \mathrm{dom}(\mathbf{H}_{\alpha}) \cap C_c(\mathcal{G})$. In view of (3.2.20), we get

$$\Gamma_0^{\mathcal{V}} f = \mathrm{R}_{\mathcal{V}} \widetilde{\Gamma}_0^{\mathcal{V}} f, \qquad \Gamma_1^{\mathcal{V}} f = \mathrm{R}_{\mathcal{V}}^{-1} (\widetilde{\Gamma}_1^{\mathcal{V}} - \mathrm{Q}_{\mathcal{V}} \widetilde{\Gamma}_0^{\mathcal{V}}) f,$$

for all $f \in \mathrm{dom}(\mathbf{H}_{\max}) \cap C_c(\mathcal{G})$, where

$$\mathrm{R}_{\mathcal{V}} = U_{\mathcal{G}} \mathrm{R}_{\mathcal{E}} U_{\mathcal{G}}^{-1}, \qquad \mathrm{Q}_{\mathcal{V}} = U_{\mathcal{G}} \mathrm{Q}_{\mathcal{E}} U_{\mathcal{G}}^{-1},$$

$\mathrm{R}_{\mathcal{E}} = \oplus_{e\in\mathcal{E}}\mathrm{R}_e^{1/2}$, $\mathrm{Q}_{\mathcal{E}} = \oplus_{e\in\mathcal{E}}\mathrm{Q}_e$ are defined by (3.2.2) and $U_{\mathcal{G}}$ is given by (3.2.17). Hence $f \in \mathrm{dom}(\mathbf{H}'_\alpha)$ if and only if $f \in \mathrm{dom}(\mathbf{H}_{\max}) \cap C_c(\mathcal{G})$ satisfies

$$D\Gamma_1^{\mathcal{V}} f = C\Gamma_0^{\mathcal{V}} f,$$

where

$$D = \widetilde{D}\mathrm{R}_{\mathcal{V}}, \qquad C = (\widetilde{C} - \widetilde{D}\mathrm{Q}_{\mathcal{V}})\mathrm{R}_{\mathcal{V}}^{-1}.$$

The operators D and C are well defined on $\mathcal{H}_{\mathcal{V},c}$, which consists of vectors of $\mathcal{H}_{\mathcal{V}}$ having only finitely many non-zero coordinates.

(ii) Define the linear relation

$$\Theta'_\alpha = \big\{(f,g) \in \mathcal{H}_{\mathcal{V},c} \times \mathcal{H}_{\mathcal{V},c} \,|\, Cf = Dg\big\} \tag{3.2.25}$$

and let $\mathbf{H}_{\Theta'_\alpha}$ be the corresponding restriction given by (3.2.22). By construction, Θ'_α is symmetric and hence so is $\mathbf{H}_{\Theta'_\alpha}$ (see Theorem A.4(i)). Moreover, $\mathbf{H}'_\alpha \subseteq \mathbf{H}_{\Theta'_\alpha}$ and it is straightforward to check that $\mathbf{H}_{\Theta'_\alpha} \subseteq \mathbf{H}^0_\alpha$. Then by Theorem A.4(i), $\Theta^0_\alpha := \overline{\Theta'_\alpha}$ is the boundary relation parameterizing (via (3.2.22)) the minimal operator $\mathbf{H}^0_\alpha$.

(iii) To proceed further, let $f = (f_v)_{v\in\mathcal{V}} \in \mathcal{H}_{\mathcal{V}}$, where $f_v = (f_{v,\vec{e}})_{\vec{e}\in\vec{\mathcal{E}}_v}$. For each $v \in \mathcal{V}$, let us denote by P_v the orthogonal projection in $\mathcal{H}_{\mathcal{V}}$ onto $\mathcal{H}_v$, the subspace consisting of elements $f = (f_u)_{u\in\mathcal{V}} \in \mathcal{H}_{\mathcal{V}}$ with all entries equal zero except f_v, that is,

$$(P_v f)_u = (\delta_{vu} f_{u,\vec{e}})_{\vec{e}\in\vec{\mathcal{E}}_u}, \qquad \delta_{vu} = \begin{cases} 1, & u = v,\\ 0, & u \neq v.\end{cases}$$

By construction, the operators $\widetilde{C}$, $\widetilde{D}$, $\mathrm{R}_{\mathcal{V}}$ (and hence D) commute with P_v. In particular,

$$\mathrm{R}_{\mathcal{V}} = \bigoplus_{v\in\mathcal{V}} \mathrm{R}_v, \qquad \mathrm{R}_v = \mathrm{diag}\left(\sqrt{r(e)}\right)_{\vec{e}\in\vec{\mathcal{E}}_v}, \tag{3.2.26}$$

and

$$D = \bigoplus_{v\in\mathcal{V}} D_v, \qquad D_v = \widetilde{D}_v\mathrm{R}_v = \widetilde{D}_v \cdot \mathrm{diag}\left(\sqrt{r(e)}\right)_{\vec{e}\in\vec{\mathcal{E}}_v}. \tag{3.2.27}$$

However, the form of $\mathrm{Q}_{\mathcal{V}}$ (and hence of C) is a bit more complicated:

$$\mathrm{Q}_{\mathcal{V}} = \widetilde{\mathrm{Q}}^0 - \bigoplus_{v\in\mathcal{V}} \mathrm{Q}_v, \qquad \mathrm{Q}_v = \mathrm{diag}\left(\frac{\nu(e)}{|e|}\right)_{\vec{e}\in\vec{\mathcal{E}}_v}, \tag{3.2.28}$$

where

$$(\widetilde{\mathrm{Q}}^0 f)_{v,\vec{e}} = \frac{\nu(e)}{|e|} f_{u,-\vec{e}}, \tag{3.2.29}$$

and $u \in \mathcal{V}$ and $-\vec{e} \in \vec{\mathcal{E}}_u$ are given by

$$u := \begin{cases} e_\tau, & \vec{e} \in \vec{\mathcal{E}}_v^+,\\ e_\imath, & \vec{e} \in \vec{\mathcal{E}}_v^-,\end{cases} \qquad -\vec{e} := \begin{cases} (-,e), & \vec{e} \in \vec{\mathcal{E}}_v^+,\\ (+,e), & \vec{e} \in \vec{\mathcal{E}}_v^-.\end{cases}$$

The operators P_vC and P_vD are finite rank and hence admit a bounded extension onto $\mathcal{H}_{\mathcal{V}}$. By abusing the notation, we shall denote these extensions by P_vC and P_vD as well. It is straightforward to verify that $f \in \mathrm{dom}(\mathbf{H}_{\max})$ satisfies (2.4.5) exactly when

$$P_v D\Gamma_1^{\mathcal{V}} f = P_v C\Gamma_0^{\mathcal{V}} f. \tag{3.2.30}$$

Therefore, combining the definition of $\mathbf{H}_\alpha$ (see (2.4.14)) with (A.2.3), we conclude that the boundary relation Θ_α parameterizing $\mathbf{H}_\alpha$ in the sense of (3.2.22) is explicitly given by

$$\Theta_\alpha = \{(f,g) \in \mathcal{H}_\mathcal{V} \times \mathcal{H}_\mathcal{V} \,|\, P_v C f = P_v D g \text{ for all } v \in \mathcal{V}\}. \tag{3.2.31}$$

In particular, by Theorem A.4(i), $\Theta_\alpha = (\Theta_\alpha')^* = (\Theta_\alpha^0)^*$.

(iv) By (3.2.25), $\mathrm{mul}(\Theta_\alpha') = \ker(D)$ (notice that we consider D as the operator defined only on $\mathcal{H}_{\mathcal{V},c}$ and hence $\ker(D)$ is not closed). On the other hand, (3.2.31) implies that

$$\mathrm{mul}(\Theta_\alpha) = \{f \in \mathcal{H}_\mathcal{V} \,|\, P_v D f = 0 \text{ for all } v \in \mathcal{V}\}, \tag{3.2.32}$$

and hence

$$\mathrm{mul}(\Theta_\alpha) = \overline{\mathrm{mul}(\Theta_\alpha')} = \mathrm{mul}(\Theta_\alpha^0).$$

Therefore, Θ_α^0 is densely defined on $\mathcal{H}_\mathcal{V}^{\mathrm{op}} := \mathrm{mul}(\Theta_\alpha)^\perp$ and hence admits the decomposition (A.1.1), that is,

$$\Theta_\alpha^0 = \Theta_{\mathrm{op}}^0 \oplus \Theta_{\mathrm{mul}}, \qquad \Theta_{\mathrm{mul}} = \{0\} \times \mathrm{mul}(\Theta_\alpha), \tag{3.2.33}$$

where Θ_{op}^0 is the graph of a densely defined closed symmetric operator acting in $\mathcal{H}_\mathcal{V}^{\mathrm{op}}$. Next observe that

$$\mathcal{H}_\mathcal{V}^{\mathrm{op}} = \mathrm{mul}(\Theta_\alpha)^\perp = \ker(D)^\perp = \overline{\mathrm{ran}(D^*)} = \mathrm{span}\{\mathbf{f}^v\}_{v\in\mathcal{V}},$$

where $\mathbf{f}^v = (\mathbf{f}_u^v)_{u\in\mathcal{V}} \in \mathcal{H}_v$ is given by

$$\mathbf{f}_u^v = (\mathbf{f}_{u,\vec{e}}^v)_{\vec{e}\in\vec{\mathcal{E}}_u}, \qquad \mathbf{f}_{u,\vec{e}}^v = \begin{cases} \sqrt{r(e)}, & u = v, \\ 0\;, & u \neq v. \end{cases} \tag{3.2.34}$$

By construction, $\mathbf{f}^v \perp \mathbf{f}^u$ whenever $v \neq u$ and

$$\|\mathbf{f}^v\|^2 = \sum_{\vec{e}\in\vec{\mathcal{E}}_v} r(e) = m(v) \tag{3.2.35}$$

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

Let us now show that $\mathbf{f}^v \in \mathrm{dom}(\Theta_\alpha^0)$ for every $v \in \mathcal{V}$. It is straightforward to calculate that

$$(P_u C\mathbf{f}^v)_u = \big(P_u(\widetilde{C} - \widetilde{D}\mathrm{Q}_\mathcal{V})\mathrm{R}_\mathcal{V}^{-1}\mathbf{f}^v\big)_u = \begin{cases} \big(\underbrace{0,0,\dots,0,\, \alpha(v) + \sum_{w\in\mathcal{V}} b(v,w)}_{\deg(v)}\big), & u = v, \\ \big(\underbrace{0,0,\dots,0,-b(u,v)}_{\deg(u)}\big), & u \neq v,\ u \sim v, \\ 0, & u \neq v,\ u \not\sim v, \end{cases}$$

where $b \colon \mathcal{V} \times \mathcal{V} \to [0,\infty)$ is the weight function given by (3.1.6). Moreover, for $g \in \mathcal{H}_{\mathcal{V},c}$ we have

$$(P_u D g)_u = (P_u \widetilde{D}\mathrm{R}_\mathcal{V} g)_u = \big(\underbrace{0,0,\dots,0, \sum_{\vec{e}\in\vec{\mathcal{E}}_u} \sqrt{r(e)}\, g_{u,\vec{e}}}_{\deg(u)}\big).$$

Therefore, define $\mathbf{g}^v = (\mathbf{g}^v_u)_{u\in\mathcal{V}} \in \mathcal{H}^{\mathrm{op}}_{\mathcal{V}}$ by

$$\mathbf{g}^v_u = (\sqrt{r(e)})_{\vec{e}\in\vec{\mathcal{E}}_u} \times \begin{cases} \frac{1}{m(v)}(\alpha(v) + \sum_{w\sim v} b(v,w)), & u = v, \\ -\frac{b(u,v)}{m(u)}, & u \neq v,\ u \sim v, \\ 0, & u \neq v,\ u \not\sim v. \end{cases} \tag{3.2.36}$$

Clearly, this implies the following equality

$$C\mathbf{f}^v = D\mathbf{g}^v,$$

and hence $\mathbf{f}^v \in \mathrm{dom}(\Theta'_\alpha) \subseteq \mathrm{dom}(\Theta^0_\alpha)$. Moreover, (3.2.36) immediately implies that

$$\mathbf{g}^v = \frac{1}{m(v)}\Big(\alpha(v) + \sum_{u\sim v} b(u,v)\Big)\mathbf{f}^v - \sum_{u\sim v} \frac{b(u,v)}{m(u)}\mathbf{f}^u =: \Theta^0_{\mathrm{op}}\mathbf{f}^v. \tag{3.2.37}$$

Noting that by construction the family $(\mathbf{f}^v)_{v\in\mathcal{V}}$ is an orthogonal basis in $\mathcal{H}^{\mathrm{op}}_{\mathcal{V}}$ and taking into account (3.2.35), the above equality implies that the operator part Θ^0_{op} of Θ^0_α is unitarily equivalent to the minimal operator $\widetilde{\mathbf{h}}^0_\alpha$ defined in $\ell^2(\mathcal{V})$ by

$$(\widetilde{\tau} f)(v) = \frac{1}{\sqrt{m(v)}}\left(\sum_{u\in\mathcal{V}} b(v,u)\Big(\frac{f(v)}{\sqrt{m(v)}} - \frac{f(u)}{\sqrt{m(u)}}\Big) + \frac{\alpha(v)}{\sqrt{m(v)}} f(v)\right), \tag{3.2.38}$$

for each vertex $v \in \mathcal{V}$. More specifically, as usual we define the operator $\widetilde{\mathbf{h}}^0_\alpha$ in $\ell^2(\mathcal{V})$ as the closure in $\ell^2(\mathcal{V})$ of the pre-minimal operator

$$\begin{array}{rccc} \widetilde{\mathbf{h}}'_\alpha\colon & \mathrm{dom}(\widetilde{\mathbf{h}}'_\alpha) & \to & \ell^2(\mathcal{V}) \\ & f & \mapsto & \widetilde{\tau} f \end{array}, \tag{3.2.39}$$

where $\mathrm{dom}(\mathbf{h}'_\alpha) := C_c(\mathcal{V})$. It remains to notice that the operators $\widetilde{\mathbf{h}}^0_\alpha$ and $\mathbf{h}^0_\alpha$ are unitarily equivalent. Indeed, it is easy to verify that $\mathbf{h}'_\alpha = \mathcal{U}^{-1}\widetilde{\mathbf{h}}'_\alpha\mathcal{U}$, where

$$\begin{array}{rccc} \mathcal{U}\colon & \ell^2(\mathcal{V};m) & \to & \ell^2(\mathcal{V}) \\ & f & \mapsto & \sqrt{m} f \end{array}, \tag{3.2.40}$$

is an isometric isomorphism. ☐

Remark 3.12. In fact, one can write down explicitly the isometric isomorphism $\Phi\colon \ell^2(\mathcal{V};m) \to \mathcal{H}^{\mathrm{op}}_{\mathcal{V}}$ relating $\Theta^{\mathrm{op}}_\alpha$ and $\mathbf{h}^0_\alpha$. Indeed, we proved that the collection of vectors $(\mathbf{f}^v)_{v\in\mathcal{V}}$ given by (3.2.34) forms an orthogonal basis in $\mathcal{H}^{\mathrm{op}}_{\mathcal{V}}$. Moreover, their norms are given by (3.2.35), which immediately implies that the map

$$\begin{array}{rccc} \Phi\colon & \ell^2(\mathcal{V};m) & \to & \mathcal{H}^{\mathrm{op}}_{\mathcal{V}} \\ & a & \mapsto & \sum_{v\in\mathcal{V}} a_v \mathbf{f}^v \end{array} \tag{3.2.41}$$

is an isometric isomorphism. In particular, this implies the following representation:

$$\Theta^{\mathrm{op}}_\alpha = \big\{(\Phi f, \Phi\mathbf{h}^0_\alpha f) \,|\, f \in \mathrm{dom}(\mathbf{h}^0_\alpha)\big\}. \tag{3.2.42}$$

3.2.4. Proof of Theorem 3.1. Now we have all the ingredients to finish the proof of the main result of this section. It is analogous to the proof of Theorem 2.9 in [**67**] and we provide the details for the sake of completeness.

Proof of Theorem 3.1. Consider the vertex-based boundary triplet $\Pi_{\mathcal{V}}$. Using Proposition 3.11, item (i) follows from Theorem A.4(iii).

Next, observe that

$$\mathrm{H}_{e,\max} \upharpoonright \ker(\Gamma_{0,e}) =: \mathrm{H}^F_e$$

is the Friedrichs extension of $\mathrm{H}_{e,\min} = (\mathrm{H}_{e,\max})^*$, and hence we conclude that

$$\mathbf{H}_{\max} \upharpoonright \ker(\Gamma_0) = \bigoplus_{e\in\mathcal{E}} \mathrm{H}_e^F \tag{3.2.43}$$

is the Friedrichs extension of $\mathbf{H}_{\min} = (\mathbf{H}_{\max})^*$. Moreover,

$$\sigma(\mathrm{H}_e^F) = \Big\{ \frac{\pi^2 n^2}{\eta(e)^2} \,\Big|\, n \in \mathbb{Z}_{\geq 1} \Big\}, \tag{3.2.44}$$

and hence

$$\inf \sigma(\mathbf{H}^F) = \inf_{e\in\mathcal{E}} \inf \sigma(\mathrm{H}_e^F) = \inf_{e\in\mathcal{E}} \frac{\pi^2}{\eta(e)^2} = \frac{\pi^2}{(\sup_{e\in\mathcal{E}} \eta(e))^2}. \tag{3.2.45}$$

Now item (ii) follows from Theorem A.9 and Corollary 3.9; items (iii)–(iv) as well as items (vi) and (viii) follow from Theorem A.7 by taking into account Corollary 3.9; item (vii) follows from Theorem A.10.

Finally, (3.2.43) and (3.2.44) imply that the spectrum of $\mathbf{H}^F$ is purely discrete if and only if $\#\{e \in \mathcal{E} \mid \eta(e) > \varepsilon\}$ is finite for every $\varepsilon > 0$. Moreover, $\mathcal{H}_F$ can be written in the form (3.2.22) with $\Theta_{\mathrm{mul}} = \{0\} \times \mathcal{H}_{\mathcal{V}}$. By Theorem A.4(iv), the difference of resolvents satisfies

$$(\mathbf{H}_\alpha - \mathrm{i})^{-1} - (\mathbf{H}^F - \mathrm{i})^{-1} \in \mathfrak{S}_\infty$$

exactly when $(\Theta_\alpha - \mathrm{i})^{-1} - (\Theta_{\mathrm{mul}} - \mathrm{i})^{-1}$ is a compact operator. It remains to notice that $(\Theta_{\mathrm{mul}} - \mathrm{i})^{-1} = \mathbb{O}_{\mathcal{H}_{\mathcal{V}}}$. □

We finish this section with the following remark.

Remark 3.13. Notice that (3.2.22) establishes a bijective correspondence between the set $\mathrm{Ext}(\mathbf{H}_{\min})$ of proper extensions of $\mathbf{H}_{\min}$ and the set of all linear relations in $\mathcal{H}_{\mathcal{V}}$. In fact, Theorem 3.1 extends to all operators $\mathbf{H}_\Theta$ and it relates basic spectral properties of the self-adjoint extension $\mathbf{H}_\Theta$ and the corresponding boundary relation Θ (see, e.g., [**67**, Theorem 2.9]). In particular, this would be helpful in the treatment of the case when $\mathbf{H}^0$ has nontrivial deficiency indices (cf. Theorem 3.1(ii)–(viii)) and this will be done in the next section.

Remark 3.14. The above remark indicates that the machinery developed in this section enables us to consider all possible (self-adjoint) vertex conditions (for instance, two other important families are δ'-couplings and symmetrized δ'-couplings). Moreover, one may include more general differential expressions including magnetic Schrödinger operators. However, the main difficulty is the search for a suitable boundary operator, which usually requires separate considerations, and then the study of its properties (cf., e.g., [**141**, § 5-6]). Let us mention that there are strong indications that one may connect spectral properties (in the sense of Theorem 3.1) of magnetic Schrödinger operators on metric graphs with those of weighted magnetic Schrödinger operators on graphs (see [**34**, § 3.5]). Moreover, it seems to us that one may also establish similar connections between Laplacians with δ'-couplings and symmetrized δ'-couplings and "weighted" Hodge Laplacians on graphs, respectively, signless Laplacians on graphs (cf. [**178**]). However, all these require separate considerations and will be done elsewhere.

3.3. Spectral properties: metric graphs and models

We restrict ourselves to the case $\alpha \equiv 0$, that is, in this section we shall consider Kirchhoff Laplacians only. Our main aim now is to look at Corollary 3.2 from the continuous-to-discrete perspective. Let $(\mathcal{G}, \mu, \nu)$ be a given weighted metric graph, that is, $\mathcal{G}$ is a locally finite metric graph (as a metric space) and μ, ν are two edge weights on $\mathcal{G}$. With each model $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ of $(\mathcal{G}, \mu, \nu)$ we can associate a weighted graph Laplacian

$$(\tau f)(v) = \frac{1}{m(v)} \sum_{u \in \mathcal{V}} b(v,u)(f(v) - f(u)), \quad v \in \mathcal{V}, \tag{3.3.1}$$

where m and b are defined by (3.1.5) and (3.1.6), respectively. Thus we have the minimal Kirchhoff Laplacian $\mathbf{H}^0$ on $\mathcal{G}$ and the family of minimal graph Laplacians $\mathbf{h}^0$ associated with the models of $(\mathcal{G}, \mu, \nu)$. In this situation Corollary 3.2(i) immediately implies the following results.

COROLLARY 3.15. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph and let $\mathbf{H}^0$ be the corresponding minimal Kirchhoff Laplacian. Then:*

(i) *For each model of $(\mathcal{G}, \mu, \nu)$, the deficiency indices of $\mathbf{H}^0$ and $\mathbf{h}^0$ are equal,*

$$\mathrm{n}_{\pm}(\mathbf{H}^0) = \mathrm{n}_{\pm}(\mathbf{h}^0). \tag{3.3.2}$$

(ii) *If $\mathbf{H}^0$ is self-adjoint, then $\mathbf{h}^0$ is self-adjoint for each model. And conversely, $\mathbf{H}^0$ is self-adjoint exactly when $\mathbf{h}^0$ is self-adjoint for one (and hence for all) models of $(\mathcal{G}, \mu, \nu)$.*

In order to preserve the equivalences further, the next results require a careful choice of a model, which motivates the following definition.

DEFINITION 3.16. For a given model $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ of $(\mathcal{G}, \mu, \nu)$, the quantity $\eta^*(\mathcal{E})$ defined by (3.1.2) is called *the intrinsic size of the model.* A model has *finite intrinsic size* if $\eta^*(\mathcal{E}) < \infty$. Otherwise, $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ is called a model of *infinite intrinsic size.*

A weighted metric graph $(\mathcal{G}, \mu, \nu)$ has *finite intrinsic size* if all its models are of finite intrinsic size. Otherwise, $(\mathcal{G}, \mu, \nu)$ has *infinite intrinsic size.*

We define the *essential intrinsic size* of a given model by

$$\eta^*_{\mathrm{ess}}(\mathcal{E}) := \inf_{\widetilde{\mathcal{E}}} \sup_{e \in \mathcal{E} \setminus \widetilde{\mathcal{E}}} \eta(e), \tag{3.3.3}$$

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

REMARK 3.17. A few remarks are in order.

(i) The above definition becomes transparent when $\mu = \nu$. Indeed, in this case $\eta(e) = |e|$ for all $e \in \mathcal{E}$ and the intrinsic size of a model is simply the length of its "longest" edge, that is, $\eta^*(\mathcal{E}) = \ell^*(\mathcal{E})$, where

$$\ell^*(\mathcal{E}) = \sup_{e \in \mathcal{E}} |e|. \tag{3.3.4}$$

In particular, such a model has infinite intrinsic size exactly when there is an arbitrarily long edge. Similarly,

$$\eta^*_{\mathrm{ess}}(\mathcal{E}) = \ell^*_{\mathrm{ess}}(\mathcal{E}) := \inf_{\widetilde{\mathcal{E}}} \sup_{e \in \mathcal{E} \setminus \widetilde{\mathcal{E}}} |e|, \tag{3.3.5}$$

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

(ii) The function r in (3.1.5) is given by (3.1.3) if the model has finite size and by (3.1.4) if it has infinite size.

(iii) The definition of essential intrinsic size can be understood as follows. For any compact subgraph $\widetilde{\mathcal{G}} \subset \mathcal{G}$ and every $\varepsilon > 0$, one can always find an edge in $\mathcal{E} \setminus \widetilde{\mathcal{E}}$ whose intrinsic length is at least $\eta^*_{\mathrm{ess}}(\mathcal{E}) - \varepsilon$. Moreover, for any $\varepsilon > 0$, there is a compact subgraph $\widetilde{\mathcal{G}}$ such that the intrinsic length of every edge $e \in \mathcal{E} \setminus \widetilde{\mathcal{E}}$ is smaller than $\eta^*_{\mathrm{ess}}(\mathcal{E}) + \varepsilon$. In particular, $\eta^*_{\mathrm{ess}}(\mathcal{E}) = 0$ means that for any $\varepsilon > 0$ there is a compact subgraph $\widetilde{\mathcal{G}}$ such that all edges in $\mathcal{E} \setminus \widetilde{\mathcal{E}}$ have intrinsic length less than ε.

Corollary 3.18. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph such that the corresponding minimal Kirchhoff Laplacian $\mathbf{H}^0$ is self-adjoint, $\mathbf{H}^0 = \mathbf{H}$. Then:*

(i) *The operator $\mathbf{H}$ is positive definite, $\lambda_0(\mathbf{H}) > 0$, if and only if there is a model of finite intrinsic size such that the corresponding operator $\mathbf{h}$ is positive definite, $\lambda_0(\mathbf{h}) > 0$.*

(ii) $\lambda_0^{\mathrm{ess}}(\mathbf{H}) > 0$ *exactly when there is a model of finite intrinsic size such that* $\lambda_0^{\mathrm{ess}}(\mathbf{h}) > 0$.

(iii) *If $(\mathcal{G}, \mu, \nu)$ has infinite intrinsic size, then $\lambda_0(\mathbf{H}) = \lambda_0^{\mathrm{ess}}(\mathbf{H}) = 0$ and, moreover, $\lambda_0(\mathbf{h}) = \lambda_0^{\mathrm{ess}}(\mathbf{h}) = 0$ for all models with finite intrinsic size.*

(iv) *The spectrum of $\mathbf{H}$ is purely discrete if and only if there is a model with zero essential intrinsic size, $\eta^*_{\mathrm{ess}}(\mathcal{E}) = 0$ and the spectrum of the corresponding graph Laplacian $\mathbf{h}$ is purely discrete.*

(v) *If there is a model with $\eta^*_{\mathrm{ess}}(\mathcal{E}) > 0$, then the essential spectrum of $\mathbf{H}$ is not empty and, moreover, so is the essential spectrum of $\mathbf{h}$ for each model with $\eta^*_{\mathrm{ess}}(\widetilde{\mathcal{E}}) = 0$.*

Proof. By Corollary 3.15, $\mathbf{h}$ is self-adjoint, $\mathbf{h} = \mathbf{h}^0$ for each model of a given weighted metric graph. Moreover, both operators are nonnegative. Then (i) and (ii) follow immediately from Corollary 3.2(iii)–(iv) since one can always find a model with finite intrinsic size. The same argument together with Theorem 3.1(v) proves items (iv)–(v).

Thus it remains to show (iii). In fact we only need to prove the first claim that $\lambda_0(\mathbf{H}) = \lambda_0^{\mathrm{ess}}(\mathbf{H}) = 0$ if there is a model of infinite size. However, the Friedrichs extension $\mathbf{H}^F$ has zero spectral gap, see (3.2.45), and hence so does every nonnegative self-adjoint restriction of $\mathbf{H}_{\max}$.[†] □

Remark 3.19. Notice that one can always find a model with $\eta^*_{\mathrm{ess}}(\mathcal{E}) = 0$ by refining (even if $(\mathcal{G}, \mu, \nu)$ has infinite intrinsic size). Indeed, for each model the edge set $\mathcal{E}$ is countable and hence one can obtain a new model satisfying $\eta^*_{\mathrm{ess}}(\widetilde{\mathcal{E}}) = 0$ by "cutting" an edge into equally short pieces; then the next edge into shorter ones, and so on.

Let us stress the following fact. The above results demonstrate that a Kirchhoff Laplacian shares some properties with the corresponding graph Laplacians for each model (e.g., self-adjointness), however, for some properties the class of models must be sufficiently good in a certain sense. For instance, strict positivity of spectra/essential spectra requires models having finite intrinsic size, $\eta^*(\mathcal{E}) < \infty$.

[†]In fact, following line by line the argument of M. Solomyak in [**193**, Theorem 5.1], one can show in this case that the whole semi-axis $[0, \infty)$ belongs to the spectrum of $\mathbf{H}$.

Discreteness (that is, compactness of resolvents) requires even a more refined choice (essential intrinsic size must be zero, $\eta^*_{\mathrm{ess}}(\mathcal{E}) = 0$). On the other hand, Corollary 3.18 demonstrates that if the set of models is in a certain sense too wide (for instance, there are models having infinite size), then the corresponding Kirchhoff Laplacian can't have the required property (e.g., positive spectral gap). However, in the latter case the absence of a required property is shared with all graph Laplacians arising from all reasonable models.

We would like to finish with a result which sheds light on the situation when the deficiency indices of $\mathbf{H}^0$ are nontrivial. However, first we need the following useful fact.

LEMMA 3.20. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph together with the minimal Kirchhoff Laplacian $\mathbf{H}^0$. If $\mathrm{n}_\pm(\mathbf{H}^0) > 0$, then for each model the map*

$$\begin{aligned} \widetilde{\mathbf{h}} \quad \mapsto \quad \widetilde{\mathbf{H}} = \mathbf{H}_{\widetilde{\Theta}} &:= \mathbf{H}_{\max} \restriction \{f \in \mathrm{dom}(\mathbf{H}_{\max}) \,|\, (\Gamma_0^{\mathcal{V}} f, \Gamma_1^{\mathcal{V}} f) \in \widetilde{\Theta}\} \\ \widetilde{\Theta} &:= \Theta_{\mathrm{mul}} \oplus \big\{(\Phi f, \Phi\widetilde{\mathbf{h}} f) \,|\, f \in \mathrm{dom}(\widetilde{\mathbf{h}})\big\} \end{aligned} \tag{3.3.6}$$

is a bijection between the sets $\mathrm{Ext}_S(\mathbf{h}^0)$ and $\mathrm{Ext}_S(\mathbf{H}^0)$ of self-adjoint extensions of $\mathbf{h}^0$ and $\mathbf{H}^0$. Here $\{\mathcal{H}_{\mathcal{V}}, \Gamma_0^{\mathcal{V}}, \Gamma_1^{\mathcal{V}}\}$ is the vertex-based boundary triplet defined in Section 3.2.2, the map Φ and the multivalued part Θ_{mul} are given by (3.2.41) *and, respectively,* (3.2.32).

PROOF. The existence of a bijection is a trivial consequence of von Neumann's formulas in view of (3.3.2), however, we would like to give another proof based on the use of the boundary triplets approach, which enables us to connect self-adjoint extensions of $\mathbf{H}^0$ and $\mathbf{h}^0$ in a rather transparent way.

Take a self-adjoint extension $\widetilde{\mathbf{H}} \in \mathrm{Ext}(\mathbf{H}^0)$ of $\mathbf{H}^0$. Then for a chosen model it admits the representation (3.2.22), that is, there exists a self-adjoint linear relation $\widetilde{\Theta}$ in $\mathcal{H}_{\mathcal{V}}$ such that[†]

$$\mathrm{dom}(\widetilde{\mathbf{H}}) = \big\{f \in \mathrm{dom}(\mathbf{H}_{\max}) \,|\, (\Gamma_0^{\mathcal{V}} f, \Gamma_1^{\mathcal{V}} f) \in \widetilde{\Theta}\big\}. \tag{3.3.7}$$

By Theorem A.4(i), $\widetilde{\Theta}$ is a self-adjoint extension of the linear relation Θ^0 parameterizing $\mathbf{H}^0$ via (3.2.23). As it was mentioned in the proof of Proposition 3.11, Θ^0 admits the representation (3.2.33). Similarly, $\widetilde{\Theta}$ admits analogous decomposition. Moreover, the multivalued parts of Θ^0 and $\widetilde{\Theta}$ coincides, that is, $\Theta_{\mathrm{mul}} = \widetilde{\Theta}_{\mathrm{mul}}$, since both Θ_{mul} and $\widetilde{\Theta}_{\mathrm{mul}}$ are self-adjoint relations (or since $\mathrm{mul}(\Theta^0) = \mathrm{mul}(\Theta)$). Therefore, $\widetilde{\Theta}_{\mathrm{op}}$ is a self-adjoint extension of Θ^0_{op} in $\mathcal{H}^{\mathrm{op}}_{\mathcal{V}}$. Taking into account (3.2.42), every self-adjoint extension of Θ^0 has the form

$$\widetilde{\Theta} = \Theta_{\mathrm{mul}} \oplus \big\{(\Phi f, \Phi\widetilde{\mathbf{h}} f) \,|\, f \in \mathrm{dom}(\widetilde{\mathbf{h}})\big\},$$

where $\widetilde{\mathbf{h}}$ is a self-adjoint extension of $\mathbf{h}^0$. □

REMARK 3.21. In fact, one can rewrite the map (3.3.6) in a more convenient form and this will be done in Chapter 4 (see Lemma 4.7 below).

Lemma 3.20 provides us with a map establishing a 1-to-1 correspondence between self-adjoint extensions of $\mathbf{H}^0$ and $\mathbf{h}^0$. It turns out that their spectral properties are closely connected as well:

[†]Taking into account Theorem A.4, in fact $\widetilde{\Theta}$ is given by $\widetilde{\Theta} = \{(\Gamma_0^{\mathcal{V}} f, \Gamma_1^{\mathcal{V}} f) \,|\, f \in \mathrm{dom}(\widetilde{\mathbf{H}})\}$.

THEOREM 3.22. *Let* $(\mathcal{G}, \mu, \nu)$ *be a weighted metric graph together with a fixed model. Suppose*

$$\mathrm{n}_{\pm}(\mathbf{H}^0) > 0,$$

and $\widetilde{\mathbf{H}} \in \mathrm{Ext}_S(\mathbf{H}_0)$. *If* $\widetilde{\mathbf{h}} \in \mathrm{Ext}_S(\mathbf{h}_0)$ *is the self-adjoint extension corresponding to* $\widetilde{\mathbf{H}}$ *via* (3.3.6), *then:*

(i) $\widetilde{\mathbf{H}}$ *is lower semibounded if and only if* $\widetilde{\mathbf{h}}$ *is lower semibounded.*
(ii) $\widetilde{\mathbf{H}}$ *is nonnegative if and only if* $\widetilde{\mathbf{h}}$ *is nonnegative.*
(iii) *The total multiplicities of negative spectra of* $\widetilde{\mathbf{H}}$ *and* $\widetilde{\mathbf{h}}$ *coincide,*

$$\kappa_-(\widetilde{\mathbf{H}}) = \kappa_-(\widetilde{\mathbf{h}}).$$

(iv) *The spectrum of* $\widetilde{\mathbf{H}}$ *is purely discrete if and only if the model satisfies* $\eta^*_{\mathrm{ess}}(\mathcal{E}) = 0$ *and the spectrum of* $\widetilde{\mathbf{h}}$ *is purely discrete.*

If additionally the corresponding model has finite intrinsic size, $\eta^*(\mathcal{E}) < \infty$, *then:*

(v) $\widetilde{\mathbf{H}}$ *is positive definite if and only if* $\widetilde{\mathbf{h}}$ *is positive definite.*
(vi) *If, in addition, the extension* $\widetilde{\mathbf{H}}$ *is lower semibounded, then* $\lambda_0^{\mathrm{ess}}(\widetilde{\mathbf{H}}) > 0$ ($\lambda_0^{\mathrm{ess}}(\widetilde{\mathbf{H}}) = 0$) *exactly when* $\lambda_0^{\mathrm{ess}}(\widetilde{\mathbf{h}}) > 0$ (*respectively,* $\lambda_0^{\mathrm{ess}}(\widetilde{\mathbf{h}}) = 0$).
(vii) *Moreover, the following equivalence*

$$\widetilde{\mathbf{H}}^- \in \mathfrak{S}_p(L^2) \quad \Longleftrightarrow \quad \widetilde{\mathbf{h}}^- \in \mathfrak{S}_p(\ell^2),$$

holds for all $p \in (0, \infty]$. *In particular, negative spectra of* $\widetilde{\mathbf{H}}$ *and* $\widetilde{\mathbf{h}}$ *are discrete simultaneously.*

The proof is an immediate corollary of Lemma 3.20 and Remark 3.13 and we leave it to the reader.

REMARK 3.23. In fact, Theorem 3.22 specifies the properties of the map (3.3.6) when it is further restricted to certain subclasses of self-adjoint extensions. Namely, items (i)–(iii) say that (3.3.6) is a bijection between the sets of semibounded/nonnegative/ self-adjoint extensions. According to items (v) and (vi), (3.3.6) is a bijection between self-adjoint extensions having a positive spectral gap/positive essential spectral gap, however, only if the corresponding model of a weighted metric graph has finite intrinsic size.

REMARK 3.24 (Laplacians with δ-couplings). It is not difficult to notice that Lemma 3.20 extends to the operator $\mathbf{H}^0_\alpha$ with $\alpha \not\equiv 0$ in an obvious way. Taking into account that the representation (3.3.6) is the key to prove Theorem 3.22, it is then straightforward to see that the analog of Theorem 3.22 holds true for the operator $\mathbf{H}_\alpha$ with non-trivial α.

3.3.1. Historical remarks. The fact that the boundary triplets machinery is a convenient tool to investigate finite and infinite metric graphs was realized in the 2000s (the literature is enormous and we only refer to [**34**], [**66**], [**179**], which also contain further references). However, in all these studies it was assumed that edge lengths admit a uniform positive lower bound ($\inf_{e\in\mathcal{E}} \eta(e) > 0$ in our notation). Notice that in contrast to the finite intrinsic size assumption (which can always be achieved by subdividing edges), this "uniform positive lower bound" assumption, which is rather common in the quantum graph literature [**24**], [**179**], is indeed a restriction. The main obstacle on this way is to construct a boundary triplet for the maximal operator $\mathbf{H}_{\max}$. A convenient approach to construct such a triplet was proposed by M.M. Malamud and H. Neidhardt in [**156**] (see Theorem A.11). This technique was applied in [**141**] to investigate 1d Schrödinger operators with local point interactions on discrete sets and then in [**67**] to Laplacians on unweighted metric graphs ($\mu = \nu \equiv 1$).

CHAPTER 4

Connections between parabolic properties

This chapter is dedicated to correspondences between Kirchhoff Laplacians and discrete graph Laplacians on the level of Markovian extensions and parabolic properties (e.g., recurrence, stochastic completeness, on-diagonal heat kernel estimates).

4.1. Markovian extensions

As in Section 3.3, let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph (as a metric space). The discussion below is independent of the choice of a concrete model, however, one can, of course, choose a model $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ and look then at $(\mathcal{G}, \mu, \nu)$ as its metric realization. Let also $\mathbf{H}^0$ be the corresponding minimal Kirchhoff Laplacian in $L^2(\mathcal{G}; \mu)$. We start by collecting some basic properties of *Markovian extensions*, that is, of self-adjoint extensions whose quadratic form is a Dirichlet form (see Appendix B for definitions and further facts). First of all, recall that $H^1(\mathcal{G})$ is the weighted Sobolev space defined by (2.4.19). When equipped with the graph norm (2.4.20), it turns into a Hilbert space. It is clear that the energy form

$$\mathfrak{Q}[f] = \int_{\mathcal{G}} |\nabla f(x)|^2 \nu(\mathrm{d}x), \tag{4.1.1}$$

when restricted to $\mathrm{dom}(\mathfrak{Q}_N) = H^1(\mathcal{G})$, is a Dirichlet form on $L^2(\mathcal{G}; \mu)$ and hence the corresponding Neumann Laplacian $\mathbf{H}_N$ is a Markovian extension of $\mathbf{H}^0$. Moreover, the quadratic form $\mathfrak{Q}_D$ of the Friedrichs extension of $\mathbf{H}^0$, which coincides with the Dirichlet Laplacian $\mathbf{H}_D$, is the restriction of $\mathfrak{Q}$ to the subspace $H^1_0(\mathcal{G})$. Recall that $H^1_0(\mathcal{G})$ is defined as the closure of $\mathrm{dom}(\mathbf{H}) \cap C_c(\mathcal{G})$ with respect to $\|\cdot\|_{H^1(\mathcal{G})}$ and hence $\mathfrak{Q}_D$ is a regular Dirichlet form. It is well known that the Dirichlet and Neumann Laplacians play a rather distinctive role among the Markovian extensions of $\mathbf{H}^0$.

LEMMA 4.1. *If $\widetilde{\mathbf{H}}$ is a Markovian extension of $\mathbf{H}^0$, then $\mathrm{dom}(\widetilde{\mathbf{H}}) \subset H^1(\mathcal{G})$ and*

$$\mathbf{H}_N \le \widetilde{\mathbf{H}} \le \mathbf{H}_D, \tag{4.1.2}$$

where the inequalities are understood in the sense of forms.[‡] *Moreover, the following statements are equivalent:*

(i) $\mathbf{H}^0$ *admits a unique Markovian extension,*
(ii) $\mathbf{H}_D = \mathbf{H}_N$,
(iii) $H^1_0(\mathcal{G}) = H^1(\mathcal{G})$,
(iv) *the Gaffney Laplacian* $\mathbf{H}_G$ *is self-adjoint.*

[‡]We shall write $A \le B$ for two nonnegative 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 $f \in \mathrm{dom}(\mathfrak{t}_B)$. The latter is also equivalent to the fact that $(A+I)^{-1} - (B+I)^{-1}$ is a positive operator.

PROOF. The proof of [**97**, Theorem 5.2] carries over to our setting (see also the proof of [**77**, Theorem 3.3.1]). □

An analogous result holds true for weighted graph Laplacians (see [**97**]). Namely, fix a model $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ and let $\mathbf{h}^0$ be the graph Laplacian defined in $\ell^2(\mathcal{V}; m)$ by (3.1.7) with the coefficients (3.1.5) and (3.1.6) (notice that $\alpha \equiv 0$). In most of this chapter we are going to consider exactly this graph Laplacian, which is related to the Kirchhoff Laplacian. We shall see in Chapter 6 that this is not at all a restriction. Following the considerations in Section 2.2, we can introduce the Dirichlet $\mathbf{h}_D$ and the Neumann $\mathbf{h}_N$ Laplacians. Namely, define the energy form by

$$\mathfrak{q}[\mathbf{f}] := \frac{1}{2} \sum_{u,v\in\mathcal{V}} b(u,v)|\mathbf{f}(u) - \mathbf{f}(v)|^2, \tag{4.1.3}$$

with the edge weight

$$b(u,v) = \begin{cases} \sum_{\vec{e}\in\vec{\mathcal{E}}_u:\, e\in\mathcal{E}_v} \frac{\nu(e)}{|e|}, & u \neq v, \\ 0, & u = v, \end{cases} \qquad (u,v) \in \mathcal{V}\times\mathcal{V}, \tag{4.1.4}$$

and denote by $\mathrm{dom}(\mathfrak{q}_N)$ the space of all $\ell^2(\mathcal{V}; m)$-functions $\mathbf{f}$ such that $\mathfrak{q}[\mathbf{f}]$ is finite. Clearly, the restriction $\mathfrak{q}_N$ of $\mathfrak{q}$ to $\mathrm{dom}(\mathfrak{q}_N)$ is a Dirichlet form. The corresponding self-adjoint operator $\mathbf{h}_N$ is a Markovian extension of $\mathbf{h}^0$ and we refer to it as the *Neumann extension*. Moreover, the Friedrichs extension $\mathbf{h}_D$ is also a Markovian extension of $\mathbf{h}^0$ and we call it the *Dirichlet extension*. Its quadratic form $\mathfrak{q}_D$ is obtained by restricting $\mathfrak{q}_N$ to the domain $\mathrm{dom}(\mathfrak{q}_D)$, which is the closure of $\mathrm{dom}(\mathbf{h}^0)$ with respect to the graph norm

$$\|\cdot\|^2_{H^1(\mathcal{V})} := \mathfrak{q}[\cdot] + \|\cdot\|^2_{\ell^2(\mathcal{V};m)}.$$

Let us also denote

$$H^1(\mathcal{V}) = H^1(\mathcal{V}, m; b) := \mathrm{dom}(\mathfrak{q}_N), \tag{4.1.5}$$

and

$$H^1_0(\mathcal{V}) = H^1_0(\mathcal{V}, m; b) := \mathrm{dom}(\mathfrak{q}_D). \tag{4.1.6}$$

The analog of Lemma 4.1 for the discrete operator $\mathbf{h}^0$ now reads (see [**97**, Theorem 5.2]): *If* $\widetilde{\mathbf{h}}$ *is a Markovian extension of* $\mathbf{h}^0$, *then* $\mathrm{dom}(\widetilde{\mathbf{h}}) \subseteq H^1(\mathcal{V})$ *and*

$$\mathbf{h}_N \leq \widetilde{\mathbf{h}} \leq \mathbf{h}_D. \tag{4.1.7}$$

4.2. Brownian motion and random walks

The framework of Dirichlet forms relates the energy forms (4.1.1) and (4.1.3) with stochastic processes (*Brownian motions* and, respectively, *random walks*) and we will review certain connections known on this level. We will not need these stochastic results in the sequel and hence restrict to a rather informal discussion. However, in our opinion this viewpoint is conceptually important and gives a good motivation for subsequent considerations.

We follow the setup in Section 4.1: $(\mathcal{G}, \mu, \nu)$ is a weighted metric graph and $\mathfrak{Q}_D$ is the corresponding (strongly local) Dirichlet form in $L^2(\mathcal{G})$. Moreover, we fix a model of $(\mathcal{G}, \mu, \nu)$ and consider the corresponding form $\mathfrak{q}_D$ in $\ell^2(\mathcal{V}; m)$ associated with (4.1.3) and (4.1.4), where $m\colon \mathcal{V} \to (0, \infty)$ is the vertex weight (3.1.5). By definition, both $\mathfrak{Q}_D$ and $\mathfrak{q}_D$ are regular Dirichlet forms and hence they correspond to two stochastic processes $(X^{\mathcal{G}}_t)_{t\geq 0}$ and $(X^{\mathcal{V}}_t)_{t\geq 0}$ (see Remark B.3).

The stochastic process $(X_t^{\mathcal{V}})_{t\ge 0}$ defined by $\mathfrak{q}_D$ is a *continuous-time random walk* (see [**12**, Rem. 5.7], [**134**, Sections 0.10 and 2.5] and [**172**] for details and further information). Roughly speaking, a particle starting at some vertex $v \in \mathcal{V}$ first waits for a random waiting time, which is exponentially distributed with parameter

$$\frac{1}{m(v)}\sum_{u\in\mathcal{V}} b(u,v) = \mathrm{Deg}(v), \qquad v\in\mathcal{V}, \tag{4.2.1}$$

(which is called the weighted degree in Section 2.2), and then jumps to a randomly chosen vertex $u \in \mathcal{V}$. Here, the probability of jumping from v to u is given by

$$p(u,v) = \frac{b(u,v)}{\sum_{u\in\mathcal{V}} b(u,v)}, \qquad u,v\in\mathcal{V}. \tag{4.2.2}$$

Repeating the same steps for the vertex u and continuing in this manner, we end up with a continuous-time random walk. Notice that the expected waiting time of the particle at the vertex v equals $1/\mathrm{Deg}(v)$. In particular, according to Lemma 2.9, the boundedness of $\mathbf{h}_D$ is equivalent to the existence of a uniform positive lower bound for expected waiting times.

On the other hand, the stochastic process $(X_t^{\mathcal{G}})_{t\ge 0}$ associated with $\mathfrak{Q}_D$ is a *Brownian motion* on a metric graph (see, e.g., [**70**, Section 2], [**63**, Section 2] and [**152**, Section 2]). It admits the following informal description: assume the particle starts at the vertex $v \in \mathcal{V}$. Let $\mathcal{B} = (B_t)_{t\ge 0}$ denote the standard Brownian motion on $\mathbb{R}$ started at the origin. For each excursion of $\mathcal{B}$, we randomly pick an oriented edge $\vec{e} \in \vec{\mathcal{E}}_v$ with probability

$$P(v,\vec{e}) = \frac{\nu(e)}{\sum_{\vec{e}\in\vec{\mathcal{E}}_v}\nu(e)}, \qquad \vec{e}\in\mathcal{E}_v.$$

The excursions are then performed successively in the corresponding edges $e \in \mathcal{E}_v$, starting from v (for a loop edge, the orientation of $\vec{e}$ needs to be taken into account), however with different speeds. Namely, if $\vec{e}_1$ is the first chosen edge, then in the first excursion the particle is at position $|B_{\nu(e_1)t/\mu(e_1)}|$ instead of $|B_t|$ inside e_1 and so on. This is performed until we reach a new vertex $u \in \mathcal{V}\setminus\{v\}$. Then we repeat the construction with u as the starting vertex and continue in the same manner.

To make the connection between the two processes $(X_t^{\mathcal{G}})_{t\ge 0}$ and $(X_t^{\mathcal{V}})_{t\ge 0}$, we briefly recall the results of [**70**]. Denote by T the *first hitting time* of the Brownian motion, that is, the first time that the Brownian motion started at some vertex hits a different vertex. Then the expected value of T, if the Brownian motion starts at $v \in \mathcal{V}$, is given by (see [**70**, Theorem 2.2])

$$\mathbb{E}^v T = \frac{\sum_{\vec{e}\in\vec{\mathcal{E}}_v}|e|\mu(e)}{\sum_{w\neq v}\sum_{e\in\mathcal{E}_w\cap\mathcal{E}_v}\frac{\nu(e)}{|e|}}, \qquad v\in\mathcal{V}. \tag{4.2.3}$$

Then the next natural question is which of the neighboring vertices gets hit at the time T. By [**70**, Theorem 2.1], if the Brownian motion starts at $v \in \mathcal{V}$, then for each $u \sim v$, $u \neq v$, the probability of being this next vertex is precisely

$$\mathbb{P}^v(X_T^{\mathcal{G}} = u) = \frac{\sum_{e\in\mathcal{E}_u\cap\mathcal{E}_v}\frac{\nu(e)}{|e|}}{\sum_{w\neq v}\sum_{e\in\mathcal{E}_w\cap\mathcal{E}_v}\frac{\nu(e)}{|e|}}. \tag{4.2.4}$$

Comparing (4.2.1) with (4.2.3) and (4.2.2) with (4.2.4), we see that if m is defined by (3.1.5) with the weight $r(e)$ given by (3.1.3) and b by (3.1.6), they coincide. In fact, the above discussion shows that to a certain extent the continuous-time random walk associated with $\mathfrak{q}_D$ is a discretization of the Brownian motion defined by $\mathfrak{Q}_D$. This can be taken as a first indication for connections between parabolic properties. However, we also stress that already the second moments of the hitting and waiting times differ (see [**70**, Theorem 2.3]).

4.3. Correspondence between quadratic forms

A more straightforward approach to establish connections between weighted Kirchhoff Laplacians and weighted graph Laplacians is to compare their quadratic forms. Fix a model $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ of $(\mathcal{G}, \mu, \nu)$ and consider the space of *continuous edgewise affine functions on* $\mathcal{G}$,

$$\mathrm{CA}(\mathcal{G}\backslash\mathcal{V}) := \big\{ f \in C(\mathcal{G}) \,\big|\, f|_e \text{ is affine for each edge } e \in \mathcal{E} \big\}. \tag{4.3.1}$$

The importance of $\mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ stems from the fact that it contains the kernel $\ker(\mathbf{H})$ of the maximal Kirchhoff Laplacian $\mathbf{H}$, as well as all harmonic functions on $\mathcal{G}$, as a subspace (see Section 6.5.2). Clearly, for each refinement of a given model the corresponding space of edgewise affine functions is larger.

Every function $f \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ can be identified with its values $f|_{\mathcal{V}} = (f(v))_{v\in\mathcal{V}}$ at the vertices. And conversely, we can identify each $\mathbf{f} \in C(\mathcal{V})$ with a continuous edgewise affine function $f \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ such that $\mathbf{f} = f|_{\mathcal{V}} = \big(f(v)\big)_{v\in\mathcal{V}}$. This suggests to define the map

$$\begin{array}{cccc} \imath_{\mathcal{V}}\colon & C(\mathcal{G}) & \longrightarrow & C(\mathcal{V}) \\ & f & \mapsto & f|_{\mathcal{V}}. \end{array} \tag{4.3.2}$$

Notice that this map is linear. Moreover, it is bijective when restricted to $\mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$. In the following we shall denote by $\imath_{\mathcal{V}}^{-1}$ the inverse of its restriction to $\mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$. Clearly, when restricted to bounded edgewise affine functions, $\imath_{\mathcal{V}}$ is a bijection onto $\ell^\infty(\mathcal{V})$. The situation is not so trivial when $1 \le p < \infty$, as the next result shows. Recall that (see Definition 3.16) a model of a weighted metric graph has finite intrinsic size if

$$\eta^*(\mathcal{E}) = \sup_{e\in\mathcal{E}} \eta(e) = \sup_{e\in\mathcal{E}} |e|\sqrt{\frac{\mu(e)}{\nu(e)}} < \infty. \tag{4.3.3}$$

Moreover, we define the vertex weight m by (3.1.5) with r given by (3.1.3) for models having finite intrinsic size and by (3.1.4) otherwise.

Lemma 4.2. *If* $f \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V}) \cap L^p(\mathcal{G};\mu)$, $1 \le p < \infty$, *then* $\mathbf{f} = \imath_{\mathcal{V}}(f) \in \ell^p(\mathcal{V}; m)$, *where m is the vertex weight* (3.1.5), (3.1.3)–(3.1.4). *If additionally the underlying model has finite intrinsic size, then the inclusion* $\mathbf{f} \in \ell^p(\mathcal{V}; m)$ *implies that the corresponding continuous edgewise affine function* $f = \imath_{\mathcal{V}}^{-1}(\mathbf{f})$ *belongs to* $L^p(\mathcal{G};\mu)$ *and, moreover,*

$$\|f\|^p_{L^p(\mathcal{G};\mu)} \le \|\mathbf{f}\|^p_{\ell^p(\mathcal{V};m)} \le 4^p \|f\|^p_{L^p(\mathcal{G};\mu)}. \tag{4.3.4}$$

Proof. Consider the case $p = 1$ first. Then

$$\frac{\ell}{4}\big(|f(0)| + |f(\ell)|\big) \le \int_0^\ell |f(x)|\mathrm{d}x \le \frac{\ell}{2}\big(|f(0)| + |f(\ell)|\big), \tag{4.3.5}$$

for each affine function on $\mathcal{I}_\ell = [0, \ell]$ and hence

$$\begin{aligned}\|f\|_{L^1(\mathcal{G};\mu)} &= \int_{\mathcal{G}} |f(x)|\mu(\mathrm{d}x) = \sum_{e\in\mathcal{E}} \int_e |f(x)|\mu(\mathrm{d}x) \\ &\geq \frac{1}{4} \sum_{e\in\mathcal{E}} |e|\mu(e)(|f(e_\imath)| + |f(e_\tau)|),\end{aligned}$$

whenever $f \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$. However, by (3.1.3)–(3.1.4),

$$r(e) \leq |e|\mu(e) \tag{4.3.6}$$

for all $e \in \mathcal{E}$, and hence (3.1.5) implies the estimate

$$\|f\|_{L^1(\mathcal{G};\mu)} \geq \frac{1}{4}\|\imath_{\mathcal{V}}(f)\|_{\ell^1(\mathcal{V};m)} = \frac{1}{4}\|\mathbf{f}\|_{\ell^1(\mathcal{V};m)}. \tag{4.3.7}$$

The case $p > 1$ easily follows from the above considerations. Indeed, applying Hölder's inequality to the left-hand side in (4.3.5) together with the simple inequality

$$(a + b)^p \geq a^p + b^p, \qquad a, b, \geq 0,\ p \geq 1,$$

we get from (4.3.5) the following estimate for edgewise affine functions

$$4^p \int_e |f(x)|^p \mu(\mathrm{d}x) \geq |e|\mu(e)\big(|f(e_\imath)|^p + |f(e_\tau)|^p\big), \qquad e \in \mathcal{E}. \tag{4.3.8}$$

Summing up over all edges and taking into account (4.3.6), we finally arrive at the estimate

$$4^p\|f\|^p_{L^p(\mathcal{G};\mu)} \geq \|\imath_{\mathcal{V}}(f)\|^p_{\ell^p(\mathcal{V};m)} = \|\mathbf{f}\|^p_{\ell^p(\mathcal{V};m)}. \tag{4.3.9}$$

This proves the first claim as well as the second inequality in (4.3.4).

Assume now that the model has finite intrinsic size. Then r is defined by (3.1.3) and hence for $f = \imath_{\mathcal{V}}^{-1}(\mathbf{f}) \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ we get

$$\begin{aligned}\|f\|^p_{L^p(\mathcal{G})} &= \sum_{e\in\mathcal{E}} \int_e |f(x)|^p \mu(\mathrm{d}x) \\ &\leq \sum_{e\in\mathcal{E}} |e|\mu(e) \max_{x\in e} |f(x)|^p \\ &\leq \sum_{e\in\mathcal{E}} |e|\mu(e)(|f(e_\imath)|^p + |f(e_\tau)|^p) \\ &\leq \sum_{v\in\mathcal{V}} |\mathbf{f}(v)|^p m(v) = \|\mathbf{f}\|^p_{\ell^p(\mathcal{V};m)}.\end{aligned}$$

This clearly implies the first estimate in (4.3.4) and finishes the proof. □

REMARK 4.3. A few remarks are in order.

(i) Considering $\mathrm{CA}(\mathcal{G}\backslash\mathcal{V}) \cap L^p(\mathcal{G};\mu)$ as a Banach space with the corresponding L^p norm, the above result actually says that $\imath_{\mathcal{V}}$ is a bounded linear operator from $\mathrm{CA}(\mathcal{G}\backslash\mathcal{V}) \cap L^p(\mathcal{G};\mu)$ to $\ell^p(\mathcal{V};m)$ for all $1 \leq p < \infty$ (however, for $p = \infty$ this claim is trivial) and this is true for each model of a given weighted metric graph. However, this map has a bounded inverse exactly when the model has finite intrinsic size.

(ii) The estimate in (4.3.4) is not optimal. In particular, in the case $p = 2$ the arguments from [**67**, Rem. 3.8] (see also [**146**, § 2.5]) show that

$$2\|f\|^2_{L^2(\mathcal{G};\mu)} \le \|\mathbf{f}\|^2_{\ell^2(\mathcal{V};m)} \le 6\|f\|^2_{L^2(\mathcal{G};\mu)},$$

for any model of finite intrinsic size (for models of infinite intrinsic size, only the second inequality is valid).

(iii) Let us also mention that if $f \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ is nonnegative, $f \ge 0$, then the second inequality in (4.3.5) turns into equality. Therefore, if the underlying model has finite intrinsic size, we end up with the equality

$$\|f\|_{L^1(\mathcal{G};\mu)} = \frac{1}{2}\|\imath_{\mathcal{V}}(f)\|_{\ell^1(\mathcal{V};m)} = \frac{1}{2}\|\mathbf{f}\|_{\ell^1(\mathcal{V};m)} \tag{4.3.10}$$

for all $0 \le f \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V}) \cap L^1(\mathcal{G};\mu)$.

The crucial fact for our further considerations is the observation that the above results can be extended to the H^1 setting:

Corollary 4.4. *If $f \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V}) \cap H^1(\mathcal{G})$, then $\mathbf{f} = \imath_{\mathcal{V}}(f)$ belongs to $H^1(\mathcal{V})$ and*

$$\mathfrak{Q}[f] = \mathfrak{q}[\mathbf{f}]. \tag{4.3.11}$$

Conversely, if $\mathbf{f} \in H^1(\mathcal{V})$ and the underlying model has finite intrinsic size, then $f = \imath_{\mathcal{V}}^{-1}(\mathbf{f}) \in H^1(\mathcal{G})$.

Proof. Taking into account the relationship established in Lemma 4.2, we only need to mention that for $f \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ the energy forms (4.1.1) and (4.1.3) coincide upon identification (4.3.2):

$$\begin{aligned}\mathfrak{Q}[f] = \int_{\mathcal{G}} |\nabla f(x)|^2 \nu(\mathrm{d}x) &= \sum_{e\in\mathcal{E}} \int_e |\nabla f(x)|^2 \nu(\mathrm{d}x)\\ &= \sum_{e\in\mathcal{E}} \frac{\nu(e)}{|e|} |f(e_\imath) - f(e_\tau)|^2 \\ &= \frac{1}{2}\sum_{u,v\in\mathcal{V}} b(v,u)|\mathbf{f}(v) - \mathbf{f}(u)|^2 = \mathfrak{q}[\mathbf{f}].\end{aligned} \tag{4.3.12}$$

□

Every continuous function f on $\mathcal{G}$ can be uniquely decomposed as

$$f = f_{\mathrm{lin}} + f_0, \tag{4.3.13}$$

where both f_{lin} and f_0 are continuous functions on $\mathcal{G}$, however, f_{lin} is edgewise affine on $\mathcal{G}$, $f_{\mathrm{lin}} \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ and f_0 vanishes at all vertices, that is,

$$f_{\mathrm{lin}}|_{\mathcal{V}} = f|_{\mathcal{V}}, \qquad f_0|_{\mathcal{V}} = 0.$$

Notice also the following identity $f_{\mathrm{lin}} = (\imath_{\mathcal{V}}^{-1} \circ \imath_{\mathcal{V}})(f)$ in terms of (4.3.2). Now we are in position to state the key technical result connecting the energy forms (4.1.1) and (4.1.3). For convenience matters, let us introduce the following notation

$$H^1_0(\mathcal{G}\backslash\mathcal{V}) = \{f \in H^1(\mathcal{G}) \,|\, f|_{\mathcal{V}} = 0\}.$$

Lemma 4.5. *Let $f \in H^1(\mathcal{G})$ and consider its decomposition* (4.3.13)*. If* (4.3.3) *is satisfied, then $f_0 \in H^1_0(\mathcal{G}\backslash\mathcal{V})$, $f_{\mathrm{lin}} \in H^1(\mathcal{G})$ and*

$$\mathfrak{Q}[f] = \mathfrak{Q}[f_{\mathrm{lin}}] + \mathfrak{Q}[f_0]. \tag{4.3.14}$$

Moreover, $\mathbf{f} = \imath_{\mathcal{V}}(f)$ *belongs to* $H^1(\mathcal{V})$ *and*

$$\mathfrak{Q}[f_{\mathrm{lin}}] = \mathfrak{q}[\mathbf{f}]. \tag{4.3.15}$$

PROOF. A straightforward edgewise integration by parts gives

$$\begin{aligned}\mathfrak{Q}[f] &= \sum_{e\in\mathcal{E}} \int_e |\nabla f(x)|^2 \nu(\mathrm{d}x) \\ &= \sum_{e\in\mathcal{E}} \int_e |\nabla f_{\mathrm{lin}}(x)|^2 + |\nabla f_0(x)|^2\, \nu(\mathrm{d}x) \\ &= \int_{\mathcal{G}} |\nabla f_{\mathrm{lin}}(x)|^2 \nu(\mathrm{d}x) + \int_{\mathcal{G}} |\nabla f_0(x)|^2 \nu(\mathrm{d}x) = \mathfrak{Q}[f_{\mathrm{lin}}] + \mathfrak{Q}[f_0].\end{aligned}$$

The latter implies that if f is continuous and has finite energy (i.e., it is edgewise in H^1 and $\mathfrak{Q}[f] < \infty$), then both summands on the RHS in (4.3.13) have finite energy. In particular, (4.3.14) holds for all continuous edgewise H^1 functions on $\mathcal{G}$.

Taking into account the following trivial estimate

$$\int_0^{|e|} |f(x)|^2 \mathrm{d}x \le \frac{|e|^2}{\pi^2} \int_0^{|e|} |f'(x)|^2 \mathrm{d}x,$$

which holds for any $f \in H^1_0([0,|e|])$, we get

$$\|f_0\|_{L^2(\mathcal{G};\mu)} \le \frac{\eta^*(\mathcal{E})}{\pi} \|\nabla f_0\|_{L^2(\mathcal{G};\nu)}. \tag{4.3.16}$$

Therefore, $f_0 \in L^2(\mathcal{G};\mu)$ whenever (4.3.3) holds true and f_0 has finite energy. This immediately implies that $f_{\mathrm{lin}} \in H^1(\mathcal{G})$ if so is f and (4.3.3) holds. It remains to apply Corollary 4.4. □

REMARK 4.6. The constant in (4.3.16) is optimal since so are the corresponding constants in one-dimensional inequalities for H^1_0 functions (see also (3.2.44)).

To emphasize the role of the map (4.3.2), let us provide another way to write down the correspondence between self-adjoint extensions of the minimal Kirchhoff Laplacian $\mathbf{H}^0$ and the corresponding minimal graph Laplacian $\mathbf{h}^0$established in Lemma 3.20. For a self-adjoint extension $\widetilde{\mathbf{H}} \in \mathrm{Ext}_S(\mathbf{H}^0)$ of $\mathbf{H}^0$ define the operator $\widetilde{\mathbf{h}}$ in $\ell^2(\mathcal{V};m)$ by setting

$$\widetilde{\mathbf{h}} := \mathbf{h} \restriction \mathrm{dom}(\widetilde{\mathbf{h}}), \qquad \mathrm{dom}(\widetilde{\mathbf{h}}) = \big\{\imath_{\mathcal{V}}(f) \,|\, f \in \mathrm{dom}(\widetilde{\mathbf{H}})\big\}, \tag{4.3.17}$$

where $\mathbf{h} = (\mathbf{h}^0)^*$ is the maximal graph Laplacian.

LEMMA 4.7. *Let* $\mathbf{H}^0$ *be the minimal Kirchhoff Laplacian with possibly nontrivial deficiency indices,* $\mathrm{n}_\pm(\mathbf{H}^0) \ge 0$*. If* $\widetilde{\mathbf{H}} \in \mathrm{Ext}_S(\mathbf{H}^0)$*, then the operator* $\widetilde{\mathbf{h}}$ *defined by* (4.3.17) *is a self-adjoint extension of* $\mathbf{h}^0$*. Moreover, the induced map*

$$\begin{array}{ccc}\mathrm{Ext}_S(\mathbf{H}^0) & \longrightarrow & \mathrm{Ext}_S(\mathbf{h}^0) \\ \widetilde{\mathbf{H}} & \mapsto & \widetilde{\mathbf{h}}\end{array} \tag{4.3.18}$$

is a bijection. The inverse image of a self-adjoint extension $\widetilde{\mathbf{h}}$ *of* $\mathbf{h}^0$ *is the extension*

$$\widetilde{\mathbf{H}} := \mathbf{H} \restriction \mathrm{dom}(\widetilde{\mathbf{H}}), \qquad \mathrm{dom}(\widetilde{\mathbf{H}}) = \big\{f \in \mathrm{dom}(\mathbf{H}) \,|\, \imath_{\mathcal{V}}(f) \in \mathrm{dom}(\widetilde{\mathbf{h}})\big\}. \tag{4.3.19}$$

PROOF. First of all, let us show that the map is well defined, that is, $\widetilde{\mathbf{h}}$ is indeed a self-adjoint restriction of $\mathbf{h}$. Recall that $\widetilde{\mathbf{H}}$ admits the representation (3.3.7) and, moreover, by Lemma 3.20, there is a self-adjoint extension $\widehat{\mathbf{h}} \in \mathrm{Ext}_S(\mathbf{h}_0)$ such that

$$\widetilde{\Theta} = \Theta_{\mathrm{mul}} \oplus \big\{(\Phi f, \Phi\widehat{\mathbf{h}} f) \,|\, f \in \mathrm{dom}(\widehat{\mathbf{h}})\big\}.$$

The Kirchhoff conditions at vertices imply that (see (3.2.14) and (3.2.34), (3.2.41))

$$\Gamma_0^{\mathcal{V}} f = \sum_{v\in\mathcal{V}} f(v)\mathbf{f}^v = \Phi(\imath_{\mathcal{V}}(f)) \tag{4.3.20}$$

for all $f \in \mathrm{dom}(\mathbf{H})$. Therefore, by (3.3.7), $\mathrm{dom}(\widehat{\mathbf{h}}) = \Phi^{-1}(\mathrm{dom}(\widetilde{\Theta})) = \mathrm{dom}(\widetilde{\mathbf{h}})$. Thus, by (4.3.17), $\widetilde{\mathbf{h}} = \widehat{\mathbf{h}} \in \mathrm{Ext}_S(\mathbf{h}^0)$. Moreover, this also implies that the map (4.3.18) coincides with the inverse of the map (3.3.6) and hence (4.3.18) is a bijection by Lemma 3.20.

It remains to prove the last claim. However, by definition, we have

$$\begin{aligned}\mathrm{dom}(\widetilde{\mathbf{H}}) &\subseteq \big\{f \in \mathrm{dom}(\mathbf{H}) \,|\, \imath_{\mathcal{V}}(f) \in \mathrm{dom}(\widetilde{\mathbf{h}})\big\}\\ &= \big\{f \in \mathrm{dom}(\mathbf{H}_{\max}) \,|\, (\Gamma_0^{\mathcal{V}} f, \Gamma_1^{\mathcal{V}} f) \in \Theta,\ \imath_{\mathcal{V}}(f) \in \mathrm{dom}(\widetilde{\mathbf{h}})\big\}.\end{aligned}$$

Taking into account the decomposition

$$\Theta = \Theta_{\mathrm{mul}} \oplus \big\{(\Phi\mathbf{f}, \Phi\,\mathbf{h}\mathbf{f}) \,|\, \mathbf{f} \in \mathrm{dom}(\mathbf{h})\big\},$$

as well as (4.3.20), it is clear that (4.3.19) coincides with (3.3.6), which proves the claim. $\square$

REMARK 4.8. Since the map (4.3.17)–(4.3.18) coincides with the inverse of the map (3.3.6), Theorem 3.22 (see also Remark 3.23) implies that (4.3.17) remains to be a bijection when it is further restricted to certain subclasses of self-adjoint extensions (e.g., semibounded, nonnegative etc.).

It turns out that the simple correspondence in Lemma 4.7 also prevails on the level of quadratic forms.

COROLLARY 4.9. *Suppose* $\widetilde{\mathbf{H}} \in \mathrm{Ext}_S(\mathbf{H}^0)$ *is a self-adjoint extension of* $\mathbf{H}^0$ *and let* $\widetilde{\mathbf{h}} \in \mathrm{Ext}_S(\mathbf{h}^0)$ *be the self-adjoint extension of* $\mathbf{h}^0$ *defined by* (4.3.17). *Then*

$$\langle \widetilde{\mathbf{H}} f, f\rangle_{L^2(\mathcal{G};\mu)} = \langle \widetilde{\mathbf{h}}\,\mathbf{f}, \mathbf{f}\rangle_{\ell^2(\mathcal{V};m)} + \int_{\mathcal{G}} |\nabla f_0(x)|^2\,\nu(\mathrm{d}x) \tag{4.3.21}$$

for all $f \in \mathrm{dom}(\widetilde{\mathbf{H}})$, *where* $\mathbf{f} = \imath_{\mathcal{V}}(f)$ *and* f_0 *is the function defined by* (4.3.13). *In particular,* f_0 *has finite energy,* $\mathfrak{Q}[f_0] = \|\nabla f_0\|^2_{L^2(\mathcal{G};\nu)} < \infty$ *for every* $f \in \mathrm{dom}(\widetilde{\mathbf{H}})$.

PROOF. Take $f \in \mathrm{dom}(\widetilde{\mathbf{H}})$ and consider $\mathbf{f} = \imath_{\mathcal{V}}(f)$, which belongs to $\mathrm{dom}(\widetilde{\mathbf{h}})$ by definition. Using the same notation as in the proof of Lemma 3.20 and Lemma 4.7, we conclude from (4.3.20) that

$$\langle \widetilde{\mathbf{h}}\,\mathbf{f}, \mathbf{f}\rangle_{\ell^2(\mathcal{V};m)} = \langle \widetilde{\mathbf{h}}\Phi^{-1}\Gamma_0^{\mathcal{V}} f, \Phi^{-1}\Gamma_0^{\mathcal{V}} f\rangle_{\ell^2(\mathcal{V};m)} = \langle \Gamma_1^{\mathcal{V}} f, \Gamma_0^{\mathcal{V}} f\rangle_{\mathcal{H}_{\mathcal{V}}} = \langle \Gamma_1^{\mathcal{E}} f, \Gamma_0^{\mathcal{E}} f\rangle_{\mathcal{H}_{\mathcal{E}}}.$$

Here, $\Pi_{\mathcal{E}}$ and $\Pi_{\mathcal{V}}$ denote the edge-based and vertex-based boundary triplets introduced in Theorem 3.5 and Corollary 3.8 in Section 3.2.2. Next, decompose

$f \in \mathrm{dom}(\widetilde{\mathbf{H}})$ as $f = f_0 + f_{\mathrm{lin}}$ (see (4.3.13)). A straightforward edgewise integration by parts gives (see (3.2.4))

$$\begin{aligned}\langle \widetilde{\mathbf{H}} f, f\rangle_{L^2(\mathcal{G})} &= \sum_{e\in\mathcal{E}} -\langle \Delta f, f\rangle_{L^2(e;\mu)} \\ &= \sum_{e\in\mathcal{E}} \langle \Gamma_{1,e} f, \Gamma_{0,e} f\rangle_{\mathbb{C}^2} + \langle \nabla f_0, \nabla f\rangle_{L^2(e;\nu)} \\ &= \sum_{e\in\mathcal{E}} \langle \Gamma_{1,e} f, \Gamma_{0,e} f\rangle_{\mathbb{C}^2} + \sum_{e\in\mathcal{E}} \langle \nabla f_0, \nabla f\rangle_{L^2(e;\nu)} \\ &= \langle \Gamma_1^{\mathcal{E}} f, \Gamma_0^{\mathcal{E}} f\rangle_{\mathcal{H}_{\mathcal{E}}} + \sum_{e\in\mathcal{E}} \langle \nabla f_0, \nabla f\rangle_{L^2(e;\nu)}.\end{aligned}$$

Notice that we can rearrange sums. Indeed, both $(\Gamma_{0,e} f)_{e\in\mathcal{E}}$ and $(\Gamma_{1,e} f)_{e\in\mathcal{E}}$ belong to $\mathcal{H}_{\mathcal{E}}$ by Theorem 3.5 and hence the first sum is absolutely convergent. Taking into account that f_0 vanishes on $\mathcal{V}$, we get

$$\langle \nabla f_0, \nabla f\rangle_{L^2(e;\nu)} = \langle \nabla f_0, \nabla f_0\rangle_{L^2(e;\nu)} \geq 0$$

for all $e \in \mathcal{E}$, which implies that the second series is also absolutely convergent and equals the energy $\mathfrak{Q}[f_0]$ of f_0. This finishes the proof of the equality (4.3.21). $\square$

REMARK 4.10. Notice that Theorem 3.1(i) states that the sets of self-adjoint extensions of $\mathbf{H}^0$ and $\mathbf{h}^0$ are in 1-to-1 correspondence and the concept of boundary triplets provides the explicit correspondence which, however, requires a construction of a suitable boundary triplet. From this perspective, Lemma 4.7 and Corollary 4.9 connect self-adjoint extensions via quadratic forms and this approach has its roots in the pioneering works of M.G. Krein, M.I. Vishik and M.S. Birman in the 1950s on boundary value problems for elliptic PDEs (see, e.g., [**55**] for more details). However, let us emphasize that the decomposition (4.3.21) is usually established under the additional assumption that the corresponding symmetric operator is uniformly positive, see [**154**, f-la (25)] (in our setting this would mean that the Dirichlet Laplacian $\mathbf{H}_D$ has positive spectral gap).

4.4. Correspondence between Markovian extensions

According to (4.1.2) and (4.1.7), the sets $\mathrm{Ext}_M(\mathbf{H}^0)$ and $\mathrm{Ext}_M(\mathbf{h}^0)$ of Markovian extensions are nonempty. Lemma 3.20 as well as Lemma 4.7 show that first of all, the sets of self-adjoint extensions $\mathrm{Ext}_S(\mathbf{H}^0)$ and $\mathrm{Ext}_S(\mathbf{h}^0)$ are in bijection, and, what is more important, each self-adjoint extension of $\mathbf{h}^0$ can be seen as a boundary operator parameterizing the corresponding self-adjoint extension of $\mathbf{H}^0$. The further correspondence between their spectral properties indicates that one can hope that (4.3.17)–(4.3.18) induces a bijection between the sets $\mathrm{Ext}_M(\mathbf{H}^0)$ and $\mathrm{Ext}_M(\mathbf{h}^0)$ and we shall see that this is indeed the case.

It turns out that the correspondence between Markovian extensions can be conveniently explained using the notion of extended Dirichlet spaces (see Appendix B.3 for details) and we need to introduce the following function spaces. Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph together with a fixed model. Recall that the energy of a continuous, edgewise H^1-function $f\colon \mathcal{G} \to \mathbb{C}$ is given by

$$\mathfrak{Q}[f] := \|\nabla f\|^2_{L^2(\mathcal{G};\nu)} = \int_{\mathcal{G}} |\nabla f(x)|^2 \,\nu(\mathrm{d}x). \tag{4.4.1}$$

The space of *functions of finite energy* is defined as

$$\dot H^1(\mathcal{G}) := \big\{ f \in C(\mathcal{G}) \,\big|\, f|_e \in H^1(e) \text{ for all } e \in \mathcal{E}, \quad \mathfrak{Q}[f] < \infty \big\},$$

and its subspace of functions vanishing on the vertex set is denoted by $\dot H^1_0(\mathcal{G}\backslash\mathcal{V})$,

$$\dot H^1_0(\mathcal{G}\backslash\mathcal{V}) := \{ f \in \dot H^1(\mathcal{G}) \mid \imath_{\mathcal{V}}(f) \equiv 0 \}.$$

Let us stress at this point that in contrast to the Sobolev space $H^1(\mathcal{G})$ we do not require f to belong to $L^2(\mathcal{G};\mu)$ (for example, $\mathbb{1}$ always belongs to $\dot H^1(\mathcal{G})$, however, $\mathbb{1} \in H^1(\mathcal{G})$ exactly when $\mu(\mathcal{G}) < \infty$).

Since $\dot H^1(\mathcal{G}) \subset C(\mathcal{G})$, each $f \in \dot H^1(\mathcal{G})$ can be decomposed into $f = f_{\rm lin} + f_0$ as in (4.3.13) and, moreover, we easily get (see the proof of Lemma 4.5)

$$\mathfrak{Q}[f] = \mathfrak{Q}[f_{\rm lin}] + \mathfrak{Q}[f_0], \tag{4.4.2}$$

which implies that $f_{\rm lin} \in \dot H^1(\mathcal{G})$ and $f_0 \in \dot H^1_0(\mathcal{G}\backslash\mathcal{V})$ whenever $f \in \dot H^1(\mathcal{G})$. Moreover, the calculations in the proof of Corollary 4.4 imply that

$$\mathfrak{Q}[f_{\rm lin}] = \mathfrak{q}[\mathbf{f}] = \frac{1}{2}\sum_{u,v\in\mathcal{V}} b(v,u)|\mathbf{f}(v) - \mathbf{f}(u)|^2, \tag{4.4.3}$$

where $\mathbf{f} = \imath_{\mathcal{V}}(f) = \imath_{\mathcal{V}}(f_{\rm lin})$. In particular, this means that a function $\mathbf{f} \in C(\mathcal{V})$ has finite energy, $\mathfrak{q}[\mathbf{f}] < \infty$ exactly when the corresponding edgewise affine function $f_{\rm lin} = \imath_{\mathcal{V}}^{-1}(\mathbf{f}) \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ has finite energy. In contrast to the usual Sobolev space $H^1(\mathcal{G})$, the above decomposition holds for all models of a given metric graph (see Lemma 4.5) and exactly this fact makes the use of extended Dirichlet spaces very convenient. In particular a similar decomposition holds for all Markovian extensions and the corresponding extended Dirichlet spaces.

Lemma 4.11. *Let* $\widetilde{\mathbf{H}}$ *be a Markovian extension of the minimal Kirchhoff Laplacian* $\mathbf{H}^0$ *and* $\widetilde{\mathfrak{Q}}_e \colon \mathrm{dom}(\widetilde{\mathfrak{Q}}_e) \to [0,+\infty)$ *the corresponding extended Dirichlet form. Then:*

(i) $\mathrm{dom}(\widetilde{\mathfrak{Q}}_e) \subseteq \dot H^1(\mathcal{G})$.

(ii) $\dot H^1_0(\mathcal{G}\backslash\mathcal{V}) \subseteq \mathrm{dom}(\widetilde{\mathfrak{Q}}_e)$ *and for each* $f_0 \in \dot H^1_0(\mathcal{G}\backslash\mathcal{V})$

$$\widetilde{\mathfrak{Q}}_e[f_0] = \mathfrak{Q}[f_0].$$

(iii) *Each* $f \in \mathrm{dom}(\widetilde{\mathfrak{Q}}_e)$ *has an approximating sequence* $(f_n)_n \subset \mathrm{dom}(\widetilde{\mathbf{H}})$.

(iv) *If* $f = f_{\rm lin} + f_0 \in \mathrm{dom}(\widetilde{\mathfrak{Q}}_e)$, *then* $f_{\rm lin} \in \mathrm{dom}(\widetilde{\mathfrak{Q}}_e)$, $f_0 \in \dot H^1_0(\mathcal{G}\backslash\mathcal{V})$ *and*

$$\widetilde{\mathfrak{Q}}_e[f] = \widetilde{\mathfrak{Q}}_e[f_{\rm lin}] + \mathfrak{Q}[f_0].$$

Proof. (i) By Lemma 4.1, $\mathbf{H}_N \le \widetilde{\mathbf{H}}$. Moreover, it is easy to observe that the extended Dirichlet space for $\mathfrak{Q}_N$ is contained in $\dot H^1(\mathcal{G})$, which implies the desired inclusion.

(ii) For each $f_0 \in \dot H^1_0(\mathcal{G}\backslash\mathcal{V})$ there exists a sequence $(f_n)_n \subset \mathrm{dom}(\mathbf{H}) \cap C_c(\mathcal{G})$ such that each f_n vanishes in a neighborhood of all vertices and

$$\lim_{n\to\infty} \mathfrak{Q}[f_0 - f_n] = 0.$$

The claim now follows easily from Corollary 4.9.

(iii) is an immediate consequence of the fact that $\mathrm{dom}(\widetilde{\mathbf{H}})$ is a core of $\mathrm{dom}(\widetilde{\mathfrak{Q}})$ and convergence in the graph norm of $\widetilde{\mathfrak{Q}}$ implies uniform convergence on compact subsets of $\mathcal{G}$.

(iv) Take $f = f_{\rm lin} + f_0 \in \mathrm{dom}(\widetilde{\mathfrak{Q}}_e)$. By (i), $f_0 \in \dot{H}^1_0(\mathcal{G}\backslash\mathcal{V})$ and hence (ii) implies that $f_{\rm lin} \in \mathrm{dom}(\widetilde{\mathfrak{Q}}_e)$. By (iii), pick an approximating sequence $(f_n)_n \subset \mathrm{dom}(\widetilde{\mathbf{H}})$ for f with $f_n = f_{n,0} + f_{n,\rm lin}$ for each n. By the proof of (ii), there exists an approximating sequence $(g_n)_n \subset \mathrm{dom}(\mathbf{H}) \cap C_c(\mathcal{G})$ for f_0 such that $g_n|_{\mathcal{V}} \equiv 0$. Corollary 4.9 implies that $(f_{n,0})_n$ and $(g_n)_n$ are $\mathfrak{Q}$-Cauchy sequences. Moreover, it is straightforward to show that

$$\lim_{n\to\infty} \mathfrak{Q}[f_0 - f_{n,0}] = \lim_{n\to\infty} \mathfrak{Q}[f_0 - g_n] = 0.$$

Since $(f_n - g_n)_n$ is an approximating sequence for $f_{\rm lin}$, by Corollary 4.9 we get

$$\begin{aligned}\widetilde{\mathfrak{Q}}[f_{\rm lin}] &= \lim_{n\to\infty} \langle \widetilde{\mathbf{h}}\, \mathbf{f}_n, \mathbf{f}_n\rangle + \mathfrak{Q}[f_{n,0} - g_n] \\ &= \lim_{n\to\infty} \langle \widetilde{\mathbf{h}}\, \mathbf{f}_n, \mathbf{f}_n\rangle + \mathfrak{Q}[f_{n,0}] - \mathfrak{Q}[f_{n,0}] \\ &= \widetilde{\mathfrak{Q}}[f] - \mathfrak{Q}[f_0].\end{aligned}$$

This completes the proof of Lemma 4.11. □

Now we are in position to state the main result of this subsection.

THEOREM 4.12. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph together with a fixed model. Then the map defined by* (4.3.17) *induces a bijection*

$$\begin{array}{ccc}\mathrm{Ext}_M(\mathbf{H}^0) & \longrightarrow & \mathrm{Ext}_M(\mathbf{h}^0) \\ \widetilde{\mathbf{H}} & \mapsto & \widetilde{\mathbf{h}}\end{array}. \tag{4.4.4}$$

PROOF. By Lemma 4.7, the map (4.3.17) is a bijection between $\mathrm{Ext}_S(\mathbf{H}^0)$ and $\mathrm{Ext}_S(\mathbf{h}^0)$ and hence we only need to show that $\widetilde{\mathbf{H}} \in \mathrm{Ext}_S(\mathbf{H}^0)$ is Markovian exactly when so is the corresponding $\widetilde{\mathbf{h}} \in \mathrm{Ext}_S(\mathbf{h}^0)$. We divide the proof in several steps.

(i) First suppose that $\widetilde{\mathbf{H}} \in \mathrm{Ext}_M(\mathbf{H}^0)$ and $\widetilde{\mathbf{h}} \in \mathrm{Ext}_S(\mathbf{h}^0)$ is defined by (4.3.17) with the corresponding quadratic form $\widetilde{\mathfrak{q}}$ in $\ell^2(\mathcal{V}; m)$. Let us show that $\widetilde{\mathbf{h}}$ is also Markovian. Define the quadratic form

$$\widehat{\mathfrak{q}}_e[\mathbf{f}] := \widetilde{\mathfrak{Q}}_e[\imath_{\mathcal{V}}^{-1}(\mathbf{f})], \quad \mathbf{f} \in \mathrm{dom}(\widehat{\mathfrak{q}}_e) := \big\{f \in C(\mathcal{V})|\ \imath_{\mathcal{V}}^{-1}(f) \in \mathrm{dom}(\widetilde{\mathfrak{Q}}_e)\big\}, \tag{4.4.5}$$

and also its $\ell^2(\mathcal{V}; m)$ restriction (compare with (B.3.1))

$$\widehat{\mathfrak{q}} := \widehat{\mathfrak{q}}_e \restriction \mathrm{dom}(\widehat{\mathfrak{q}}), \qquad \mathrm{dom}(\widehat{\mathfrak{q}}) = \mathrm{dom}(\widehat{\mathfrak{q}}_e) \cap \ell^2(\mathcal{V}; m). \tag{4.4.6}$$

Here $\widetilde{\mathfrak{Q}}_e$ is the extended Dirichlet form of $\widetilde{\mathfrak{Q}}$. It is straightforward to prove that $\widehat{\mathfrak{q}}$ is closed, which basically follows from the fact that $\widetilde{\mathfrak{Q}}_e$ is closed under taking a.e. pointwise limits of $\widetilde{\mathfrak{Q}}_e$-Cauchy sequences. Moreover, $\widehat{\mathfrak{q}}$ inherits the Markovian property from $\widetilde{\mathfrak{Q}}_e$. Indeed, take $\mathbf{f} \in \mathrm{dom}(\widehat{\mathfrak{q}})$ and pick a normal contraction $\varphi \colon \mathbb{C} \to \mathbb{C}$. Then $f = \imath_{\mathcal{V}}^{-1}(\mathbf{f}) \in \mathrm{dom}(\widetilde{\mathfrak{Q}}_e)$ and hence $\varphi \circ \mathbf{f} = \imath_{\mathcal{V}}(\varphi \circ f)$ belongs to $\mathrm{dom}(\widehat{\mathfrak{q}})$ since $\widetilde{\mathfrak{Q}}_e$ is Markovian (see Appendix B.3). Moreover, Lemma 4.11 implies

$$\widehat{\mathfrak{q}}[\varphi\circ\mathbf{f}] = \widehat{\mathfrak{q}}_e[\varphi\circ\mathbf{f}] = \widetilde{\mathfrak{Q}}_e[\imath_{\mathcal{V}}^{-1}(\varphi\circ\mathbf{f})] \le \widetilde{\mathfrak{Q}}_e[\varphi\circ f] \le \widetilde{\mathfrak{Q}}_e[f] = \widetilde{\mathfrak{Q}}_e[\imath_{\mathcal{V}}^{-1}(\mathbf{f})] = \widehat{\mathfrak{q}}[\mathbf{f}].$$

Thus, $\widehat{\mathfrak{q}}$ is a Dirichlet form in $\ell^2(\mathcal{V}; m)$ and the corresponding self-adjoint operator $\widehat{\mathbf{h}}$ is Markovian. Hence to prove the claim it suffices to show that $\widehat{\mathbf{h}} = \widetilde{\mathbf{h}}$ (or equivalently that $\widehat{\mathfrak{q}} = \widetilde{\mathfrak{q}}$).

First of all, (4.3.17) implies that $\mathrm{dom}(\widetilde{\mathbf{h}}) \subseteq \mathrm{dom}(\widehat{\mathfrak{q}})$ and $\widetilde{\mathfrak{q}} = \widehat{\mathfrak{q}}$ on $\mathrm{dom}(\widetilde{\mathbf{h}})$ by Corollary 4.9. Therefore, $\widetilde{\mathbf{h}} \ge \widehat{\mathbf{h}}$.

To prove the converse, observe that $\widehat{\mathbf{h}} \in \mathrm{Ext}_S(\mathbf{h}^0)$. Indeed, take $\mathbf{f} \in \mathrm{dom}(\mathbf{h}')$ and $\mathbf{g} \in \mathrm{dom}(\widehat{\mathfrak{q}})$ and then pick an $f \in \mathrm{dom}(\mathbf{H}')$ with $\imath_{\mathcal{V}}(f) = \mathbf{f}$ and an approximating sequence $(g_n)_n \subset \mathrm{dom}(\widetilde{\mathbf{H}})$ for $g := \imath_{\mathcal{V}}^{-1}(\mathbf{g}) \in \mathrm{dom}(\widetilde{\mathfrak{Q}}_e) \cap \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$. Then by Lemma 4.11 (iv),

$$\widehat{\mathfrak{q}}[\mathbf{f},\mathbf{g}] = \widetilde{\mathfrak{Q}}_e[\imath_{\mathcal{V}}^{-1}(f), \imath_{\mathcal{V}}^{-1}(g)] = \widetilde{\mathfrak{Q}}_e[f, \imath_{\mathcal{V}}^{-1}(g)] = \lim_{n\to\infty} \widetilde{\mathfrak{Q}}[f, g_n] = \lim_{n\to\infty} \langle \mathbf{H}' f, g_n\rangle_{L^2}.$$

Since $\widetilde{\mathbf{H}} \geq \mathbf{H}_N$ (see Lemma 4.1), it follows that g_n converges to g uniformly on compact subsets of $\mathcal{G}$. Using integration by parts and (4.4.2),

$$\widehat{\mathfrak{q}}[\mathbf{f},\mathbf{g}] = \langle \mathbf{H}' f, g\rangle_{L^2} = \mathfrak{Q}[f,g] = \mathfrak{q}[\mathbf{f},\mathbf{g}] = \langle \mathbf{h}'\mathbf{f}, \mathbf{g}\rangle_{\ell^2},$$

which shows that $\mathbf{h}' \subseteq \widehat{\mathbf{h}}$ and hence $\widehat{\mathbf{h}} \in \mathrm{Ext}_S(\mathbf{h}^0)$.

Let $\widehat{\mathbf{H}}$ be the nonnegative self-adjoint extension of $\mathbf{H}^0$ corresponding to $\widehat{\mathbf{h}}$ via (4.3.17). Again, we infer from Lemma 4.7, Lemma 4.11(iv) and Corollary 4.9 that (see also (B.3.1))

$$\mathrm{dom}(\widehat{\mathbf{H}}) \subseteq \mathrm{dom}(\widetilde{\mathfrak{Q}}_e) \cap L^2(\mathcal{G};\mu) = \mathrm{dom}(\widetilde{\mathfrak{Q}})$$

and that $\widehat{\mathfrak{Q}} = \widetilde{\mathfrak{Q}}$ on $\mathrm{dom}(\widehat{\mathbf{H}})$. This implies that $\widehat{\mathbf{H}} \geq \widetilde{\mathbf{H}}$. However, the map between nonnegative extensions of $\mathbf{H}^0$ and $\mathbf{h}^0$ is monotonic (this can easily be deduced from Krein's resolvent formula (A.3.2)), that is, $\widetilde{\mathbf{H}}_1 \geq \widetilde{\mathbf{H}}_2$ exactly when $\widetilde{\mathbf{h}}_1 \geq \widetilde{\mathbf{h}}_2$. Hence we conclude that $\widehat{\mathbf{h}} = \widetilde{\mathbf{h}}$.

(ii) It remains to show that $\widetilde{\mathbf{H}}$ is a Markovian extension of $\mathbf{H}^0$ if $\widetilde{\mathbf{h}}$ is a Markovian extension of $\mathbf{h}^0$. The proof essentially consists in reversing the construction of the previous step. More precisely, we define the quadratic form

(4.4.7)
$$\widehat{\mathfrak{Q}}_e[f] := \widetilde{\mathfrak{q}}_e[\imath_{\mathcal{V}}(f)] + \mathfrak{Q}[f_0], \quad f \in \mathrm{dom}(\widehat{\mathfrak{Q}}_e) := \big\{ g \in \dot{H}^1(\mathcal{G}) |\ \imath_{\mathcal{V}}(g) \in \mathrm{dom}(\widetilde{\mathfrak{q}}_e)\big\}$$

and consider its restriction

$$\widehat{\mathfrak{Q}} := \widehat{\mathfrak{Q}}_e \restriction \mathrm{dom}(\widehat{\mathfrak{Q}}), \qquad \mathrm{dom}(\widehat{\mathfrak{Q}}) = \mathrm{dom}(\widehat{\mathfrak{Q}}_e) \cap L^2(\mathcal{G};\mu). \tag{4.4.8}$$

Similar to the previous step, it turns out that $\widehat{\mathfrak{Q}}$ is a Dirichlet form in $L^2(\mathcal{G};\mu)$ and the associated operator coincides with $\widetilde{\mathbf{H}}$, that is, $\widehat{\mathbf{H}} = \widetilde{\mathbf{H}}$. Let us only prove that $\widehat{\mathfrak{Q}}$ verifies the Markovian property (B.1.1) since the other claimed properties can be verified without difficulty analogous to the previous step and we omit the details.

Take $f \in \widehat{\mathfrak{Q}}$ and pick a normal contraction $\varphi\colon \mathbb{C} \to \mathbb{C}$. By [**131**, Theorem 3.12] (see also (4.1.7)), the difference $\widetilde{\mathfrak{q}}_e - \mathfrak{q}$ satisfies the Markovian condition (B.1.1) on $\mathrm{dom}(\widetilde{\mathfrak{q}}_e)$. Setting $\mathbf{f} := \imath_{\mathcal{V}}(f)$, we see that $\imath_{\mathcal{V}}(\varphi\circ f) = \varphi \circ \mathbf{f}$ and in particular $\varphi \circ f \in \mathrm{dom}(\widetilde{\mathfrak{q}})$. Moreover, it follows from (4.4.2) that

$$\begin{aligned}\widehat{\mathfrak{Q}}[f] &= \widetilde{\mathfrak{q}}_e[\mathbf{f}] + \mathfrak{Q}[f_0] = \widetilde{\mathfrak{q}}_e[\mathbf{f}] + \mathfrak{Q}[f] - \mathfrak{Q}[\imath_{\mathcal{V}}^{-1}(\mathbf{f})] = \widetilde{\mathfrak{q}}_e[\mathbf{f}] - \mathfrak{q}[\mathbf{f}] + \mathfrak{Q}[f] \\ &\geq (\widetilde{\mathfrak{q}}_e - \mathfrak{q})[\varphi\circ\mathbf{f}] + \mathfrak{Q}[\varphi\circ f] = \widehat{\mathfrak{Q}}[\varphi\circ f],\end{aligned}$$

which shows that $\widehat{\mathfrak{Q}}$ is Markovian. □

The proof of Theorem 4.12 in fact contains the following transparent correspondence between the extended Dirichlet forms (see (4.4.5)–(4.4.6) and (4.4.7)–(4.4.8)).

COROLLARY 4.13. *Let $(\mathcal{G},\mu,\nu)$ be a weighted metric graph together with a fixed model. Let also $\widetilde{\mathbf{H}}$ be a Markovian extension of $\mathbf{H}^0$ and consider the associated*

Markovian extension $\widetilde{\mathbf{h}}$ *of* $\mathbf{h}^0$ *defined by* (4.3.17). *The domains of the corresponding extended Dirichlet forms* $\widetilde{\mathfrak{Q}}_e$ *and* $\widetilde{\mathfrak{q}}_e$ *are related by*

$$\operatorname{dom}(\widetilde{\mathfrak{q}}_e) = \{\imath_{\mathcal{V}}(f) \,|\, f \in \operatorname{dom}(\widetilde{\mathfrak{Q}}_e)\} \tag{4.4.9}$$

and

$$\operatorname{dom}(\widetilde{\mathfrak{Q}}_e) = \{f \in \dot{H}^1(\mathcal{G}) \,|\, \imath_{\mathcal{V}}(f) \in \operatorname{dom}(\widetilde{\mathfrak{q}}_e)\}. \tag{4.4.10}$$

Moreover, for every function $f \in \operatorname{dom}(\widetilde{\mathfrak{Q}}_e)$,

$$\widetilde{\mathfrak{Q}}_e[f] = \widetilde{\mathfrak{q}}_e[\imath_{\mathcal{V}}(f)] + \mathfrak{Q}[f_0]. \tag{4.4.11}$$

However, the above correspondence cannot be extended to the Dirichlet forms (and form domains) without further restrictions on the underlying model.

Corollary 4.14. *Let* $(\mathcal{G}, \mu, \nu)$ *be a weighted metric graph together with a fixed model having finite intrinsic size. Let* $\widetilde{\mathbf{H}} \in \operatorname{Ext}_M(\mathbf{H}^0)$ *and* $\widetilde{\mathbf{h}} \in \operatorname{Ext}_M(\mathbf{h}^0)$ *be given by* (4.3.17). *Then the corresponding Dirichlet forms* $\widetilde{\mathfrak{Q}}$ *and* $\widetilde{\mathfrak{q}}$ *are connected by*

$$\widetilde{\mathfrak{q}}[\mathbf{f}] = \widetilde{\mathfrak{Q}}[\imath_{\mathcal{V}}^{-1}(\mathbf{f})], \qquad \mathbf{f} \in \operatorname{dom}(\widetilde{\mathfrak{q}}) = \big\{\imath_{\mathcal{V}}(f) \,|\; f \in \operatorname{dom}(\widetilde{\mathfrak{Q}})\big\}, \tag{4.4.12}$$

and

$$\begin{aligned} \operatorname{dom}(\widetilde{\mathfrak{Q}}) &= \big\{\imath_{\mathcal{V}}^{-1}(\mathbf{f}) + f_0 \,|\; \mathbf{f} \in \operatorname{dom}(\widetilde{\mathfrak{q}}), \quad f_0 \in H^1_0(\mathcal{G}\backslash\mathcal{V})\big\}, \\ \widetilde{\mathfrak{Q}}[f] &= \widetilde{\mathfrak{q}}[\mathbf{f}] + \mathfrak{Q}[f_0], \qquad f = \imath_{\mathcal{V}}^{-1}(\mathbf{f}) + f_0 \in \operatorname{dom}(\widetilde{\mathfrak{Q}}). \end{aligned} \tag{4.4.13}$$

Proof. Taking into account (B.3.1), the proof is a straightforward combination of Corollary 4.13, Lemma 4.11 and Lemma 4.5. □

Remark 4.15. It is easy to show that under the finite intrinsic size assumption (4.3.3), Corollary 4.14 holds true for nonnegative extensions $\widetilde{\mathbf{H}} \in \operatorname{Ext}_S^+(\mathbf{H}^0)$ and $\widetilde{\mathbf{h}} \in \operatorname{Ext}_S^+(\mathbf{h}^0)$ as well. However, we restrict to the special case of Markovian extensions for the sake of a streamlined exposition.

Remark 4.16. The results of this section remain valid for Laplacians with δ-couplings $\mathbf{H}^0_\alpha$ (see Section 2.4.3) and their associated discrete Laplacians $\mathbf{h}^0_\alpha$ (see (3.1.7) and Theorem 3.1), of course under the additional assumption that all strengths are nonnegative, that is, $\alpha\colon \mathcal{V} \to [0, \infty)$.

4.5. Recurrence/transience

As it was explained in Section 4.2, the connection between a Brownian motion on a metric graph and a continuous time random walk on a graph indicates a connection between the corresponding heat semigroups. The main tool to confirm this intuition is the close relationship between the energy forms established in the previous sections. We begin with the study of *recurrence* and *transience* (see Appendix B.2 for definitions and further references).

Theorem 4.17. *Let* $(\mathcal{G}, \mu, \nu)$ *be a weighted metric graph together with a fixed model. Let also* $\widetilde{\mathbf{H}}$ *be a Markovian extension of* $\mathbf{H}^0$ *and* $\widetilde{\mathbf{h}}$ *the corresponding Markovian extension of* $\mathbf{h}^0$ *(see Theorem 4.12). Then the heat semigroup* $(e^{-\widetilde{\mathbf{H}}t})_{t>0}$ *is recurrent (respectively, transient) if and only if the semigroup* $(e^{-\widetilde{\mathbf{h}}t})_{t>0}$ *is recurrent (respectively, transient).*

PROOF. The claim follows immediately from the recurrence characterization by means of extended Dirichlet spaces (see Lemma B.7) and the relationship between extended Dirichlet spaces established in Corollary 4.13. Notice also that $\mathcal{G}$ (and hence $\mathcal{G}_d$ for each model of $\mathcal{G}$) is connected and hence the corresponding Dirichlet form is irreducible, which implies the recurrence/transience dichotomy. $\square$

REMARK 4.18. Let us stress that recurrence/transience is independent of the choice of a model of a weighted metric graph (one may even allow models having infinite intrinsic size). So, the situation is analogous to the self-adjoint uniqueness (cf. Corollary 3.15): *if* $(e^{-\widetilde{\mathbf{H}}t})_{t>0}$ *is recurrent, then* $(e^{-\widetilde{\mathbf{h}}t})_{t>0}$ *is recurrent for all models of* $(\mathcal{G}, \mu, \nu)$*. And conversely,* $(e^{-\widetilde{\mathbf{H}}t})_{t>0}$ *is recurrent if* $(e^{-\widetilde{\mathbf{h}}t})_{t>0}$ *is recurrent for one (and hence for all) models of* $(\mathcal{G}, \mu, \nu)$*.*

REMARK 4.19. A similar approach connecting recurrence/transience on graphs and metric graphs was suggested in [**95**, Chapter 4].

For the two extremal Markovian extensions, the Dirichlet and Neumann Laplacians $\mathbf{H}_D$ and $\mathbf{H}_N$, we obtain the following characterizations.

COROLLARY 4.20. *Let* $(\mathcal{G}, \mu, \nu)$ *be a weighted metric graph together with a fixed model. The following statements are equivalent for the Neumann Laplacian* $\mathbf{H}_N$*:*

(i) $(e^{-\mathbf{H}_N t})_{t>0}$ *is recurrent,*
(ii) $(e^{-\mathbf{h}_N t})_{t>0}$ *is recurrent,*
(iii) $\mathbb{1} \in \mathrm{dom}(\mathfrak{Q}_N^e)$*, where* $\mathrm{dom}(\mathfrak{Q}_N^e)$ *is the extended Dirichlet space of* $\mathfrak{Q}_N$*,*
(iv) $\mathrm{dom}(\mathfrak{Q}_N^e) = \dot{H}^1(\mathcal{G})$*.*

PROOF. Since $\mathbb{1} \in \dot{H}^1(\mathcal{G})$, in view of Theorem 4.12, Theorem 4.17 and Lemma B.7, we only need to prove the implication (iii) $\Rightarrow$ (iv). The arguments leading to their proofs are well-known (see, e.g., [**134**, Prop. 6.11]), however, we repeat them for the sake of completeness.

Suppose (iii) holds true and let $(f_n)_n \subset H^1(\mathcal{G})$ be an approximating sequence for $\mathbb{1}$, that is, $\lim_{n\to\infty} f_n(x) = 1$ for a.e. $x \in \mathcal{G}$ and $\lim_{n\to\infty} \mathfrak{Q}[f_n] = 0$. Replacing f_n by $\widetilde{f}_n := 0 \vee \mathrm{Re}(f_n) \wedge 1$, if necessary, we can assume that $0 \le f_n \le 1$. Suppose also that $g \in \dot{H}^1(\mathcal{G})$ is bounded. Then $g_n := f_n g$ belongs to $H^1(\mathcal{G})$ as well for all $n \in \mathbb{Z}_{\ge 0}$. Moreover, the sequence $(g_n)_n$ converges to g pointwise a.e. on $\mathcal{G}$ and

$$\lim_{n\to\infty} \mathfrak{Q}[g - g_n] \le \lim_{n\to\infty} 2\|g\|_\infty^2 \mathfrak{Q}[f_n] + 2\int_{\mathcal{G}} (1 - f_n)^2 |\nabla g|^2 \,\nu(\mathrm{d}x) = 0.$$

Hence every bounded function $g \in \dot{H}^1(\mathcal{G})$ belongs to $\mathrm{dom}(\mathfrak{Q}_N^e)$ and satisfies $\mathfrak{Q}_N^e[g] = \mathfrak{Q}[g]$. On the other hand, for every (real-valued) function $g \in \dot{H}^1(\mathcal{G})$, the sequence defined by $g_n := (-n) \vee g_n \wedge n$, $n \in \mathbb{Z}_{\ge 0}$ converges pointwise to g and, moreover, $\lim_{n\to\infty} \mathfrak{Q}[g - g_n] = 0$. In particular, it follows that (iv) holds true. $\square$

In the case of Dirichlet Laplacians, the characterization looks slightly differently. If $\mathbf{H}^0$ admits a unique Markovian extensions, then $\mathbf{H}_D$ coincides with $\mathbf{H}_N$ and in this case the above characterization applies. It turns out that Markovian uniqueness is necessary for $(e^{-\mathbf{H}_D t})_{t>0}$ to be recurrent.

COROLLARY 4.21. *Let* $(\mathcal{G}, \mu, \nu)$ *be a weighted metric graph together with a fixed model. The following statements are equivalent for the Dirichlet Laplacian* $\mathbf{H}_D$*:*

(i) $(e^{-\mathbf{H}_D t})_{t>0}$ *is recurrent,*

(ii) $(e^{-\mathbf{h}_D t})_{t>0}$ *is recurrent,*
(iii) $\mathbb{1} \in \operatorname{dom}(\mathfrak{Q}_D^e)$*, where* $\operatorname{dom}(\mathfrak{Q}_D^e)$ *is the extended Dirichlet space of* $\mathfrak{Q}_D$*,*
(iv) $\operatorname{dom}(\mathfrak{Q}_D^e) = \dot{H}^1(\mathcal{G})$*,*
(v) $\mathbf{H}_D = \mathbf{H}_N$ *and* $\operatorname{dom}(\mathfrak{Q}_D^e) = \dot{H}^1(\mathcal{G})$*.*

PROOF. Clearly, we only need to prove that $\mathbf{H}_D = \mathbf{H}_N$ if $(e^{-\mathbf{H}_D t})_{t>0}$ is recurrent. However, $\mathfrak{Q}_D$ is a regular Dirichlet form and the corresponding fact connecting recurrence and Markovian uniqueness is rather well known (see, e.g., [**98**, Theorem 5.20]). □

REMARK 4.22. A few remarks are in order.

(i) Let us stress that Markovian uniqueness is not necessary for the Neumann Laplacian to be recurrent. Intuitively, this is explained by the fact that Neumann boundary conditions are considered as a reflecting boundary. On the other hand, one can easily construct simple examples (see, e.g., Lemma 5.13).
(ii) For the Kirchhoff Laplacian $\mathbf{H}_\alpha$ with nonzero $\alpha \geq 0$ (which is equivalent to the presence of a nonzero killing term for $\mathbf{h}_\alpha$) the corresponding Dirichlet form is always transient.
(iii) As in the manifold case (see, e.g., [**88**]), transience/recurrence for both Kirchhoff Laplacians and graph Laplacians admits several equivalent reformulations in terms of harmonic and subharmonic functions. We shall return to this issue in Section 7.4.

4.6. Stochastic completeness

The preceding sections suggest a connection between stochastic completeness of the Kirchhoff Laplacian $\mathbf{H}$ on a weighted metric graph $(\mathcal{G}, \mu, \nu)$ and its associated discrete Laplacian $\mathbf{h}$ on a fixed model. In fact, the results of [**70**], [**112**] imply that (assuming the model has finite intrinsic size and, for simplicity, that $\mathbf{H}$ and $\mathbf{h}$ are self-adjoint[‡])

$$(e^{-t\mathbf{H}})_{t>0} \text{ stochastically complete} \Rightarrow (e^{-t\mathbf{h}})_{t>0} \text{ stochastically complete.} \tag{4.6.1}$$

It can be shown by examples that the converse direction fails (even for models of finite intrinsic size). However, we are going to show that equivalence holds true in (4.6.1) if the corresponding model is in a certain sense fine enough.

THEOREM 4.23. *Let* $(\mathcal{G}, \mu, \nu)$ *be a weighted metric graph with a fixed model of finite intrinsic size. Let* $\widetilde{\mathbf{H}} \in \operatorname{Ext}_M(\mathbf{H}^0)$ *be a Markovian extension of* $\mathbf{H}^0$ *together with the corresponding extension* $\widetilde{\mathbf{h}} \in \operatorname{Ext}_M(\mathbf{h}^0)$ *defined on* $\ell^2(\mathcal{V}; m)$ *by* (4.3.17)*.*

(i) *If* $(e^{-t\widetilde{\mathbf{H}}})_{t>0}$ *is stochastically complete, then* $(e^{-t\widetilde{\mathbf{h}}})_{t>0}$ *is stochastically complete.*
(ii) *If* $(e^{-t\widetilde{\mathbf{h}}})_{t>0}$ *is stochastically complete and the model additionally satisfies*

$$\sum_{e\in\mathcal{E}} \eta(e)\sqrt{|e|\mu(e)} < \infty, \tag{4.6.2}$$

then $(e^{-t\widetilde{\mathbf{H}}})_{t>0}$ *is stochastically complete.*

[‡]It is assumed in [**70**], [**112**] that $\mathcal{G}$ is complete as a metric space with respect to the corresponding intrinsic metric, which implies the self-adjointness of both $\mathbf{H}$ and $\mathbf{h}$, see Theorem 7.1.

Notice that one can always find a model satisfying (4.6.2) since by cutting a given edge e into N equal edges, the corresponding summand $\eta(e)\sqrt{|e|\mu(e)}$ in (4.6.2) is replaced with $\frac{1}{\sqrt{N}}\eta(e)\sqrt{|e|\mu(e)}$. Taking this into account we end up with the following immediate corollary.

Corollary 4.24. *Let $(\mathcal{G},\mu,\nu)$ be a weighted metric graph and let $\widetilde{\mathbf{H}} \in \mathrm{Ext}_M(\mathbf{H}^0)$ be a Markovian extension of $\mathbf{H}^0$. Then:*

(i) $(e^{-t\widetilde{\mathbf{H}}})_{t>0}$ *is stochastically complete exactly when for each model of $(\mathcal{G},\mu,\nu)$ having finite intrinsic size the heat semigroup $(e^{-t\widetilde{\mathbf{h}}})_{t>0}$ with the generator $\widetilde{\mathbf{h}}$ defined by* (4.3.17) *is stochastically complete.*

(ii) $(e^{-t\widetilde{\mathbf{H}}})_{t>0}$ *is not stochastically complete exactly when for each model of $(\mathcal{G},\mu,\nu)$ having finite intrinsic size and satisfying* (4.6.2) *the corresponding heat semigroup $(e^{-t\widetilde{\mathbf{h}}})_{t>0}$ is not stochastically complete.*

Remark 4.25. By Corollary 4.24(i), stochastic incompleteness of $(e^{-t\widetilde{\mathbf{H}}})_{t>0}$ is equivalent to the existence of a model of finite intrinsic size such that $(e^{-t\widetilde{\mathbf{h}}})_{t>0}$ is not stochastically complete. The point of Corollary 4.24(ii) is to provide an explicit class of models for which $\widetilde{\mathbf{H}}$ and $\widetilde{\mathbf{h}}$ are simultaneously stochastically complete.

Proof of Theorem 4.23. (i) was essentially obtained in [**70**], [**112**] and we only slightly adapt the proof of [**112**, pp. 137–140] to our setting. Suppose $(e^{-t\widetilde{\mathbf{H}}})_{t>0}$ is stochastically complete and consider the operator $\widetilde{\mathbf{h}}$ (see (4.3.17)) for some fixed model of $(\mathcal{G},\mu,\nu)$ satisfying (4.3.3). By Lemma B.6, there exists a sequence $(f_n) \subset \mathrm{dom}(\widetilde{\mathfrak{Q}})$ such that $0 \le f_n \le 1$ for all $n \ge 0$, $\lim_{n\to\infty} f_n = 1$ a.e. on $\mathcal{G}$, and

$$\lim_{n\to\infty} \widetilde{\mathfrak{Q}}[f_n, g] = 0$$

for all $g \in \mathrm{dom}(\widetilde{\mathfrak{Q}}) \cap L^1(\mathcal{G};m)$. By Corollary 4.14, $\mathbf{f}_n = \imath_{\mathcal{V}}(f_n) \in \mathrm{dom}(\widetilde{\mathfrak{q}})$ and $0 \le \mathbf{f}_n \le 1$ for all $n \ge 0$. Moreover, using additionally Lemma 4.2, we see that

$$\lim_{n\to\infty} \widetilde{\mathfrak{q}}[\mathbf{f}_n, \mathbf{g}] = \lim_{n\to\infty} \widetilde{\mathfrak{Q}}[\imath_{\mathcal{V}}^{-1}(\mathbf{f}_n), \imath_{\mathcal{V}}^{-1}(\mathbf{g})] = \lim_{n\to\infty} \widetilde{\mathfrak{Q}}[f_n, \imath_{\mathcal{V}}^{-1}(\mathbf{g})] = 0$$

for all $\mathbf{g} \in \mathrm{dom}(\widetilde{\mathfrak{q}}) \cap \ell^1(\mathcal{V};m)$. Taking into account again Lemma B.6, it remains to show that $\lim_{n\to\infty} \mathbf{f}_n(v) = 1$ for all vertices $v \in \mathcal{V}$. We decompose $f_n = f_{n,\mathrm{lin}} + f_{n,0}$ as in (4.3.13), where $f_{n,\mathrm{lin}} \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ and $f_{n,0} \in H^1_0(\mathcal{G}\backslash\mathcal{V})$. Denote by g_n^e the restriction of $f_{n,0}$ to the edge $e \in \mathcal{E}$ and extended by zero to the rest of $\mathcal{G}$. Clearly g_n^e belongs to $\mathrm{dom}(\widetilde{\mathfrak{Q}}) \cap L^1(\mathcal{G})$ and taking into account Corollary 4.14, we see that

$$\lim_{n\to\infty} \int_e |\nabla g_n^e|^2\, \nu(\mathrm{d}x_e) = \lim_{n\to\infty} \widetilde{\mathfrak{Q}}[g_n^e, g_n^e] = \lim_{n\to\infty} \widetilde{\mathfrak{Q}}[f_n, g_n^e] = 0.$$

Since g_n^e has support contained in the edge e, this implies that $\lim_{n\to\infty} g_n^e(x) = 0$ for all $x \in e$ and hence $\lim_{n\to\infty} f_{n,0}(x) = 0$ for all $x \in \mathcal{G}$. Thus $\lim_{n\to\infty} f_{n,\mathrm{lin}}(x) = 1$ on $\mathcal{G}$, which implies the desired property of $(\mathbf{f}_n)$.

(ii) Suppose now that $(e^{-t\widetilde{\mathbf{h}}})_{t>0}$ is stochastically complete for some model of $(\mathcal{G},\mu,\nu)$ satisfying (4.3.3). By Lemma B.6, there exists a sequence $(\mathbf{f}_n) \subset \mathrm{dom}(\widetilde{\mathfrak{q}})$ such that $0 \le \mathbf{f}_n \le 1$, $\lim_{n\to\infty} \mathbf{f}_n(v) = 1$ for all $v \in \mathcal{V}$ and $\lim_{n\to\infty} \widetilde{\mathfrak{q}}[\mathbf{f}_n, g] = 0$ for all $g \in \mathrm{dom}(\widetilde{\mathfrak{q}}) \cap \ell^1(\mathcal{V};m)$. Define $f_n := \imath_{\mathcal{V}}^{-1}(\mathbf{f}_n) \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ and notice that (f_n) is a sequence in $\mathrm{dom}(\widetilde{\mathfrak{Q}})$ with $0 \le f_n \le 1$ and $\lim_{n\to\infty} f_n(x) = 1$ for all $x \in \mathcal{G}$.

Moreover, by Corollary 4.14 we have

$$\widetilde{\mathfrak{Q}}[f_n, g] = \widetilde{\mathfrak{Q}}[f_n, g_{\text{lin}}] = \widetilde{\mathfrak{q}}[\mathbf{f}_n, \imath_{\mathcal{V}}(g_{\text{lin}})]$$

for all $g \in \text{dom}(\widetilde{\mathfrak{Q}})$. Hence, by Lemma B.6, the stochastic completeness of $(e^{-t\widetilde{\mathbf{H}}})_{t>0}$ would follow if we could prove that $\mathbf{g} := \imath_{\mathcal{V}}(g_{\text{lin}})$ belongs to $\text{dom}(\widetilde{\mathfrak{q}}) \cap \ell^1(\mathcal{V}; m)$ for all $g \in \text{dom}(\widetilde{\mathfrak{Q}}) \cap L^1(\mathcal{G})$. Taking into account Corollary 4.14 and Lemma 4.2 with $p = 1$, it suffices to show that $g_{\text{lin}} \in L^1(\mathcal{G}; \mu)$ and the additional assumption (4.6.2) is needed exactly for this purpose. Indeed, for an edge $e \in \mathcal{E}_v$, the estimate

$$\begin{aligned}|g_{\text{lin}}(x) - g(x)| &\le |g_{\text{lin}}(x) - g_{\text{lin}}(v)| + |g(x) - g(v)| \\ &\le |e|^{1/2}\Big(\int_e |\nabla g_{\text{lin}}(x_e)|^2 \mathrm{d}x_e\Big)^{1/2} + |e|^{1/2}\Big(\int_e |\nabla g(x_e)|^2 \mathrm{d}x_e\Big)^{1/2}\end{aligned}$$

holds for all $x \in e$. Taking into account Corollary 4.14 this implies

$$\int_e |g_{\text{lin}}(x) - g(x)|\, \mu(\mathrm{d}x) \le 2\eta(e)\sqrt{|e|\mu(e)}\sqrt{\widetilde{\mathfrak{Q}}[g]}, \qquad e \in \mathcal{E},$$

and hence

$$\int_{\mathcal{G}} |g_{\text{lin}}(x)|\mu(\mathrm{d}x) \le \|g\|_{L^1(\mathcal{G};\mu)} + 2\sqrt{\widetilde{\mathfrak{Q}}[g]}\sum_{e\in\mathcal{E}} \eta(e)\sqrt{|e|\mu(e)},$$

which proves the claim. □

REMARK 4.26. A few remarks are in order.

(i) As in the manifold case (see, e.g., [**88**, Theorem 6.2]), stochastic completeness for both Kirchhoff Laplacians and graph Laplacians admits several equivalent reformulations in terms of λ-harmonic or λ-subharmonic functions and the uniqueness for the heat equation in L^∞ or ℓ^∞ (Khas'minskii-type theorems). Therefore, both Theorem 4.23 and Corollary 4.24 can be reformulated in these terms. For further details we refer to Section 7.5.

(ii) The condition (4.6.2) in Theorem 4.23 is far from being optimal. Actually, what one needs in order to prove the converse implication to (i) in Theorem 4.23 is the boundedness of $\imath_{\mathcal{V}}$ as a map from $\text{dom}(\widetilde{\mathfrak{Q}}) \cap L^1(\mathcal{G}; \mu)$ to $\text{dom}(\widetilde{\mathfrak{q}}) \cap \ell^1(\mathcal{V}; m)$.

(iii) Theorem 4.23 extends in an obvious way to the case of nontrivial δ-couplings, of course under the positivity assumption that $\alpha \ge 0$ on $\mathcal{V}$.

(iv) In [**115**] and [**114**], a "refinement" of a graph $(\mathcal{V}, m; b)$ was suggested (see [**114**, Def. 1.4] and [**115**, Def. 1.10]). It is very much similar to the construction induced by (3.1.5)–(3.1.6) when refining a weighted metric graph, however, the corresponding difference can be seen as adding loops at the end vertices of a refined edge in order to keep the same vertex weights. Moreover, the construction from [**114**], [**115**] enjoys the same important stability property w.r.t. stochastic completeness: *if a refined graph is stochastically complete, then so is the original graph* $(\mathcal{V}, m; b)$ (see [**114**, Theorem 1.5]).

4.7. Spectral estimates

Recall that in Theorem 3.22(v) we observed the following equivalence between strict positivity of spectra,

$$\lambda_0(\widetilde{\mathbf{H}}) = \inf \sigma(\widetilde{\mathbf{H}}) > 0 \qquad \Longleftrightarrow \qquad \lambda_0(\widetilde{\mathbf{h}}) = \inf \sigma(\widetilde{\mathbf{h}}) > 0$$

for a nonnegative extension $\widetilde{\mathbf{H}}$ of $\mathbf{H}^0$ on a weighted metric graph $(\mathcal{G}, \mu, \nu)$ and the associated nonnegative extension $\widetilde{\mathbf{h}}$ of $\mathbf{h}^0$ on a fixed model having finite intrinsic size. In this section we present a simple two-sided estimate between $\lambda_0(\widetilde{\mathbf{H}})$ and $\lambda_0(\widetilde{\mathbf{h}})$ based on the results of Section 4.3.

THEOREM 4.27. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph together with a fixed model. Suppose $\widetilde{\mathbf{H}} \in \mathrm{Ext}_S(\mathbf{H}^0)$ is a nonnegative extension of $\mathbf{H}^0$ and consider in $\ell^2(\mathcal{V}; m)$ the nonnegative extension $\widetilde{\mathbf{h}} \in \mathrm{Ext}_S(\mathbf{h}^0)$ of $\mathbf{h}^0$ defined by* (4.3.17). *Then*

$$\min\Big\{\lambda_0(\widetilde{\mathbf{h}}),\ \frac{1}{2}\Big(\frac{\pi}{\eta^*(\mathcal{E})}\Big)^2\Big\} \le \lambda_0(\widetilde{\mathbf{H}}) \le \min\Big\{6\lambda_0(\widetilde{\mathbf{h}}),\ \Big(\frac{\pi}{\eta^*(\mathcal{E})}\Big)^2\Big\}. \tag{4.7.1}$$

PROOF. First of all, recall from Theorem 3.22(ii) that $\widetilde{\mathbf{H}} \ge 0$ exactly when $\widetilde{\mathbf{h}} \ge 0$. Moreover, since $\widetilde{\mathbf{H}}$ is a nonnegative extension of $\mathbf{H}_{\min} = \mathbf{H}^*_{\max}$, whose Friedrichs extension $\mathbf{H}^F$ is given by (3.2.43), we conclude from (3.2.45) that

$$\lambda_0(\widetilde{\mathbf{H}}) \le \lambda_0(\mathbf{H}^F) = \frac{\pi^2}{\eta^*(\mathcal{E})^2}.$$

In particular, (4.7.1) trivially holds if the model has infinite intrinsic size since all three terms vanish in this case (see also Corollary 3.18(iii)). Hence in the following, we assume $\eta^*(\mathcal{E}) < \infty$.

Recall the following variational characterization via the Rayleigh quotient

$$\lambda_0(\widetilde{\mathbf{H}}) = \inf_{f \in \mathrm{dom}(\widetilde{\mathbf{H}})} \frac{\langle \widetilde{\mathbf{H}} f, f\rangle_{L^2(\mathcal{G};\mu)}}{\|f\|^2_{L^2(\mathcal{G};\mu)}}, \qquad \lambda_0(\widetilde{\mathbf{h}}) = \inf_{\mathbf{f} \in \mathrm{dom}(\widetilde{\mathbf{h}})} \frac{\langle \widetilde{\mathbf{h}}\, \mathbf{f}, \mathbf{f}\rangle_{\ell^2(\mathcal{V};m)}}{\|\mathbf{f}\|^2_{\ell^2(\mathcal{V};m)}}. \tag{4.7.2}$$

Turning to the upper estimate in terms of $\lambda_0(\widetilde{\mathbf{h}}_0)$, let $\mathbf{f} \in \mathrm{dom}(\widetilde{\mathbf{h}})$ be fixed. By Corollary 4.9, there is $f = f_{\mathrm{lin}} + f_0 \in \mathrm{dom}(\widetilde{\mathbf{H}})$ such that $\imath_{\mathcal{V}}(f) = \mathbf{f}$ and $f_0 \in \dot{H}^1_0(\mathcal{G}\setminus\mathcal{V})$. Moreover, by (4.3.16) and (4.3.3), $\dot{H}^1_0(\mathcal{G}\setminus\mathcal{V}) = H^1_0(\mathcal{G}\setminus\mathcal{V})$ algebraically and topologically. Modifying f by edgewise H^2-functions vanishing in a neighborhood of $\mathcal{V}$, we readily construct a sequence $(f_n) \subseteq \mathrm{dom}(\widetilde{\mathbf{H}})$, $f_n = f_{n,\mathrm{lin}} + f_{n,0}$ such that $\imath_{\mathcal{V}}(f_n) = \imath_{\mathcal{V}}(f_{n,\mathrm{lin}}) = \mathbf{f}$ and

$$\lim_{n\to\infty} \mathfrak{Q}[f_{n,0}] + \|f_{n,0}\|_{L^2(\mathcal{G};\mu)} = 0.$$

Hence we conclude from Corollary 4.9 that

$$\lambda_0(\widetilde{\mathbf{H}}) \le \lim_{n\to\infty} \frac{\langle \widetilde{\mathbf{H}} f_n, f_n\rangle_{L^2(\mathcal{G};\mu)}}{\|f_n\|^2_{L^2(\mathcal{G};\mu)}} = \frac{\langle \widetilde{\mathbf{h}}\, \mathbf{f}, \mathbf{f}\rangle_{\ell^2(\mathcal{V};m)}}{\|\imath_{\mathcal{V}}^{-1}(\mathbf{f})\|^2_{L^2(\mathcal{G};\mu)}},$$

and Remark 4.3(ii) finishes the proof of the upper estimate in (4.7.1).

It remains to prove the lower inequality in (4.7.1). By Corollary 4.9, every function $f \in \mathrm{dom}(\widetilde{\mathbf{H}})$ can be decomposed as $f = f_{\mathrm{lin}} + f_0$ with $f_{\mathrm{lin}} \in \mathrm{CA}(\mathcal{G}\setminus\mathcal{V})$ and $f_0 \in \dot{H}^1_0(\mathcal{G}\setminus\mathcal{V})$ (see also (4.3.13)). Setting $\mathbf{f} := \imath_{\mathcal{V}}(f)$, (4.3.21) together with (4.3.16) imply that

$$\begin{aligned}\langle \widetilde{\mathbf{H}} f, f\rangle_{L^2(\mathcal{G};\mu)} &\ge \langle \widetilde{\mathbf{h}}\, \mathbf{f}, \mathbf{f}\rangle_{\ell^2(\mathcal{V};m)} + \frac{\pi^2}{\eta^*(\mathcal{E})^2}\|f_0\|^2_{L^2(\mathcal{G};\mu)} \\ &\ge \lambda_0(\widetilde{\mathbf{h}})\|\mathbf{f}\|^2_{\ell^2(\mathcal{V};m)} + \frac{\pi^2}{\eta^*(\mathcal{E})^2}\|f_0\|^2_{L^2(\mathcal{G};\mu)}.\end{aligned}$$

The lower estimate in (4.7.1) now follows from Remark 4.3(ii) and the trivial inequality $\|f\|^2_{L^2(\mathcal{G};\mu)} \le 2\|f_{\mathrm{lin}}\|^2_{L^2(\mathcal{G};\mu)} + 2\|f_0\|^2_{L^2(\mathcal{G};\mu)}$. □

We shall continue the study of the positivity of spectral gaps in Section 7.3 and now we complete this section with a few remarks.

REMARK 4.28. The constant in the second estimate in (4.7.1) can be improved. For instance, a modified version of [**177**, Cor. 2.2 and Rem. 2.3] yields the bound

$$\lambda_0(\widetilde{\mathbf{H}}) \le \frac{\pi^2}{2}\lambda_0(\widetilde{\mathbf{h}}).$$

REMARK 4.29. Theorem 4.27 remains valid for Laplacians with δ-couplings $\mathbf{H}^0_\alpha$ (see Section 2.4.3) and their associated discrete Laplacians $\mathbf{h}^0_\alpha$ (see (3.1.7) and Theorem (3.1) and Remark 3.24), of course under the additional assumption that all strengths are nonnegative, that is, $\alpha\colon \mathcal{V} \to [0,\infty)$.

4.8. Ultracontractivity estimates

Theorem 4.27 shows that under the additional assumption (4.3.3), there is a connection between the decay of heat semigroups $\mathrm{e}^{-t\widetilde{\mathbf{H}}}$ and $\mathrm{e}^{-t\widetilde{\mathbf{h}}}$ since $\|\mathrm{e}^{-t\widetilde{\mathbf{H}}}\|_{L^2} = \mathrm{e}^{-t\lambda_0(\widetilde{\mathbf{H}})}$ and $\|\mathrm{e}^{-t\widetilde{\mathbf{h}}}\|_{\ell^2} = \mathrm{e}^{-t\lambda_0(\widetilde{\mathbf{h}})}$ for all $t > 0$. Our next result indicates that the connection between the decay of heat semigroups can be specified further if $\lambda_0(\mathbf{H}) = \lambda_0(\mathbf{h}) = 0$. More specifically, we are going to relate small and large time behavior of the heat kernels by studying the corresponding ultracontractivity estimates.

THEOREM 4.30. *Let $(\mathcal{G},\mu,\nu)$ be a weighted metric graph together with a fixed model having finite intrinsic size. Let also $\widetilde{\mathbf{H}} \in \mathrm{Ext}_M(\mathbf{H}^0)$ be a Markovian extension of $\mathbf{H}^0$ and consider the associated Markovian extension $\widetilde{\mathbf{h}}$ of $\mathbf{h}^0$ on $\ell^2(\mathcal{V};m)$ defined by* (4.3.17)*.*

(i) *If $(\mathrm{e}^{-t\widetilde{\mathbf{H}}})_{t>0}$ is ultracontractive and there are $D \ge 1$ and $C_1 > 0$ such that*

$$\|\mathrm{e}^{-t\widetilde{\mathbf{H}}}\|_{L^1\to L^\infty} \le C_1 t^{-D/2} \tag{4.8.1}$$

holds for all $t > 0$, then $(\mathrm{e}^{-t\widetilde{\mathbf{h}}})_{t>0}$ is ultracontractive and

$$\|\mathrm{e}^{-t\widetilde{\mathbf{h}}}\|_{\ell^1\to \ell^\infty} \le C_2 t^{-D/2} \tag{4.8.2}$$

holds for all $t > 0$ with some positive constant $C_2 > 0$.

(ii) *If there is $D > 2$ such that the heat kernel of $\widetilde{\mathbf{h}}$ satisfies* (4.8.2) *for all $t > 0$ and, in addition, the underlying model satisfies*

$$\sup_{e\in\mathcal{E}} \big(|e|\mu(e)\big)^{1-2/D}\frac{|e|}{\nu(e)} < \infty, \tag{4.8.3}$$

then the heat kernel of $\widetilde{\mathbf{H}}$ satisfies (4.8.1) *for all $t > 0$ with some positive constant $C_1 > 0$.*

PROOF. (i) Suppose that (4.8.1) holds true for all $t > 0$ with some fixed $D \ge 1$. Then, by Theorem C.4, the Nash-type inequality

$$\|f\|^{2+4/D}_{L^2(\mathcal{G};\mu)} \le C\,\widetilde{\mathfrak{Q}}[f]\,\|f\|^{4/D}_{L^1(\mathcal{G};\mu)} \tag{4.8.4}$$

holds true for all $0 \le f \in \mathrm{dom}(\widetilde{\mathfrak{Q}}) \cap L^1(\mathcal{G};\mu)$, where $\widetilde{\mathfrak{Q}}$ is the Dirichlet forms associated with $\widetilde{\mathbf{H}}$. However, restricting in (4.8.4) to edgewise affine functions and then using Corollary 4.14 and the second inequality in (4.3.4) with $p = 2$ together with the first one with $p = 1$ (see also Remark 4.3(iii)), one easily concludes that (4.8.4) implies

$$\|\mathbf{f}\|^{2+4/D}_{\ell^2(\mathcal{V};m)} \le \widetilde{C}\,\widetilde{\mathfrak{q}}[\mathbf{f}]\,\|\mathbf{f}\|^{4/D}_{\ell^1(\mathcal{V};m)}, \qquad \widetilde{C} = 4^{2+4/D}C, \tag{4.8.5}$$

for all $0 \le \mathbf{f} \in \mathrm{dom}(\widetilde{\mathfrak{q}}) \cap \ell^1(\mathcal{V};m)$, where $\widetilde{\mathfrak{q}}$ is the Dirichlet forms associated with $\widetilde{\mathbf{h}}$. By Theorem C.4, this implies (4.8.2) for all $t > 0$.

(ii) Suppose now that (4.8.2) holds true for all $t > 0$ with some fixed $D > 2$. Then, by Varopoulos's theorem (Theorem C.2), the Sobolev-type inequality

$$\|\mathbf{f}\|^2_{\ell^q(\mathcal{V};m)} \le C\,\widetilde{\mathfrak{q}}[\mathbf{f}], \qquad \mathbf{f} \in \mathrm{dom}(\widetilde{\mathfrak{q}}), \tag{4.8.6}$$

is valid, where $q = q(D) := \frac{2D}{D-2}$. Since the model satisfies (4.3.3), by Corollary 4.14, every $f \in \mathrm{dom}(\widetilde{\mathfrak{Q}})$ admits a unique decomposition $f = \imath_{\mathcal{V}}^{-1}(\mathbf{f}) + f_0$ with $\mathbf{f} \in \mathrm{dom}(\widetilde{\mathfrak{q}})$, $f_0 \in H^1_0(\mathcal{G}\setminus\mathcal{V})$ and, moreover,

$$\widetilde{\mathfrak{Q}}[f] = \widetilde{\mathfrak{q}}[\mathbf{f}] + \mathfrak{Q}[f_0] = \widetilde{\mathfrak{q}}[\mathbf{f}] + \|\nabla f_0\|^2_{L^2(\mathcal{G};\nu)}.$$

Using Lemma 4.2, the first inequality in (4.3.4) with $p = q$ together with (4.8.6) imply that

$$\|\imath_{\mathcal{V}}^{-1}(\mathbf{f})\|^2_{L^q(\mathcal{G};\mu)} \le C\,\widetilde{\mathfrak{q}}[\mathbf{f}]. \tag{4.8.7}$$

Next, using the following simple estimate

$$\Big(\int_0^\ell |f(s)|^q \mathrm{d}s\Big)^{2/q} \le \ell^{2/q} \sup_{0\le x\le \ell} |f(x)|^2 \le \ell^{1+2/q}\int_0^\ell |f'(s)|^2 \mathrm{d}s,$$

which holds true for all $f \in H^1_0(0,\ell)$ and $\ell > 0$, we obtain

$$\Big(\int_e |f(x)|^q \mu(\mathrm{d}x)\Big)^{2/q} \le |e|^{1+2/q}\frac{\mu(e)^{2/q}}{\nu(e)}\int_e |\nabla f(x)|^2 \nu(\mathrm{d}x), \qquad f \in H^1_0(\mathcal{G}\setminus\mathcal{V}),$$

for each edge $e \in \mathcal{E}$. Since $q > 2$, this immediately implies the inequality

$$\|f_0\|^2_{L^q(\mathcal{G};\mu)} \le C\,\|\nabla f_0\|^2_{L^2(\mathcal{G};\nu)}, \tag{4.8.8}$$

for all $f_0 \in H^1_0(\mathcal{G}\setminus\mathcal{V})$, where the constant $C = C(\mathcal{E},\mu,\nu)$ depends only on the model and edge weights μ,ν and is given by

$$C(\mathcal{E},\mu,\nu) = \sup_{e\in\mathcal{E}} |e|^{1+2/q}\frac{\mu(e)^{2/q}}{\nu(e)} = \sup_{e\in\mathcal{E}} (|e|\mu(e))^{1-2/D}\frac{|e|}{\nu(e)}.$$

Thus, combining (4.8.8) with (4.8.7), we arrive at the following Sobolev-type inequality

$$\|f\|^2_{L^q(\mathcal{G};\mu)} \le \widetilde{C}\,\widetilde{\mathfrak{Q}}[f], \qquad f \in \mathrm{dom}(\widetilde{\mathfrak{Q}}). \tag{4.8.9}$$

Applying Theorem C.2 once again, we conclude that $(\mathrm{e}^{-t\widetilde{\mathbf{H}}})_{t>0}$ is ultracontractive and (4.8.1) holds true for all $t > 0$. □

Remark 4.31. In the special case $\mu = \nu \equiv \mathbb{1}$ on $\mathcal{G}$, Theorem 4.30 was proved in [**67**, § 5]. However, the proof of Theorem 4.30(i) in [**67**] was based on the use of Varopoulos' Theorem and hence was restricted to the case $D > 2$. Notice that Theorem 4.30(i) with $\mu = \nu \equiv \mathbb{1}$ was observed by G. Rozenblum and M. Solomyak (see [**186**, Theorem 4.1]), however, for a different discrete Laplacian (the vertex weight m is defined in [**186**] as the vertex degree function $\deg\colon v \mapsto \#(\vec{\mathcal{E}}_v)$).

The proof of Theorem 4.30(ii) indicates that (4.8.3) is necessary for the validity of (4.8.1) for $t > 0$. As the next result shows, it is indeed necessary for all $D > 0$.

LEMMA 4.32. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph and let $\widetilde{\mathbf{H}} \in \mathrm{Ext}_M(\mathbf{H}^0)$ be a Markovian extension of $\mathbf{H}^0$. Assume also that $(\mathrm{e}^{-t\widetilde{\mathbf{H}}})_{t>0}$ is ultracontractive. If there is a model of $(\mathcal{G}, \mu, \nu)$ such that (4.8.3) fails to hold for a given $D > 0$, then*

$$\sup_{t\in(0,1)} t^{D/2}\, \|\mathrm{e}^{-t\widetilde{\mathbf{H}}}\|_{L^1\to L^\infty} = \infty. \tag{4.8.10}$$

In particular, (4.8.10) *always holds for $D \in (0, 1)$.*

PROOF. Assume the converse, that is, (4.8.1) holds for all $t \in (0, 1)$ with some fixed $D > 0$. Then, by Theorem C.4, this implies that the Nash-type inequality

$$\|f\|^{2+4/D}_{L^2(\mathcal{G};\mu)} \le C\, (\widetilde{\mathfrak{Q}}[f] + \|f\|^2_{L^2(\mathcal{G};\mu)})\, \|f\|^{4/D}_{L^1(\mathcal{G};\mu)} \tag{4.8.11}$$

holds true for all $0 \le f \in \mathrm{dom}(\widetilde{\mathfrak{Q}}) \cap L^1(\mathcal{G}; \mu)$. In particular, this inequality holds for all $0 \le f \in H^1_0(\mathcal{G}\backslash\mathcal{V}) \cap L^1(\mathcal{G}; \mu)$. It remains to apply a scaling argument. Indeed, take a positive function $0 \ne f_0 \in H^1_0([0, 1])$ with $\|f_0\|_{L^1} = 1$ and choose a model of $(\mathcal{G}, \mu, \nu)$ satisfying (4.3.3). Next define $f_e \in H^1_0(\mathcal{G}\backslash\mathcal{V})$ as $f_0(\cdot/|e|)$ on e (upon identification of $e \in \mathcal{E}$ with $\mathcal{I}_e = [0, |e|]$) and then extend it by 0 to the rest of $\mathcal{G}\backslash e$. Clearly, $0 \le f_e \in \mathrm{dom}(\widetilde{\mathfrak{Q}}) \cap L^1(\mathcal{G}; \mu)$ for all $e \in \mathcal{E}$ and

$$\|f_e\|_{L^1(\mathcal{G};\mu)} = |e|\mu(e), \quad \|f_e\|^2_{L^2(\mathcal{G};\mu)} = |e|\mu(e)\|f_0\|^2_2, \quad \mathfrak{Q}[f_e] = \frac{\nu(e)}{|e|}\|f_0'\|^2_2. \tag{4.8.12}$$

Plugging f_e into (4.8.11), we get

$$\begin{aligned} C &\ge \frac{(|e|\mu(e))^{1+2/D}\|f_0\|_2^{2+4/D}}{\big(\frac{\nu(e)}{|e|}\|f_0'\|_2^2 + |e|\mu(e)\|f_0\|_2^2\big)(|e|\mu(e))^{4/D}} \ge \frac{(|e|\mu(e))^{1-2/D}\|f_0\|_2^{2+4/D}}{\frac{\nu(e)}{|e|}\big(\|f_0'\|_2^2 + \eta^*(\mathcal{E})^2\|f_0\|_2^2\big)} \\ &= \left(\frac{\eta(e)^{2D-2}}{\mu(e)\nu(e)}\right)^{\frac{1}{D}} \frac{\|f_0\|_2^{2+4/D}}{\|f_0'\|_2^2 + \eta^*(\mathcal{E})^2\|f_0\|_2^2} \end{aligned}$$

for all $e \in \mathcal{E}$. Since $\eta^*(\mathcal{E}) < \infty$, the latter is unbounded from above if (4.8.3) fails to hold, and hence we arrive at a contradiction, which proves the first claim.

To prove the last claim it suffices to mention that $2D - 2 < 0$ if $D \in (0, 1)$ and hence we can always find a model such that (4.8.3) is not true with $D \in (0, 1)$. □

Using Theorem C.6, it is possible to extend the above connections to subexponential scales. In the next result we shall always assume that $s\colon \mathbb{R}_{>0} \to \mathbb{R}_{>0}$ *is a decreasing differentiable bijection such that its logarithmic derivative has polynomial growth* (see (C.0.9)). For instance, those are functions that behave like $t^{-d/2}$ with $d > 0$ for small t, and e^{-ct^α} with $\alpha \in (0, 1]$ for large D (notice that $\alpha > 1$ is also allowed, however, heat semigroups cannot have such a fast decay at infinity).

THEOREM 4.33. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph together with a fixed model having finite intrinsic size. Let also $\widetilde{\mathbf{H}} \in \mathrm{Ext}_M(\mathbf{H}^0)$ be a Markovian extension of $\mathbf{H}^0$ and consider the associated Markovian extension $\widetilde{\mathbf{h}}$ of $\mathbf{h}^0$ on $\ell^2(\mathcal{V}; m)$ defined by* (4.3.17).

(i) *If $(\mathrm{e}^{-t\widetilde{\mathbf{H}}})_{t>0}$ is ultracontractive and*

$$\|\mathrm{e}^{-t\widetilde{\mathbf{H}}}\|_{L^1\to L^\infty} \le s(t), \qquad t > 0, \tag{4.8.13}$$

then $(\mathrm{e}^{-t\widetilde{\mathbf{h}}})_{t>0}$ *is ultracontractive and*

$$\|\mathrm{e}^{-t\widetilde{\mathbf{h}}}\|_{\ell^1\to\ell^\infty} \le s(ct) \tag{4.8.14}$$

holds for all $t>0$ *with some positive constant* $c>0$.

(ii) *If* (4.8.13) *holds true, then there is a positive constant* $C>0$ *such that*

$$\Big(\frac{8|e|\mu(e)}{\pi^2}\Big)^2\theta_s\Big(\frac{\pi^2}{8\,|e|\mu(e)}\Big) \le 8\frac{\nu(e)}{|e|}, \qquad \theta_s := -s'\circ s^{-1}, \tag{4.8.15}$$

for all $e\in\mathcal{E}$.

Proof. (i) For simplicity we assume that $\mathbf{H}$ is self-adjoint. Our proof is based on the use of Theorem C.6 and its proof in [**45**]. First of all, by Proposition II.2 from [**45**], (4.8.13) implies that

$$\gamma_s(\|f\|^2_{L^2(\mathcal{G};\mu)}) \le \mathfrak{Q}[f], \tag{4.8.16}$$

for all $0\le f\in \mathrm{dom}(\mathfrak{Q})$ with $\|f\|_{L^1(\mathcal{G};\mu)}\le 1$. Here the function $\gamma_s\colon \mathbb{R}_{>0}\to\mathbb{R}_{>0}$ is given by

$$\gamma_s(x) := \sup_{r>0}\frac{x}{2r}\log\Big(\frac{x}{s(r)}\Big). \tag{4.8.17}$$

In particular, the latter holds for edgewise affine functions and hence restricting to $0\le f\in \mathrm{CA}(\mathcal{G}\setminus\mathcal{V})$ we get by taking into account (4.3.10) and (4.3.11) that

$$\gamma_s(4^{-1}\|\mathbf{f}\|^2_{\ell^2(\mathcal{V};m)}) \le 4\mathfrak{q}[\mathbf{f}], \tag{4.8.18}$$

for all $0\le \mathbf{f}\in\mathrm{dom}(\mathfrak{q})$ with $\|\mathbf{f}\|_{L^1(\mathcal{V};m)}\le 1$. Here we also used (4.3.4) with $p=2$ together with the monotonicity of the logarithm. Now, taking into account that $\theta_{4s}(x) = 4\theta_s(x/4)$, by [**45**, Lemma II.3], there is $\widetilde{C}>0$ such that

$$\theta(4^{-1}\|\mathbf{f}\|^2_{\ell^2(\mathcal{V};m)}) \le \widetilde{C}\mathfrak{q}[\mathbf{f}], \tag{4.8.19}$$

for all $0\le \mathbf{f}\in\mathrm{dom}(\mathfrak{q})$ with $\|\mathbf{f}\|_{\ell^1(\mathcal{V};m)}\le 1$. It remains to use Theorem C.6 once again.

(ii) By Theorem C.6, (4.8.13) implies the Nash-type inequality

$$\theta_s\big(\|f\|^2_{L^2(\mathcal{G};\mu)}\big) \le C\mathfrak{Q}[f], \tag{4.8.20}$$

for all $f\in\mathrm{dom}(\mathfrak{Q})$ with $\|f\|_{L^1(\mathcal{G};\mu)}=1$. Pick $0\le f_0\in H^1_0([0,1])$ with $\|f_0\|_1=1$. For each $e\in\mathcal{E}$, define $f_e\in H^1_0(\mathcal{G})$ as in the proof of Lemma 4.32. Plugging $f=\frac{1}{|e|\mu(e)}f_e$ into (4.8.20) and taking into account (4.8.12), we get

$$\theta_s\Big(\frac{\|f_0\|_2^2}{|e|\mu(e)}\Big) \le \frac{\nu(e)}{|e|}\Big(\frac{\|f_0'\|_2}{|e|\mu(e)}\Big)^2, \tag{4.8.21}$$

for all $e\in\mathcal{E}$ and each $0\le f_0\in H^1_0([0,1])$ with $\|f_0\|_1=1$. Finally, choosing $f_0(x)=\frac{\pi}{2}\sin(\pi x)$ in (4.8.21), we end up with (4.8.15). ☐

Remark 4.34. We are convinced that (4.8.14) together with (4.8.15) should imply the estimate (4.8.13), however, we have not succeeded in proving it by applying T. Coulhon's extension of Theorem C.4. Let us also stress that in the case of a polynomial decay our proof of Theorem 4.30(ii) is based on Varopoulos's theorem (Theorem C.2) and hence the range of the corresponding exponent is restricted to $D>2$.

CHAPTER 5

1-D Schrödinger operators with point interactions

Let us demonstrate our findings by considering the simplest possible situation: Fix $\mathcal{L} \in (0,\infty]$ and let $(x_k)_{k\geq 0} \subset \mathcal{I} := [0,\mathcal{L})$ be a strictly increasing sequence such that $x_0 = 0$ and $x_k \uparrow \mathcal{L}$. Considering (x_k) as a vertex set and the intervals $e_k = [x_k, x_{k+1}]$ as edges, we end up with the simplest infinite metric graph – an infinite *path graph*. In this case the edge weights $\mu, \nu\colon \mathcal{I} \to \mathbb{R}_{>0}$ are given by

$$\mu(x) = \sum_{k\geq 0} \mu_k \mathbb{1}_{[x_k,x_{k+1})}(x), \qquad \nu(x) = \sum_{k\geq 0} \nu_k \mathbb{1}_{[x_k,x_{k+1})}(x), \tag{5.0.1}$$

where $(\mu_k)_{k\geq 0}$ and $(\nu_k)_{k\geq 0}$ are positive real sequences. For every real sequence $\alpha = (\alpha_k)_{k\geq 0}$ conditions (2.4.5) take the form:

$$\begin{cases} f(x_k-) = f(x_k+) =: f(x_k), \\ \nu_k f'(x_k+) - \nu_{k-1} f'(x_k-) = \alpha_k f(x_k), \end{cases} \tag{5.0.2}$$

for all $k \geq 0$, where we set $f'(0-) = 0$ for notational simplicity and hence for $k = 0$ the corresponding condition is $\nu_0 f'(0) = \alpha_0 f(0)$. The corresponding (maximal) operator $\mathrm{H}_\alpha := \mathrm{H}_{\mu,\nu,\alpha}$ acting in $L^2(\mathcal{I};\mu)$ is known as the *1d Schrödinger operator with δ-interactions* on $X = (x_k)_{k\geq 0}$ (see, e.g., [**3**]), and the corresponding differential expression is given by

$$\tau = \frac{1}{\mu(x)}\Big(-\frac{\mathrm{d}}{\mathrm{d}x}\nu(x)\frac{\mathrm{d}}{\mathrm{d}x} + \sum_{k\geq 0} \alpha_k \delta(x - x_k)\Big). \tag{5.0.3}$$

REMARK 5.1. There are manifold reasons to investigate the operator H_α. First of all, it serves as a toy model in quantum mechanics. Indeed, if $\mu_k = \nu_k = 1$ for all $k \geq 0$, then (5.0.3) turn into the usual δ-coupling on X and H_α in this case is nothing but the Hamiltonian (see [**3**], [**142**])

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{k\geq 0} \alpha_n \delta_{x_n}. \tag{5.0.4}$$

Moreover, (5.0.3) naturally appears in the study of Kirchhoff Laplacians and Laplacians with δ-couplings on family preserving graphs (see Section 8.1 for further details).

5.1. The case $\alpha \equiv 0$ and Krein strings

We begin with the study of the "unperturbed" case, that is, when $\alpha \equiv 0$ and hence (5.0.3) is the classical weighted Sturm–Liouville operator

$$\tau = -\frac{1}{\mu(x)}\frac{\mathrm{d}}{\mathrm{d}x}\nu(x)\frac{\mathrm{d}}{\mathrm{d}x}. \tag{5.1.1}$$

In this situation the well developed spectral theory of Sturm–Liouville operators [**205**] and Krein strings [**118**], [**119**] leads to rather transparent and complete, although far from being trivial, answers to some spectral questions.

Let $\mathrm{H} := \mathrm{H}_{\mu,\nu}$ be the maximal operator associated with (5.1.1) in $L^2(\mathcal{I};\mu)$ and subject to the Neumann boundary condition at $x = 0$:

$$\mathrm{dom}(\mathrm{H}) = \big\{f \in L^2(\mathcal{I};\mu)\,|\, f, \nu f' \in AC_{\mathrm{loc}}[0,\mathcal{L}),\ f'(0) = 0,\ \tau f \in L^2(\mathcal{I};\mu)\big\}. \tag{5.1.2}$$

The corresponding minimal operator H^0 is defined as the closure in $L^2(\mathcal{I};\mu)$ of the pre-minimal operator H':

$$\mathrm{H}' = \mathrm{H} \restriction \mathrm{dom}(\mathrm{H}'), \qquad \mathrm{dom}(\mathrm{H}') = \mathrm{dom}(\mathrm{H}) \cap C_c(\mathcal{I}). \tag{5.1.3}$$

It is immediate to see that H and H^0 coincide with the maximal and, respectively, minimal Kirchhoff Laplacians defined in Section 2.4.1. The next result provides a rather transparent criterion for the equality $\mathrm{H} = \mathrm{H}^0$ to hold.

LEMMA 5.2. *The operator* H *is self-adjoint if and only if the series*

$$\sum_{k\ge 0} \mu_k |e_k| \Big(\sum_{j\le k} \frac{|e_j|}{\nu_j}\Big)^2 \tag{5.1.4}$$

diverges.

PROOF. The self-adjointness criterion follows from the standard limit point/limit circle classification for (5.1.1) (see, e.g., [**205**]). Namely, $\tau y = 0$ has two linearly independent solutions

$$y_1(x) \equiv 1, \qquad y_2(x) = \int_0^x \frac{\mathrm{d}s}{\nu(s)}, \qquad x \in [0,\mathcal{L}),$$

and one simply needs to verify whether or not both y_1 and y_2 belong to $L^2(\mathcal{I};\mu)$. Clearly, $y_1 \in L^2(\mathcal{I};\mu)$ exactly when the series

$$\sum_{k\ge 0} \mu_k |e_k| \tag{5.1.5}$$

converges. Moreover, it is straightforward to check that $y_2 \in L^2(\mathcal{I};\mu)$ if and only if the series (5.1.4) converges. The Weyl alternative finishes the proof. □

The above considerations suggest to introduce the following quantity:

$$\mathcal{L}_\nu := \int_{\mathcal{I}} \frac{\mathrm{d}x}{\nu(x)} = \sum_{k\ge 0} \frac{|e_k|}{\nu_k}. \tag{5.1.6}$$

Observe that $\mathcal{L}_\nu < \infty$ exactly when all solutions to $\tau y = 0$ are bounded.

COROLLARY 5.3. *If*

$$\sum_{k\ge 0} \mu_k |e_k| = \infty, \tag{5.1.7}$$

then H *is self-adjoint. Moreover, in the case* $\mathcal{L}_\nu < \infty$*,* (5.1.7) *is also necessary for the self-adjointness.*

REMARK 5.4. A few remarks are in order.

(i) Notice that the condition (5.1.7) admits two transparent geometric reformulations. Namely, equipping the set $X = \{x_k\}_{k\geq 1}$ with weights $m\colon x_k \mapsto \mu_{k-1}|e_{k-1}| + \mu_k|e_k|$, and considering the path graph ($x_k \sim x_n$ exactly when $|k-n| = 1$) as a metric space (X, ϱ_m) equipped with the path metric ϱ_m (see Section 6.4.2 for a detailed definition), then condition (5.1.7) is equivalent to
   (a) infinite total volume: $m(X) = \sum_{k\geq 0} m(x_k) = \mu_0|e_0| + 2\sum_{k\geq 1}\mu_k|e_k|$,
   (b) completeness of (X, ϱ_m).

   In particular, Lemma 5.2 implies that completeness of (X, ϱ_m) is only sufficient for H to be self-adjoint (cf. Theorem 7.7). Moreover, observe that in the case of a path graph both conditions (a) and (b) become also necessary for the self-adjointness exactly when the constant $\mathcal{L}_\nu$ is finite, that is, when all solutions to $\tau y = 0$ are bounded.

(ii) It is an interesting and, in fact, very difficult question to decide about the self-adjointness by looking at the geometry of a given metric graph. Lemma 5.2 demonstrates that even in the simplest case of a weighted path graph its solution involves nontrivial tools.

Despite the well developed spectral theory of Sturm–Liouville operators, it turns out that the detailed spectral analysis of the operator (5.1.2) is already a difficult task even with this very special class of weights (5.0.1). However, in one particular situation the analysis is rather straightforward.

Lemma 5.5. *If the series* (5.1.4) *is convergent, then the deficiency indices of* H^0 *equal* 1 *and the self-adjoint extensions of* H^0 *form a one-parameter family* H_θ, *where* $\theta \in [0,\pi)$ *and*

$$\mathrm{dom}(\mathrm{H}_\theta) := \big\{f \in \mathrm{dom}(\mathrm{H}) \mid \cos(\theta) f_\nu(\mathcal{L}) + \sin(\theta) f'_\nu(\mathcal{L}) = 0\big\}. \tag{5.1.8}$$

Here $f_\nu(\mathcal{L}) = \lim_{x\to\mathcal{L}}(f(x) - \nu(x)f'(x)y_2(x))$ *and* $f'_\nu(\mathcal{L}) = \lim_{x\to\mathcal{L}}\nu(x)f'(x)$.

Moreover, the spectrum of H_θ *is purely discrete, bounded from below, and eigenvalues (if ordered in the non-decreasing order) obey the Weyl law:*

$$\lim_{n\to\infty}\frac{n}{\sqrt{\lambda_n(\mathrm{H}_\theta)}} = \frac{1}{\pi}\int_0^{\mathcal{L}}\sqrt{\frac{\mu(x)}{\nu(x)}}\,\mathrm{d}x = \frac{1}{\pi}\sum_{k\geq 0}|e_k|\sqrt{\frac{\mu_k}{\nu_k}}. \tag{5.1.9}$$

Proof. The first claim is standard (see, e.g., [**205**]). The second one follows from, e.g., [**84**, Chapter 6.7]. □

Remark 5.6. (i) Using the definition (3.1.1) of the intrinsic edge length, we set

$$\eta_k := \eta(e_k) = |e_k|\sqrt{\frac{\mu_k}{\nu_k}} \tag{5.1.10}$$

for all $k \in \mathbb{Z}_{\geq 0}$, and then the RHS (5.1.9) is nothing but

$$\frac{1}{\pi}\sum_{k\geq 0}\eta(e_k) = \frac{1}{\pi}\times\text{intrinsic length of }\mathcal{I}.$$

(ii) If y_2 is bounded, then $f_\nu(\mathcal{L})$ can be replaced by $\lim_{x\to\mathcal{L}} f(x)$.

The next result mostly follows from the work of I.S. Kac and M.G. Krein [**117**], [**118**] on spectral theory of Krein strings. Recall that $\lambda_0(A)$ and $\lambda_0^{\mathrm{ess}}(A)$ denote the bottoms of the spectrum, respectively, of the essential spectrum of a self-adjoint operator A.

LEMMA 5.7. *Suppose that the series* (5.1.4) *diverges, i.e., the operator* H *is self-adjont. Then:*

(i) **Positive spectral gap**: $\lambda_0(\mathrm{H}) > 0$ *if and only if*

$$\mathcal{L}_\nu = \sum_{k\geq 0} \frac{|e_k|}{\nu_k} < \infty \qquad \text{and} \qquad \sup_{n\geq 0} \sum_{k\leq n} \mu_k |e_k| \sum_{k\geq n} \frac{|e_k|}{\nu_k} < \infty. \tag{5.1.11}$$

(ii) **Positive essential spectral gap**: $\lambda_0^{\mathrm{ess}}(\mathrm{H}) > 0$ *if and only if either* (5.1.11) *holds true or*

$$\sum_{k\geq 0} \frac{|e_k|}{\nu_k} = \infty \qquad \text{and} \qquad \sup_{n\geq 0} \sum_{k\leq n} \frac{|e_k|}{\nu_k} \sum_{k\geq n} \mu_k |e_k| < \infty. \tag{5.1.12}$$

(iii) **Discreteness**: *The spectrum of* H *is purely discrete if and only if* either $\sum_{k\geq 0} \frac{|e_k|}{\nu_k} < \infty$ *and*

$$\lim_{n\to\infty} \sum_{k\leq n} \mu_k |e_k| \sum_{k\geq n} \frac{|e_k|}{\nu_k} = 0, \tag{5.1.13}$$

or $\sum_{k\geq 0} \mu_k |e_k| < \infty$ *and*

$$\lim_{n\to\infty} \sum_{k\leq n} \frac{|e_k|}{\nu_k} \sum_{k\geq n} \mu_k |e_k| = 0, \tag{5.1.14}$$

PROOF. Let us only give a sketch of the proof (details can be found in, e.g., [**146**]). First observe that 0 is an eigenvalue of H exactly when $y_1 = \mathbb{1} \in L^2(\mathcal{I};\mu)$, that is, exactly when the series (5.1.5) converges. Taking this fact into account together with the divergence of (5.1.4), to prove (i), (ii) and (iii) it suffices to observe that by using a simple change of variables, the operator H is unitarily equivalent to the minimal operator $\widetilde{H}$ defined in the Hilbert space $L^2([0,\mathcal{L}_\nu);\mu_g)$ by the differential expression

$$\widetilde{\tau} = -\frac{1}{\mu_g(x)} \frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

and subject to the Neumann boundary condition at $x = 0$. Here

$$\mu_g := (\mu \cdot \nu) \circ g^{-1}, \tag{5.1.15}$$

where the function $g\colon [0,\mathcal{L}) \to [0,\infty)$ is given by

$$g(x) = \int_0^x \frac{ds}{\nu(s)}, \qquad \mathcal{L}_\nu := g(\mathcal{L}) = \int_0^{\mathcal{L}} \frac{ds}{\nu(s)}. \tag{5.1.16}$$

Notice that g is strictly increasing, locally absolutely continuous on $[0,\mathcal{L})$ and maps $[0,\mathcal{L})$ onto $[0,\mathcal{L}_\nu)$. Hence its inverse $g^{-1}\colon [0,\mathcal{L}_\nu) \to [0,\mathcal{L})$ is also strictly increasing and locally absolutely continuous on $[0,\mathcal{L})$. Now the remaining claims follow from the results of M.G. Krein and I.S. Kac (see Theorems 1 and 3 in [**117**] or [**118**, Section 11] and [**119**]). □

REMARK 5.8. A few remarks are in order.

(i) Using the quantities in (5.1.11) and (5.1.12) one can obtain sharp estimates on $\lambda_0(\mathrm{H})$ and $\lambda_0^{\mathrm{ess}}(\mathrm{H})$ (cf., e.g., [**146**], [**193**]).

(ii) If the spectrum of H is discrete, then it consists of simple eigenvalues such that $0 \le \lambda_0(\mathrm{H}) < \lambda_1(\mathrm{H}) < \lambda_2(\mathrm{H}) < \dots$ and the Weyl type asymptotics (5.1.9) holds true. If the RHS in (5.1.9) is infinite (i.e., $\mathcal{I} = [0, \mathcal{L})$ has infinite intrinsic length), then there are criteria (see [**119**]) to decide whether the series
$$\sum_{n\ge 1} \frac{1}{\lambda_n(\mathrm{H})^\gamma}$$
converges with some $\gamma > 1/2$ (the series diverges for all $\gamma \in (0, 1/2]$).

If the spectrum of H is not discrete, the study of spectral types of H is a highly nontrivial problem. However, we would like to mention only one result on the absolutely continuous spectrum established recently in [**25**].

LEMMA 5.9 ([**25**]). *Assume that $\mathcal{I} = [0, \mathcal{L})$ has infinite intrinsic length,*
$$\int_0^{\mathcal{L}} \sqrt{\frac{\mu(x)}{\nu(x)}}\,\mathrm{d}x = \sum_{k\ge 0} |e_k| \sqrt{\frac{\mu_k}{\nu_k}} = \sum_{k\ge 0} \eta_k = \infty, \tag{5.1.17}$$
and define the increasing sequence $(t_n)_{n\ge 0} \subset [0, \mathcal{L})$ by setting
$$\int_0^{t_n} \sqrt{\frac{\mu(x)}{\nu(x)}}\,\mathrm{d}x = n, \qquad n \in \mathbb{Z}_{\ge 0}.$$
If
$$\sum_{n\ge 0} \Big(\int_{t_n}^{t_n+2} \mu(x)\mathrm{d}x \int_{t_n}^{t_n+2} \frac{\mathrm{d}x}{\nu(x)} - 4 \Big) < \infty, \tag{5.1.18}$$
then $\sigma_{\mathrm{ac}}(\mathrm{H}) = [0, \infty)$.

REMARK 5.10. The operator H also plays an important role in the analysis of Kirchhoff Laplacians on family preserving graphs $(\mathcal{G}, \mu, \nu)$, which are known to reduce to Sturm-Liouville operators (see [**29**], [**30**]). In this situation, the weights admit the following description in terms of graph parameters of $\mathcal{G}$ (for simplicity we restrict to the case when the weights in Section 2.1 are constant on $\mathcal{G}$ and hence $\mu = \nu \equiv const$ in (5.0.1)):

- $|e_k|$ is the length of edges between the consecutive combinatorial spheres S_k and S_{k+1},
- $\mu_k = \nu_k$ is the number of edges between the consecutive combinatorial spheres S_k and S_{k+1},
- the series (5.1.5) equals the total volume of the metric graph $\mathcal{G}$.

For instance, for radially symmetric antitrees $\mu_k = s_k s_{k+1}$, where $(s_k)_{k\ge 0} \subseteq \mathbb{Z}_{\ge 1}$ are the antitree sphere numbers [**29**], [**146**] (see also Section 8.1 for weighted metric antitrees); for radially symmetric trees $\mu_k = b_0 \dots b_k$, where $(b_k)_{k\ge 0} \subseteq \mathbb{Z}_{\ge 1}$ are the tree branching numbers [**193**].

In conclusion, let us quickly discuss parabolic properties of Markovian extensions of H^0. We begin with the characterization of Markovian uniqueness. Recall that the Gaffney Laplacian H_G is defined (see Lemma 2.18) as the restriction of H to H^1 functions, that is,
$$\mathrm{dom}(\mathrm{H}_G) = \{ f \in \mathrm{dom}(\mathrm{H}) \,|\, f' \in L^2(\mathcal{I}; \nu) \}. \tag{5.1.19}$$

LEMMA 5.11. *The operator* H_G *is self-adjoint if and only if* $y_2 = \int_0^x \frac{ds}{\nu(s)}$ *does not belong to* $H^1(\mathcal{I})$*, that is, either the series* (5.1.4) *diverges or* $\mathcal{L}_\nu = \infty$*. If* H_G *is not self-adjoint, then its Markovian restrictions form a one parameter family*

$$\mathrm{dom}(\mathrm{H}_\theta) := \big\{f \in \mathrm{dom}(\mathrm{H}_G) \,|\, \cos(\theta) f(\mathcal{L}) + \sin(\theta) f_\nu'(\mathcal{L}) = 0\big\}, \quad \theta \in [0, \pi/2]. \tag{5.1.20}$$

Here $f(\mathcal{L}) = \lim_{x\to\mathcal{L}} f(x)$ *and* $f_\nu'(\mathcal{L}) = \lim_{x\to\mathcal{L}} \nu(x) f'(x)$*.*

PROOF. If H_G is not self-adjoint, then so is H and hence, by Lemma 5.2, the series (5.1.4) converges. On the other hand, all self-adjoint extensions in this case are parameterized by (5.1.8). For each $\theta \neq \frac{\pi}{2}$, $\mathrm{dom}(\mathrm{H}_\theta)$ contains functions such that $f_\nu'(\mathcal{L}) = 1$, that is, $f'(x) = \frac{1}{\nu(x)}(1 + o(1))$ as $x \to \mathcal{L}$. However, if $\mathcal{L}_\nu = \infty$, then $f' \notin L^2(\mathcal{I};\nu)$, which implies that H_G admits a unique self-adjoint restriction corresponding to $\theta = \frac{\pi}{2}$. The latter contradicts our assumption that H_G is not self-adjoint since in this case H_G admits at least two different self-adjoint restrictions H_D and H_N. □

REMARK 5.12. Notice that the self-adjointness of H_G is equivalent to the equality $H^1(\mathcal{I}) = H_0^1(\mathcal{I})$, where $H^1(\mathcal{I}) = \{f \in AC_{\mathrm{loc}}(\mathcal{I}) \,|\, f \in L^2(\mathcal{I};\mu),\ f' \in L^2(\mathcal{I};\nu)\}$ and $H_0^1(\mathcal{I}) = \overline{H^1(\mathcal{I}) \cap C_c(\mathcal{I})}^{\|\cdot\|_{H^1}}$.

The next result provides a characterization of transience/recurrence of Markovian restrictions of H_G.

LEMMA 5.13. *Let* H_G *be the Gaffney Laplacian* (5.1.19)*.*

(i) *If* H_G *is self-adjoint, then it is recurrent if and only if* $\mathcal{L}_\nu = \infty$*.*
(ii) *If* H_G *is not self-adjoint and* H_θ *is its Markovian restriction* (5.1.20)*, then* H_θ *is recurrent if and only if* $\theta = \pi/2$*.*

PROOF. It is not difficult to show that H_G (or its Markovian restriction when H_G is not self-adjoint) is transient exactly when the Green's function of H_G is well defined at the zero energy, that is, one needs to look at the limit of the resolvent $(\mathrm{H}_G - z)^{-1}$ when $z \uparrow 0$. It remains to use the form of the resolvent of a second order linear differential operator. □

Finally, let us state the stochastic completeness criterion, which essentially goes back to W. Feller [**69**].

LEMMA 5.14. *Let* H_G *be the Gaffney Laplacian* (5.1.19)*.*

(i) *If* H_G *is self-adjoint, then it is stochastically incomplete if and only if*

$$\mathcal{L}_\nu < \infty, \qquad \textit{and} \qquad \frac{1}{\nu(x)} \int_0^x \mu(s) \mathrm{d}s \in L^1(\mathcal{I}). \tag{5.1.21}$$

(ii) *If* H_G *is not self-adjoint and* H_θ *is its Markovian restriction* (5.1.20)*, then* H_θ *is stochastically complete if and only if* $\theta = \pi/2$*.*

PROOF. (i) If H_G is self-adjoint, then stochastic completeness is equivalent to the fact that for some (and hence for all) $\lambda > 0$ the boundary value problem

$$(\nu(x) y')' = \lambda \mu(x) y, \qquad y'(0) = 0. \tag{5.1.22}$$

has only a trivial nonnegative bounded solution on $\mathcal{I}$. Integrating (5.1.22) with $\lambda = 1$ yields

$$y'(x) = \frac{1}{\nu(x)} \int_0^x y(s)\mu(s)\mathrm{d}s, \quad x \in [0, \mathcal{L}).$$

Since a solution to (5.1.22) is unique up to a scalar multiple, we can assume that $y(0) = 1$. Clearly, $y \in L^\infty(\mathcal{I})$ exactly when $y' \in L^1(\mathcal{I})$. Thus, if y is bounded, then (5.1.21) necessarily holds true. Conversely, taking into account that y is nondecreasing, we get

$$0 \le y'(x) \le \frac{y(x)}{\nu(x)} \int_0^x \mu(s)\mathrm{d}s =: y(x)b(x), \quad x \in [0, \mathcal{L}).$$

Since $w' = wb$ has a bounded solution on $\mathcal{I}$ satisfying $w(0) = 1$ whenever $b \in L^1(\mathcal{I})$, and taking into account that $y \le w$ on $\mathcal{I}$, this completes the proof of sufficiency.

(ii) If H_G is not self-adjoint, then each Markovian restriction H_θ of H_G has purely discrete, nonnegative spectrum. Moreover, each eigenvalue of H_θ is simple. Thus the claim is an immediate consequence of the spectral theorem and the definition of stochastic completeness. □

5.2. Connection via boundary triplets

If $\alpha \ne 0$ and, in particular, if α takes negative values on X, the analysis of H_α, the maximal operator associated with (5.0.3) in $L^2(\mathcal{I};\mu)$[‡], becomes more involved. In particular, we shall see that there is no transparent self-adjointness criterion.

Consider the interval $\mathcal{I} = [0, \mathcal{L})$ together with the sequence $X = (x_k)_{k\ge0}$ as a metric path graph: $\mathcal{V} = \mathbb{Z}_{\ge0}$ is a vertex set, and $k \sim n$ exactly when $|k-n| = 1$; the length of the edge e_k connecting k with $k+1$ equals $|e_k| := x_{k+1} - x_k$. Following (3.1.3)–(3.1.6) and using (5.1.10), we define the weight $r\colon \mathbb{Z}_{\ge0} \to \mathbb{R}_{>0}$:

- if $\eta^*(X) := \sup_{k\ge0} \eta_k < \infty$, then

$$r(k) = |e_k|\mu_k, \qquad k \ge 0, \tag{5.2.1}$$

- if $\eta^*(X) = \infty$, we set

$$r(k) = \begin{cases} |e_k|\mu_k, & \eta_k \le 1, \\ \sqrt{\mu_k\nu_k}, & \eta_k > 1. \end{cases} \tag{5.2.2}$$

Next, we define the weights $m\colon \mathbb{Z}_{\ge0} \to (0,\infty)$ and $b\colon \mathbb{Z}_{\ge0} \times \mathbb{Z}_{\ge0} \to [0,\infty)$ by

$$m(k) = \begin{cases} r(0), & k = 0, \\ r(k-1) + r(k), & k \ge 1, \end{cases} \tag{5.2.3}$$

and

$$b(k,n) = \begin{cases} \frac{\nu_{\min(n,k)}}{|x_k - x_n|}, & |n-k| = 1, \\ 0, & |n-k| \ne 1. \end{cases} \tag{5.2.4}$$

[‡]The precise definitions of H_α and the corresponding minimal operator H^0_α are given in Section 2.4.1, see (2.4.14), (2.4.15) and take into account (5.0.2).

First, we can associate the minimal $\mathbf{h}_\alpha^0$ and the maximal $\mathbf{h}_\alpha$ operators in the weighted Hilbert space $\ell^2(\mathbb{Z}_{\geq 0}; m)$ with the discrete Schrödinger-type expression

$$(\tau f)(k) := \frac{1}{m(k)}\Big(\sum_{n\geq 0} b(k,n)(f(k)-f(n)) + \alpha_k f(k)\Big), \quad k \in \mathbb{Z}_{\geq 0}. \tag{5.2.5}$$

Next, using the map (3.2.40), we can consider in $\ell^2(\mathbb{Z}_{\geq 0})$ the minimal $\widetilde{\mathbf{h}}_\alpha^0$ and the maximal $\widetilde{\mathbf{h}}_\alpha$ operators, which are unitarily equivalent to $\mathbf{h}_\alpha^0$ and, respectively, $\mathbf{h}_\alpha$. The corresponding difference expression (3.2.38) is the following second order difference expression

$$(\tilde{\tau}_\alpha f)(k) = \begin{cases} a_0 f(0) - b_0 f(1), & k = 0, \\ -b_{k-1} f(k-1) + a_k f(k) - b_k f(k+1), & k \geq 1, \end{cases} \tag{5.2.6}$$

where

$$a_k = \frac{1}{m(k)}\Big(\alpha_k + \frac{\nu_{k-1}}{|e_{k-1}|} + \frac{\nu_k}{|e_k|}\Big), \qquad b_k = \frac{\nu_k}{|e_k|\sqrt{m(k)m(k+1)}}, \tag{5.2.7}$$

for all $k \geq 0$ with $\nu_{-1}/|e_{-1}| = 0$ for notational simplicity. Hence the operator $\widetilde{\mathbf{h}}_\alpha$ is nothing but the maximal operator associated in $\ell^2(\mathbb{Z}_{\geq 0})$ with the Jacobi (tri-diagonal) matrix

$$J = \begin{pmatrix} a_0 & -b_0 & 0 & 0 & \dots \\ -b_0 & a_1 & -b_1 & 0 & \dots \\ 0 & -b_1 & a_2 & -b_2 & \dots \\ 0 & 0 & -b_2 & a_3 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}. \tag{5.2.8}$$

Therefore, Theorem 3.1 establishes connections between the operator (5.0.3) and spectral theory of Jacobi (tri-diagonal) matrices. We would like to present only one claim regarding self-adjointness.

THEOREM 5.15. *Let $\widetilde{\mathbf{h}}_\alpha^0$ be the minimal operator defined in $\ell^2(\mathbb{Z}_{\geq 0})$ by the Jacobi matrix* (5.2.8) *with Jacobi parameters* (5.2.7). *Then the deficiency indices of H_α^0 and $\widetilde{\mathbf{h}}_\alpha^0$ are equal and*

$$\mathrm{n}_+(\mathrm{H}_\alpha^0) = \mathrm{n}_-(\mathrm{H}_\alpha^0) = \mathrm{n}_\pm(\widetilde{\mathbf{h}}_\alpha^0) \leq 1. \tag{5.2.9}$$

In particular, H_α is self-adjoint if and only if $\widetilde{\mathbf{h}}_\alpha$ is self-adjoint.

Applying spectral theory of Jacobi matrices and using Theorem 3.1 we would be able to investigate spectral properties of the operators H_α and this approach was taken in [**141**, § 5.2] for the case $\mu = \nu \equiv \mathbb{1}$. Let us only provide some simple self-adjointness criteria.

LEMMA 5.16. *Let H_α be the maximal operator defined by* (5.0.3) *in $L^2(\mathcal{I}; \mu)$.*

(i) *If the series*

$$\sum_{k\geq 0} \eta_k^2 = \sum_{k\geq 0} |e_k|^2 \frac{\mu_k}{\nu_k} \tag{5.2.10}$$

diverges, then H_α is self-adjoint for any α.

(ii) *If $\mathcal{I}$ has infinite intrinsic length, i.e.,* (5.1.17) *holds, and $\alpha\colon X \to \mathbb{R}$ is such that $\widetilde{\mathbf{h}}_\alpha^0$ is bounded from below, then H_α is self-adjoint and bounded from below.*

PROOF. (i) By the Carleman test [**2**, Problem I.1], $\widetilde{\mathbf{h}}_\alpha^0$ is self-adjoint if the series

$$\sum_{k\geq 0}\frac{1}{b_k} \tag{5.2.11}$$

diverges. However,

$$\frac{1}{b_k} = \frac{|e_k|\sqrt{m(k)m(k+1)}}{\nu_k} \geq \frac{|e_k|r(k)}{\nu_k} \geq \begin{cases}\eta_k^2, & \eta_k\leq 1,\\ 1, & \eta_k>1.\end{cases} \tag{5.2.12}$$

Therefore, (5.2.11) diverges if so is (5.2.10). It remains to apply Theorem 5.15.

(ii) By the Wouk test [**2**, Problem I.4], $\widetilde{\mathbf{h}}_\alpha^0$ is self-adjoint if it is bounded from below and

$$\sum_{k\geq 0}\frac{1}{\sqrt{b_k}} = \infty.$$

It remains to take into account (5.2.12) and then apply Theorem 5.15. □

REMARK 5.17. One can apply other self-adjointness tests (see, e.g, [**2**, Chap. I]) to J with the Jacobi parameters given by (5.2.7) in order to get various self-adjointness conditions for the operator H_α (cf., e.g., [**141**, § 5]). For instance, Berezanskii's test [**2**, Prob. I.5] would lead to examples with nontrivial deficiency indices even if (5.1.17) is satisfied.

5.3. Jacobi matrices and Krein–Stieltjes strings as boundary operators

The results in the previous subsection connect spectral properties of Sturm–Liouville operators with a certain family of Jacobi matrices. The natural question arising in this context is:

How large is the class of Jacobi matrices with Jacobi parameters (5.2.7)?

The next result shows that for each choice of Jacobi parameters $(a_k, b_k)_{k\geq 0}$ one can find weights μ, ν and strengths α such that (5.2.7) holds.

PROPOSITION 5.18. *For every symmetric Jacobi (tri-diagonal) matrix* (5.2.8) *normalized by the condition $b_k>0$ for all $k\geq 0$ there exist lengths $(|e_k|)_{k\geq 0}\subset\mathbb{R}_{>0}$, weights $(\nu_k)_{k\geq 0}\subset\mathbb{R}_{>0}$ and strengths $(\alpha_k)_{k\geq 0}\subset\mathbb{R}$ such that:*

(i) **Normalization:** *lengths $(|e_k|)_{k\geq 0}$ and weights $(\nu_k)_{k\geq 0}$ satisfy*

$$\eta_k = \frac{|e_k|}{\sqrt{\nu_k}} \leq 1 \tag{5.3.1}$$

for all $k\geq 0$.

(ii) **Jacobi parameters** *have the form*

$$a_k = \frac{1}{|e_{k-1}|+|e_k|}\Big(\alpha_k + \frac{\nu_{k-1}}{|e_{k-1}|} + \frac{\nu_k}{|e_k|}\Big), \tag{5.3.2}$$

$$b_k = \frac{\nu_k}{|e_k|\sqrt{(|e_{k-1}|+|e_k|)(|e_k|+|e_{k+1}|)}}, \tag{5.3.3}$$

for all $k\geq 0$.

(iii) **Boundary operator:** *the minimal operator* $\widetilde{\mathbf{h}}$ *associated in* $\ell^2(\mathbb{Z}_{\ge 0})$ *with the matrix* (5.2.8) *having Jacobi parameters* (5.3.2)–(5.3.3) *serves as a boundary operator (in the sense of Proposition 3.11) for the minimal operator* $\mathrm{H}^0 = \mathrm{H}^0_{\mathbb{1},\nu,\alpha}$ *defined by the differential expression*

$$\tau_{\nu,\alpha} = -\frac{\mathrm{d}}{\mathrm{d}x}\nu(x)\frac{\mathrm{d}}{\mathrm{d}x} + \sum_{k\ge 0}\alpha_k\delta(x-x_k), \tag{5.3.4}$$

in the Hilbert space $L^2(\mathcal{I})$. *Here* $\mathcal{I} = [0,\mathcal{L})$ *and the weight* $\nu\colon \mathcal{I}\to\mathbb{R}_{>0}$ *is defined by*

$$x_k = \sum_{j=0}^{k-1}|e_j|, \qquad \mathcal{L} = \sum_{k\ge 0}|e_k|, \qquad \nu(x) = \sum_{k\ge 0}\nu_k \mathbb{1}_{[x_k,x_{k+1})}(x). \tag{5.3.5}$$

Proof. Since $\alpha_k \in \mathbb{R}$ in (5.2.7) can be chosen arbitrary, the main difficulty is of course to show that every sequence $(b_k)_{k\ge 0}$ of positive real numbers can be realized as (5.2.7). Let $(b_k)_{k\ge 0} \subset (0,\infty)$ be given. First set $|e_0| = 1$ and hence by (5.3.3) holds for $k=0$ if

$$|e_1| = \frac{\nu_0^2}{b_0^2} - 1.$$

If $b_0 < 1$, we set $\nu_0 = 1$ and define $|e_1|$ by the above equation, otherwise, we set $\nu_0 = \sqrt{2}b_0 > 1$ and $|e_1| = 1$. Clearly, both (5.3.1) and (5.3.3) hold true for $k=0$.

Next we proceed inductively. Assume we have already defined positive numbers $\nu_0,\dots,\nu_{n-1}$ and $|e_0|,\dots,|e_n|$ such that (5.3.3) holds for $k=0,\dots,n-1$. Set

$$s_n := \frac{|e_n|}{\sqrt{|e_{n-1}|+|e_n|}\sqrt{|e_n|+1}}. \tag{5.3.6}$$

If $s_n \le b_n$, we set

$$|e_{n+1}| = 1, \qquad \nu_n = \frac{b_n}{s_n}|e_n|^2 \ge |e_n|^2, \tag{5.3.7}$$

and otherwise we choose

$$|e_{n+1}| = \frac{s_n^2}{b_n^2}(1+|e_n|) - |e_n| > 1, \qquad \nu_n = |e_n|^2. \tag{5.3.8}$$

Clearly, by construction, both (5.3.1) and (5.3.3) hold true for $k=n$. Therefore, proceeding inductively, we obtain sequences of lengths $(|e_k|)_{k\ge 1}$ and weights $(\nu_k)_{k\ge 1}$ such that (5.3.3) holds together with (5.3.1). □

Remark 5.19. A few remarks are in order.

(i) Combining Proposition 5.18 with Theorem 3.1, we conclude that basic spectral theory of Jacobi matrices (e.g., self-adjointness, semiboundedness etc.) can be included into the spectral theory of Sturm–Liouville operators of the form (5.3.4)–(5.3.5).

(ii) The choice of lengths and weights is not unique. Indeed, taking into account that (3.1.1)–(3.1.6) are invariant under the scaling $|e| \to |e|c(e)$, $\mu(e) \to \frac{\mu(e)}{c(e)}$, and $\nu(e) \to \nu(e)c(e)$ for any $c\colon \mathcal{E}\to(0,\infty)$, one can rescale parameters and construct lengths and weights with the following properties:
- $|e_k| \le 1$ and $\mu_k = \nu_k$ for all $k\ge 0$ (hence $\mu = \nu$ in (5.0.3)),
- $\nu_k = 1$ and $|e_k|^2\mu_k \le 1$ for all $k \ge 0$ (hence $\nu \equiv 1$ in (5.0.3)),

- $|e_k| = 1$ and $\mu_k \le \nu_k$ for all $k \ge 0$ (hence $X = \mathbb{N}$ in (5.0.3)).

(iii) Let us also stress that for Jacobi (tri-diagonal) matrices (5.2.8) still there is no self-adjointness criterion formulated in closed form in terms of Jacobi parameters (there are only various necessary and sufficient conditions). This in particular means that even in the simplest case of a weighted path graph one cannot hope for a transparent self-adjointness criterion formulated in terms of weights and interaction strengths.

If $\alpha \ge 0$, then the Hamiltonian H_α generates a Markovian semigroup in $L^2(\mathcal{I};\mu)$ (assume, for a moment, that H_α is self-adjoint). However, the boundary operator $\widetilde{\mathbf{h}}_\alpha$ does not reflect the parabolic properties of H_α (it is not difficult to see that the semigroup generated by $\widetilde{\mathbf{h}}_\alpha$ in $\ell^2(\mathbb{Z}_{\ge 0})$ is positivity preserving, however, in general it is not ℓ^∞ contractive). From this perspective, let us look at the minimal operator $\mathbf{h}^0$ defined in $\ell^2(\mathbb{Z}_{\ge 0}; m)$ by (5.2.5) with the coefficients (5.2.3) and (5.2.4) and $\alpha \equiv 0$. It serves as the boundary operator for the Sturm–Liouville operator H, however, it also captures the parabolic properties of H (see Chapter 4). Following the setting of Section 2.2, every weight function b given by (5.2.4) defines an infinite path graph. Since the coefficients of b depend only on the weight ν and edge lengths, it is clear that every weighted path graph can be obtained via (5.2.4). However, the difference expression (5.2.5) (see (3.1.7)) also contains the vertex weight m defined by (5.2.3). Thus, we can reformulate the question posed at the very beginning of Section 5.3 as follows:

Does every path graph b over $(\mathbb{Z}_{\ge 0}, m)$ arise as a boundary operator for H?

Taking into account Proposition 5.18, the answer may look a bit surprising.

PROPOSITION 5.20. *Let $m\colon \mathbb{Z}_{\ge 0} \to (0,\infty)$ and $b\colon \mathbb{Z}_{\ge 0} \times \mathbb{Z}_{\ge 0} \to [0,\infty)$ be positive weights such that b defines an infinite path graph (i.e., $b(k,n) = b(n,k) > 0$ exactly when $|k-n| = 1$). Then the minimal operator $\mathbf{h}^0$ associated in $\ell^2(\mathbb{Z}_{\ge 0}; m)$ with the weighted Laplacian*

$$(\tau f)(k) := \frac{1}{m(k)} \sum_{n \ge 0} b(n,k)(f(k) - f(n)), \quad k \in \mathbb{Z}_{\ge 0}, \tag{5.3.9}$$

arises as a boundary operator for some Sturm–Liouville operator (5.1.1) *with the weights* (5.0.1) *if and only if*

$$\sum_{k=0}^{n} (-1)^{n-k} m(k) > 0 \tag{5.3.10}$$

for all $n \ge 0$.

PROOF. The necessity of (5.3.10) follows from (5.2.3) since $m(0) = r(0) > 0$ and for all $n \ge 1$ we have

$$\sum_{k=0}^{n} (-1)^{n-k} m(k) = (-1)^n m(0) + \sum_{k\ge 1}^{n} (-1)^{n-k}\big(r(k-1) + r(k)\big) = r(n) > 0.$$

To prove sufficiency, suppose that $m\colon \mathbb{Z}_{\ge 0} \to (0,\infty)$ satisfies (5.3.10) and set $b(k) := b(k,k+1)$, $k \ge 0$. Thus the LHS (5.3.10) defines a positive sequence

$r\colon \mathbb{Z}_{\geq 0} \to (0,\infty)$. Setting

$$|e_k| := \begin{cases} \sqrt{\frac{r(k)}{b(k)}}, & r(k) \leq b(k), \\ \frac{r(k)}{b(k)}, & r(k) > b(k), \end{cases} \qquad \mu(k) := \begin{cases} \sqrt{r(k)b(k)}, & r(k) \leq b(k), \\ r(k), & r(k) > b(k), \end{cases}$$

for all $k \geq 0$, we end up with a suitable and, in fact unique, choice of the weight function

$$\mu(x) = \sum_{k\geq 0} \mu(k)\mathbb{1}_{[x_k, x_{k+1})}, \qquad x_k = \sum_{j=0}^{k-1} |e_j|,$$

such that the minimal operator $\mathbf{h}^0$ associated in $\ell^2(\mathbb{Z}; m)$ with (5.3.9) is the boundary operator for H^0 associated with (5.1.1) (with the weights $\mu = \nu$). $\square$

REMARK 5.21. Surprisingly enough, we are not able to obtain all difference expressions of the form (3.1.7) even in the simplest case of a path graph. The main restriction is the form of the weight function m. More precisely, the *formal Laplacian* L associated to a path graph b over the measure space $(\mathbb{Z}_{\geq 0}, m)$ can be obtained via (5.2.3), (5.2.4) only if the weight function m belongs to the image of the cone of strictly positive functions $C^+(\mathbb{Z}_{\geq 0})$ under the map $\mathrm{I} + \mathcal{S}$, where $\mathcal{S}$ is the right shift operator defined on $C(\mathbb{Z}_{\geq 0})$ by

$$\mathcal{S}\colon \big(f(k)\big)_{k\geq 0} \mapsto \big(f(k-1)\big)_{k\geq 0}, \tag{5.3.11}$$

where $f(-1) := 0$ for notational simplicity. Indeed, with this notation (5.2.3) takes the form

$$m = (\mathrm{I} + \mathcal{S})r,$$

and then the validity of (5.3.10) for all $n \geq 0$ is exactly the inclusion $m \in C^+(\mathbb{Z}_{\geq 0})$.

REMARK 5.22 (Krein–Stieltjes strings). Set

$$\ell_k = \frac{1}{b(k,k+1)} = \frac{|e_k|}{\nu_k}, \qquad \xi_k = \sum_{j=0}^{k-1} \ell_j, \qquad \omega_k = m(k)$$

for all $k \geq 0$. Next define the positive measure ω on $[0,\ell)$, where $\ell := \sum_{k\geq 0} \ell_k$, by

$$\omega([0,\xi)) := \sum_{\xi_k \leq \xi} \omega_k.$$

If $\alpha_k = 0$ for all $k \geq 0$, then the spectral problem $\tau f = zf$ associated with the difference expression (5.2.5), (5.2.3), (5.2.4) admits a mechanical interpretation (see [**2**, Appendix], [**118**, § 13]): it describes small oscillations of a string of length ℓ with mass density ω. The corresponding spectral problem can be written as

$$-y'' = z\omega y, \quad \xi \in [0,\ell), \tag{5.3.12}$$

which is similar to the form of (5.1.1), however, the coefficient ω is a measure bearing point masses only. Strings whose mass density has the above form are usually called *Krein–Stieltjes strings* (the corresponding finite difference expressions appear in the study of the Stieltjes moment problem and their mechanical interpretation was observed by M.G. Krein [**118**]). Thus, the results of this section establish a connection between two classes of strings: strings whose mass density is piecewise constant and Krein–Stieltjes strings. However, Proposition 5.20 says that we can't cover the whole class of Krein–Stieltjes strings.

CHAPTER 6

Graph Laplacians as boundary operators

The results in the preceding chapters lead to the following question: *which graph Laplacians may arise as boundary operators (in the sense of Chapters 3 and 4) for a Kirchhoff Laplacian on a weighted metric graph?*

Let us be more specific in stating the above problem. Suppose a vertex set $\mathcal{V}$ is given. Each graph Laplacian (2.2.3) is determined by the vertex weight $m\colon \mathcal{V} \to (0,\infty)$, edge weight function $b\colon \mathcal{V}\times\mathcal{V} \to [0,\infty)$ having the properties (i), (ii) and (iv) of Section 2.2, and the killing term $c\colon \mathcal{V} \to [0,\infty)$. We always assume that the underlying graphs are connected. With each such b we can associate a locally finite simple graph $\mathcal{G}_b = (\mathcal{V}, \mathcal{E}_b)$ as described in Remark 2.7.

Definition 6.1. A *cable system* for a graph b over $(\mathcal{V}, m)$ is a model of a weighted metric graph $(\mathcal{G}, \mu, \nu)$ having $\mathcal{V}$ as its vertex set and such that the functions defined by (3.1.1)–(3.1.5) and (3.1.6) coincide with m and, respectively, b. If in addition the underlying graph $(\mathcal{V}, \mathcal{E})$ of the model coincides with $\mathcal{G}_b = (\mathcal{V}, \mathcal{E}_b)$, then the cable system is called *minimal*.

Remark 6.2. Notice that the underlying combinatorial graph $(\mathcal{V}, \mathcal{E})$ of a cable system for $(\mathcal{V}, m; b)$ can always be obtained from the simple graph $\mathcal{G}_b = (\mathcal{V}, \mathcal{E}_b)$ by adding loops and multiple edges.

Since the killing term c is nothing but the strength of δ-couplings at the vertices in (3.1.7), we can restrict our considerations to the case $c \equiv 0$:

Problem 6.1. *Which locally finite graphs $(\mathcal{V}, m; b)$ have a minimal cable system?*

The case of a path graph shows that the answer to the above problem is not trivial (see Proposition 5.20). However, we stress that a general cable system may have loops and multiple edges and thus the simplicity assumption on the model of $(\mathcal{G}, \mu, \nu)$ (that is, the minimality of a cable system for $(\mathcal{V}, m; b)$) might be too restrictive. In fact, as discussed in Remark 2.11 and Remark 2.12, we can allow multi-graphs and this leads us to another question:

Problem 6.2. *Which locally finite graphs $(\mathcal{V}, m; b)$ have a cable system?*

Once the above problems will be resolved, the next natural question (also in context with possible applications) is:

Problem 6.3. *How can one describe all cable systems of a locally finite graph b over $(\mathcal{V}, m)$?*

On the other hand, there is another closely connected class of second order difference operators on graphs, however, acting in $\ell^2(\mathcal{V})$. In particular, the operator defined in $\ell^2(\mathcal{V})$ by the difference expression (3.2.38) is a special case of

$$(\tau f)(v) = \beta(v)f(v) - \sum_{u\in\mathcal{V}} q(u,v)f(u), \qquad v \in \mathcal{V},$$

where $\beta\colon \mathcal{V} \to \mathbb{R}$ and q is a graph over $\mathcal{V}$ satisfying the properties (i), (ii) and (iv) of Section 2.2. This leads to a similar problem:

PROBLEM 6.4. *Given a graph q over $\mathcal{V}$, which of the above difference expressions arise as boundary operators for Laplacians with δ-couplings on a weighted metric graph $(\mathcal{G},\mu,\nu)$ over $\mathcal{G}_q = (\mathcal{V},\mathcal{E}_q)$?*

Despite an obvious similarity and a clear connection between these problems, as we learned in Section 5.3, they have very different answers even in the case of a path graph (see Proposition 5.18 and Proposition 5.20).

REMARK 6.3. Taking into account an obvious analogy between the above second order difference expression and Jacobi matrices, it is tempting to call them *Jacobi matrices on graphs* (cf., e.g., [**8**], [**9**], [**10**]).

6.1. Examples

Before studying Problems 6.1–6.4, let us first give several illustrative examples.

EXAMPLE 6.4 (Normalized Laplacians/Simple random walks). Let $\mathcal{G}_d = (\mathcal{V},\mathcal{E})$ be a locally finite simple graph. Let also $|\cdot|\colon \mathcal{E} \to (0,\infty)$ be given and define edge weights $\mu,\nu\colon \mathcal{E} \to (0,\infty)$ by setting

$$\mu\colon e \mapsto \frac{1}{|e|}, \qquad\qquad \nu\colon e \mapsto |e|. \tag{6.1.1}$$

Notice that the intrinsic edge length is constant on $\mathcal{E}$, that is,

$$\eta(e) = |e|\sqrt{\frac{\mu(e)}{\nu(e)}} = 1$$

for all $e \in \mathcal{E}$ in this case, and hence (3.1.3), (3.1.5) and (3.1.6) give

$$m(v) = \sum_{u\sim v} |e|\mu(e) = \deg(v), \qquad v \in \mathcal{V}, \tag{6.1.2}$$

and

$$b(u,v) = \begin{cases} 1, & u \sim v, \\ 0, & u \not\sim v, \end{cases} \qquad (u,v) \in \mathcal{V}\times\mathcal{V}. \tag{6.1.3}$$

The corresponding graph Laplacian (3.1.7) (with $\alpha \equiv 0$) has the form

$$(L_{\mathrm{norm}}f)(v) := \frac{1}{\deg(v)}\sum_{u\sim v} f(v) - f(u) = f(v) - \frac{1}{\deg(v)}\sum_{u\sim v} f(u), \tag{6.1.4}$$

for all $v \in \mathcal{V}$. It is known in the literature as a *normalized Laplacian* (or *physical Laplacian*). This operator has a venerable history. In particular, it appears as the generator of the simple random walk on $\mathcal{G}_d = (\mathcal{V},\mathcal{E})$, where "simple" refers to the fact that the probabilities to move from v to a neighboring vertex are all equal to $\frac{1}{\deg(v)}$ (see, e.g., [**209**]). ♢

EXAMPLE 6.5 (Electrical networks/Random walks). Again, let $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ be a locally finite simple graph. Suppose $|\cdot|\colon \mathcal{E} \to \{1\}$, that is, the corresponding metric graph $\mathcal{G}$ is equilateral (each $e \in \mathcal{E}$ can be identified with a copy of the interval $[0,1]$). Next, suppose that the edge weights $\mu, \nu\colon \mathcal{E} \to (0,\infty)$ coincide, that is, $\mu(e) = \nu(e)$ for all $e \in \mathcal{E}$. Then

$$\eta(e) = \sqrt{\frac{\mu(e)}{\nu(e)}} = 1$$

for all $e \in \mathcal{E}$ and hence, by (3.1.3), (3.1.5) and (3.1.6),

$$b(u,v) = \begin{cases} \mu(e_{u,v}), & u \sim v, \\ 0, & u \not\sim v, \end{cases} \qquad m(v) = m_b(v) := \sum_{e \in \mathcal{E}_v} \mu(e). \tag{6.1.5}$$

The corresponding graph Laplacian (3.1.7) (with $\alpha \equiv 0$) is given explicitly by

$$(L_b f)(v) := \frac{1}{m_b(v)} \sum_{u \sim v} b(u,v)(f(v) - f(u)), \qquad v \in \mathcal{V}, \tag{6.1.6}$$

and arises in the study of random walks on $\mathcal{G}_d$ (a.k.a. reversible Markov chains), where the jump probabilities are defined by (see, e.g., [**12**, Chap. 1.2], [**89**])

$$p(u,v) = \frac{b(u,v)}{\sum_{x \in \mathcal{V}} b(u,x)}, \qquad u, v \in \mathcal{V}.$$

On the other hand, considering informally an electrical network as a set of wires (edges) and nodes (vertices), we can interpret $b(u,v)$ as a *conductance* of a wire $e_{u,v}$ connecting u with v, $r(u,v) = \frac{1}{b(u,v)}$ is the *resistance* of $e_{u,v}$ and $m(v)$ is the *total conductance* at v. Thus, the corresponding weighted Laplacian L_b arises in the study of *pure resistor networks* (see [**12**], [**192**], [**209**]).

Therefore, *every electrical network operator/generator of a random walk (reversible Markov chains) on a locally finite graph arises as a boundary operator for a Kirchhoff Laplacian on a weighted metric graph.* Notice also that by Lemma 2.9 the corresponding graph Laplacian is bounded (in fact, its norm is at most 2). ◊

REMARK 6.6. The construction in Example 6.5 connecting a random walk on a graph with a Brownian motion on a weighted metric graph can be found in [**202**].

The above examples show that a very important class of graph Laplacians arises as boundary operators (in the sense of Proposition 3.11) for Laplacians on weighted metric graphs. However, as we shall see next, the answer to Problem 6.1 is far from trivial.

EXAMPLE 6.7 (Combinatorial Laplacians on antitrees). Again, let $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ be a locally finite simple graph. Set $m = \mathbb{1}$ on $\mathcal{V}$ and define a graph b over $(\mathcal{V}, m)$ by

$$b(u,v) = \begin{cases} 1, & u \sim v \\ 0, & u \not\sim v, \end{cases} \qquad (u,v) \in \mathcal{V} \times \mathcal{V}. \tag{6.1.7}$$

Notice in particular that the associated combinatorial graph $(\mathcal{V}, \mathcal{E}_b)$ coincides with $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$. The corresponding graph Laplacian acts in $\ell^2(\mathcal{V})$ and is given by

$$(L_{\mathrm{comb}} f)(v) := \sum_{u \sim v} f(v) - f(u) = \deg(v) f(v) - \sum_{u \sim v} f(u). \tag{6.1.8}$$

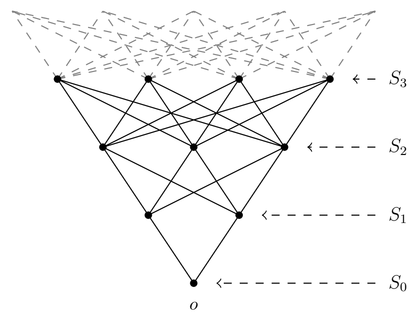

FIGURE 6.1. Example of an antitree with $s_n = \#S_n = n + 1$.

This operator is known as the *combinatorial Laplacian*† and $A = (b(u, v))_{u,v\in\mathcal{V}}$ is nothing but the adjacency matrix of the graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$.

Suppose additionally that our graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ is a rooted *antitree* (see [**210**], [**47**], [**146**] and also Section 8.1), that is, fix a root vertex $o \in \mathcal{V}$ and then order the graph with respect to the combinatorial spheres S_n, $n \in \mathbb{Z}_{\ge 0}$ (S_n consists of all vertices $v \in \mathcal{V}$ such that the combinatorial distance from v to the root o, that is, the combinatorial length of the shortest path connecting v with o, equals n; notice that $S_0 = \{o\}$). The graph $\mathcal{G}_d$ is called an *antitree* if it is simple and 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 Fig. 6.1). In this particular situation (a combinatorial Laplacian on an infinite antitree) the next result provides a complete answer to Problem 6.1.

PROPOSITION 6.8. *Let $\mathcal{A} = (\mathcal{V}, \mathcal{E})$ be an (infinite) antitree with sphere numbers $s_n := \#S_n$, $n \in \mathbb{Z}_{\ge 0}$. Then the corresponding combinatorial Laplacian* (6.1.8) *on $\mathcal{A}$ arises as a boundary operator for a minimal Kirchhoff Laplacian on a weighted metric antitree if and only if*

$$\sum_{k=0}^{n} (-1)^k s_{n-k} > 0 \tag{6.1.9}$$

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

We shall give the proof of this result in Section 6.2. Let us only mention the similarity between (6.1.9) and (5.3.10), which is, in fact, not at all surprising in view of connections between Laplacians on family preserving graphs and Jacobi matrices (see [**30**]). ♢

6.2. Life without loops I: Graph Laplacians

We begin with Problem 6.1. Its importance stems from the fact that every regular Dirichlet form over $(\mathcal{V}, m)$ arises as the energy form $\mathfrak{q}_D$ for some graph (b, c) over $(\mathcal{V}, m)$ (see [**130**, Theorem 7]).

Suppose a connected locally finite graph (b, c) over $(\mathcal{V}, m)$ is given. Let $\mathcal{G}_b = (\mathcal{V}, \mathcal{E}_b)$ be the simple graph associated with (b, c): $u \sim v$ exactly when $b(u, v) \ne 0$

†Seems, there is no agreement how to call this difference operator and sometimes the name 'physical Laplacian' is used instead. However, taking into account its obvious connection with the adjacency matrix, the name 'combinatorial Laplacian' looks more appropriate to us.

(see Remark 2.7). Then for each weighted metric graph $(\mathcal{G},\mu,\nu)$ over $(\mathcal{V},\mathcal{E}_b)$ the functions defined by (3.1.1)–(3.1.5) and (3.1.6) take the following form:

$$m_{\mathcal{G}}(v) = \sum_{u\colon b(u,v)\neq 0} r(e_{u,v}), \tag{6.2.1}$$

where r is defined by (3.1.1), (3.1.3)–(3.1.4), and

$$b_{\mathcal{G}}(u,v) = \begin{cases} \frac{\nu(e_{u,v})}{|e_{u,v}|}, & b(u,v)>0,\\ 0, & b(u,v)=0.\end{cases} \tag{6.2.2}$$

Comparing the form of the boundary operator (3.1.7) with (2.2.3), it is clear that the killing term c is nothing but the strength of δ-couplings at the vertices and hence we can restrict our considerations to the case $c\equiv 0$. In fact, the next result shows that Problem 6.1 can be reduced to a description of all possible vertex weights m:

PROPOSITION 6.9. *A locally finite graph $(\mathcal{V},m;b)$ admits a minimal cable system if and only if there is a function $r_b\colon\mathcal{E}_b\to(0,\infty)$ such that*

$$m(v) = \sum_{e\in\mathcal{E}_v} r_b(e) \tag{6.2.3}$$

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

PROOF. Necessity immediately follows from (6.2.1). Let us prove sufficiency. Suppose there is $r_b\colon\mathcal{E}_b\to(0,\infty)$ such that (6.2.3) holds true for all $v\in\mathcal{V}$. First of all, we set $|e_{u,v}|\equiv 1$ and $\nu(e_{u,v}) := b(u,v)$ for all edges $e_{u,v}\in\mathcal{E}_b$. Moreover, if $\sup_{u,v} r_b(e_{u,v})/b(u,v)<\infty$, we define $\mu(e_{u,v}) = r_b(e_{u,v})$ and otherwise set

$$\mu(e_{u,v}) = \begin{cases} r_b(e_{u,v}), & r_b(e_{u,v})\le b(u,v),\\ \frac{r_b(e_{u,v})^2}{b(u,v)}, & r_b(e_{u,v})> b(u,v),\end{cases}$$

for each $e_{u,v}\in\mathcal{E}_b$. It is then straightforward to check that the corresponding functions defined by (3.1.1)–(3.1.5) and (3.1.6) coincide with m and b. □

In fact, the above result shows that the answer to Problem 6.1 is analogous to the answer in the case of a path graph (see Proposition 5.20 and Remark 5.21). Indeed, let $\mathcal{G}_d = (\mathcal{V},\mathcal{E})$ be a simple locally finite graph and consider the map $D\colon C(\mathcal{V})\to C(\mathcal{E})$ given by

$$(Df)(e_{u,v}) = f(u)+f(v). \tag{6.2.4}$$

If we define the Hilbert space $\ell^2(\mathcal{E})$ as follows

$$\ell^2(\mathcal{E}) = \Big\{\phi\colon\mathcal{E}\to\mathbb{C}\mid \sum_{e\in\mathcal{E}}|\phi(e)|^2<\infty\Big\},$$

then D defines a possibly unbounded operator from $\ell^2(\mathcal{V})$ to $\ell^2(\mathcal{E})$ (in fact, D is bounded if and only if the graph $\mathcal{G}_d$ has bounded geometry, $\sup_{v\in\mathcal{V}}\deg(v)<\infty$). Its (formal) adjoint $D^*\colon C(\mathcal{E})\to C(\mathcal{V})$ is given by

$$(D^*\phi)(v) = \sum_{e\in\mathcal{E}_v}\phi(e),\quad v\in\mathcal{V}. \tag{6.2.5}$$

Comparing this formula with (6.2.3), we immediately arrive at the following result:

COROLLARY 6.10. *A locally finite graph $(\mathcal{V},m;b)$ admits a minimal cable system if and only if m belongs to the image of the positive cone $C^+(\mathcal{E})$ under the map D^*.*

REMARK 6.11. Taking into account Example 6.5, Corollary 6.10 admits the following reformulation: *A locally finite graph* $(\mathcal{V}, m; b)$ *admits a minimal cable system if and only if there are resistances* $R\colon \mathcal{E}_b \to \mathbb{R}_{>0}$ *such that total conductances on* $\mathcal{V}$ *coincide with* m.

Let us apply the above result to antitrees in order to prove Proposition 6.8.

PROOF OF PROPOSITION 6.8. By Proposition 6.9, we need to show that for a given antitree $\mathcal{A} = (\mathcal{V}, \mathcal{E})$ with sphere numbers $(s_n)_{n\geq 0}$ the condition (6.1.9) holds for all $n \geq 0$ if and only if there is a strictly positive function $r\colon \mathcal{E} \to (0,\infty)$ such that $\sum_{e\in\mathcal{E}_v} r(e) = 1$ for all $v \in \mathcal{V}$.

Suppose first that (6.1.9) holds for all $n \geq 0$. Then setting

$$r(e) := \frac{1}{s_n s_{n+1}} \sum_{k=0}^{n} (-1)^k s_{n-k},$$

for all $e \in \mathcal{E}_n$, where $\mathcal{E}_n$ the set of edges connecting the spheres S_n and S_{n+1}, we get for each $v \in S_n$, $n \geq 0$:

$$\begin{aligned}\sum_{e\in\mathcal{E}_v} r(e) &= \sum_{e\in\mathcal{E}_n\cap\mathcal{E}_v} r(e) + \sum_{e\in\mathcal{E}_{n-1}\cap\mathcal{E}_v} r(e)\\ &= s_{n+1}\frac{1}{s_n s_{n+1}} \sum_{k=0}^{n} (-1)^k s_{n-k} + s_{n-1}\frac{1}{s_{n-1} s_n} \sum_{k=0}^{n-1} (-1)^k s_{n-1-k} = 1.\end{aligned}$$

Conversely, suppose $r\colon \mathcal{E} \to (0,\infty)$ is such that $D^* r = \mathbb{1}_{\mathcal{V}}$. Then we have

$$\sum_{e\in\mathcal{E}_0} r(e) = \sum_{e\in\mathcal{E}_o} r(e) = 1 = \#S_0 = s_0,$$

and hence

$$\begin{aligned}0 < \sum_{e\in\mathcal{E}_n} r(e) &= \sum_{v\in S_n}\sum_{e\in\mathcal{E}_v} r(e) - \sum_{e\in\mathcal{E}_{n-1}} r(e)\\ &= s_n - \sum_{e\in\mathcal{E}_{n-1}} r(e)\\ &= \sum_{k=0}^{n} (-1)^k s_{n-k}\end{aligned}$$

for all $n \geq 0$, where the last equality follows immediately by induction. □

REMARK 6.12. A few remarks are in order.

(i) Proposition 6.8 can be generalized to family preserving graphs (see [**30**] for definitions).

(ii) We stress that, by the above results, the combinatorial Laplacian on an infinite path graph $\mathcal{G}_d = \mathbb{Z}_{\geq 0}$ has no minimal cable system. Indeed, every infinite path graph is an antitree with sphere numbers $s_n = 1$ for all $n \geq 0$ and (6.1.9) clearly fails to hold in this case (see also Proposition 5.20).

Despite its simple form, for a given vertex weight it is not so easy to verify the conditions in Proposition 6.9 and Corollary 6.10. In particular, returning to Example 6.7, the corresponding vertex weight m is a constant function, $m = \mathbb{1}_{\mathcal{V}}$, and one may ask: *for which graphs* $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ *the constant function* $\mathbb{1}_{\mathcal{V}}$ *belongs* *to* $D^*(C^+(\mathcal{E}))$*?* The answer to this question is provided by the following elegant result:

LEMMA 6.13. *Let* $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ *be a simple graph satisfying Hypotheses 2.1. Then* $\mathbb{1}_\mathcal{V} \in D^*(C^+(\mathcal{E}))$ *if and only if for each* $e \in \mathcal{E}$ *there is a disjoint cycle cover of* $\mathcal{G}_d$ *containing* e *in one of its cycles.*

Recall that a *disjoint cycle cover* of $\mathcal{G}_d$ is a collection of vertex-disjoint cycles in $\mathcal{G}_d$ such that every vertex in $\mathcal{G}_d$ lies on some edge in one of the cycles. Here, by a cycle of length $n \in \mathbb{Z}_{\geq 2}$ in a simple graph $\mathcal{G}_d$, we mean a path $\mathcal{P} = (v_k)_{k=0}^n$ such that $v_0 = v_n$ and all other vertices are distinct. Notice that this definition differs slightly from the one given in Section 2.1.1, that is, in the present section we allow for a moment cycles of length two (consisting of "going back and forth" along one fixed edge).

REMARK 6.14. Lemma 6.13 is due to G. Zaimi and was published in *MathOverflow*[†] as the answer to a question posed by M. Folz. It is curious to mention that Folz came up in [**70**] with a problem similar to Problem 6.1 when studying stochastic completeness of weighted graphs and attempting to prove a volume growth test by employing connections between Dirichlet forms on graphs and metric graphs, which allow to transfer the results from strongly local Dirichlet forms to Dirichlet forms on graphs [**70**], [**71**] (see Sections 4.2 and 4.6 for further information).

REMARK 6.15. Notice that in the case of finite graphs, for each $e \in \mathcal{E}$ there is a disjoint cycle cover containing e in one of its cycles if and only if removing an edge decreases the permanent of the corresponding adjacency matrix. The appearance of permanents is not at all surprising since

$$(D^*Df)(v) = \sum_{u\sim v} f(v) + f(u) = \deg(v)f(v) + \sum_{u\sim v} f(u)$$

is the so-called *signless Laplacian*. Here the second summand is the usual adjacency matrix.

6.3. Life with loops

As we have seen in Section 6.2, a minimal cable system for $(\mathcal{V}, m; b)$ may not exist. Moreover, to verify its existence is a rather complicated task even in some simple cases. It turns out that the situation changes once we drop the minimality assumption. In particular, we obtain an affirmative answer to Problem 6.2:

THEOREM 6.16. *Every locally finite graph* $(\mathcal{V}, m; b)$ *has a cable system.*

PROOF. The proof is by construction. As before, denote by $\mathcal{G}_b = (\mathcal{V}, \mathcal{E}_b)$ the simple graph associated with b (see Remark 2.7). Let $\mathcal{G}_{\text{loop}} = (\mathcal{V}, \mathcal{E}_{\text{loop}})$ be the (combinatorial) graph obtained from $\mathcal{G}_b = (\mathcal{V}, \mathcal{E}_b)$ by adding a loop $e_v = e_{v,v}$ at each vertex $v \in \mathcal{V}$. More precisely, its edge set is given by

$$\mathcal{E}_{\text{loop}} = \mathcal{E}_b \cup \{e_v |\, v \in \mathcal{V}\}.$$

[†]`https://mathoverflow.net/questions/59117/`: *Assigning positive edge weights to a graph so that the weight incident to each vertex is 1*, (2011).

Next, define the edge weight $p\colon \mathcal{E}_{\mathrm{loop}} \to (0,\infty)$ by

$$p(e_{u,v})^2 = \begin{cases} \frac{1}{2\max\{1,\mathrm{Deg}(u),\mathrm{Deg}(v)\}}, & u \neq v, \\ 1, & u = v, \end{cases} \tag{6.3.1}$$

where Deg is the weighted degree function (2.2.8). The edge lengths are then defined by $|\cdot| = p(\cdot)$ on $\mathcal{E}_{\mathrm{loop}}$ and the edge weights μ and ν are given by

$$\mu(e_{u,v}) = \nu(e_{u,v}) = \begin{cases} b(u,v)p(u,v), & u \neq v, \\ m(v) - \sum_{u\sim v} b(u,v)p(e_{u,v})^2, & u = v. \end{cases} \tag{6.3.2}$$

By construction, $\mu(e_v) = \nu(e_v) > 0$ and hence we indeed obtain well-defined weights $\mu, \nu\colon \mathcal{E}_{\mathrm{loop}} \to (0,\infty)$. Moreover, it it easy to check that $(\mathcal{G}_{\mathrm{loop}}, |\cdot|, \mu, \nu)$ is a cable system for $(\mathcal{V}, m; b)$. $\square$

Remark 6.17. A few remarks are in order:

(i) The above construction is taken from [**70**, Rem. 2, p. 2107], where it was suggested in context with synchronizing Brownian motions and random walks on graphs. However, we stress that, due to the presence of a loop at every vertex, this cable system is never minimal.

(ii) After establishing existence of cable systems, the next natural question is their uniqueness. In fact, every locally finite graph b over $(\mathcal{V}, m)$ has a large number of cable systems. In particular, the above cable system is a special case of a general construction using different metrizations of discrete graphs. These connections will be discussed in the next section.

6.4. Intrinsic metrics

In this section we discuss connections between *intrinsic metrics* for the Kirchhoff Laplacian on a weighted metric graph $(\mathcal{G}, \mu, \nu)$ and the associated discrete Laplacian on a fixed model. Notice that we cannot expect a close link between the properties of the length metric ϱ_0 (see Section 2.1) and Kirchhoff Laplacians on weighted metric graphs since ϱ_0 does not depend on μ and ν. However, it is known that the spectral properties of an operator associated to a (regular) Dirichlet form relate closely to its associated *intrinsic metrics* (see, e.g., [**73**], [**195**] for precise definitions and further references).

Historically, intrinsic metrics appear first in context with strongly local forms (see [**51**, Chap. 3.2], [**26**]). More precisely, to each strongly local, regular Dirichlet form there is an associated intrinsic metric and this notion allows to generalize many results known for the Laplace–Beltrami operator on a Riemannian manifold and the Riemannian metric (see [**195**], [**196**], [**197**] for details and further references).

A rather general notion of intrinsic metrics for arbitrary (regular) Dirichlet forms was introduced in [**73**]. With its help, a variety of results could be recovered also in the non-local setting (see, e.g., [**18**], [**73**], [**111**], [**114**], [**127**] and the references therein). One of the crucial differences is that it is no longer possible to associate a unique intrinsic metric to a general Dirichlet form. More precisely, if the Dirichlet form is strongly local, then the classical intrinsic metric is intrinsic in the sense of [**73**]. Moreover, it is in a certain sense the largest one among all such metrics (see [**73**, Theorem 6.1]) and hence provides a canonical choice. For a non-local Dirichlet form (including the setting of graph Laplacians), there is in general no largest intrinsic metric and hence it is not possible to make a canonical choice.

6.4.1. Intrinsic metrics on metric graphs. We define the intrinsic metric ϱ of a weighted metric graph $(\mathcal{G},\mu,\nu)$ as the (largest) intrinsic metric of its Dirichlet Laplacian $\mathbf{H}_D$ (in particular, note that $\mathfrak{Q}_D$ is a strongly local, regular Dirichlet form). By [**195**, eq. (1.3)] (see also [**73**, Theorem 6.1]), ϱ_{intr} is given by

$$\varrho_{\mathrm{intr}}(x,y) = \sup\big\{f(x)-f(y)\,|\, f\in\widehat{\mathcal{D}}_{\mathrm{loc}}\big\},\qquad x,y\in\mathcal{G},$$

where the function space $\widehat{\mathcal{D}}_{\mathrm{loc}}$ is defined as

$$\widehat{\mathcal{D}}_{\mathrm{loc}} = \big\{f\in H^1_{\mathrm{loc}}(\mathcal{G})\;\big|\;\nu(x)|\nabla f(x)|^2\le\mu(x)\ \text{ for a.e. } x\in\mathcal{G}\big\}.$$

It turns out that ϱ_{intr} admits a rather explicit description. First of all, the above suggest to define the *intrinsic weight* $\eta\colon\mathcal{G}\to(0,\infty)$,

$$\eta=\eta_{\mu,\nu} := \sqrt{\frac{\mu}{\nu}}\quad\text{on }\ \mathcal{G}. \tag{6.4.1}$$

This weight gives rise to a new measure on $\mathcal{G}$ whose density w.r.t. the Lebesgue measure is exactly η (as in the case of the edge weights on a metric graph, we abuse the notation and denote with η both the edge weight and the corresponding measure).

Recall from Remark 2.2 that a path $\mathcal{P}$ in $\mathcal{G}$ is a continuous and piecewise injective map $\mathcal{P}\colon I\to\mathcal{G}$ defined on an interval $I\subseteq\mathbb{R}$. In case that $\mathcal{I}=[a,b]$ is compact, we call $\mathcal{P}$ a path with starting point $x:=\mathcal{P}(a)$ and endpoint $y:=\mathcal{P}(b)$. The *(intrinsic) length* of such a path $\mathcal{P}$ in $\mathcal{G}$ is defined as

$$|\mathcal{P}|_\eta := \sum_j\int_{\mathcal{P}((t_j,t_{j+1}))}\eta(\mathrm{d}s), \tag{6.4.2}$$

where $a=t_0<\dots<t_n=b$ is any partition of $\mathcal{I}=[a,b]$ such that $\mathcal{P}$ is injective on each interval (t_j,t_{j+1}) (clearly, $|\mathcal{P}|_\eta$ is well-defined).

LEMMA 6.18. *The metric ϱ_η defined by*

$$\varrho_\eta(x,y) := \inf_{\mathcal{P}}|\mathcal{P}|_\eta = \inf_{\mathcal{P}}\int_{\mathcal{P}}\eta(\mathrm{d}s),\qquad x,y\in\mathcal{G}, \tag{6.4.3}$$

where the infimum is taken over all paths $\mathcal{P}$ from x to y, coincides with the intrinsic metric on $(\mathcal{G},\mu,\nu)$ (w.r.t. $\mathfrak{Q}_D$), that is, $\varrho_{\mathrm{intr}}=\varrho_\eta$.

Notice that in the case $\mu=\nu$, η coincides with the Lebesgue measure and hence ϱ_η is nothing but the length metric ϱ_0 on $\mathcal{G}$.

PROOF. The proof is straightforward and can be found in, e.g., [**95**, Prop. 2.21], however, we decided to present it for the sake of completeness. First, observe that for any two points x,y on $\mathcal{G}$ and every path $\mathcal{P}$ from x to y, the following estimate

$$|f(x)-f(y)|\le\int_{\mathcal{P}}|\nabla f|\mathrm{d}s\le\int_{\mathcal{P}}\sqrt{\frac{\mu}{\nu}}\,\mathrm{d}s=\int_{\mathcal{P}}\eta(\mathrm{d}s)=|\mathcal{P}|_\eta \tag{6.4.4}$$

holds true for every $f\in\widehat{\mathcal{D}}_{\mathrm{loc}}$, and hence $\varrho_{\mathrm{intr}}\le\varrho_\eta$. On the other hand, define $f\in H^1_{\mathrm{loc}}(\mathcal{G})$ by fixing some $y\in\mathcal{G}$ and then set $f(x)=\varrho_\eta(x,y)$, $x\in\mathcal{G}$. It is immediate to see that f is edgewise absolutely continuous and $|\nabla f|=\sqrt{\frac{\mu}{\nu}}$ a.e. on $\mathcal{G}$. Therefore,

$f \in \widehat{\mathcal{D}}_{\mathrm{loc}}$. Moreover, for each $x \in \mathcal{G}$ we clearly have $\varrho_\eta(x, y) = f(x) - f(y) = f(x)$, which finishes the proof. $\square$

REMARK 6.19. According to the above definition of the intrinsic weight, we get for a path $\mathcal{P}_e$ consisting of a single edge $e \in \mathcal{E}$

$$|\mathcal{P}_e|_\eta = \int_e \eta(\mathrm{d}s) = |e|\sqrt{\frac{\mu(e)}{\nu(e)}} = \eta(e),$$

which connects the intrinsic path metric $\varrho_{\mathrm{intr}} = \varrho_\eta$ on $(\mathcal{G}, \mu, \nu)$ with the notion of the intrinsic edge length (3.1.1).

6.4.2. Intrinsic metrics on discrete graphs. The idea to use different metrics on graphs can be traced back at least to [**52**] and versions of metrics adapted to weighted discrete graphs have appeared independently in several works, see, e.g., [**70**], [**71**], [**90**], [**163**]. Let us now recall the definition of intrinsic metrics for graph Laplacians, where we follow [**18**], [**73**], [**127**].

For a given connected graph b over $(\mathcal{V}, m)$, a symmetric function $p\colon \mathcal{V} \times \mathcal{V} \to [0, \infty)$ such that $p(u, v) > 0$ exactly when $b(u, v) > 0$ is called a *weight function* for $(\mathcal{V}, m; b)$. Every weight function p generates a *path metric* ϱ_p on $\mathcal{V}$ with respect to the graph b via

$$\varrho_p(u, v) := \inf_{\mathcal{P}=(v_0,\dots,v_n)\colon\, u=v_0,\ v=v_n} \sum_k p(v_{k-1}, v_k). \tag{6.4.5}$$

Here the infimum is taken over all paths in b connecting u and v, that is, all sequences $\mathcal{P} = (v_0, \dots, v_n)$ such that $v_0 = u$, $v_n = v$ and $b(v_{k-1}, v_k) > 0$ for all $k \in \{1, \dots, n\}$. We stress that we always assume that b is locally finite (see Section 2.2) and hence $\varrho_p(u, v) > 0$ whenever $u \neq v$.

EXAMPLE 6.20. Let us provide a few important examples.

(i) *Combinatorial distance*: Let $p\colon \mathcal{V} \times \mathcal{V} \to \{0, 1\}$ be given by

$$p(u, v) = \begin{cases} 1, & b(u, v) \neq 0, \\ 0, & b(u, v) = 0. \end{cases} \tag{6.4.6}$$

Then the corresponding path metric is nothing but the combinatorial distance ϱ_{comb} (also known as the *word metric* in the context of Cayley graphs) on a graph b over $\mathcal{V}$.

(ii) *Natural path metric*: Define $p_b\colon \mathcal{V} \times \mathcal{V} \to [0, \infty)$ by

$$p_b(u, v) = \begin{cases} 1/b(u, v), & b(u, v) \neq 0, \\ 0, & b(u, v) = 0. \end{cases} \tag{6.4.7}$$

Then the corresponding path metric ϱ_b depends only on the graph b and not on the weight function m, and hence one may call it as a *natural path metric*. Notice also that the edge weight (6.4.7) can be interpreted as resistances (see Example 6.5).

(iii) *Star path metric*: Let $m\colon \mathcal{V} \to (0, \infty)$ be a vertex weight. Set

$$p_m(u, v) = \begin{cases} m(u) + m(v), & b(u, v) \neq 0, \\ 0, & b(u, v) = 0. \end{cases} \tag{6.4.8}$$

Then the corresponding path metric ϱ_m is called the *star metric* on the graph b over $\mathcal{V}$. The following two choices of m are of particular interest: the vertex weight

$$m_b(v) := \sum_{u\in\mathcal{V}} b(u,v), \qquad v\in\mathcal{V}, \tag{6.4.9}$$

corresponds to a simple random walk on graph b (see Remark 2.11). Another choice

$$m_{1/b}(v) := \sum_{u\sim v} \frac{1}{b(u,v)}, \qquad v\in\mathcal{V}. \tag{6.4.10}$$

appears in [**67**]. In particular, if $b\colon \mathcal{V}\times\mathcal{V}\to\{0,1\}$, then both m_b and $m_{1/b}$ coincide with the combinatorial degree function deg. In both cases the vertex weight can be considered as a weight (or length) of the corresponding star $\mathcal{E}_v$ at $v\in\mathcal{V}$, which explains the name.

Recall (see [**73**] and also [**113**], [**127**]) the following important notion:

Definition 6.21. A metric ϱ on $\mathcal{V}$ is called *intrinsic* with respect to $(\mathcal{V},m;b)$ if

$$\sum_{u\in\mathcal{V}} b(u,v)\varrho(u,v)^2 \le m(v) \tag{6.4.11}$$

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

Similarly, a weight function $p\colon \mathcal{V}\times\mathcal{V}\to[0,\infty)$ is called an *intrinsic weight* for $(\mathcal{V},m;b)$ if

$$\sum_{u\in\mathcal{V}} b(u,v)p(u,v)^2 \le m(v), \qquad v\in\mathcal{V}.$$

If p is an intrinsic weight, then the associated path metric ϱ_p is called *strongly intrinsic* (it is obviously intrinsic in the sense of Definition 6.21).

Remark 6.22. For any given locally finite graph $(\mathcal{V},m;b)$ an intrinsic metric always exists (see [**113**, Example 2.1], [**127**] and also [**44**]). Indeed, we obtain an intrinsic weight by setting

$$p(u,v) = \begin{cases} \frac{1}{\sqrt{\max\{1,\mathrm{Deg}(u),\mathrm{Deg}(v)\}}}, & b(u,v)\neq 0,\\ 0, & b(u,v)=0,\end{cases} \tag{6.4.12}$$

where Deg is the weighted degree function (2.2.8), and hence the corresponding path metric $\varrho=\varrho_p$ is strongly intrinsic. We are going to provide further examples in the next sections.

Example 6.23. Let us continue with Example 6.20.

(i) If a graph $b\colon \mathcal{V}\times\mathcal{V}\to\{0,1\}$ is locally finite and $m=\deg$ on $\mathcal{V}$, then the combinatorial distance ϱ_{comb} on $\mathcal{V}$ is intrinsic.

(ii) If $m=m_{1/b}$, then the path metric ϱ_b is intrinsic. Moreover, the weight p_b is intrinsic as well.

(iii) Let us stress that the star path metric ϱ_m is not intrinsic in general since it does not contain any information on b except the underlying combinatorial structure.

REMARK 6.24. Let us emphasize that the combinatorial distance ϱ_{comb} is not intrinsic for the combinatorial Laplacian L_{comb} ($m \equiv \mathbb{1}$ on $\mathcal{V}$ in this case). However, ϱ_{comb} is equivalent to an intrinsic path metric if and only if deg is bounded on $\mathcal{V}$, that is, the corresponding graph has bounded geometry. If $\sup_{\mathcal{V}} \deg(v) = \infty$, then L_{comb} is unbounded in $\ell^2(\mathcal{V})$ and it turned out that ϱ_{comb} is not a suitable metric on $\mathcal{V}$ to study the properties of L_{comb} (in particular, this has led to certain controversies in the past, see [**133**], [**210**]).

6.4.3. Connections between discrete and continuous. Consider a weighted metric graph $(\mathcal{G}, \mu, \nu)$ and its intrinsic metric ϱ_η defined in Section 6.4.1. With each model of $(\mathcal{G}, \mu, \nu)$ we can associate the vertex set $\mathcal{V}$ together with the vertex weight $m\colon \mathcal{V} \to (0, \infty)$ and the graph $b\colon \mathcal{V} \times \mathcal{V} \to [0, \infty)$, see (3.1.1)–(3.1.6). The next result shows that the intrinsic metric ϱ_η of $(\mathcal{G}, \mu, \nu)$ gives rise to a particular intrinsic metric for $(\mathcal{V}, m; b)$.

LEMMA 6.25. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph and ϱ_η its intrinsic metric. Fix further a model of $(\mathcal{G}, \mu, \nu)$ having finite intrinsic size and define the metric $\varrho_{\mathcal{V}}$ on $\mathcal{V}$ as a restriction of ϱ_η onto $\mathcal{V} \times \mathcal{V}$,*

$$\varrho_{\mathcal{V}}(u, v) := \varrho_\eta(u, v), \qquad (u, v) \in \mathcal{V} \times \mathcal{V}. \tag{6.4.13}$$

Then:

(i) *$\varrho_{\mathcal{V}}$ is an intrinsic metric for $(\mathcal{V}, m; b)$.*
(ii) *$(\mathcal{G}, \varrho_\eta)$ is complete as a metric space exactly when $(\mathcal{V}, \varrho_{\mathcal{V}})$ is complete.*

PROOF. (i) Fix a model of $(\mathcal{G}, \mu, \nu)$ and consider the edge weight function $p_\eta\colon \mathcal{V} \times \mathcal{V} \to [0, \infty)$ given by

$$p_\eta(u, v) = \begin{cases} \min_{e \in \mathcal{E}_{u,v}} \eta(e), & u \sim v \text{ and } u \neq v, \\ 0, & \text{else}, \end{cases} \qquad (u, v) \in \mathcal{V} \times \mathcal{V}. \tag{6.4.14}$$

Here $\mathcal{E}_{u,v}$ denotes the set of edges between u and v (recall that we allow multigraphs). Using (3.1.1)–(3.1.6), notice that for every $v \in \mathcal{V}$,

$$\begin{aligned} \sum_{u \in \mathcal{V}} b(u, v) p_\eta(u, v)^2 &= \sum_{u \in \mathcal{V} \setminus \{v\}} \sum_{e \in \mathcal{E}_{u,v}} \frac{\nu(e)}{|e|} p_\eta(u, v)^2 \\ &\leq \sum_{u \in \mathcal{V} \setminus \{v\}} \sum_{e \in \mathcal{E}_{u,v}} \frac{\nu(e)}{|e|} \eta(e)^2 \\ &= \sum_{u \in \mathcal{V} \setminus \{v\}} \sum_{e \in \mathcal{E}_{u,v}} |e| \mu(e) \\ &\leq m(v), \end{aligned}$$

where in the last inequality we used the fact that $(\mathcal{G}, \mu, \nu)$ has finite intrinsic size. Hence p_η is an intrinsic weight for $(\mathcal{V}, m; b)$. It remains to notice that each path $\mathcal{P}$ without self-intersections from $u \in \mathcal{V}$ to $v \in \mathcal{V}$ in the metric graph $\mathcal{G}$ can be identified with a path $\mathcal{P}_d = (e_{u,v_1}, \dots, e_{v_{n-1},v})$ in the fixed model from $u = v_0$ to $v = v_n$ without self-intersections. With respect to this identification,

$$|\mathcal{P}|_\eta = \sum_{k=1}^{n} \eta(e_{v_{k-1},v_k})$$

which immediately implies that $\varrho_{p_\eta} = \varrho_\eta|_{\mathcal{V}\times\mathcal{V}}$ (notice that both the infima in (6.4.3) and (6.4.5) can be taken over paths without self-intersections).

(ii) The remaining equivalence of the metric space completeness is straightforward to verify directly (one can also immediately observe it by comparing geodesic completeness on both metric spaces and then using the corresponding versions of the Hopf–Rinow theorems, see Section 6.4.5). $\square$

REMARK 6.26. Notice that the proof also implies that (6.4.14) is an intrinsic weight for $(\mathcal{V}, m; b)$ and $\varrho_{\mathcal{V}} = \varrho_{p_\eta}$ is the corresponding strongly intrinsic path metric.

Let us mention that Lemma 6.25 also has an interpretation in terms of *quasi-isometries* (see, e.g., [**12**, Def. 1.12], [**173**, Sec. 1.3], [**184**]).

DEFINITION 6.27. A map $\phi\colon X_1 \to X_2$ between two metric spaces (X_1, ϱ_1) and (X_2, ϱ_2) is called *a quasi-isometry* if there are constants $a, R > 0$ and $b \geq 0$ such that

$$a^{-1}(\varrho_1(x,y) - b) \leq \varrho_2(\phi(x), \phi(y)) \leq a(\varrho_1(x,y) + b), \tag{6.4.15}$$

for all $x, y \in X_1$ and, moreover,

$$\bigcup_{x\in X_1} B_R(\phi(x); \varrho_1) = X_2. \tag{6.4.16}$$

One can check that quasi-isometries define an equivalence relation between metric spaces. It turns out that the map $\imath_{\mathcal{V}}$ defined in Section 4.3 is closely related with a quasi-isometry between weighted graphs and metric graphs:

LEMMA 6.28. *Assume the conditions of Lemma 6.25. Then the map*

$$\varphi\colon \mathcal{V} \to \mathcal{G}, \qquad \varphi(v) = v \tag{6.4.17}$$

defines a quasi-isometry between the metric spaces $(\mathcal{G}, \varrho_\eta)$ and $(\mathcal{V}, \varrho_{\mathcal{V}})$. Moreover, the map φ is bi-Lipschitz (i.e., b in (6.4.15) *can be set equal to* 0*).*

PROOF. The proof is a straightforward check of (6.4.15) and (6.4.16) for the map ϕ with $a = 1$, $b = 0$ and $R = \eta^*(\mathcal{E})$ and we leave it to the reader. $\square$

REMARK 6.29. The notion of quasi-isometries was introduced in the works of M. Gromov [**92**] and M. Kanai [**121**], [**122**]. It is well-known in context with Riemannian manifolds and (combinatorial) graphs that roughly isometric spaces share many important properties: e.g., geometric properties (such as volume growth and isoperimetric inequalities) [**121**], parabolicity/transience [**46**], [**121**], [**158**], Nash inequalities [**46**], Liouville-type theorems for harmonic functions of finite energy [**46**], [**104**], [**105**], [**149**], [**158**], [**191**] and parabolic/elliptic Harnack inequalities [**14**], [**15**], [**46**], [**101**]. However, we stress that most of these connections also require additional conditions on the local geometry of the spaces. Typically, one imposes a bounded geometry assumption for manifolds [**121**] and bounded geometry/controlled weights assumptions for graphs [**12**], [**15**], [**192**, Chap. VII].

Some of our conclusions are reminiscent of this notion (see, e.g., Theorem 4.17, Theorem 4.30 and Proposition 7.38), but in fact our results go beyond this framework. For instance, the strong/weak Liouville property (i.e., all positive/bounded harmonic functions are constant) is not preserved under bi-Lipschitz maps in general [**153**]. However, the equivalence holds true for our setting (this is a trivial consequence of Lemma 6.46 below). In addition, we stress that in contrast to the above works, we do not require any additional local conditions (e.g., bounded geometry). On the other hand, our results connect only two particular roughly isometric spaces $(\mathcal{G}, \varrho_\eta)$ and $(\mathcal{V}, \varrho_\mathcal{V})$ and not the whole equivalence class of roughly isometric weighted graphs or weighted metric graphs.

By Lemma 6.25, each cable system having finite intrinsic size† gives rise to an intrinsic metric $\varrho_\mathcal{V}$ for $(\mathcal{V}, m; b)$ using a simple restriction to vertices. In view of Problems 6.1–6.2, it is natural to ask which intrinsic metrics on graphs can be obtained as restrictions of intrinsic metrics on weighted metric graphs. It turns out that a rather large class can be covered in this way. Before stating the result, let us recall one more definition.

Definition 6.30. Let b be a locally finite graph over $\mathcal{V}$. A metric ϱ on $\mathcal{V}$ has *finite jump size* (with respect to b) if

$$s(\varrho) := \sup\{\varrho(u,v) \,|\, u,v \in \mathcal{V} \text{ with } b(u,v) > 0\} \tag{6.4.18}$$

is finite.

Lemma 6.31. *Let $(\mathcal{V}, m; b)$ be a locally finite graph and let $\rho\colon \mathcal{V}\times\mathcal{V} \to [0,\infty)$ be an intrinsic path metric having finite jump size $s(\varrho) < \infty$. Then there is a cable system for $(\mathcal{V}, m; b)$ satisfying $\eta^*(\mathcal{E}) \le \max\{s(\varrho), 1\}$ and such that $\rho_\mathcal{V} = \rho$. Moreover, $(\mathcal{V}, \varrho_\mathcal{V})$ is complete exactly when the corresponding weighted metric graph $(\mathcal{G}, \mu, \nu)$ of the cable system equipped with its intrinsic metric ϱ_η is complete.*

Proof. Our proof follows closely the ideas of [**112**, p. 128] and [**70**]. The edge set $\mathcal{E}$ of the cable system $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu_\mathcal{E}, \nu_\mathcal{E})$ is defined as follows: first of all, we create an edge $e = e_{u,v}$ between each pair of vertices $u, v \in \mathcal{V}$ with $b(u,v) > 0$. Moreover, we add a loop edge at each vertex $v \in \mathcal{V}$ satisfying

$$\sum_{u\in\mathcal{V}\setminus\{v\}} b(u,v)\varrho(u,v)^2 < m(v).$$

Notice that the resulting combinatorial graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ does not have any multiple edges. Specifying now the edge lengths and weight, assume first that $e_{u,v} \in \mathcal{E}$ is a non-loop edge, that is, $u \ne v$. Then we set

$$|e_{u,v}| = \varrho(u,v), \qquad \mu(e_{u,v}) = \nu(e_{u,v}) = \varrho(u,v)b(u,v).$$

If $e \in \mathcal{E}$ is a loop at the vertex $v \in \mathcal{V}$, then we define

$$|e| = 1, \qquad \mu(e) = \nu(e) = m(v) - \sum_{u\in\mathcal{V}\setminus\{v\}} b(u,v)\varrho(u,v)^2 > 0.$$

By definition, $\eta(e_{u,v}) = |e_{u,v}| = \varrho(u,v)$ for each non-loop edge $e_{u,v}$ and it is straightforward to check that $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu_\mathcal{E}, \nu_\mathcal{E})$ is a cable system for $(\mathcal{V}, m; b)$. Moreover, since ϱ is a path metric, we easily infer that $\varrho = \varrho_\mathcal{V}$ (see Remark 6.26 (ii)). □

Remark 6.32. A few remarks are in order.

(i) Notice that an intrinsic path metric with jump size $s(\varrho) \le 1$ indeed exists for every graph $(\mathcal{V}, m; b)$ (e.g., take the path metric in Remark 6.22).

†Since by definition a cable system is a model of a weighted metric graph, the notion of intrinsic size (see Definition 3.16) immediately extends to cable systems.

(ii) We stress that not every intrinsic metric is a path metric. However, in some sense intrinsic path metrics correspond to particularly large intrinsic metrics. Namely, for every intrinsic metric ϱ, the choice $p(u,v) := \varrho(u,v)$ whenever $b(u,v) > 0$ defines an intrinsic weight and the corresponding path metric clearly satisfies $\varrho \le \varrho_p$ on $\mathcal{V} \times \mathcal{V}$.

6.4.4. Description of cable systems. The results of the previous sections naturally lead us to Problem 6.3. It does not seem realistic to obtain a complete answer to this question since the class of all cable systems of $(\mathcal{V}, m; b)$ is rather large. Hence our strategy will be to restrict to a certain class of "well-behaved" cable systems and obtain a precise description of those.

DEFINITION 6.33. A cable system $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ for a graph b over $(\mathcal{V}, m)$ is called *canonical* if it satisfies the following additional assumptions:

(i) the underlying graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ has no multiple edges,
(ii) the edge weights μ and ν coincide,

$$\mu(e) = \nu(e), \qquad e \in \mathcal{E}, \tag{6.4.19}$$

(iii) $|e| = 1$ whenever e is a loop and, moreover, $\sup_{e\in\mathcal{E}} |e| < \infty$.

The set of canonical cable systems of $(\mathcal{V}, m; b)$ is denoted by $\mathrm{Cab} = \mathrm{Cab}(\mathcal{V}, m; b)$.

Notice that conditions (ii) and (iii) imply that canonical cable systems have finite intrinsic size since in this case intrinsic edge length coincides with the edge length and hence $\eta^*(\mathcal{E}) = \sup_{e\in\mathcal{E}} |e|$.

The importance of canonical cable systems stems from the fact that the intrinsic metric ϱ_η of the corresponding weighted metric graph coincides with the length metric ϱ_0. Moreover, it turns out that canonical cable systems can be described in terms of intrinsic metrics. More precisely, denote by $\mathrm{W}(\mathcal{V}, m; b)$ the set of intrinsic weights for $(\mathcal{V}, m; b)$ having *finite jump size*, that is, all intrinsic weights $p\colon \mathcal{V}\times\mathcal{V} \to \mathbb{R}_{\ge 0}$ satisfying

$$\sup_{u,v\colon b(u,v)>0} p(u,v) < \infty. \tag{6.4.20}$$

We already observed that for every canonical cable system, the choice

$$p(u,v) = \begin{cases} |e_{u,v}| & \text{if } u \ne v \text{ and } u \sim v, \\ 0 & \text{else}, \end{cases} \tag{6.4.21}$$

defines an intrinsic weight on $(\mathcal{V}, m; b)$ (see Remark 6.26). Hence (6.4.21) defines a map

$$\Psi\colon\ \mathrm{Cab}(\mathcal{V}, m; b) \to \mathrm{W}(\mathcal{V}, m; b). \tag{6.4.22}$$

In fact this leads to a one-to-one correspondence between canonical cable systems and intrinsic weights.

THEOREM 6.34. *Suppose b is a locally finite connected graph over $(\mathcal{V}, m)$. Then the map Ψ defined by* (6.4.21) *and* (6.4.22) *is a bijection between the set of canonical cable systems of* $(\mathcal{V}, m; b)$ *and intrinsic weights of* $(\mathcal{V}, m; b)$ *having finite jump size.*

PROOF. As noticed above, the map Ψ is well-defined and, moreover, its surjectivity was established in Lemma 6.31. More precisely, if we replace $\varrho(u,v)$ by $p(u,v)$ in its proof, we obtain an explicit construction of a canonical cable system for every $p \in \mathrm{W}(\mathcal{V}, m; b)$.

To prove the injectivity of Ψ, we essentially invert the construction in Lemma 6.31. Let $C = (\mathcal{V}, \mathcal{E}, |\cdot|, \mu)$ be a canonical cable system for $(\mathcal{V}, m; b)$. First of all, notice that the non-loop edges of $\mathcal{E}$ are determined by (3.1.6): there is an edge $e_{u,v}$ between $u \neq v$ exactly when $b(u, v) > 0$. Moreover, if $\Psi(C) = p$, then the equalities (6.4.21) and (3.1.6) imply that

$$|e_{u,v}| = p(u, v), \qquad\qquad \mu(e) = b(u, v)p(u, v)$$

for each non-loop edge $e_{u,v}$ between $u \neq v$. However, this means that the location of the loop edges of $\mathcal{E}$ is determined by (3.1.5) and the finite intrinsic size assumption. Namely, it is easy to see that they are attached to exactly those vertices $v \in \mathcal{V}$ with

$$m(v) - \sum_{u : b(u,v)>0} b(u, v)p(u, v)^2 = m(v) - \sum_{u : b(u,v)>0} |e_{u,v}|\mu(e_{u,v}) > 0.$$

This proves that the edge set $\mathcal{E}$ of C is uniquely determined by $p = \Psi(C)$. Moreover, since we required that $|e| = 1$ for loop edges, it follows that

$$2\mu(e_v) = m(v) - \sum_{u : b(u,v)>0} b(u, v)p(u, v)^2 > 0$$

if there is a loop e_v at a vertex $v \in \mathcal{V}$. This shows that the weight function $\mu \colon \mathcal{E} \to (0, \infty)$ is determined by $p = \Psi(C)$ as well and the injectivity of Ψ is proven. □

REMARK 6.35. Notice that from a cable system $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ of $(\mathcal{V}, m; b)$ we can construct further ones by scaling, that is, we set

$$|e|' = c(e)|e|, \qquad \mu'(e) = c(e)^{-1}\mu(e), \qquad \nu'(e) = c(e)\nu(e), \qquad e \in \mathcal{E},$$

for some $(c(e))_{e\in\mathcal{E}} \subseteq (0, \infty)$. The corresponding Kirchhoff Laplacians and energy forms are (unitarily) equivalent as well. Among these equivalent cable systems there is a unique one satisfying $\mu \equiv \nu$ and this explains condition (ii) in Definition 6.33 (cf. also [**95**, Def. 2.18]). Conditions (ii) and (iii) exclude similar constructions (i.e., by replacing single edges with multiple ones and different normalizations of loop edges) and simplify the definition of m (see (3.1.1)–(3.1.5)).

6.4.5. Interlude: the Hopf–Rinow theorem on graphs. As it was already mentioned in Remark 2.1, a metric graph $\mathcal{G}$ equipped with its length metric ϱ_0 is a length metric space (or simply a length space, see [**36**] for definitions). Clearly, equipping a weighted metric graph $(\mathcal{G}, \mu, \nu)$ with the intrinsic metric ϱ_η, which is defined by (6.4.3), turns $\mathcal{G}$ into a length space as well. A path $\mathcal{P}$ in $\mathcal{G}$, a continuous and piecewise injective map $\mathcal{P} \colon I \to \mathcal{G}$ defined on an interval $I \subseteq \mathbb{R}$, is called *geodesic* if it is locally a distance minimizer, i.e., for each $x \in I$ there is a neighborhood $B(x) \subset I$ of x such that $\mathcal{P}|_{B(x)}$ is a shortest path (w.r.t. the corresponding length metric). In the following it would be convenient to assume that each geodesic is parameterized by its arc-length.

Complete lengths spaces enjoy a number of very important properties. For instance, if $(\mathcal{G}, \varrho_\eta)$ is complete as a metric space (recall that we always assume $\mathcal{G}$ to be locally finite), then it is *a geodesic metric space* meaning that any two points $x, y \in \mathcal{G}$ can be connected by a minimal geodesic, that is, by a shortest path (see, e.g., [**36**, Theorem 2.5.23]). Moreover, the classical Hopf–Rinow theorem, which connects completeness with geodesic completeness, as well as with compactness of closed distance balls, extends from the smooth setting of Riemannian manifolds to locally compact length spaces [**36**, Theorem 2.5.28], and in the case of metric graphs it reads as follows.

THEOREM 6.36 (Hopf–Rinow's theorem on metric graphs). *Let $\mathcal{G}$ be a locally finite connected weighted metric graph and let ϱ be a path metric on $\mathcal{G}$.*[†] *The following assertions are equivalent:*

(i) *$(\mathcal{G}, \varrho)$ is complete,*
(ii) *$(\mathcal{G}, \varrho)$ is boundedly compact (every closed metric ball in $(\mathcal{G}, \varrho)$ is compact),*
(iii) *every geodesic $\mathcal{P}\colon [0, a) \to \mathcal{G}$ extends to a continuous path $\overline{\mathcal{P}}\colon [0, a] \to \mathcal{G}$.*

It is natural to expect that the Hopf–Rinow theorem extends to the case of locally finite weighted graphs and this was done in [**165**] and [**113**, Theorem A.1] (see also [**127**]).

THEOREM 6.37 (Hopf–Rinow's theorem on graphs). *Let b be a locally finite graph over $\mathcal{V}$ and let ϱ be a path metric for $(\mathcal{V}; b)$. The following assertions are equivalent:*

(i) *$(\mathcal{V}, \varrho)$ is complete as a metric space,*
(ii) *every closed metric ball in $(\mathcal{V}, \varrho)$ is finite,*
(iii) *every infinite geodesic has infinite length.*[‡]

REMARK 6.38. A few remarks are in order.

(i) Taking into account the connection between weighted graphs and cable systems, it is not difficult to derive Theorem 6.37 from Theorem 6.36. For instance, if additionally ϱ is intrinsic for $(\mathcal{V}, m; b)$ and has finite jump size, then by Theorem 6.34 there is a canonical cable system $(\mathcal{G}, \mu, \mu)$ such that ϱ coincides with the restriction of $\varrho_\eta = \varrho_0$ onto $\mathcal{V}\times\mathcal{V}$. By Lemma 6.25(ii), $(\mathcal{V}, \varrho)$ is complete if and only if so is $(\mathcal{G}, \varrho_\eta)$ and hence it remains to apply Theorem 6.36. Notice that this approach was used in [**165**, p. 24].
(ii) For a version of the discrete Hopf–Rinow theorem for graphs which are *not locally finite* see the recent [**135**].

6.4.6. Volume growth. We finish this section with a simple but useful estimate between the volume of balls with respect to the intrinsic metrics ϱ_η and $\varrho_\mathcal{V}$. For any $x \in \mathcal{G}$ and $r > 0$, we denote an intrinsic distance ball of radius r by

$$B_r(x) := B_r(x; \varrho_\eta) = \{y \in \mathcal{G} \mid \varrho_\eta(x, y) < r\}. \tag{6.4.23}$$

Similarly, for any vertex $v \in \mathcal{V}$ and $r > 0$, the ball of radius r in the induced metric $\varrho_\mathcal{V}$ on $\mathcal{V}$ is denoted by

$$B_r^\mathcal{V}(v) := B_r^\mathcal{V}(v; \varrho_\mathcal{V}) = \{u \in \mathcal{V} \mid \varrho_\mathcal{V}(u, v) < r\}. \tag{6.4.24}$$

In particular, we have the obvious relation $B_r^\mathcal{V}(v; \varrho_\mathcal{V}) = B_r(v; \varrho_\eta) \cap \mathcal{V}$ for every $r > 0$ and vertex $v \in \mathcal{V}$.

LEMMA 6.39. *Assume the conditions of Lemma 6.25. Then*

$$\mu\big(B_r(v; \varrho_\eta)\big) \le m\big(B_r^\mathcal{V}(v; \varrho_\mathcal{V})\big) \le 2\mu\big(B_{r+\eta^*(\varepsilon)}(v; \varrho_\eta)\big) \tag{6.4.25}$$

for every $r > 0$ and vertex $v \in \mathcal{V}$.

[†]In fact, we are going to use this result with only two particular metrics on $\mathcal{G}$: the length metric ϱ_0 and the intrinsic path metric ϱ_η.

[‡]In a discrete measure space, paths are parameterized by the combinatorial distance and "infinite geodesic" simply means that as a path it has infinite combinatorial length.

Proof. First of all, notice that

$$m\big(B_r^{\mathcal{V}}(v)\big) = \sum_{u\in B_r^{\mathcal{V}}(v)}\sum_{\vec{e}\in\vec{\mathcal{E}}_u}\mu(e)|e| = \sum_{e\in\vec{\mathcal{E}}}\mu(e)|e|\Big(\mathbb{1}_{B_r(v)}(e_\imath)+\mathbb{1}_{B_r(v)}(e_\tau)\Big),$$

where as always $\mathbb{1}_{B_r(v)}$ denotes the characteristic function of the subset $B_r(v)\subseteq\mathcal{G}$. This implies the first inequality since clearly

$$m\big(B_r^{\mathcal{V}}(v)\big) \ge \sum_{e\in\mathcal{E}\colon\, e\cap B_r(v)\neq\varnothing}\mu(e)|e| \ge \sum_{e\in\mathcal{E}}\mu(e\cap B_r(v)) = \mu(B_r(v)).$$

Conversely, every edge $e\in\mathcal{E}$ with at least one endpoint in $B_r(v)$ is contained in the larger ball $B_{r+\eta^*(\mathcal{E})}(v)$. In particular,

$$m\big(B_r^{\mathcal{V}}(v)\big) \le 2\sum_{e\in\mathcal{E}}\mu\big(e\cap B_{r+\eta^*(\mathcal{E})}(v)\big) \le 2\mu(B_{r+\eta^*(\mathcal{E})}(v)),$$

and the proof is complete. □

Remark 6.40. On the one hand, Lemma 6.39 establishes connections between volume growth of large balls in $(\mathcal{G},\varrho_\eta)$ and $(\mathcal{V},\varrho_{\mathcal{V}})$ (e.g., their polynomial/subexponential/exponential growth rates are the same) and, in fact, this phenomenon is well-known in context with quasi-isometries (indeed, a volume growth is one of the most important quasi-isometric invariants). On the other hand, Lemma 6.39 indicates a connection between small scales too and this is usually not a part of the quasi-isometric setting.

6.5. Harmonic functions on graphs

6.5.1. Harmonic functions on weighted graphs. Let us begin by briefly recalling basic definitions. Assume that b is a connected graph over $(\mathcal{V},m)$ satisfying the assumptions (i)–(iii) of Section 2.2 (at this point there is no need to assume that b is locally finite). Also, by L we denote the corresponding formal Laplacian (2.2.3) (the killing term c is assumed to be identically zero).

Definition 6.41. A function $f\colon\mathcal{V}\to\mathbb{C}$ is called *harmonic* (*subharmonic, superharmonic*) w.r.t. $(\mathcal{V},m;b)$ (or, simply, L-harmonic, L-subharmonic, L-superharmonic) if f belongs to $\mathcal{F}_b(\mathcal{V})$ and satisfies

$$(Lf)(v)=0, \qquad \Big((Lf)(v)\le 0, \quad (Lf)(v)\ge 0\Big) \tag{6.5.1}$$

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

If $f\in\mathcal{F}_b(\mathcal{V})$ satisfies (6.5.1) on a subset $Y\subseteq\mathcal{V}$, then it is called *harmonic on* Y (*subharmonic on* Y, etc.) w.r.t. $(\mathcal{V},m;b)$.

Remark 6.42. Let us emphasize that the notion of harmonic/subharmonic/superharmonic functions is independent of the weight m and hence one can simply set $m\equiv 1$ in Definition 6.41 and say *harmonic/subharmonic/superharmonic w.r.t.* $(\mathcal{V};b)$. On the other hand, when considering the maximal Laplacian $\mathbf{h}$ (see (2.2.5)) in the Hilbert space $\ell^2(\mathcal{V};m)$, its kernel consists of L-harmonic functions which belong to $\ell^2(\mathcal{V};m)$, and this subspace of course depends on the weight m.

The following fact is trivial in the setting of weighted graphs.

LEMMA 6.43. *Suppose $f \in \mathcal{F}_b(\mathcal{V})$ solves $Lf + \lambda f = 0$ for some $\lambda \in \mathbb{R}_{\geq 0}$.*[†] *Then $|f|$ is subharmonic w.r.t. $(\mathcal{V}, m; b)$. If in addition f is real-valued, then both f_+ and f_- are subharmonic w.r.t. $(\mathcal{V}, m; b)$. Here $f_\pm = (|f| \pm f)/2$.*

PROOF. First observe that $Lf + \lambda f = 0$ means that

$$f(v)\Big(\sum_{u\in\mathcal{V}} b(u,v) + \lambda m(v)\Big) = \sum_{u\in\mathcal{V}} b(u,v)f(u)$$

for all $v \in \mathcal{V}$. Since the second factor on the LHS is positive, we get

$$|f(v)|\Big(\sum_{u\in\mathcal{V}} b(u,v) + \lambda m(v)\Big) = \Big|\sum_{u\in\mathcal{V}} b(u,v)f(u)\Big| \leq \sum_{u\in\mathcal{V}} b(u,v)|f(u)|,$$

which immediately implies that

$$\begin{aligned}(L|f|)(v) &= \frac{1}{m(v)}\sum_{u\in\mathcal{V}} b(u,v)(|f(v)| - |f(u)|)\\ &= \frac{1}{m(v)}\Big(|f(v)|\sum_{u\in\mathcal{V}} b(u,v) - \sum_{u\in\mathcal{V}} b(u,v)|f(u)|\Big)\\ &\leq -\lambda|f(v)|.\end{aligned}$$

Therefore, $L|f| \leq -\lambda|f| \leq 0$ and hence $|f|$ is subharmonic w.r.t. $(\mathcal{V}, m; b)$. It remains to notice that for real-valued f by linearity we have

$$Lf_\pm = \frac{1}{2}\big(L|f| \pm Lf\big) \leq \frac{1}{2}\big(-\lambda|f| \mp \lambda f\big) \leq 0. \qquad \square$$

6.5.2. Harmonic functions on metric graphs. In the case of metric graphs, one can start with the definition for strongly local Dirichlet forms (see, e.g., [**195**]).

DEFINITION 6.44. A function $f\colon \mathcal{G} \to \mathbb{R}$ is called *harmonic* w.r.t. $(\mathcal{G}, \mu, \nu)$ if $f \in H^1_{\mathrm{loc}}(\mathcal{G})$ and

$$\int_{\mathcal{G}} \nabla f(x)\nabla g(x)\nu(\mathrm{d}x) = 0, \tag{6.5.2}$$

for all $0 \leq g \in H^1_c(\mathcal{G}) = H^1(\mathcal{G}) \cap C_c(\mathcal{G})$.

If for an open subset $Y \subseteq \mathcal{G}$, (6.5.2) holds for all $0 \leq g \in H^1(\mathcal{G}) \cap C_c(Y)$ with compact support in Y, then f is called *harmonic* on Y.

Replacing the equality in (6.5.2) by the inequality " $\leq$ " (resp., by " $\geq$ "), one gets the definition of a *subharmonic* (resp., *superharmonic*) function on $Y \subseteq \mathcal{G}$ w.r.t. $(\mathcal{G}, \mu, \nu)$.

REMARK 6.45. We stress that the notion of harmonic/subharmonic/superharmonic functions is independent of the weight $\mu\colon \mathcal{G} \to (0, \infty)$ (since this obviously holds for the space $H^1_{\mathrm{loc}}(\mathcal{G})$) and hence we could also call them harmonic/subharmonic/superharmonic functions w.r.t. $(\mathcal{G}, \nu)$. However, for our purposes we will mainly be interested in functions which additionally belong to $L^p(\mathcal{G}; \mu)$ and of course these spaces do depend on the edge weight μ.

If it is clear from the context which graph (weighted graph or weighted metric graph) is meant, we shall simply say harmonic, subharmonic, etc. Notice also that on each edge the structure of the corresponding Sobolev space is very well understood and hence we can rewrite the above definition in a more convenient

[†]Usually, for $\lambda > 0$ such a function is called λ-harmonic.

form. Recall (see Section 4.3) that for each fixed model of $(\mathcal{G}, \mu, \nu)$, $\mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ denotes the space of continuous edgewise affine functions on $\mathcal{G}$.

LEMMA 6.46. *A function $f\colon \mathcal{G} \to \mathbb{R}$ is harmonic w.r.t. $(\mathcal{G}, \mu, \nu)$ exactly when $f \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ for some model of $(\mathcal{G}, \mu, \nu)$ and, moreover, f satisfies Kirchhoff conditions at each vertex $v \in \mathcal{V}$.*

PROOF. Clearly, we only need to prove the "only if" claim. Fix an arbitrary model of $(\mathcal{G}, \mu, \nu)$. Upon choosing test functions $g \in H^1_c(\mathcal{G})$ whose support is contained in single edges, it is straightforward to see that f is affine on each edge $e \in \mathcal{E}$ (indeed, one simply needs to use the fact that a distributional solution to $f'' = 0$ is a classical solution). Next, for each vertex $v \in \mathcal{V}$, choosing test functions supported in a sufficiently small vicinity of v, a straightforward integration by parts shows that f must satisfy Kirchhoff conditions at $v \in \mathcal{V}$. □

REMARK 6.47. Let us stress that by Lemma 6.46 the set of harmonic functions is independent of the choice of a model of $\mathcal{G}$.

Using the same arguments one can easily show the following result:

LEMMA 6.48. *A function $f \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ is subharmonic (superharmonic) w.r.t. $(\mathcal{G}, \mu, \nu)$ exactly when*

$$\sum_{\vec{e}\in\vec{\mathcal{E}}_v} \nu(e)\partial_{\vec{e}} f(v) \ge 0, \qquad \Big(\sum_{\vec{e}\in\vec{\mathcal{E}}_v} \nu(e)\partial_{\vec{e}} f(v) \le 0\Big) \tag{6.5.3}$$

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

REMARK 6.49. (i) Similar to the discrete situation, Definition 6.44 can be reformulated in terms of the Laplacian Δ (see (2.4.3)). More specifically, the LHS in (6.5.2) allows us to define Δ on locally H^1 functions in a standard way (as a distribution on the test function space $H^1_c(\mathcal{G})$). Then a locally H^1 function f is called harmonic (resp., subharmonic, superharmonic) if $\Delta f = 0$ on $\mathcal{G}$ (resp., Δf is a nonpositive/nonnegative distribution on $\mathcal{G}$). This definition becomes transparent for edgewise affine functions. If $f \in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ for some model of $(\mathcal{G}, \mu, \nu)$, then a straightforward integration by parts shows that, as a distribution,

$$\Delta f = \sum_{v\in\mathcal{V}} \Big(\sum_{\vec{e}\in\vec{\mathcal{E}}_v} \nu(e)\partial_{\vec{e}} f(v)\Big)\delta_v. \tag{6.5.4}$$

Comparing (6.5.4) with Lemma 6.46 and Lemma 6.48, one concludes that f is harmonic (subharmonic or superharmonic) exactly when $\Delta f = 0$ ($\Delta f \ge 0$ or $\Delta f \le 0$).

(ii) We stress that there are sub-/superharmonic functions which are not edgewise affine. For instance, it is easy to check that a continuous, edgewise H^2-function f is subharmonic exactly when f satisfies (6.5.3) and is subharmonic on every edge. However, for our purposes it will suffice to consider only edgewise affine sub-/superharmonic functions.

It is not difficult to notice that the above results immediately connect harmonic, subharmonic, and superharmonic functions on graphs and on metric graphs.

LEMMA 6.50. *Let* $(\mathcal{G},\mu,\nu)$ *be a weighted metric graph together with a fixed model. Let also* $(\mathcal{V},m;b)$ *be the corresponding weighted graph defined by* (3.1.3)–(3.1.6). *Then* $f\in \mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ *is harmonic (resp., subharmonic, superharmonic) if and only if* $\mathbf{f}=\imath_{\mathcal{V}}(f)=f|_{\mathcal{V}}$ *is harmonic (resp., subharmonic, superharmonic) w.r.t.* $(\mathcal{V},m;b)$. *Here the map* $\imath_{\mathcal{V}}$ *is defined by* (4.3.2).

PROOF. Notice that for an edgewise affine function f, its slope at v on an oriented edge $\vec{e}\in\vec{\mathcal{E}}_v$ having vertices v and u is simply given by

$$\partial_{\vec{e}}f(v)=\frac{f(u)-f(v)}{|e|}.$$

Thus, comparing (6.5.4) with (3.1.6) and then using Lemma 6.46 (resp., Lemma 6.48), one finishes the proof. □

We also need the following analog of Lemma 6.43.

LEMMA 6.51. *Suppose* $f\in H^1_{\mathrm{loc}}(\mathcal{G})$ *solves* $\Delta f=\lambda f$ *for some* $\lambda\in\mathbb{R}_{\ge 0}$ *and, moreover, satisfies Kirchhoff conditions at all the vertices. Then* $|f|$ *is subharmonic. If in addition* f *is real-valued, then both* f_+ *and* f_- *are subharmonic.*

PROOF. Due to linearity, we can assume without loss of generality that f is real-valued. Fix some model of $(\mathcal{G},\mu,\nu)$. Then the equality $\Delta f=\lambda f$ implies that f is a classical solution to $\nu(e)f''=\lambda\mu(e)f$ on each edge $e\in\mathcal{E}$ (upon an identification of e with the interval $\mathcal{I}_e=[0,|e|]$). Hence it is easy to show that $|f|''\ge\lambda\frac{\mu(e)}{\nu(e)}|f|$, where the inequality is understood in the distributional sense (e.g., use the Kato inequality [**182**, Theorem X.27]). It remains to notice that

$$\sum_{\vec{e}\in\vec{\mathcal{E}}_v}\nu(e)\partial_{\vec{e}}|f|(v)\ge 0,$$

for all vertices $v\in\mathcal{V}$. Since f is continuous at $v\in\mathcal{V}$, in the case $f(v)\ne 0$, $|f|$ coincides with $\operatorname{sign}(f(v))f$ in a small vicinity of v and hence Kirchhoff conditions would imply that

$$\sum_{\vec{e}\in\vec{\mathcal{E}}_v}\nu(e)\partial_{\vec{e}}|f|(v)=\sum_{\vec{e}\in\vec{\mathcal{E}}_v}\nu(e)\partial_{\vec{e}}f(v)=0$$

at every such vertex. If $f(v)=0$, then it is straightforward to see that in this case

$$0=\sum_{\vec{e}\in\vec{\mathcal{E}}_v}\nu(e)\partial_{\vec{e}}f(v)\le\sum_{\vec{e}\in\vec{\mathcal{E}}_v}\nu(e)\partial_{\vec{e}}|f|(v),$$

which finishes the proof. □

The following result is a standard characterization via the mean value property.

LEMMA 6.52 (Mean value property). *Let* $f\in\mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ *be real-valued. Then* f *is harmonic (subharmonic, superharmonic) if and only if for each* $v\in\mathcal{V}$

$$\frac{1}{\mu(B_r(v;\varrho_\eta))}\int_{B_r(v;\varrho_\eta)}f(x)\mu(\mathrm{d}x)=f(v),\qquad\Big(\ge f(v),\qquad\le f(v)\Big)\tag{6.5.5}$$

for all sufficiently small $r>0$. *Here* ϱ_η *is the intrinsic metric on* $(\mathcal{G},\mu,\nu)$ *and* $B_r(v;\varrho_\eta)$ *is the distance ball in* $(\mathcal{G},\varrho_\eta)$ *of radius* $r>0$ *with the center at* v.

PROOF. In fact, the mean value property is a straightforward consequence of Lemma 6.46 (resp., and Lemma 6.48). Indeed, suppose $r > 0$ is such that the corresponding distance ball $B_\eta(v;r)$ is isomorphic to a star-shaped set (2.1.4). Then taking into account that f is edgewise affine, we easily get

$$\begin{aligned}\int_{B_r(v;\varrho_\eta)} f(x)\mu(\mathrm{d}x) &= \sum_{e\in\mathcal{E}_v}\int_{e\cap B_r(v;\varrho_\eta)} f(x_e)\mu(\mathrm{d}x_e)\\ &= \sum_{\vec{e}\in\vec{\mathcal{E}}_v}\frac{1}{2}\Big(2f(v)+\partial_{\vec{e}}f(v)\frac{r|e|}{\eta(e)}\Big)\frac{r|e|}{\eta(e)}\mu(e)\\ &= f(v)r\sum_{\vec{e}\in\vec{\mathcal{E}}_v}\sqrt{\mu(e)\nu(e)}+\frac{r^2}{2}\sum_{\vec{e}\in\vec{\mathcal{E}}_v}\nu(e)\partial_{\vec{e}}f(v).\end{aligned}$$

It remains to notice that

$$\mu(B_r(v;\varrho_\eta)) = \sum_{\vec{e}\in\vec{\mathcal{E}}_v}\mu(e)\frac{r|e|}{\eta(e)} = r\sum_{\vec{e}\in\vec{\mathcal{E}}_v}\sqrt{\mu(e)\nu(e)}. \qquad \square$$

REMARK 6.53. We stress that the mean-value property on weighted metric graphs holds only locally. That is, even for a harmonic function f on $(\mathcal{G},\mu,\nu)$, the equality (6.5.5) can fail when the integral is taken over a ball $B_r(v;\varrho_\eta)$ with large radius r. Indeed, problems arise already if $B_r(v;\varrho_\eta)$ contains more than one vertex of degree ≥ 3 and the latter is not at all surprising since these vertices can be considered as singularities of one-dimensional manifolds (see Remark 2.4).

6.5.3. Liouville-type properties on graphs. An important question is which subspaces of harmonic functions are trivial, that is, which conditions ensure the uniqueness of solutions to the Helmholz equation

$$\Delta u = \lambda u.$$

Such results are referred to as *Liouville-type theorems.* In Riemannian geometry L^p-Liouville theorems for harmonic functions were studied for example by S.T. Yau [**214**], L. Karp [**123**], P. Li and R. Schoen [**151**] and many others. Karp's and Yau's theorems were later generalized by K.-T. Sturm [**195**] to the setting of strongly local, regular Dirichlet forms. In particular, in the case of metric graphs Sturm's result reads as follows (cf. Corollary 1(a) in [**195**]).

THEOREM 6.54 (Yau's L^p-Liouville theorem on metric graphs [**195**]). *If $(\mathcal{G},\mu,\nu)$ is a locally finite weighted metric graph such that $(\mathcal{G},\varrho_\eta)$ is complete, then every nonnegative subharmonic function which belongs to $L^p(\mathcal{G};\mu)$ for some $p\in(1,\infty)$ is identically zero. In particular, if $f\in L^p(\mathcal{G};\mu)$ is harmonic, then $f\equiv 0$.*

In the case of weighted graphs, Liouville-type theorems have been investigated in, e.g., [**106**], [**183**], [**162**], [**108**] and the analogs of Yau's and Karp's theorems were established quite recently by B. Hua and M. Keller [**111**].

THEOREM 6.55 (Yau's L^p-Liouville theorem on graphs [**111**]). *Let b be a locally finite connected graph over $(\mathcal{V},m)$ and let ϱ be an intrinsic path metric of finite jump size. If $(\mathcal{V},\varrho)$ is complete as a metric space, then every nonnegative L-subharmonic function which belongs to $\ell^p(\mathcal{V};m)$ for some $p\in(1,\infty)$ is identically zero. In particular, if $f\in\ell^p(\mathcal{V};m)$ is L-harmonic, then $f\equiv 0$.*

REMARK 6.56. We stated Corollary 1.2 from [**111**] in a weaker form in order to simplify considerations. In fact, the assumption that ϱ is a path metric can be weakened. More precisely, the conclusion remains valid for a general intrinsic metric ϱ of finite jump size such that ϱ generates the discrete topology on $\mathcal{V}$ and $(\mathcal{V}, \varrho)$ is complete (the latter follows by a simple comparison argument with the path metric ϱ_p constructed in Remark 6.32(ii)).

In fact, the connection between intrinsic metrics on weighted graphs and cable systems shows that Theorem 6.55 easily follows from Theorem 6.54:

PROOF OF THEOREM 6.55. Let ϱ be an intrinsic path metric for $(\mathcal{V}, m; b)$ having finite jump size. Then by Lemma 6.31 there is a canonical cable system $(\mathcal{G}, \mu, \mu)$ such that ϱ coincides with the restriction of $\varrho_\eta = \varrho_0$ onto $\mathcal{V} \times \mathcal{V}$. Clearly, $(\mathcal{V}, \varrho)$ is complete if and only if so is $(\mathcal{G}, \varrho_\eta)$.

Take now a nonnegative function $\mathbf{f}\colon \mathcal{V} \to \mathbb{R}_{\geq 0}$ which is L-subharmonic. By Lemma 6.50, the corresponding function $f = \imath_{\mathcal{V}}^{-1}(\mathbf{f})$ is nonnegative and subharmonic w.r.t. $(\mathcal{G}, \mu, \nu)$. If $\mathbf{f} \in \ell^p(\mathcal{V}; m)$ for some $p \in (1, \infty)$, then $f \in L^p(\mathcal{G}; \mu)$ according to Lemma 4.2. Applying Theorem 6.54, we conclude that f is trivial and hence so is $\mathbf{f} = \imath_{\mathcal{V}}(f)$. □

REMARK 6.57. Using the same line of reasoning and also connections between volume growth of metric graphs and weighted graphs (see Lemma 6.39), one can easily connect, for example, Karp's L^p Liouville theorems for metric graphs and weighted graphs (see Section 7.4), Grigor'yan's L^1 theorem, etc.

6.6. Life without loops II: Jacobi matrices on graphs

This section deals with Problem 6.4. For a given $\beta\colon \mathcal{V} \to \mathbb{R}$ and a connected graph q over $\mathcal{V}$ satisfying the properties (i), (ii) and (iv) of Section 2.2, consider a second order symmetric difference expression

$$(\tau f)(v) = \beta(v) f(v) - \sum_{u \in \mathcal{V}} q(u,v) f(u), \qquad v \in \mathcal{V}. \tag{6.6.1}$$

Alternatively, its action can be described by the infinite symmetric matrix $\mathrm{H} = (h_{uv})_{u,v\in\mathcal{V}}$ given by

$$h_{uv} = \begin{cases} \beta(v), & u = v, \\ -q(u,v), & u \neq v. \end{cases}$$

As described in Section 2.2, we can associate in $\ell^2(\mathcal{V})$ the minimal and maximal operator with the difference expression (6.6.1).

REMARK 6.58. Every difference operator (6.6.1) is a Schrödinger-type operator on $\ell^2(\mathcal{V})$ in the sense of Remark 2.10: the weight function $m = \mathbb{1}_{\mathcal{V}}$ on $\mathcal{V}$ and its coefficients are explicitly given by

$$b(u,v) = q(u,v), \qquad\qquad c(v) = \beta(v) - \sum_{u\in\mathcal{V}} q(u,v). \tag{6.6.2}$$

Symmetric difference expressions (6.6.1) are also known as *Jacobi matrices on graphs* (see, e.g., [**8**], [**9**], [**10**]).

On the other hand, every Schrödinger-type operator in $\ell^2(\mathcal{V}; m)$ is unitarily equivalent (by means of the map $\mathcal{U}\colon \ell^2(\mathcal{V}; m) \to \ell^2(\mathcal{V})$ defined by (3.2.40)) to a Schrödinger operator in $\ell^2(\mathcal{V})$ and hence from this perspective the class of Schrödinger-type operators on $\ell^2(\mathcal{V})$ is sufficiently large.

The next result answers Problem 6.4 in the affirmative.

THEOREM 6.59. *Let $q\colon \mathcal{V}\times\mathcal{V}\to[0,\infty)$ be a locally finite connected graph over $\mathcal{V}$ and let $\mathcal{G}_q=(\mathcal{V},\mathcal{E}_q)$ be the underlying simple graph (see Remark 2.7). Then there exist edge weights $\nu\colon\mathcal{E}_q\to(0,\infty)$ and edge lengths $|\cdot|\colon\mathcal{E}_q\to(0,\infty)$ such that*

$$|e|^2\le\nu(e) \tag{6.6.3}$$

for all $e\in\mathcal{E}_q$, and

$$q(u,v)=\frac{\nu(e_{u,v})}{|e_{u,v}|\big(\sum_{e\in\mathcal{E}_u}|e|\big)^{1/2}\big(\sum_{e\in\mathcal{E}_v}|e|\big)^{1/2}}, \tag{6.6.4}$$

for all $e_{u,v}\in\mathcal{E}_q$.

Notice that the difference expression (3.2.38) is a special case of (6.6.1):

$$\beta(v)=\frac{1}{m(v)}\Big(\alpha(v)+\sum_{u\in\mathcal{V}}b(u,v)\Big),\qquad q(u,v)=\frac{b(u,v)}{\sqrt{m(u)}\sqrt{m(v)}}. \tag{6.6.5}$$

Moreover, the minimal operator $\widetilde{\mathbf{h}}_\alpha$ associated with (6.6.1), (6.6.5) shares many of its basic spectral properties with the Laplacian $\mathbf{H}_\alpha$ (see Theorem 3.1 and its proof), however, there is in general no connection between their parabolic properties. Theorem 6.59 implies the following result.

COROLLARY 6.60. *Every second-order difference operator* (6.6.1) *arises as a boundary operator of a Laplacian with δ-couplings. More precisely, there is a weighted metric graph $(\mathcal{G},\mu,\nu)$ such that for its simple model $(\mathcal{V},\mathcal{E}_q,|\cdot|,\mu,\nu)$ and a function $\alpha\colon\mathcal{V}\to\mathbb{R}$ the relations* (6.6.5) *holds true, where the graph $(\mathcal{V},m;b)$ is given by* (3.1.1)–(3.1.5) *and* (3.1.6).

The proof of Theorem 6.59 is based on the following two lemmas, however, first we need to recall a few basic notions. A connected simple graph $(\mathcal{V},\mathcal{E})$ without cycles is called *a tree*. We shall denote trees by $\mathcal{T}$. Notice that for any two vertices u, v on a tree $\mathcal{T}$ there is exactly one path $\mathcal{P}$ connecting u and v, and hence the combinatorial distance on $\mathcal{T}$ is exactly the number of edges in the path 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*. Each vertex $v\in\mathcal{V}(\mathcal{T})$ having degree 1 is called a *leaf.*

LEMMA 6.61. *Let $\mathcal{T}=(\mathcal{V},\mathcal{E})$ be a locally finite infinite tree. Then there is an infinite subtree $\mathcal{T}_\infty=(\mathcal{V}_\infty,\mathcal{E}_\infty)\subseteq\mathcal{T}$ such that $\mathcal{T}_\infty$ has at most one leaf and $\mathcal{T}$ is obtained by attaching to each vertex $v\in\mathcal{V}_\infty$ a (possibly empty) finite tree $\mathcal{T}_v$.*

PROOF. The proof is by construction, which can informally be considered as "cutting away" finite subtrees from a given tree. Fix a root $o\in\mathcal{V}$ for $\mathcal{T}$ and order the vertices of $\mathcal{T}$ according to combinatorial spheres. The latter also introduces a natural orientation on $\mathcal{T}$: for every edge e its initial vertex $e_\imath$ belongs to the smaller combinatorial sphere.

Next, let us define the standard partial ordering on $\mathcal{T}$. For two edges $e,\widetilde{e}\in\mathcal{E}$, we write $\widetilde{e}\prec e$, if the path from the root o to the terminal vertex e_τ of e passes through $\widetilde{e}$. For any $e\in\mathcal{E}$, denote by $\mathcal{T}_e\subseteq\mathcal{T}$ the subtree with the edge set

$$\mathcal{E}(\mathcal{T}_e)=\{\widetilde{e}\in\mathcal{E}\mid e\prec\widetilde{e}\}.$$

Since " $\prec$ " is transitive on $\mathcal{E}$, $e \in \mathcal{T}_{\tilde{e}}$ implies that $\mathcal{T}_e \subseteq \mathcal{T}_{\tilde{e}}$. Moreover, define

$$\mathcal{E}_v^\infty = \{e \in \mathcal{E}_v^+ \,|\, \mathcal{T}_e \text{ is infinite}\}, \tag{6.6.6}$$

where $\mathcal{E}_v^+$ is the sets of outgoing edges at v, see (2.1.1), and then for each $v \in \mathcal{V}$ denote by $\mathcal{T}_v$ the (possibly empty) finite subtree of $\mathcal{T}$ with the edge set

$$\mathcal{E}(\mathcal{T}_v) = \bigcup_{e \in \mathcal{E}_v^+ \setminus \mathcal{E}_v^\infty} \mathcal{E}(\mathcal{T}_e). \tag{6.6.7}$$

After all these lengthy preparations, we finally begin our construction. For every edge $e \in \mathcal{E}_o^+ = \mathcal{E}_o$ consider the subtree $\mathcal{T}_e$. Since $\mathcal{T}$ is infinite, there is at least one edge $e \in \mathcal{E}_o^+$ such that the corresponding subtree $\mathcal{T}_e$ is infinite and hence the set $\mathcal{E}_o^\infty$ is non-empty. Denote the set of terminal vertices of all edges $e \in \mathcal{E}_o^\infty$ by $\mathcal{V}_1^\infty$. Notice that $\mathcal{V}_1^\infty$ is a subset of the first combinatorial sphere S_1. Next for each $v \in \mathcal{V}_1^\infty$ consider the corresponding edge sets $\mathcal{E}_v^\infty$. Again all of them are non-empty since, by construction, each $\mathcal{T}_e$ is infinite. The union of all terminal vertices of $e \in \mathcal{E}_v^\infty$ with $v \in \mathcal{V}_1^\infty$ is denoted by $\mathcal{V}_2^\infty$. Clearly, $\mathcal{V}_2^\infty$ is a non-empty subset of the second combinatorial sphere S_2. Continuing this process, we end up with an infinite sequence of vertex sets $\mathcal{V}_n^\infty \subseteq S_n$, $n \geq 1$. Since our initial tree $\mathcal{T}$ is infinite but locally finite, every vertex set $\mathcal{V}_n^\infty$, $n \geq 1$ is non-empty.

Now we define $\mathcal{T}_\infty$ as the subtree of $\mathcal{T}$ with the vertex set $\mathcal{V}_\infty := \{o\} \cup \{\mathcal{V}_n^\infty\}_{n \geq 1}$. It follows from our construction that $\mathcal{T}_\infty$ is an infinite tree with the only possible leaf o (this happens exactly when $\#\mathcal{E}_o^\infty = 1$). Moreover, it is immediate to see that attaching to each $v \in \mathcal{V}_\infty$ the finite subtree $\mathcal{T}_v$ defined by (6.6.7) we recover the given tree $\mathcal{T}$. $\square$

The next result proves Theorem 6.59 for trees:

LEMMA 6.62. *Let q be a locally finite graph over $\mathcal{V}$ such that the associated simple graph $\mathcal{G}_q$ (see Remark 2.7) is an infinite tree $\mathcal{T} = (\mathcal{V}, \mathcal{E})$. Then there exist edge weights $\nu\colon \mathcal{E} \to (0,\infty)$ and edge lengths $|\cdot|\colon \mathcal{E} \to (0,\infty)$ such that* (6.6.3) *and* (6.6.4) *hold true for all $e \in \mathcal{E}$.*

PROOF. We divide the proof in several steps.

(i) First of all, notice that the existence of ν and $|\cdot|$ satisfying (6.6.3) and (6.6.4) for all $e \in \mathcal{E}$ is equivalent to the existence of edge lengths $|\cdot|$ satisfying

$$T(e_{u,v}) := \frac{|e_{u,v}|}{\big(\sum_{e \in \mathcal{E}_u} |e|\big)^{1/2} \big(\sum_{e \in \mathcal{E}_v} |e|\big)^{1/2}} \leq q(u,v), \tag{6.6.8}$$

for each $u \sim v$, since in this case a suitable choice of the edge weight ν is simply given by

$$\nu(e) := |e|^2 \frac{q(e)}{T(e)}, \qquad e \in \mathcal{E}. \tag{6.6.9}$$

Here and below we use the obvious notation $q(e_{u,v}) = q(u,v)$ for each $e = e_{u,v} \in \mathcal{E}$.

(ii) Next, by Lemma 6.61, we can find an infinite rooted subtree $\mathcal{T}_\infty = (\mathcal{V}_\infty, \mathcal{E}_\infty)$ of $\mathcal{T}$ such that $\mathcal{T}_\infty$ has at most one leaf at its root o and such that $\mathcal{T}$ is obtained by attaching to each $v \in \mathcal{V}_\infty$ a (possibly empty) finite tree $\mathcal{T}_v$. Clearly,

$$\mathcal{E} \setminus \mathcal{E}_\infty = \bigcup_{v \in \mathcal{V}_\infty} \mathcal{E}(\mathcal{T}_v).$$

(iii) We start by assigning edge lengths to each finite non-empty subtree $\mathcal{T}_v$, $v \in \mathcal{V}_\infty$. Consider $\mathcal{T}_v$ as a rooted tree with the root at v, $o(\mathcal{T}_v) = v$. Let $h(v)$ be the height of $\mathcal{T}_v$, i.e., the maximal combinatorial distance of a vertex in $\mathcal{T}_v$ to v. For $n \in \{1, \dots, h(v)\}$, denote by $\mathcal{E}^n(\mathcal{T}_v)$ the set of edges $e \in \mathcal{E}(\mathcal{T}_v)$ between the combinatorial spheres $S_{n-1}(\mathcal{T}_v)$ and $S_n(\mathcal{T}_v)$ of $\mathcal{T}_v$. We will assign lengths for the sets $\mathcal{E}^n(\mathcal{T}_v)$ inductively in n starting from the top of $\mathcal{T}_v$ and going downwards to $o(\mathcal{T}_v)$. More precisely, we define positive reals $\ell_1, \dots, \ell_{h(v)}$ by first setting $\ell_{h(v)} = 1$ and, if $h(v) > 1$, inductively

$$\ell_{k-1} := \max_{e \in \mathcal{E}^k(\mathcal{T}_v)} \frac{\ell_k}{q(e)^2} = \frac{\ell_k}{(\min_{e \in \mathcal{E}^k(\mathcal{T}_v)} q(e))^2}$$

for all $k \in \{2, \dots, h(v)\}$. Next, we put $|e| := \ell_k$ for all $e \in \mathcal{E}^k(\mathcal{T}_v)$, $k \in \{1, \dots, h(v)\}$. Clearly, with this choice of lengths we have

$$\begin{aligned} T(e) &= \frac{\ell_k}{\left(\sum_{e \in \mathcal{E}_{e_\imath}} |e|\right)^{1/2} \left(\sum_{e \in \mathcal{E}_{e_\tau}} |e|\right)^{1/2}} \\ &\leq \frac{\ell_k}{\left(\sum_{e \in \mathcal{E}^-_{e_\imath}} |e|\right)^{1/2} \left(\sum_{e \in \mathcal{E}^-_{e_\tau}} |e|\right)^{1/2}} \leq \sqrt{\ell_k/\ell_{k-1}} \leq q(e) \end{aligned}$$

for all $e \in \mathcal{E}^k(\mathcal{T}_v)$ and $k \in \{2, \dots, h(v)\}$.

(iv) It remains to define edge lengths for edges in $\mathcal{T}_\infty$ such that (6.6.8) then holds true on $\mathcal{E}_\infty$ and also on each non-empty edge set $\mathcal{E}^1(\mathcal{T}_v)$, $v \in \mathcal{V}$. Again, we will assign edge lengths inductively for the sets $\mathcal{E}^n(\mathcal{T}_\infty)$, but now moving "upwards" the tree $\mathcal{T}_\infty$. Here $\mathcal{E}^n(\mathcal{T}_\infty)$, $n \geq 1$ is the set of edges $e \in \mathcal{E}_\infty$ between the combinatorial spheres $S_{n-1}(\mathcal{T}_\infty)$ and $S_n(\mathcal{T}_\infty)$ in $\mathcal{T}_\infty$.

For $n = 1$, we set $|e| = 1$ for all $e \in \mathcal{E}^1(\mathcal{T}_\infty)$ if $\mathcal{E}^1(\mathcal{T}_\infty) = \mathcal{E}_o^\infty = \mathcal{E}_o$ (that is, if $\mathcal{T}_o$ is empty). Otherwise, we define

$$\widetilde{\ell}_1 := \max_{e \in \mathcal{E}^1(\mathcal{T}_o)} \frac{|e|}{q(e)^2} = \frac{\ell_1(o)}{(\min_{e \in \mathcal{E}^1(\mathcal{T}_o)} q(e))^2},$$

and then set $|e| = \widetilde{\ell}_1$ for all $e \in \mathcal{E}^1(\mathcal{T}_\infty)$. Hence for each $e \in \mathcal{E}^1(\mathcal{T}_o)$ we get

$$\begin{aligned} T(e) &= \frac{\ell_1(o)}{\left(\sum_{e \in \mathcal{E}_o} |e|\right)^{1/2} \left(\sum_{e \in \mathcal{E}_{e_\tau}} |e|\right)^{1/2}} \\ &\leq \frac{\ell_1(o)}{\left(\sum_{e \in \mathcal{E}^1(\mathcal{T}_o)} |e|\right)^{1/2} \left(\sum_{e \in \mathcal{E}^1(\mathcal{T}_\infty)} |e|\right)^{1/2}} \\ &\leq \sqrt{\ell_1(o)/\widetilde{\ell}_1} \leq q(e). \end{aligned}$$

Now assume we have already defined edge lengths for edges in $\mathcal{E}^k(\mathcal{T}_\infty)$ for all $k \leq n$, such that (6.6.8) holds true on each

$$\widetilde{\mathcal{E}}^k := \mathcal{E}^{k-1}(\mathcal{T}_\infty) \cup \bigcup_{v \in S_{k-1}} \mathcal{E}^1(\mathcal{T}_v)$$

for $k \leq n$. Now we define again

$$\widetilde{\ell}_{n+1} := \max_{e \in \widetilde{\mathcal{E}}^{n+1}} \frac{|e|}{q(e)^2},$$

and then we set $|e| = \widetilde{\ell}_{n+1}$ for all $e \in \mathcal{E}^{n+1}(\mathcal{T}_\infty)$. By our choice of the root, every vertex $v \in S_n(\mathcal{T}_\infty)$ is adjacent to at least one $e \in \mathcal{E}^{n+1}(\mathcal{T}_\infty)$. Hence $T(\tilde{e}) \le q(\tilde{e})$ for all $\tilde{e}$ in $\widetilde{\mathcal{E}}^{n+1}$. Since $\bigcup_{n\ge 1} \mathcal{E}^n(\mathcal{T}_\infty) = \mathcal{E}_\infty$, by induction we obtain edge lengths on $\mathcal{E}$ such that (6.6.8) holds true for all $e \in \mathcal{E}$. $\square$

Now we are ready to prove Theorem 6.59 and Corollary 6.60.

Proof of Theorem 6.59. As in the proof of Lemma 6.62, it suffices to show the existence of lengths $|\cdot|$ satisfying (6.6.8) since in this case a suitable choice of edge weights is provided by (6.6.9). The main idea behind our construction is the observation that we assign weights and lengths to edges, and hence we can "transform" in a suitable way our graph to a tree and then apply Lemma 6.62 .

Suppose that $\mathcal{T}$ is a spanning tree for the underlying combinatorial graph $\mathcal{G}_q$. Denote the edge set of $\mathcal{T}$ by $\mathcal{E}(\mathcal{T}) \subseteq \mathcal{E}_q$. Now we decouple each remaining edge $e_{u,v} \in \mathcal{E}_q \setminus \mathcal{E}(\mathcal{T})$ at exactly one vertex (say, v) and thereby transform it to a leaf attached to the remaining vertex u.

Applying this to all edges $e \in \mathcal{E}_q \setminus \mathcal{E}(\mathcal{T})$ yields a new graph $\widetilde{\mathcal{G}}_q$. Clearly, $\widetilde{\mathcal{G}}_q$ is a tree and its edge set $\widetilde{\mathcal{E}}_q$ can be identified in the above way with $\mathcal{E}_q$. Hence every choice of edge lengths $|\cdot|$ on $\mathcal{G}_q$ corresponds to a respective choice on $\widetilde{\mathcal{G}}_q$. Moreover, by construction we have

$$T_{\mathcal{G}_q}(e) \le T_{\widetilde{\mathcal{G}}_q}(e)$$

for all $e \in \mathcal{E}_q$, where $T_{\widetilde{\mathcal{G}}_q}(e)$ and $T_{\mathcal{G}_q}(e)$ are given by (6.6.8). More precisely, within the identification we have $\widetilde{\mathcal{E}}_v \subseteq \mathcal{E}_v$ for every $v \in \mathcal{V}$ and $\widetilde{\mathcal{E}}_{v_e} = \{e\}$ for each of the new vertices v_e, $e \in \mathcal{E}_q \setminus \mathcal{E}(\mathcal{T})$. Hence

$$T_{\mathcal{G}_d}(e_{u,v}) = \frac{|e_{u,v}|}{\left(\sum_{e\in\mathcal{E}_u} |e|\right)^{1/2}\left(\sum_{e\in\mathcal{E}_v} |e|\right)^{1/2}} \le \frac{\sqrt{|e_{u,v}|}}{\left(\sum_{e\in\mathcal{E}_u} |e|\right)^{1/2}} = T_{\widetilde{\mathcal{G}}_d}(e_{u,v})$$

for every $e_{u,v} \in \mathcal{E}_q \setminus \mathcal{E}(\mathcal{T})$ and similar for each $e \in \mathcal{E}(\mathcal{T})$. Thus every choice of edge lengths satisfying (6.6.8) for $\widetilde{\mathcal{G}}_q$ defines a suitable choice of edge lengths for $\mathcal{G}_q$. It remains to apply Lemma 6.62. $\square$

Proof of Corollary 6.60. We simply need to set $\mu(e) = 1$ for each $e \in \mathcal{E}_q$ and then choose ν and $|\cdot|$ as in Theorem 6.59. By construction, this implies $\eta(e) \le 1$ for all edges $e \in \mathcal{E}_q$. Taking into account (6.6.4), it follows that q coincides with (6.6.5). Moreover, choosing the function $\alpha\colon \mathcal{V} \to \mathbb{R}$ in a suitable way, we can achieve that β coincides with (6.6.5) as well. $\square$

Remark 6.63. A few remarks are in order.

(i) Theorem 6.59 can be seen as an extension of Proposition 5.18 to an arbitrary locally finite graph.

(ii) According to the proof of Theorem 3.1, the graph Laplacian $\mathbf{h}^0_\alpha$ associated in $\ell^2(\mathcal{V}; m)$ with (3.1.7) is unitarily equivalent (by means of the map $\mathcal{U}\colon \ell^2(\mathcal{V}; m) \to \ell^2(\mathcal{V})$ defined by (3.2.40)) to the minimal symmetric operator $\widetilde{\mathbf{h}}^0_\alpha$ defined in $\ell^2(\mathcal{V})$ by (6.6.1) with the coefficients (6.6.5) and therefore, by Theorem 3.1, $\widetilde{\mathbf{h}}^0_\alpha$ shares its basis spectral properties with the Laplacian $\mathbf{H}^0_\alpha$. However, the map $\mathcal{U}$ does not preserve the Dirichlet form structure (e.g., the quadratic form of $\widetilde{\mathbf{h}}^0_\alpha$ may fail to be a Dirichlet form even if $\alpha \equiv 0$) and hence there is in general no connection between their parabolic properties.

6.7. Further comments and open problems

We would like to conclude this part with a few comments.

1. The results of this chapter suggest to view connections between weighted graphs and metric graphs from geometric perspective. Namely, it is proved that with every weighted locally finite graph $(\mathcal{V}, m; b)$ one can always associate at least one cable system, that is, a weighted metric graph $(\mathcal{G}, \mu, \nu)$ such that for one of its models the weight m and the graph b are expressed via (3.1.1)–(3.1.5) and (3.1.6). Next, $(\mathcal{G}, \mu, \nu)$ is always equipped with the intrinsic path metric ϱ_η and it turns out that the induced metric $\varrho_\mathcal{V} = \varrho_\eta|_{\mathcal{V}\times\mathcal{V}}$ is intrinsic w.r.t. the corresponding graph $(\mathcal{V}, m; b)$. Moreover, the spaces $(\mathcal{V}, \varrho_\mathcal{V})$ and $(\mathcal{G}, \varrho_\eta)$ are quasi-isometric and this fact connects their large scale geometric properties. However, their local combinatorial structures are also connected in an obvious way and these facts together provide a partial explanation for the close connections between graph Laplacians and metric graph Laplacians established in Chapters 3 and 4. Notice also that $(\mathcal{G}, \varrho_\eta)$ is a length space, a widely studied class of metric spaces, and this provides a lot of tools and techniques. This is reminiscent of the following common practice in geometric group theory: a finitely generated group can be turned into a length space by viewing its Cayley graph as an equilateral metric graph equipped with the length metric ϱ_0; moreover, the word metric ϱ_{comb} in this case is nothing but the induced metric $\varrho_0|_{\mathcal{V}\times\mathcal{V}}$.

2. It is hard to overestimate the role of intrinsic metrics in the progress achieved for weighted graph Laplacians during the last decade. Surprisingly, the above described procedure to construct an intrinsic metric for $(\mathcal{V}, m; b)$ in fact provides a way to obtain all finite jump size intrinsic path metrics on $(\mathcal{V}, m; b)$. Moreover, upon some normalization assumptions on cable systems (e.g., canonical cable systems) the correspondence between intrinsic weights on $(\mathcal{V}, m; b)$ and cable systems becomes bijective (Theorem 6.34).

3. Let us also briefly mention the following perspective on the results of Chapter 6 and on Problems 6.1–6.4. Suppose a vertex set $\mathcal{V}$ is given and consider a weighted metric graph $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu_\mathcal{E}, \nu_\mathcal{E})$ over $\mathcal{V}$, i.e., a model of a weighted metric graph having $\mathcal{V}$ as its vertex set. To this weighted metric graph, the equations (3.1.5) and (3.1.6) associate a vertex weight $m\colon \mathcal{V} \to (0, \infty)$ and an edge weight function $b\colon \mathcal{V}\times\mathcal{V} \to [0, \infty)$ with the properties (i)–(iv) of Section 2.2. In other words, we obtain a map

$$\Phi_\mathcal{V}\colon \quad \mathrm{Graph}_{\mathrm{metr}}(\mathcal{V}) \quad\to\quad \mathrm{Graph}_{\mathrm{discr}}(\mathcal{V}), \tag{6.7.1}$$

where $\mathrm{Graph}_{\mathrm{metr}}$ and $\mathrm{Graph}_{\mathrm{metr}}$ denote the sets of all connected, locally finite weighted metric graphs and connected, locally finite weighted graphs over $\mathcal{V}$, respectively.

From this point of view, the results in Chapter 3 and Chapter 4 say that the map $\Phi_\mathcal{V}$ connects the basic spectral and parabolic properties of the respective Laplacian-type operators, as well as spectral properties of Laplacians with δ-couplings on weighted metric graphs and Schrödinger operators on weighted discrete graphs. Moreover, the results of Section 6.4 connect certain basic geometric features (see also Proposition 7.38). In terms of this map, the results of Sections 6.2–6.3 and Section 6.4.4 can be formulated as follows:

- the map $\Phi_{\mathcal{V}}$ is surjective (see Theorem 6.16).
- when restricted to simple metric graphs, the map $\Phi_{\mathcal{V}}$ is no longer surjective (Section 6.2).
- Unfortunately, the map $\Phi_{\mathcal{V}}$ is not injective, that is, the correspondence between weighted metric and weighted discrete graphs is not one-to-one. However, after restricting $\Phi_{\mathcal{V}}$ further to the class of canonical weighted metric graphs over $\mathcal{V}$, we can at least describe the preimage $\Phi_{\mathcal{V}}^{-1}(m,b)$ of a locally finite graph $(\mathcal{V},m;b)$ using intrinsic weights (see Theorem 6.34 and the map Ψ given by (6.4.22)).

4. The results of Section 6.6 show that similar connections work for Jacobi matrices on graphs. We decided not to proceed in this direction and demonstrate it by only one application in the next chapter. More specifically, in Section 7.1.3 we briefly discuss the self-adjointness problem for the minimal operator associated with (6.6.1) in $\ell^2(\mathcal{V})$ and prove the analogs of some classical self-adjointness tests for the usual Jacobi matrices, which also improve several recent results (Theorem 7.17).

5. Taking into account the said above, the following problems remain open.

PROBLEM 6.5. *Given a locally finite b graph over* $(\mathcal{V},m)$*, is there an efficient way to decide whether it admits a minimal cable system?*

This problem can be reformulated in other terms (e.g., given a simple graph, how can one describe the image of the positive cone $C^+(\mathcal{E})$ under the map D^*?).

Of course, stated this way, Problem 6.5 is too complicated to obtain a complete answer and hence it makes sense either to restrict to some classes of weights (for constant weights the answer is given by means of a disjoint cycle cover) or to particular classes of graphs (seems, for antitrees the answer depends on sphere numbers in a rather nontrivial way).

Taking into account the fact that each graph admits an infinite family of cable systems, one can specify the above problem:

PROBLEM 6.6. *Given a locally finite b graph over* $(\mathcal{V},m)$*, is there an efficient procedure/algorithm to construct a cable system with certain desirable properties?*

The same kind of questions can be asked about Jacobi matrices on graphs:

PROBLEM 6.7. *Given a Jacobi matrix* (6.6.1) *on a graph, is there an efficient procedure/algorithm to construct a weighted metric graph such that Jacobi parameters admit the representation* (6.6.5)*?*

The direction "from $(\mathcal{V},m;b)$ to cable system" seems to be rather nontrivial despite the fact that we have provided some constructions. Namely, Problems 6.6 and 6.7 are of practical importance since it is desirable to get as accurate information as possible regarding the properties of the obtained cable system. For instance, in Theorem 7.19 it is desirable to know the qualitative behavior of the corresponding length function $|\cdot|$, however, even for the usual Jacobi matrix it is not trivial to get this information out of its Jacobi parameters (see (5.3.2)).

CHAPTER 7

From Continuous to Discrete and Back

Our main goal in this chapter is to employ the established connections between graph Laplacians and metric graph Laplacians in order to prove new results for Laplacians on metric graphs as well as to provide another perspective on recent results for weighted graph Laplacians.

7.1. Self-adjointness

In this section we provide sufficient conditions for the self-adjoint uniqueness, that is, the self-adjointness of both the minimal and the maximal Kirchhoff Laplacians and hence the equality $\mathbf{H}^0 = \mathbf{H}$.

7.1.1. Kirchhoff Laplacians. We begin our study with the case $\alpha \equiv 0$. The next result is an immediate corollary of Sturm's extension of Yau's L^p-Liouville theorem for strongly local Dirichlet forms [**195**], see Theorem 6.54.

THEOREM 7.1. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph and let ϱ_η be the corresponding intrinsic metric defined in Section 6.4.1. If $(\mathcal{G}, \varrho_\eta)$ is complete as a metric space, then the minimal Kirchhoff Laplacian $\mathbf{H}^0$ is self-adjoint and $\mathbf{H}^0 = \mathbf{H}$.*

PROOF. Assume that $\mathbf{H}^0$ is not self-adjoint. Since $\mathbf{H}^0$ is nonnegative, this means that $\ker(\mathbf{H} + \mathrm{I}) \neq \{0\}$, that is, there is $0 \neq f \in \mathrm{dom}(\mathbf{H})$ such that $\Delta f = f$ (see [**182**, Theorem X.26]). However, by Lemma 6.51, $|f|$ is subharmonic. Moreover, $|f| \in L^2(\mathcal{G}; \mu)$ since $f \in \mathrm{dom}(\mathbf{H})$. On the other hand, if $(\mathcal{G}, \varrho_\eta)$ is complete as a metric space, then Theorem 6.54 implies that $f \equiv 0$. This contradiction completes the proof. □

REMARK 7.2. A few remarks are in order.

(i) A different proof of Theorem 7.1 can be found in [**95**, Theorem 3.49]. Moreover, one more proof is provided by Theorem 7.9 below.
(ii) Simple examples show that the completeness with respect to the intrinsic path metric is only sufficient. Indeed, take a path graph and assume for simplicity that $\mu = \nu$. In this case, the intrinsic metric ϱ_η coincides with the natural path metric ϱ_0 and hence completeness is equivalent to the infinite length of the path. However, by Lemma 5.2, the self-adjointness of the Kirchhoff Laplacian is equivalent to the divergence of the series (5.1.4). For another example see [**67**, Example 4.14].
(iii) Notice also that by the Hopf–Rinow theorem for metric graphs (see Theorem 6.36) completeness of $(\mathcal{G}, \varrho_\eta)$ is equivalent to bounded compactness (compactness of distance balls), as well as to geodesic completeness.

As an immediate corollary of Theorem 7.1 and the results in Section 6.4, we obtain the analog of the above result for graph Laplacians, which was first established in [**113**, Theorem 2]:

COROLLARY 7.3 ([**113**]). *Let b be a locally finite graph over $(\mathcal{V}, m)$ and let ϱ be an intrinsic metric which generates the discrete topology on $\mathcal{V}$. If $(\mathcal{V}, \varrho)$ is complete as a metric space, then $\mathbf{h}^0$ is self-adjoint and $\mathbf{h}^0 = \mathbf{h}$.*

PROOF. We prove the claim in three steps.

(i) Assume first that ϱ is an intrinsic path metric of finite jump size such that $(\mathcal{V}, \varrho)$ is complete. Then, by Lemma 6.31 there is a cable system $(\mathcal{G}, \mu, \nu)$ for $(\mathcal{V}, m; b)$ such that $\rho = \rho_{\mathcal{V}}$ and $(\mathcal{G}, \varrho_\eta)$ is complete as a metric space. Hence the corresponding minimal Kirchhoff Laplacian $\mathbf{H}^0$ is self-adjoint by Theorem 7.1 and it remains to apply Theorem 3.1(i).

(ii) Suppose now that $\varrho = \varrho_p$ is a general intrinsic path metric with weight function $p \geq 0$ such that $(\mathcal{V}, \varrho)$ is complete. By the discrete Hopf–Rinow Theorem 6.37, the completeness is equivalent to the fact that

$$\sum_{n\geq 0} p(v_n, v_{n+1}) = \infty \tag{7.1.1}$$

for any infinite path $\mathcal{P} = (v_0, v_1, v_2, \dots)$ (i.e., $b(v_n, v_{n+1}) > 0$ for all $n \geq 0$, see (6.4.5)). However, introducing the new weight function $\tilde{p} := \min\{1, p\}$, we arrive at another path metric $\tilde{\varrho} := \varrho_{\tilde{p}}$, which is strongly intrinsic with respect to $(\mathcal{V}, m; b)$ (by construction) and, moreover, has jump size at most 1. It is not hard to show (e.g., by employing the Hopf–Rinow theorem 6.37 once again) that $(\mathcal{V}, \varrho)$ is complete exactly when so is $(\mathcal{V}, \tilde{\varrho})$ and this finishes the proof in this case.

(iii) Finally, assume that ϱ is an intrinsic metric which generates the discrete topology on $\mathcal{V}$ and such that $(\mathcal{V}, \varrho)$ is complete. We show how to associate with ϱ an intrinsic path metric $\tilde{\varrho}$ on $\mathcal{V}$ such that $(\mathcal{V}, \tilde{\varrho})$ is complete as well. Consider the weight $p\colon \mathcal{V}\times\mathcal{V} \to [0, \infty)$ given by $p(x, y) := \varrho(x, y)$ whenever $x \sim y$ and $p(x, y) = 0$ if $x \not\sim y$. By construction, p is an intrinsic weight and the associated intrinsic path metric $\tilde{\varrho} = \varrho_p$ satisfies $\rho \leq \tilde{\varrho}$. Moreover, since both $\tilde{\varrho}$ and ϱ generate the discrete topology on $\mathcal{V}$, the completeness of $(\mathcal{V}, \tilde{\varrho})$ follows by comparison. This completes the proof in the general case. □

REMARK 7.4. In the context of manifolds, Theorem 7.1 and Corollary 7.3 are known as Gaffney-type theorems.

The following results can be seen as a demonstration of the "from discrete to continuous" approach. First one can replace the completeness condition by a weaker one formulated in terms of the weighted degree function.

LEMMA 7.5. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph. Suppose that for some model of finite intrinsic size the weighted degree function* (2.2.8) *with the vertex and edge weights defined by* (3.1.5) *and* (3.1.6) *is bounded on finite radius metric balls of $(\mathcal{V}, \varrho_{\mathcal{V}})$. Then the minimal Kirchhoff Laplacian $\mathbf{H}^0$ is self-adjoint. In particular, $\mathbf{H}^0$ is self-adjoint if* Deg *is bounded on $\mathcal{V}$.*

Here $\varrho_{\mathcal{V}}$ is the restriction of ϱ_η onto $\mathcal{V} \times \mathcal{V}$ defined by (6.4.13).

PROOF. If Deg is bounded on $\mathcal{V}$, then, by Lemma 2.9, the corresponding graph Laplacian $\mathbf{h}^0$ is bounded and hence self-adjoint. Therefore, by Theorem 3.1(i), the minimal Kirchhoff Laplacian $\mathbf{H}^0$ is also self-adjoint.

Assume now that Deg is bounded on distance balls of $(\mathcal{V}, \varrho_{\mathcal{V}})$. By Lemma 6.25 (see also Remark 6.26(i)), $\varrho_{\mathcal{V}}$ is intrinsic and hence applying Theorem 1 from [**113**] we conclude that $\mathbf{h}^0$ is self-adjoint. It remains to apply Theorem 3.1(i). □

Remark 7.6. Notice that Lemma 7.5 improves Theorem 7.1. Indeed, the assumption of Lemma 7.5 is satisfied if $(\mathcal{G}, \varrho_\eta)$ is complete since in this case distance balls in $(\mathcal{V}, \varrho_{\mathcal{V}})$ are finite by the Hopf–Rinow theorem 6.37.

Theorem 7.7. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph. Assume that for some model of $(\mathcal{G}, \mu, \nu)$, the vertex set $\mathcal{V}$ equipped with the star metric ϱ_m (defined by* (6.4.8) *and* (3.1.5)*) is a complete metric space. Then the minimal Kirchhoff Laplacian $\mathbf{H}^0$ is self-adjoint.*

Proof. By Theorem 3.1(i) (see also Corollary 3.15), $\mathbf{H}^0$ is self-adjoint if and only if $\mathbf{h}^0$ is self-adjoint for some model of $(\mathcal{G}, \mu, \nu)$. However, by [**130**, Theorem 6], the minimal graph Laplacian defined by (3.3.1) in $\ell^2(\mathcal{V}; m)$ is self-adjoint if

$$\sum_{n\geq 0} m(v_n) = \infty \tag{7.1.2}$$

for any infinite path $\mathcal{P} = (v_0, v_1, v_2, \dots)$. However, our graph is locally finite and hence, by Theorem 6.37, the latter is equivalent to completeness of $(\mathcal{V}, \varrho_m)$ with respect to the star path metric (6.4.8). □

Remark 7.8. A few remarks are in order.

(i) Theorem 7.7 can be seen as an extension of Corollary 5.3 to the graph setting (see also Remark 5.4). In turn, Corollary 5.3 shows that completeness w.r.t. the star path metric ϱ_m is only sufficient even in the simplest case of a path graph. It would be of great interest to find (at least some) conditions which would guarantee the necessity of completeness w.r.t. the star path metric for the self-adjointness of both $\mathbf{H}^0$ and $\mathbf{h}^0$.

(ii) It is not hard to see that the completeness conditions in Theorem 7.1 and Theorem 7.7 are different. For example, if $\mu = \nu$, then the intrinsic metric ϱ_η coincides with the natural path metric ϱ_0 and hence the completeness in Theorem 7.1 is independent of the weight μ. On the other hand, the completeness in Theorem 7.7 is independent of the weight ν. However, in certain cases, Theorem 7.1 is a corollary of Theorem 7.7 (e.g., if $\mu = \nu \equiv 1$, see [**67**, § 4.2]).

7.1.2. Laplacians with δ-couplings. We begin with the following result proved recently in [**143**], which says that completeness combined with semiboundedness guarantees self-adjointness:

Theorem 7.9 (The Glazman–Povzner–Wienholtz theorem on metric graphs). *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph such that $(\mathcal{G}, \varrho_\eta)$ is complete. Assume that $\alpha\colon \mathcal{V} \to \mathbb{R}$ is such that the minimal Laplacian $\mathbf{H}^0_\alpha$ is bounded from below. Then $\mathbf{H}^0_\alpha$ is self-adjoint and $\mathbf{H}^0_\alpha = \mathbf{H}_\alpha$.*

Remark 7.10. A few remarks are in order.

(i) The proof of Theorem 7.9, which also provides another proof of Theorem 7.1, can be found in [**143**] (see Theorem 5.1 there). The claim in Theorem 7.9 remains valid if we add an additive potential $V\colon \mathcal{G} \to \mathbb{R}$ to the operator $\mathbf{H}^0_\alpha$, which preserves the semiboundedness. Of course, some regularity assumptions on V must be imposed (e.g., $V \in L^2_{\mathrm{loc}}(\mathcal{G})$), however, it is proved in [**143**, Theorem 5.1] that one may even allow distributional potentials $V \in H^{-1}_{\mathrm{loc}}(\mathcal{G})$.

(ii) It is tempting to replace in Theorem 7.9 the completeness w.r.t. ϱ_η by the one w.r.t. the star path metric ϱ_m. However, simple counterexamples show that it is not possible in general (see Remark 7.18(ii) and also the detailed discussion in [**143**, § 6]).

(iii) In the simplest case of a path graph Theorem 7.9 was first proved in [**4**] (see Theorem I.1 and Rem. III.2 there). However, notice also that in this case Theorem 7.9 is nothing but Lemma 5.16(ii) (take into account also Remark 3.24).

(iv) The Glazman–Povzner–Wienholtz theorem has a venerable history. To the best of our knowledge (see also [**28**, Appendix D.1] for further information), for Schrödinger operators in $\mathbb{R}^N$ the result was conjectured by I.M. Glazman and proved by A.Ya. Povzner in 1952 [**180**]. However, this paper was published in Russian and was not widely known in the West until its English translation in 1967. For instance, P. Hartman (1948) and F. Rellich (1951) proved a one-dimensional version of this result, and F. Rellich in his invited address at the ICM in Amsterdam (1954) posed a multi-dimensional result as an open problem, which was solved later by his student E. Wienholtz [**207**].

As an immediate application of Theorem 7.9 and the results connecting metric graphs with weighted graphs, we arrive at the following version of the Glazman–Povzner–Wienholtz theorem for weighted graphs (see [**143**, Theorem 6.1]).

Theorem 7.11 (The Glazman–Povzner–Wienholtz theorem on graphs). *Let b be a locally finite graph over $(\mathcal{V}, m)$ and assume that there exists an intrinsic metric ϱ which generates the discrete topology on $\mathcal{V}$ and such that $(\mathcal{V}, \varrho)$ is complete. Assume also that $\alpha\colon \mathcal{V} \to \mathbb{R}$ is such that the minimal Schrödinger operator $\mathbf{h}_\alpha^0$ is bounded from below in $\ell^2(\mathcal{V}; m)$. Then $\mathbf{h}_\alpha^0$ is self-adjoint and $\mathbf{h}_\alpha^0 = \mathbf{h}_\alpha$.*

Proof. Arguing as in the proof of Corollary 7.3, it suffices to consider the case when ϱ is an intrinsic path metric of finite jump size. Then applying Lemma 6.31, we obtain a cable system $(\mathcal{G}, \mu, \nu)$ for $(\mathcal{V}, m; b)$ such that $\rho = \rho_{\mathcal{V}}$ and $(\mathcal{G}, \varrho_\eta)$ is complete. Moreover, by Theorem 3.22(i) and Remark 3.24, the corresponding operator $\mathbf{H}_\alpha^0$ is bounded from below. Applying Theorem 7.9, we conclude that $\mathbf{H}_\alpha^0$ is self-adjoint. It remains to apply Theorem 3.1(i). □

Remark 7.12. To the best of our knowledge the Glazman–Povzner–Wienholtz theorem for graphs was established first in [**165**, Theorem 1.3] and [**199**, Theorem 6.1] (however, under the additional bounded geometry assumption on $(\mathcal{V}, b)$) and then independently in [**7**, Theorem 1] and [**94**, Theorem 2.16] (the latter allows non-locally finite graphs, see also [**187**]).

Usually, it is not an easy task to find necessary and sufficient conditions which guarantee semiboundedness. We begin with the simplest situation.

Lemma 7.13. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph together with a fixed model. Assume that the weighted degree function* (2.2.8) *with the vertex and edge weights defined by* (3.1.5) *and* (3.1.6) *is bounded on $\mathcal{V}$. Then the Laplacian $\mathbf{H}_\alpha$ with δ-couplings on $\mathcal{V}$ is self-adjoint for any $\alpha\colon \mathcal{V} \to \mathbb{R}$. Moreover, $\mathbf{H}_\alpha$ is bounded from below exactly when*

$$\inf_{v\in\mathcal{V}} \frac{\alpha(v)}{m(v)} > -\infty, \tag{7.1.3}$$

Proof. It suffices to notice that $\mathbf{h}_\alpha = \mathbf{h} + \frac{\alpha}{m}$. Indeed, $\frac{\alpha}{m}$ is a multiplication operator in $\ell^2(\mathcal{V};m)$ and hence it is self-adjoint since α is real-valued. Moreover, it is bounded from below exactly when (7.1.3) holds true. Since $\mathbf{h}$ is a bounded operator by Lemma 2.9, and both self-adjointness and semiboundedness are stable under bounded perturbations, we complete the proof by applying Theorem 3.1. □

As an immediate corollary we arrive at the following result.

Corollary 7.14. *Let $(\mathcal{G},\mu,\nu)$ be a weighted metric graph together with a fixed model. If*

$$\eta_*(\mathcal{G}) := \inf_{e\in\mathcal{E}} \eta(e) > 0, \tag{7.1.4}$$

then $\mathbf{H}_\alpha$ is self-adjoint for any $\alpha\colon \mathcal{V}\to\mathbb{R}$. Moreover, it is bounded from below exactly when (7.1.3) *is satisfied.*

Proof. Without loss of generality we can assume that the model is simple and has finite intrinsic size (we can "cut" each loop and multiple edge in the middle, and also each long edge by adding inessential vertices; clearly, this would not change $\mathbf{H}_\alpha$ and also the corresponding conditions (7.1.3) and (7.1.4) would hold true as well). Since (7.1.4) means that

$$|e|\mu(e) > \eta_*(\mathcal{G})^2\,\frac{\nu(e)}{|e|}$$

for all $e\in\mathcal{E}$ by (7.1.4), it follows that

$$\mathrm{Deg}(v) = \frac{\sum_{e\in\mathcal{E}_v}\frac{\nu(e)}{|e|}}{\sum_{e\in\mathcal{E}_v}|e|\mu(e)} \le \frac{\sum_{e\in\mathcal{E}_v}\frac{\nu(e)}{|e|}}{\sum_{e\in\mathcal{E}_v}\eta_*(\mathcal{G})^2\,\frac{\nu(e)}{|e|}} = \frac{1}{\eta_*(\mathcal{G})^2} < \infty,$$

and hence Lemma 7.13 applies. □

Remark 7.15. The most common restriction imposed in the quantum graphs literature is that $\mu=\nu\equiv 1$ and $\inf_{\mathcal{E}}|e|>0$ on $\mathcal{G}$ (see, e.g., [**24**]). For non-trivial weights, a similar assumption is sometimes imposed: $\mu=\nu$ on $\mathcal{G}$ and $\inf_{\mathcal{E}}|e|>0$, $\inf_{\mathcal{E}}\mu(e)>0$. Clearly, in both cases (7.1.4) holds true and Corollary 7.14 applies.

If the weighted degree Deg is unbounded on $\mathcal{V}$, then one needs to proceed more carefully.

Lemma 7.16. *Let $(\mathcal{G},\mu,\nu)$ be a weighted metric graph together with a fixed model. Assume that at least one of the following conditions is satisfied:*

- *$(\mathcal{G},\varrho_\eta)$ is complete as a metric space,*
- *$(\mathcal{V},\varrho_m)$ is complete as a metric space, where ϱ_m is the star path metric.*

If $\alpha\colon\mathcal{V}\to\mathbb{R}$ satisfies (7.1.3)*, then $\mathbf{H}^0_\alpha$ is self-adjoint and bounded from below.*

Proof. If $(\mathcal{G},\varrho_\eta)$ is complete as a metric space, then according to Theorem 7.9 it suffices to show that $\mathbf{H}^0_\alpha$ is bounded from below. However, this easily follows from Theorem 3.22(i) (take into account also Remark 3.24), since (7.1.3) implies that $\mathbf{h}^0_\alpha$ is lower semibounded.

If $(\mathcal{V},\varrho_m)$ is complete as a metric space, combining (7.1.3) with [**130**, Prop. 3.1] implies that $\mathbf{h}^0_\alpha$ is self-adjoint and lower semibounded. By Theorem 3.1, $\mathbf{H}^0_\alpha$ is self-adjoint and lower semibounded as well. □

7.1.3. Jacobi matrices on graphs. Of course, the results from the previous two subsections immediately apply to Jacobi matrices on graphs – Schrödinger-type operators in $\ell^2(\mathcal{V})$ (that is, the vertex weight m is constant). Let us quickly recall the setup (see Section 6.6). For a given $\beta\colon \mathcal{V} \to \mathbb{R}$ and a connected graph q over $\mathcal{V}$ satisfying the properties (i), (ii) and (iv) of Section 2.2, consider a second order symmetric difference expression

$$(\tau f)(v) = \beta(v)f(v) - \sum_{u\in\mathcal{V}} q(u,v)f(u), \qquad v \in \mathcal{V}. \tag{7.1.5}$$

As described in Section 2.2, we can associate in $\ell^2(\mathcal{V})$ the minimal $J^0 = J^0_{q,\beta}$ and maximal operator $J = J_{q,\beta}$ with the difference expression (7.1.5).

THEOREM 7.17. *If at least one of the following conditions is satisfied*

(i) *There is $C \ge 0$ such that*

$$\beta(v) - \sum_{u\in\mathcal{V}} q(u,v) \ge -M \tag{7.1.6}$$

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

(ii) *The minimal operator J^0 is bounded from below and $(\mathcal{V}, \varrho_p)$ is complete as a metric space, where ϱ_p is the path metric with the edge weights*

$$p(u,v) = \frac{1}{\sqrt{q(u,v)\,\max(\deg(u),\deg(v))}} \tag{7.1.7}$$

whenever $q(u,v) > 0$ and 0 otherwise,

then the operator J is self-adjoint and $J^0 = J$.

PROOF. (i) If $m \equiv \mathbb{1}_{\mathcal{V}}$, then the corresponding star path metric ϱ_m is nothing but the combinatorial distance on $\mathcal{V}$. Taking into account that $(\mathcal{V}, \varrho_{\mathrm{comb}})$ is complete (this can be either verified directly or by using the Hopf–Rinow theorem 6.37), it remains to apply Lemma 7.16 since $\alpha(v)$ in this case coincides with the LHS(7.1.6).

(ii) is a straightforward application of the Glazman–Povzner–Wienholtz theorem on graphs. Indeed, choosing $m \equiv \mathbb{1}_{\mathcal{V}}$, $b = q$ and $\alpha(v) = \mathrm{LHS}(7.1.6)$, we get that $J^0_{q,\beta} = \mathbf{h}^0_\alpha$ in $\ell^2(\mathcal{V}) = \ell^2(\mathcal{V}; m)$. It remains to notice that the weight (7.1.7) is intrinsic:

$$\sum_{u\sim v} q(u,v)p(u,v)^2 = \sum_{u\sim v} \frac{1}{\max(\deg(u),\deg(v))} \le \sum_{u\sim v} \frac{1}{\deg(v)} = 1,$$

for all $v \in \mathcal{V}$. It remains to apply Theorem 7.11. □

REMARK 7.18. A few remarks are in order.

(i) Theorem 7.17 can be seen as an extension of Wouk's tests for Jacobi matrices to the graph setting (compare (i) and (ii) with [**212**, Theorem 3(c) and Theorem 3(d)], see also [**2**, Problems I.3 and I.4]). On the other hand, Wouks test [**212**, Theorem 3(d)] can be seen as the analog of a one-dimensional predecessor of the Glazman–Povzner–Wienholtz theorem proved by P. Hartman (1948) and F. Rellich (1951) (see [**143**, Rem. 6.5] for further details).

(ii) It is well known that even for Jacobi matrices (5.2.8) one cannot replace (7.1.6) by the semiboundedness of the minimal operator J^0. This, in particular, implies that one cannot replace the intrinsic path metric by the star path metric ϱ_m in the completeness assumption of Glazman–Povzner-Wienholtz theorems.

(iii) Under the additional bounded degree assumption, $\sup_{\mathcal{V}} \deg(v) < \infty$, the above result was established in [**199**, Theorem 6.1] and [**165**, Theorem 1.3].

Let us give one more sufficient condition for self-adjointness. Recall that, according to Theorem 6.59, for any locally finite graph q over $\mathcal{V}$ one can find edge lengths $|\cdot|$ and weights ν satisfying (6.6.3) and (6.6.4). For a given $|\cdot|\colon \mathcal{E}_q \to (0,\infty)$, define the vertex weight $m\colon \mathcal{V} \to (0,\infty)$ by setting

$$m_q(v) = \sum_{u\sim v} |e_{u,v}|, \qquad v \in \mathcal{V}. \tag{7.1.8}$$

Taking into account (6.6.4), let us also introduce the graph $b = b_q$ over $\mathcal{V}$ by setting

$$b_q(u,v) = \begin{cases} \frac{\nu(e_{u,v})}{|e_{u,v}|}, & q(u,v) > 0, \\ 0, & q(u,v) = 0. \end{cases} \tag{7.1.9}$$

THEOREM 7.19. *Let q be a locally finite graph over $\mathcal{V}$ and $\beta\colon \mathcal{V} \to \mathbb{R}$. Suppose that $|\cdot|\colon \mathcal{E}_q \to (0,\infty)$ and $\nu\colon \mathcal{E}_q \to (0,\infty)$ are edge lengths and weights satisfying* (6.6.3) *and such that q admits the representation* (6.6.4). *If at least one of the following conditions is satisfied*

(i) *$(\mathcal{V}, \varrho_m)$ is complete, where ϱ_m is the star path metric (see Example 6.20(iii)) with $m = m_q$, and there is $M \ge 0$ such that*

$$\beta(v) - \sum_{u\in\mathcal{V}} q(u,v)\sqrt{\frac{m(u)}{m(v)}} \ge -M \tag{7.1.10}$$

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

(ii) *The minimal operator J^0 is bounded from below and $(\mathcal{V}, \varrho_b)$ is complete, where ϱ_b is the natural path metric (see Example 6.20(ii)) with $b = b_q$,*

then the operator J is self-adjoint and $J^0 = J$.

PROOF. Notice that the minimal operator J^0 is unitarily equivalent to the operator $\mathbf{h}^0_\alpha$ acting in $\ell^2(\mathcal{V}; m)$ and associated with the graph $(\mathcal{V}, m; b)$ whose coefficients are defined via (6.6.5), that is,

$$b(u,v) = b_q(u,v) = q(u,v)\sqrt{m(u)m(v)}, \qquad \alpha(v) = \beta(v)m_q(v) - \sum_{u\in\mathcal{V}} b_q(u,v).$$

If condition (i) is satisfied, then we simply need to apply Lemma 7.16(ii) to $\mathbf{h}^0_\alpha$.

Assume now that (ii) holds true. Observe that the natural path metric ϱ_b is intrinsic w.r.t. $(\mathcal{V}, m; b)$:

$$\sum_{u\sim v} b(u,v)p_b(u,v)^2 = \sum_{u\sim v} \frac{\nu(e_{u,v})}{|e_{u,v}|}\frac{|e_{u,v}|^2}{\nu(e_{u,v})} = \sum_{u\sim v} |e_{u,v}| = m(v), \quad v \in \mathcal{V}.$$

It remains to apply Theorem 7.11. ∎

7.1.4. Semiboundedness and criticality theory on graphs. Condition (7.1.3) means that the semiboundedness is preserved if the strength $\alpha\colon \mathcal{V} \to \mathbb{R}$ is not too negative. In fact, (7.1.3) can be improved by using the concept of relatively bounded perturbations (see, e.g., [**125**], [**182**]). Assume for a moment that $\alpha\colon \mathcal{V} \to (-\infty, 0]$ is non-positive. Then α is called *form bounded* with respect to $\mathbf{h}^0$ if there are $\varepsilon \geq 0$ and $\gamma \geq 0$ such that

$$\sum_{v\in\mathcal{V}} |\alpha(v)||f(v)|^2 \leq \frac{\varepsilon}{2} \sum_{u,v\in\mathcal{V}} b(u,v)|f(u)-f(v)|^2 + \gamma \sum_{v\in\mathcal{V}} m(v)|f(v)|^2 \tag{7.1.11}$$

for all $f \in C_c(\mathcal{V})$. If (7.1.11) holds with some $\varepsilon < 1$, then α is called *strongly form bounded.* Notice that (7.1.11) is nothing but

$$\Big\langle \frac{|\alpha|}{m} f, f \Big\rangle_{\ell^2(\mathcal{V};m)} \leq \varepsilon\, \mathfrak{q}[f] + \gamma \|f\|^2_{\ell^2(\mathcal{V};m)}.$$

Clearly, if α satisfies (7.1.3), then we can take $\varepsilon = 0$ in (7.1.11), which further means that the multiplication operator α is bounded in $\ell^2(\mathcal{V};m)$. The importance of this concept stems from the KLMN theorem (see, e.g., [**182**]): *if $\alpha\colon \mathcal{V} \to (-\infty, 0]$ is strongly form bounded, then the form $\mathfrak{q}_\alpha = \mathfrak{q} + \alpha$ defined as a form sum with* $\mathrm{dom}(\mathfrak{q}_\alpha) = \mathrm{dom}(\mathfrak{q})$ *is closed and bounded from below.* Combining this result further with the Glazman–Povzner–Wienholtz theorem for graphs, we would be able to get the self-adjoint uniqueness for Laplacians with δ-couplings once the negative part of α satisfies (7.1.11) and $(\mathcal{G}, \varrho_\eta)$ is complete.

To proceed further, let us recall the following notion from [**138**]. For convenience reasons, for each real-valued function $\omega\colon \mathcal{V} \to \mathbb{R}$, we shall denote the corresponding quadratic form by the same letter, that is,

$$\omega[f] := \sum_{v\in\mathcal{V}} \omega(v)|f(v)|^2, \qquad f \in C_c(\mathcal{V}).$$

Definition 7.20 ([**138**]). Let b be a connected, locally finite graph over $(\mathcal{V}, m)$ and let $\mathfrak{q} = \mathfrak{q}_{b,0}$ be the corresponding energy form in $\ell^2(\mathcal{V}, m)$. For $\lambda \geq 0$, the weight $\omega\colon \mathcal{V} \to [0,\infty)$ is called λ-*critical* w.r.t. $(\mathcal{V}, m; b)$ (for $\lambda = 0$, it is simply called *critical*) if

- the form $\mathfrak{q} + \lambda m - \omega$ is nonnegative on $C_c(\mathcal{V})$, that is, $(\mathfrak{q} + \lambda m)[f] \geq \omega[f]$ for all $f \in C_c(\mathcal{V})$,
- for each weight $\widetilde{\omega}\colon \mathcal{V} \to [0,\infty)$ satisfying $\widetilde{\omega} \geq \omega$, the form $\mathfrak{q} + \lambda m - \widetilde{\omega}$ is not nonnegative on $C_c(\mathcal{V})$.

If the last property does not hold true (i.e., there is $\widetilde{\omega}$ such that $0 \not\equiv \widetilde{\omega} - \omega \geq 0$ and the form $\mathfrak{q} + \lambda m - \widetilde{\omega}$ is nonnegative), then the weight ω is called λ-subcritical.

Combining the notion of criticality with the Glazman–Povzner–Wienholtz theorem for graphs, we arrive at the following extension of Lemma 7.16.

Lemma 7.21. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph together with a fixed model and let $(\mathcal{V}, m; b)$ be the corresponding weighted graph* (3.1.5)–(3.1.6). *If $(\mathcal{G}, \varrho_\eta)$ is complete and $\alpha\colon \mathcal{V} \to \mathbb{R}$ is such that $\alpha_- := (|\alpha| - \alpha)/2$ is λ-subcritical for some $\lambda \geq 0$, then the operator $\mathbf{H}_\alpha$ is self-adjoint and bounded from below.*

Conversely, if $\alpha\colon \mathcal{V} \to (-\infty, 0]$ is such that $\mathbf{H}^0_\alpha$ is bounded from below, then there is $\lambda \geq 0$ such that the weight $-\alpha$ is λ-subcritical for $\mathbf{h}^0$.

PROOF. If $\alpha\colon \mathcal{V}\to\mathbb{R}$ satisfies the assumptions of Lemma 7.21, then taking into account that the form $\mathfrak{q}+\lambda m-\alpha_-$ is nonnegative on $C_c(\mathcal{V})$, we conclude that

$$\mathfrak{q}_\alpha[f] \ge \mathfrak{q}_{-\alpha_-}[f] := \mathfrak{q}[f] - \alpha_-[f] \ge -\lambda\|f\|^2_{\ell^2(\mathcal{V};m)}$$

for all $f\in C_c(\mathcal{V})$. Therefore, the form $\mathfrak{q}_\alpha$ is bounded from below on $C_c(\mathcal{V})$ and hence so is the operator $\mathbf{h}^0_\alpha$. By Theorem 3.1(ii) (see also Theorem 3.22 and Remark 3.24), the operator $\mathbf{H}^0_\alpha$ is bounded from below. It remains to apply Theorem 7.9.

To prove the last claim it suffices to notice that the semiboundedness of $\mathbf{h}^0_\alpha$, which is equivalent to the semiboundedness of $\mathbf{H}^0_\alpha$, means that there is $\lambda>0$ such that $\mathbf{h}^0_\alpha+\lambda\ge 0$, where the inequality is understood in the sense of forms. It is straightforward to see that $-\alpha$ is $(\lambda+1)$-subcritical for $\mathbf{h}_0$ □

REMARK 7.22. A few remarks are in order.

(i) The notion of criticality is closely connected with the notion of recurrence (see, e.g., [**138**, Rem. 5.8]). In particular, for $\lambda=0$, $\mathbf{h}_0$ is critical exactly when it is recurrent.

(ii) A characterization of criticality is presented in [**138**, Theorem 5.3]. However, for a concrete graph b over $\mathcal{V}$ it is a highly nontrivial task to find critical and (especially) λ-critical weights. One of the approaches is to employ positive λ-harmonic/superharmonic functions, which also leads to *optimal Hardy weights*, however, this requires an explicit form or at least a rather qualified knowledge of their asymptotic behavior (see [**137**]).

(iii) Let us stress that the Glazman–Povzner–Wienholtz theorem enables us to avoid the use of the KLMN theorem, however, the price to pay is the completeness assumption on $(\mathcal{G},\varrho_\eta)$.

7.2. Markovian uniqueness and finite energy extensions

In this section we briefly address the question of uniqueness of Markovian extension for the minimal Kirchhoff Laplacian $\mathbf{H}_0$. Notice that by Lemma 4.1 the latter is equivalent to the self-adjointness of the Gaffney Laplacian $\mathbf{H}_G$. We also stress that the self-adjoint uniqueness implies Markovian uniqueness, and hence the results obtained in the previous section provide various sufficient conditions for the Markovian uniqueness as well. In particular, completeness of $\mathcal{G}$ (with respect to particular choices of path metrics) is sufficient for the Markovian uniqueness.

7.2.1. Markovian uniqueness and graph ends. Surprisingly enough, in some cases of interest it is possible to provide a complete characterization of the Markovian uniqueness in purely geometric terms. Intuitively, this problem (as well as the self-adjoint uniqueness) is closely related to finding appropriate boundary notions for infinite graphs. For unweighted metric graphs, that is, with $\mu=\nu\equiv\mathbb{1}$, the question was studied in [**144**], [**147**] using graph ends, a graph boundary notion going back to H. Freudenthal and R. Halin (see Section 2.1.3). For this purpose recall the following notion introduced in [**144**].

DEFINITION 7.23. A topological end $\gamma\in\mathfrak{C}(\mathcal{G})$ of a metric graph $\mathcal{G}$ equipped with the edge weight μ has *finite volume* (w.r.t. to μ) if there is a sequence $\mathcal{U}=(U_n)$ representing γ such that

$$\mu(U_n) = \int_{U_n}\mu(\mathrm{d}x) < \infty \tag{7.2.1}$$

for some n. Otherwise γ has *infinite volume*.

The set of all finite volume ends is denoted by $\mathfrak{C}_0(\mathcal{G};\mu)$ and we equip it with the induced topology from the end space $\mathfrak{C}(\mathcal{G})$.

The above notion leads to a complete characterization of the Markovian uniqueness in the unweighted setting $\mu = \nu \equiv \mathbb{1}$ (see [**144**, Cor. 3.12]): *all ends of the metric graph have infinite volume.* In the present section, we briefly recall the results of [**144**], [**147**] and also extend them to the following simple situation.

THEOREM 7.24. *Let $(\mathcal{G},\mu,\nu)$ be a weighted metric graph whose weight functions $\mu,\nu\colon \mathcal{G}\to(0,\infty)$ are uniformly positive, that is,*

$$\frac{1}{\mu},\ \frac{1}{\nu} \in L^\infty(\mathcal{G}). \tag{7.2.2}$$

Then the deficiency indices of the minimal Gaffney Laplacian $\mathbf{H}_{G,\min}$ are equal to the number of finite volume graph ends,

$$\mathrm{n}_\pm(\mathbf{H}_{G,\min}) = \#\mathfrak{C}_0(\mathcal{G};\mu). \tag{7.2.3}$$

Moreover, the following statements are equivalent:

(i) $\mathbf{H}^0$ *admits a unique Markovian extension,*
(ii) $\mathbf{H}_D = \mathbf{H}_N$,
(iii) *the Gaffney Laplacian $\mathbf{H}_G$ is self-adjoint,*
(iv) $H^1_0(\mathcal{G},\mu,\nu) = H^1(\mathcal{G},\mu,\nu)$,
(v) *all graph ends have infinite volume (w.r.t. μ), that is, $\mathfrak{C}_0(\mathcal{G};\mu)=\varnothing$.*

Before giving the proof of Theorem 7.24, we recall a few standard facts on Sobolev spaces in dimension one. First of all, for every $\mathcal{I}=[0,a)$, $a\in(0,\infty]$ the embedding of $H^1(\mathcal{I})$ into $C_b(\mathcal{I}) = C(\mathcal{I})\cap L^\infty(\mathcal{I})$ is bounded and

$$\sup_{x\in\mathcal{I}} |f(x)|^2 \le C_a \int_{\mathcal{I}} |f(x)|^2 + |f'(x)|^2\,\mathrm{d}x \tag{7.2.4}$$

holds for all $f\in H^1(\mathcal{I})$, where $C_a = \sqrt{\coth(a)}$ (see [**159**]). Moreover, the limit $\lim_{x\to a} f(x)$ exists for every function $f\in H^1(\mathcal{I})$ (see, e.g., [**31**, Theorem 8.2] for bounded intervals and [**31**, Cor. 8.9] in the unbounded case).

Returning to our setting, assume that $(\mathcal{G},\mu,\nu)$ is a weighted metric graph. Suppose further that $\mathcal{P}$ is a path in $\mathcal{G}$. Notice that we can first identify $\mathcal{P}$ with a subset of $\mathcal{G}$, and then further with an interval $\mathcal{I}_\mathcal{P} = [0,|\mathcal{P}|)$ of length

$$|\mathcal{P}| := \int_\mathcal{P} \mathrm{d}x,$$

where the integral is taken over the subset $\mathcal{P}\subseteq\mathcal{G}$ w.r.t. the (unweighted) Lebesgue measure on $\mathcal{G}$ (cf. (6.4.2)). The restriction $f|_\mathcal{P}$ of a function $f\in H^1(\mathcal{G},\mu,\nu)$ to $\mathcal{P}\subseteq\mathcal{G}$ can be identified with a function on $\mathcal{I}_\mathcal{P} = [0,|\mathcal{P}|)$. Notice that, in case that (7.2.2) is satisfied, $f|_\mathcal{P}$ belongs to the (unweighted) Sobolev space $H^1(\mathcal{I}_\mathcal{P})$. In particular, (7.2.2) implies the following crucial property of H^1-functions: if $\mathcal{R} = (e_{v_n,v_{n+1}})_{n\ge0}$ is a ray, then

$$f(\gamma_\mathcal{R}) := \lim_{n\to\infty} f(v_n) \tag{7.2.5}$$

exists. Moreover, for each topological end $\gamma\in\mathfrak{C}(\mathcal{G})$ this limit is independent of the choice of the ray $\mathcal{R}$ in the corresponding graph end ω_γ. 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 $f(\gamma_{\mathcal{R}}) = f(\gamma_{\mathcal{R}''}) = f(\gamma_{\mathcal{R}'})$. Taking into account the relationship between topological ends and graph ends (see Section 2.1.3), this enables us to introduce the following notion.

DEFINITION 7.25. Assume that the weights μ, ν satisfy (7.2.2). Then for every $f \in H^1(\mathcal{G}, \mu, \nu)$ and a (topological) end $\gamma \in \mathfrak{C}(\mathcal{G})$, we define

$$f(\gamma) := f(\gamma_{\mathcal{R}}), \tag{7.2.6}$$

where $\mathcal{R}$ is any ray belonging to the corresponding graph end ω_γ.

As is easily verified, the values $f(\gamma)$, $\gamma \in \mathfrak{C}(\mathcal{G})$ are independent of the choice of the model of $(\mathcal{G}, \mu, \nu)$. It turns out that we obtain a continuous extension of f to the end compactification $\widehat{\mathcal{G}} = \mathcal{G} \cup \mathfrak{C}(\mathcal{G})$.

PROPOSITION 7.26. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph satisfying* (7.2.2). *Then for every function $f \in H^1(\mathcal{G}, \mu, \nu)$, its extension $f \colon \widehat{\mathcal{G}} \to \mathbb{C}$ is continuous.*

PROOF. Let $\gamma \in \mathfrak{C}(\mathcal{G})$ be a topological end represented by a sequence of open subsets $\mathcal{U} = (U_n)$. To prove that $f \colon \widehat{\mathcal{G}} \to \mathbb{C}$ is continuous in γ, we have to show that (see Section 2.1.3 for the definition of the topology on $\widehat{\mathcal{G}}$)

$$\lim_{n\to\infty} \sup_{x \in U_n} |f(x) - f(\gamma)| = 0.$$

As is readily verified (for instance, we can always refine the fixed model of $(\mathcal{G}, \mu, \nu)$), it suffices to prove this statement for vertices $v \in \mathcal{V}$, that is, to establish that

$$\lim_{n\to\infty} \sup_{v \in \mathcal{V} \cap U_n} |f(v) - f(\gamma)| = 0. \tag{7.2.7}$$

In order to obtain (7.2.7), we distinguish two cases. Assume first that each of the open sets U_n contains a ray $\mathcal{R}_n \subseteq U_n$ with length $|\mathcal{R}_n| > 1$. As is easily verified, then each vertex $v \in U_n$ is contained in a path without self-intersections $\mathcal{P}_v \subseteq U_n$ of length $|\mathcal{P}_v| \geq 1/2$. Since $\bigcap_n U_n = \varnothing$, it follows from (7.2.4) and assumption (7.2.2) that

$$\lim_{n\to\infty} \sup_{v \in \mathcal{V} \cap U} |f(v)|^2 \leq \lim_{n\to\infty} C_{1/2} \int_{U_n} |f(x)|^2 + |\nabla f(x)|^2 \,\mathrm{d}x = 0.$$

Clearly this also implies $f(\gamma) = 0$ and hence proves (7.2.7) in the first case.

On the other hand, suppose that there exists a set U_N such that all rays $\mathcal{R} \subseteq U_N$ have length $|\mathcal{R}| \leq 1$. Since every vertex $v \in U_n$, $n \geq N$ is contained in some ray $\mathcal{R}_v \subseteq U_n$ with $\mathcal{R}_v \in \omega_\gamma$, we have

$$\sup_{v \in \mathcal{V} \cap U_n} |f(v) - f(\gamma)| \leq \sup_{v \in \mathcal{V} \cap U_n} \int_{\mathcal{R}_v} |\nabla f(x)| \mathrm{d}x \leq \Big(\int_{U_n} |\nabla f(x)|^2 \mathrm{d}x \Big)^{1/2}$$

and assumption (7.2.2) again implies that (7.2.7) holds true. □

This leads to a description of $H^1_0(\mathcal{G}, \mu, \nu) = \overline{H^1_c(\mathcal{G})}^{\|\cdot\|_{H^1(\mathcal{G},\mu,\nu)}}$ as the space of H^1-functions with vanishing boundary values.

THEOREM 7.27. *Assume that* (7.2.2) *holds true. Then*

$$H^1_0(\mathcal{G}, \mu, \nu) = \big\{ f \in H^1(\mathcal{G}, \mu, \nu) |\, f(\gamma) = 0 \textit{ for all } \gamma \in \mathfrak{C}(\mathcal{G}) \big\}.$$

PROOF. First of all, notice that $\sup_{x\in\widehat{\mathcal{G}}}|f(x)| \le C\|f\|_{H^1(\mathcal{G},\mu,\nu)}$ for every function $f \in H^1(\mathcal{G},\mu,\nu)$ and some uniform constant $C > 0$ (this follows, e.g., from the closed graph theorem). On the other hand, if $f \in H^1(\mathcal{G},\mu,\nu)$ has compact support, then $f(\gamma) = 0$ for all graph ends $\gamma \in \mathfrak{C}(\mathcal{G})$. This proves the first inclusion "$\subseteq$".

The proof of the converse inclusion "$\supseteq$" follows line to line the proof of [**144**, Theorem 3.12] (see also the proof of [**82**, Theorem 4.14]). First of all, we may assume that $f \in H^1(\mathcal{G},\mu,\nu)$ is non-negative and vanishes on $\mathfrak{C}(\mathcal{G})$. Then for every $s > 0$, the following set

$$A_s = \{x \in \mathcal{G} |\, f(x) \ge s\}$$

is a compact subset of $\mathcal{G}$. In particular, defining $\phi_n\colon \mathbb{R}_{\ge 0} \to \mathbb{R}_{\ge 0}$ by

$$\phi_n(s) = \begin{cases} s - \frac{1}{n}, & \text{if } s \ge \frac{1}{n}, \\ 0, & \text{if } s < \frac{1}{n}, \end{cases} \tag{7.2.8}$$

the composition $f_n := \phi_n \circ f$ has compact support in $\mathcal{G}$. Moreover, $|\phi_n(s)| \le |s|$ and $|\phi_n(s) - \phi_n(t)| \le |s - t|$ for all $s, t \ge 0$ and hence f_n belongs to $H^1_0(\mathcal{G},\mu,\nu)$ for all n. As is easily verified, $\lim_{n\to\infty} f_n = f$ in $H^1(\mathcal{G},\mu,\nu)$, which finishes the proof. □

To prove the main results of this section, we also need the following lemma.

LEMMA 7.28. *Let $(\mathcal{G},\mu,\nu)$ be a weighted metric graph satisfying* (7.2.2). *Then for any finite collection of distinct finite volume ends $(\gamma_i)_{i=1}^N$, there is a function $g \in \mathrm{dom}(\mathbf{H}_N)$ with $g(\gamma_1) = 1$ and $g(\gamma_2) = \cdots = g(\gamma_N) = 0$.*

PROOF. Fix a representing sequence of open subsets $\mathcal{U}^i = (U^i_n)$ for each of the topological ends γ_i, $i = 1,\dots,N$. Without loss of generality, we may suppose that $U := U^1_0$ has measure $\mu(U) < \infty$ and $U \cap U^i_0 = \varnothing$ for all $i = 2,\dots,N$. Moreover, since ∂U is compact, the edge set $\mathcal{E}_0 = \{e \in \mathcal{E} |\, e \cap \partial U \ne \varnothing\}$ is finite and hence its union $K := \bigcup_{e\in\mathcal{E}_0} e$ is a compact subset of $\mathcal{G}$. Clearly, we can easily construct a function $g \in H^1(\mathcal{G},\mu,\nu) \cap \mathrm{dom}(\mathbf{H})$ which satisfies $g \equiv 1$ on U, $\{x \,|\, \nabla g(x) \ne 0\} \subseteq K$ and $g \equiv 0$ on $\mathcal{G} \setminus (U \cup K)$. Notice that in this step we need the finite volume property of γ_1 to ensure that $g \in L^2(\mathcal{G};\mu)$. Taking into account that $U \cap U^i_0 = \varnothing$ for $i = 2,\dots,N$, it is easily verified that g has the claimed boundary values in the graph ends γ_i, $i = 1,\dots,N$.

It remains to prove that g belongs to $\mathrm{dom}(\mathbf{H}_N)$. However, since g satisfies the Kirchhoff conditions on $\mathcal{G}$ and is (componentwise) constant on $\mathcal{G} \setminus K$, integration by parts gives

$$\begin{aligned} \mathfrak{Q}_N[g,h] &= \int_{\mathcal{G}} \nabla g(x) \nabla h(x)^* \,\nu(\mathrm{d}x) = \int_K \nabla g(x)\nabla h(x)^*\,\nu(\mathrm{d}x) \\ &= -\int_K \Delta g(x) h^*(x)\,\mu(\mathrm{d}x) = -\int_{\mathcal{G}} \Delta g(x) h^*(x)\,\mu(\mathrm{d}x) \end{aligned}$$

for every function $h \in H^1(\mathcal{G},\mu,\nu)$. In particular, g belongs to $\mathrm{dom}(\mathbf{H}_N)$ by the first representation theorem (see, e.g., [**125**, Chapter 6]). □

After these preparations we proceed with the proof of Theorem 7.24.

PROOF OF THEOREM 7.24. First of all, since $\mathbf{H}_N$ is a self-adjoint extension of $\mathbf{H}_{G,\min}$, the second von Neumann formula (cf. [**188**, Theorem 13.10]) implies

$$\mathrm{n}_\pm(\mathbf{H}_{G,\min}) = \dim\big(\mathrm{dom}(\mathbf{H}_N)/\,\mathrm{dom}(\mathbf{H}_{G,\min})\big).$$

The lower estimate "$\geq$" in (7.2.3) then follows immediately from Lemma 7.28, Theorem 7.27 and the fact that $\mathrm{dom}(\mathbf{H}_{G,\min}) \subseteq H^1_0(\mathcal{G},\mu,\nu)$. This, in particular, implies the equality if $\#\mathfrak{C}_0(\mathcal{G};\mu) = \infty$. Hence we only need to prove (7.2.3) if $\#\mathfrak{C}_0(\mathcal{G};\mu) < \infty$.

In this case, by Lemma 7.28, for every finite volume end $\gamma \in \mathfrak{C}_0(\mathcal{G};\mu)$, we can fix a function $g_\gamma \in \mathrm{dom}(\mathbf{H}_N)$ with $g_\gamma(\gamma) = 1$ and $g_\gamma(\gamma') = 0$ for all $\gamma' \in \mathfrak{C}_0(\mathcal{G};\mu)$, $\gamma' \neq \gamma$. Then every function $f \in \mathrm{dom}(\mathbf{H}_N)$ can be written as

$$f = f - \sum_{\gamma\in\mathfrak{C}_0(\mathcal{G};\mu)} f(\gamma)g_\gamma + \sum_{\gamma\in\mathfrak{C}_0(\mathcal{G};\mu)} f(\gamma)g_\gamma =: f_0 + f_{\mathfrak{C}_0}.$$

Clearly, f_0 belongs to $\mathrm{dom}(\mathbf{H}_N)$ and $f_0(\gamma) = 0$ at all finite volume graph ends $\gamma \in \mathfrak{C}(\mathcal{G})$. In fact, $f_0(\gamma) = 0$ for all graph ends (including ends of infinite volume) since f_0 extends continuously to the end compactification (see Proposition 7.26) and belongs to $L^2(\mathcal{G};\mu)$. Therefore, by Theorem 7.27, f_0 belongs to $H^1_0(\mathcal{G},\mu,\nu)$ and, comparing (2.4.24) with (2.4.25), this implies that $f_0 \in \mathrm{dom}(\mathbf{H}_{G,\min})$ and, moreover, that $\mathrm{dom}(\mathbf{H}_N)$ admits the following decomposition

$$\mathrm{dom}(\mathbf{H}_N) = \mathrm{dom}(\mathbf{H}_{G,\min}) \dot{+} \mathrm{span}\left\{g_\gamma \,|\, \gamma \in \mathfrak{C}_0(\mathcal{G};\mu)\right\}. \tag{7.2.9}$$

In particular, we conclude that

$$\mathrm{n}_\pm(\mathbf{H}_{G,\min}) = \dim\left(\mathrm{dom}(\mathbf{H}_N)/\,\mathrm{dom}(\mathbf{H}_{G,\min})\right) = \#\mathfrak{C}_0(\mathcal{G};\mu),$$

The remaining equivalences follow from Lemma 4.1 (see also Lemma 2.15 and (2.4.25)). □

Let us stress that finite volume graph ends do not provide a characterization of Markovian uniqueness for general weighted graphs $(\mathcal{G},\mu,\nu)$. This was already observed in the simple case of weighted path graphs in Section 5.1 (see in particular Lemma 5.11). Notice that $\mathbb{Z}_{\geq 0}$ has only one graph end γ and it has finite volume exactly when the sum in (5.1.5) converges. Hence, by Lemma 5.11, the Gaffney Laplacian $\mathbf{H}_G$ is self-adjoint if either the quantity $\mathcal{L}_\nu = \infty$ (and in this case the volume of the graph end is irrelevant) or $\mathcal{L}_\nu < \infty$ and γ has infinite volume.

On the other hand, the result for path graphs suggests that finite volume ends can be used under a suitable generalization of the condition $\mathcal{L}_\nu < \infty$ from Lemma 5.11. It turns out that this guess is indeed correct and we outline the idea in the following. For any path $\mathcal{P}$ in $\mathcal{G}$, we define its ν-length as (cf. (6.4.2))

$$|\mathcal{P}|_{1/\nu} = \int_{\mathcal{P}} \frac{\mathrm{d}s}{\nu(s)},$$

where the integral is taken over the corresponding subset $\mathcal{P} \subseteq \mathcal{G}$. Moreover, for any subset $U \subseteq \mathcal{G}$, its *ν-diameter at infinity* is defined as

$$D_{1/\nu}(U) := \sup\nolimits_{\mathcal{P}\subseteq U} |\mathcal{P}|_{1/\nu},$$

where the supremum is taken over all paths $\mathcal{P}$ without self-intersection in U. Suppose $\gamma \in \mathfrak{C}(\mathcal{G})$ is a topological end represented by a sequence of open subsets $\mathcal{U} = (U_n)$. Then we define its ν-diameter† by

$$D_{1/\nu}(\gamma) = \inf_n D_{1/\nu}(U_n) = \lim_{n\to\infty} D_{1/\nu}(U_n).$$

†Let us stress that $D_{1/\nu}(U)$ does not coincide with the standard definition of the diameter for metric spaces.

REMARK 7.29. As is readily verified, the value of $D_{1/\nu}(\gamma)$ is independent of the choice of the representing sequence $\mathcal{U} = (U_n)$.

It turns out that the conclusions of Theorem 7.2.2 are also valid under the assumption

$$D_{1/\nu}(\gamma) < \infty \qquad \text{for all graph ends } \gamma \in \mathfrak{C}(\mathcal{G}) \tag{7.2.10}$$

instead of (7.2.2). For instance, it is easy to see that for each $f \in H^1(\mathcal{G}, \mu, \nu)$ and ray $\mathcal{R}$,

$$\int_{\mathcal{R}} |\nabla f| \, \mathrm{d}s < \infty$$

and in particular, the limits in (7.2.5) exist. A careful analysis of the rest of the proof for Theorem 7.2.2 shows that it can be carried over as well and we omit the details.

REMARK 7.30. Assumption (7.2.10) can be seen as a generalization of the condition $\mathcal{L}_\nu < \infty$ in Lemma 5.11. On the other hand, neither of the conditions (7.2.2) and (7.2.10) implies the other one.

7.2.2. Markovian and finite energy extensions. Let us now briefly comment on the problem of describing the self-adjoint restrictions of the Gaffney Laplacian $\mathbf{H}_G$. This class of extensions is called *finite energy extensions* in [**144**] and by Lemma 2.18, these are exactly the self-adjoint extensions $\widetilde{\mathbf{H}}$ of the minimal operator $\mathbf{H}_0$ satisfying $\mathrm{dom}(\widetilde{\mathbf{H}}) \subset H^1(\mathcal{G}, \mu, \nu)$. Their importance stems from the fact that they contain all Markovian extensions (see Lemma 4.1). Moreover, the kernels of their heat semigroups and resolvents are well-behaved (the results of [**144**, § 5] extend verbatim if at least one of the assumptions (7.2.2) or (7.2.10) is satisfied).

The preceding sections suggest to describe finite energy extensions in terms of finite volume graph ends. It turns out that, if (7.2.2) or (7.2.10) holds true and in addition $\#\mathfrak{C}_0(\mathcal{G};\mu) < \infty$, this is indeed possible. Namely, in this case the maximal Gaffney Laplacian $\mathbf{H}_G$ is closed (this can be proved analogous to [**147**, Theorem 3.12(i)]). Moreover, these assumptions allow to introduce a suitable notion of a normal derivative for finite volume graph ends $\gamma \in \mathfrak{C}_0(\mathcal{G};\mu)$ (modifying the notions in [**144**, § 6] using the weights). This leads to a complete description of all Markovian extensions of the minimal Laplacian $\mathbf{H}_0$ and all self-adjoint restrictions of the maximal Gaffney Laplacian $\mathbf{H}_G$ in terms of certain boundary conditions on finite volume graph ends (analogous to [**144**, § 6.3] and [**147**, Rem. 3.13(ii)]). The proofs of these claims can easily be carried over from [**144**], [**147**], however, the full exposition reads a bit technical and hence we do not develop it here.

If $\#\mathfrak{C}_0(\mathcal{G};\mu) = \infty$, that is, the deficiency indices of the minimal Gaffney Laplacian are infinite, then even in the unweighted case $\mu = \nu \equiv \mathbb{1}$ the above methods are not sufficient for a description of finite energy extensions. We stress that in this case the Gaffney Laplacian $\mathbf{H}_G$ is not closed in general (see [**147**, § 4]) and, moreover, in many interesting cases (see [**147**, § 4]), its closure equals the maximal Laplacian $\mathbf{H}$, $\overline{\mathbf{H}}_G = \mathbf{H}$ (which is further equivalent to the equality of the minimal Kirchhoff and Gaffney Laplacians), and hence the problem is essentially as difficult as the description of self-adjoint extensions of the minimal Laplacian $\mathbf{H}^0$.

We would also like to stress that, by Theorem 4.12 and Theorem 6.16, the problem of describing Markovian extensions is equivalent for weighted metric and discrete graphs. Moreover, for weighted graph Laplacians, a description of Markovian extensions was obtained in [**131**] in terms of Dirichlet forms (in the wide sense) on the corresponding Royden boundary (see, e.g., [**82**], [**132**], [**192**] for details and definitions) equipped with a harmonic measure (in fact, on the so-called harmonic boundary, which is a subset). It should also be stressed that there is no finiteness assumption on the deficiency indices of the Gaffney Laplacian in [**131**]. However, let us emphasize that this description is by means of quadratic forms and not via boundary conditions. Moreover, the correspondence between Markovian extensions and Dirichlet forms (in the wide sense) on the boundary is in general not one-to-one and hence also does not lead to a complete characterization of the Markovian uniqueness. On the other hand, if the weighted graph $(\mathcal{V}, m; b)$ has finite total mass, $m(\mathcal{V}) < \infty$, it becomes a bijection and in this case the Royden boundary should be the correct concept to study Markovian extensions.

In general, the Royden boundary of a graph $(\mathcal{V}, m; b)$ can be rather big and hard to describe (see [**213**] for the toy model $\mathcal{G}_d = \mathbb{Z}$). Its relationship to the standard one-point compactification is closely connected to the Liouville property for finite energy harmonic functions [**132**, Theorem 6.2]. However, in the special case that $\sum_{u,v} 1/b(u, v) < \infty$, the Royden boundary coincides with the space of graph ends and several other graph boundaries (see [**82**, § 4.6] for details). Hence, under the additional assumption that $m(\mathcal{V}) < \infty$, we recover precisely the space of finite volume ends (in the discrete setting). Moreover, one can show that under either of the assumptions (7.2.10) and (7.2.2), the space of finite volume ends $\mathfrak{C}_0(\mathcal{G}; \mu)$ of a weighted metric graph $(\mathcal{G}, \mu, \nu)$ can be embedded into the Royden boundary of the discrete graph $(\mathcal{V}, m; b)$ for any model (the weights are defined by (3.1.5) and (3.1.6)). However, in general it seems that these two boundaries do not compare.

7.2.3. A few more comments. Let us point out that, by Theorem 4.12 and Theorem 6.16, the problem of characterizing Markovian uniqueness is equivalent for Laplacians on weighted metric graphs and graph Laplacians. Moreover, for weighted metric graphs $(\mathcal{G}, \mu, \nu)$ this question was studied in [**95**, Chapter 2] using metric completions (w.r.t. to several different metrics). In the parallel settings of discrete graphs and manifolds, results were obtained in terms of polarity of metric boundaries in [**113**] and [**91**], [**160**], [**161**]. These techniques obviously apply to weighted metric graphs as well (alternatively, the results from [**113**] can also be transferred using the correspondence between H^1-spaces and intrinsic metrics, see Section 4.3 and Section 6.4). However, none of these approaches leads to a complete description of the uniqueness of Markovian extensions (e.g., the characterization in [**113**, Theorem 3] requires finite capacity of the metric boundary).

An important concept in context with graphs is the construction of boundaries by employing C^*-algebra techniques (this includes both Royden and Kuramochi boundaries, see [**82**], [**124**], [**132**], [**166**], [**192**] for further details and references). Under the assumptions (7.2.2) or (7.2.10), finite volume graph ends can also be constructed by using this method. Indeed, $\mathcal{A} := H^1(\mathcal{G}, \mu, \nu) \subset C_b(\mathcal{G})$ is a subalgebra by Proposition 7.26 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, describing $\widetilde{X}$ for some concrete C^*-algebra is a rather complicated task. However, it turns out that in our situation $\widetilde{X}$ coincides with $\widetilde{\mathcal{G}} := \mathcal{G} \cup \mathfrak{C}_0(\mathcal{G}; \mu)$. Indeed, $\widetilde{\mathcal{G}} = \mathcal{G} \cup \mathfrak{C}_0(\mathcal{G}; \mu)$ equipped with the induced topology of the end compactification $\widehat{\mathcal{G}}$ is a locally compact Hausdorff space. Proposition 7.26 together with Theorem 7.27 shows that each function $f \in H^1(\mathcal{G},\mu,\nu)$ has a unique continuous extension to $\widetilde{\mathcal{G}}$ and this extension belongs to $C_0(\widetilde{\mathcal{G}})$. Moreover, by Lemma 7.28, $H^1(\mathcal{G},\mu,\nu)$ 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.

7.3. Spectral estimates

The aim of this section is to obtain spectral estimates for Laplacians on a weighted metric graph $(\mathcal{G},\mu,\nu)$. For simplicity, we restrict to the Dirichlet Laplacian $\mathbf{H}_D$ and present estimates for the bottom of its spectrum,

$$\lambda_0(\mathbf{H}_D) := \inf \sigma(\mathbf{H}_D).$$

We also recall from Theorem 4.27 that if $(\mathcal{G},\mu,\nu)$ has infinite intrinsic size, that is, there is a model with $\eta^*(\mathcal{E}) = \infty$, then $\lambda_0(\mathbf{H}_D) = 0$ (in fact, this holds true for all Markovian and all nonnegative extensions of the minimal Kirchhoff Laplacian). Therefore, without loss of generality we can restrict our considerations in this section to the case when

$$(\mathcal{G},\mu,\nu) \textit{ has finite intrinsic size.}$$

Let us mention that for weighted metric graphs of finite intrinsic size we can define the so-called *minimal model* whose vertex set consists of all points having degree not equal to 2 as well as all points with degree 2 which are not inessential.

7.3.1. Isoperimetric estimates.

We begin with estimates for $\lambda_0(\mathbf{H}_D)$ in terms of *isoperimetric constants*. Our exposition follows closely [**145**], where the special case of unweighted metric graphs (i.e., $\mu = \nu \equiv \mathbb{1}$) was considered.

Assume that we have fixed a model of $(\mathcal{G},\mu,\nu)$ with underlying combinatorial graph $\mathcal{G}_d = (\mathcal{V},\mathcal{E})$. Then clearly every finite subgraph $\mathcal{K} = (\mathcal{V}(\mathcal{K}),\mathcal{E}(\mathcal{K}))$ of $\mathcal{G}_d$ can be identified with a compact subset of $\mathcal{G}$. Moreover, its volume with respect to μ and its topological boundary are given by

$$\mu(\mathcal{K}) = \sum_{e\in\mathcal{E}(\mathcal{K})} \mu(e), \qquad \partial\mathcal{K} = \{v \in \mathcal{V}(\mathcal{K}) |\ \deg_{\mathcal{K}}(v) < \deg_{\mathcal{G}}(v)\}. \tag{7.3.1}$$

We introduce the *boundary area* of $\mathcal{K}$ as

$$\operatorname{area}(\partial\mathcal{K}) = \operatorname{area}(\partial\mathcal{K},\mu,\nu) = \sum_{v\in\partial\mathcal{K}} \sum_{\vec{e}\in\vec{\mathcal{E}}_v(\mathcal{K})} \sqrt{\mu\nu}(e). \tag{7.3.2}$$

DEFINITION 7.31. The *isoperimetric constant* of a weighted metric graph $(\mathcal{G},\mu,\nu)$ is defined as

$$\operatorname{Ch}(\mathcal{G}) = \operatorname{Ch}(\mathcal{G},\mu,\nu) := \inf_{\mathcal{K}} \frac{\operatorname{area}(\partial\mathcal{K})}{\mu(\mathcal{K})}, \tag{7.3.3}$$

where the infimum is taken over all finite, connected subgraphs $\mathcal{K} = (\mathcal{V}(\mathcal{K}),\mathcal{E}(\mathcal{K}))$ of a fixed model of $(\mathcal{G},\mu,\nu)$.

The above definition of $\operatorname{Ch}(\mathcal{G})$ is given in terms of a fixed model of $(\mathcal{G},\mu,\nu)$, however, we have the following simple fact.

LEMMA 7.32. *The isoperimetric constant* $\operatorname{Ch}(\mathcal{G})$ *does not depend on the choice of the model.*

PROOF. First of all, it is not difficult to see that (7.3.3) remains unchanged under refinement of the model (see Section 2.4.3). Namely, any subgraph in a refined model can be completed to a subgraph in a coarser model by adding the "remaining parts" of edges. It is also clear that this procedure decreases the quotient in (7.3.3). Hence for two given models of $(\mathcal{G},\mu,\nu)$, we can take their common refinement (take all the vertices of both models as the vertex set) and hence the claim follows. $\square$

The next result provides Cheeger and Buser-type estimates on weighted metric graphs.

THEOREM 7.33. *For a weighted metric graph* $(\mathcal{G},\mu,\nu)$,

$$\frac{1}{4}\mathrm{Ch}(\mathcal{G})^2 \le \lambda_0(\mathbf{H}_D) \le \frac{\pi^2}{2\eta_*(\mathcal{G})}\mathrm{Ch}(\mathcal{G}), \tag{7.3.4}$$

where $\eta_*(\mathcal{G})$ *is defined by* (7.1.4) *with* $\mathcal{E}$ *being the edge set of the minimal model.*

PROOF. (i) *Cheeger's estimate.* First of all, recall that $\lambda_0(\mathbf{H}_D)$ is given by the variational characterization

$$\lambda_0(\mathbf{H}_D) = \inf_{0\neq f\in H^1_0(\mathcal{G})} \frac{\|\nabla f\|^2_{L^2(\mathcal{G};\nu)}}{\|f\|^2_{L^2(\mathcal{G};\mu)}}. \tag{7.3.5}$$

Hence the lower estimate in (7.3.4) will follow from the inequality

$$\mathrm{Ch}(\mathcal{G})\|f\|_{L^2(\mathcal{G};\mu)} \le 2\,\|\nabla f\|_{L^2(\mathcal{G};\nu)}, \qquad f\in H^1_0(\mathcal{G}). \tag{7.3.6}$$

Without loss of generality we can assume that f is real-valued, compactly supported and smooth on all edges $e\in\mathcal{E}$. Recall also that for any compactly supported, continuous and edgewise $\mathcal{C}^1$-function $h\colon \mathcal{G}\to[0,\infty)$, the following co-area formulae hold true (see, e.g., [**145**, Lemma 3.6]):

$$\int_{\mathcal{G}} h(x)\mu(\mathrm{d}x) = \int_0^\infty \mu(\Omega_h(t))\,\mathrm{d}t$$
$$\int_{\mathcal{G}} |\nabla h(x)|\,\omega(\mathrm{d}x) = \int_0^\infty \mathrm{area}(\partial\Omega_h(t))\,\mathrm{d}t$$

where $\Omega_h(t) := \{x\in\mathcal{G}\,|\,h(x)>t\}$ for all $t\ge 0$, $\omega := \sqrt{\mu\nu}$, $\omega(\mathrm{d}x) := \sqrt{\mu\nu(x)}\mathrm{d}x$, and

$$\mathrm{area}(\partial\Omega_h(t)) := \sum_{x\in\partial\Omega_h(t)} \omega(x).$$

Notice that for almost every $t>0$, the boundary $\partial\Omega_h(t)$ contains no vertices and hence the above integral is well-defined. Indeed, every $x\in\partial\Omega_h(t)$ satisfies $h(x)=t$ and hence the claim follows from the countability of the vertex set.

Moreover, if $\partial\Omega_h(t)\cap\mathcal{V}=\varnothing$, then we can associate with $\Omega_h(t)$ the subgraph $\mathcal{K}_t\subseteq\mathcal{G}_d$ consisting of all edges $e\in\mathcal{E}$ with $\Omega_h(t)\cap e\neq\varnothing$ and their endpoints. It is then easily verified that (see also [**145**, proof of Lemma 3.7])

$$\frac{\mathrm{area}(\partial\Omega_h(t))}{\mu(\Omega_h(t))} \ge \frac{\mathrm{area}(\mathcal{K}_t)}{\mu(\mathcal{K}_t)} \ge \mathrm{Ch}(\mathcal{G}). \tag{7.3.7}$$

By choosing $h=f^2$, we conclude from the co-area formulae that

$$\mathrm{Ch}(\mathcal{G})\|f\|^2_{L^2(\mathcal{G};\mu)} \le 2\int_{\mathcal{G}} |\nabla f(x) f(x)|\,\omega(\mathrm{d}x) \le 2\|f\|_{L^2(\mathcal{G};\mu)}\|\nabla f\|_{L^2(\mathcal{G};\nu)},$$

where the last inequality follows from the Cauchy–Schwarz inequality.

(ii) *Buser's estimate.* Consider the minimal model of $(\mathcal{G},\mu,\nu)$. The edge set of a finite connected subgraph $\mathcal{K}=(\mathcal{V}(\mathcal{K}),\mathcal{E}(\mathcal{K}))$ can be split into

$$\mathcal{E}(\mathcal{K})=\mathcal{E}_0\cup\mathcal{E}_1\cup\mathcal{E}_2,$$

where $\mathcal{E}_0$, $\mathcal{E}_1$ and $\mathcal{E}_2$ denote the mutually disjoint sets of edges of $\mathcal{E}(\mathcal{K})$ with, respectively, all endpoints in $\mathcal{V}(\mathcal{K})\setminus\partial\mathcal{K}$, exactly one endpoint in $\partial\mathcal{K}$ (and hence exactly one endpoint in $\mathcal{V}(\mathcal{K})\setminus\partial\mathcal{K}$), and all endpoints in $\partial\mathcal{K}$.† Notice in particular that

$$\operatorname{area}(\partial\mathcal{K})=\sum_{e\in\mathcal{E}_1}\sqrt{\mu\nu}(e)+2\sum_{e\in\mathcal{E}_2}\sqrt{\mu\nu}(e).$$

Consider the test function $f\colon\mathcal{G}\to\mathbb{R}$ defined by

$$f|_e=\begin{cases}1, & e\in\mathcal{E}_0,\\ \sin\left(\frac{\pi}{|e|}|\cdot-e_\imath|\right), & e\in\mathcal{E}_2,\\ \sin\left(\frac{\pi}{2|e|}|\cdot-u|\right), & e=e_{u,v}\in\mathcal{E}_1 \text{ with } u\in\partial\mathcal{K},\\ 0, & e\notin\mathcal{E}(\mathcal{K}).\end{cases}$$

By construction, f belongs to $H^1_c(\mathcal{G})$ and its support coincides with $\mathcal{K}$. Moreover,

$$\begin{aligned}\|f\|^2_{L^2(\mathcal{G};\mu)}&=\sum_{e\in\mathcal{E}_0}\mu(e)|e|+\sum_{e\in\mathcal{E}_1\cup\mathcal{E}_2}\frac{\mu(e)|e|}{2}\ge\frac{\mu(\mathcal{K})}{2},\\ \|\nabla f\|^2_{L^2(\mathcal{G};\nu)}&=\frac{\pi^2}{8}\sum_{e\in\mathcal{E}_1}\frac{\nu(e)}{|e|}+\frac{\pi^2}{2}\sum_{e\in\mathcal{E}_2}\frac{\nu(e)}{|e|}\\ &=\frac{\pi^2}{8}\sum_{e\in\mathcal{E}_1}\frac{\sqrt{\mu\nu}(e)}{\eta(e)}+\frac{\pi^2}{2}\sum_{e\in\mathcal{E}_2}\frac{\sqrt{\mu\nu}(e)}{\eta(e)}\le\frac{\pi^2}{4\eta_*(\mathcal{G})}\operatorname{area}(\partial\mathcal{K}),\end{aligned}$$

and then using (7.3.5), we arrive at the second inequality in (7.3.4). □

In a similar way, one can obtain isoperimetric estimates for $\lambda_0^{\mathrm{ess}}(\mathbf{H}_D)$, the bottom of the essential spectrum of $\mathbf{H}_D$. More precisely, for any finite, connected subgraph $\mathcal{K}=(\mathcal{V}(\mathcal{K}),\mathcal{E}(\mathcal{K}))$ of our fixed model, define

$$H^1_0(\mathcal{G}\setminus\mathcal{K}):=\{f\in H^1_0(\mathcal{G})|\ \operatorname{supp}(f)\subseteq\mathcal{G}\setminus\mathcal{K}\}.$$

Then a standard Persson-type argument (or Glazman's decomposition principle in the Russian literature, see [**83**]) implies that

$$\lambda_0^{\mathrm{ess}}(\mathbf{H}_D)=\sup_{\mathcal{K}}\inf_{f\in H^1_0(\mathcal{G}\setminus\mathcal{K})}\frac{\|\nabla f\|^2_{L^2(\mathcal{G};\nu)}}{\|f\|^2_{L^2(\mathcal{G};\mu)}},\tag{7.3.8}$$

where the supremum is taken over all finite, connected subgraphs $\mathcal{K}$ of $\mathcal{G}$. Setting $\mathcal{K}_1\le\mathcal{K}_2$ exactly when $\mathcal{K}_1$ is a subgraph of $\mathcal{K}_2$, we can see the set of all finite, connected subgraphs of $\mathcal{G}$ as a directed set. Moreover, if $\mathcal{K}_1\le\mathcal{K}_2$, then

$$H^1_0(\mathcal{G}\setminus\mathcal{K}_2)\subseteq H^1_0(\mathcal{G}\setminus\mathcal{K}_1),$$

and hence (7.3.8) can be rewritten as

$$\lambda_0^{\mathrm{ess}}(\mathbf{H}_D)=\lim_{\mathcal{K}}\inf_{f\in H^1_0(\mathcal{G}\setminus\mathcal{K})}\frac{\|\nabla f\|^2_{L^2(\mathcal{G};\nu)}}{\|f\|^2_{L^2(\mathcal{G};\mu)}},\tag{7.3.9}$$

†Loop edges in $\mathcal{E}(\mathcal{K})$ are considered either as elements of $\mathcal{E}_2$ or $\mathcal{E}_0$, depending on their vertex belonging to $\partial\mathcal{K}$ or not.

where the limit is taken over all finite, connected subgraphs $\mathcal{K}$ of $\mathcal{G}$ in the sense of nets. Thus, Theorem 7.33 together with (7.3.9) suggest that, roughly speaking, $\lambda_0^{\mathrm{ess}}(\mathcal{G})$ is related to the isoperimetric behavior of $(\mathcal{G},\mu,\nu)$ "at infinity". This leads to the following definition:

DEFINITION 7.34. Let $(\mathcal{G},\mu,\nu)$ be a weighted metric graph together with a fixed model. For any finite, connected subgraph $\mathcal{K}=(\mathcal{V}(\mathcal{K}),\mathcal{E}(\mathcal{K}))$ of $\mathcal{G}$, define

$$\mathrm{Ch}_{\mathcal{K}}(\mathcal{G}) = \inf_{\mathcal{K}'\subseteq\mathcal{G}\setminus\mathcal{K}} \frac{\mathrm{area}(\partial\mathcal{K}')}{\mu(\mathcal{K}')}$$

where the infimum is over all finite, connected subgraphs $\mathcal{K}'$ of $\mathcal{G}$ with $\mathcal{K}'\subseteq\mathcal{G}\setminus\mathcal{K}$. The *isoperimetric constant at infinity* of $(\mathcal{G},\mu,\nu)$ is given by

$$\mathrm{Ch}^{\mathrm{ess}}(\mathcal{G}) := \sup_{\mathcal{K}} \mathrm{Ch}_{\mathcal{K}}(\mathcal{G}) = \lim_{\mathcal{K}} \mathrm{Ch}_{\mathcal{K}}(\mathcal{G}) \tag{7.3.10}$$

where both the supremum and the net limit are taken over all finite, connected subgraphs $\mathcal{K}$ of $\mathcal{G}$.

It turns out that (e.g., by an argument as in Lemma 7.32) the definition of $\mathrm{Ch}^{\mathrm{ess}}(\mathcal{G})$ does not depend on the choice of the model of $(\mathcal{G},\mu,\nu)$. Moreover, we obtain the following estimates:

THEOREM 7.35. *Let $\mathcal{E}$ be the edge set of the minimal model of $(\mathcal{G},\mu,\nu)$ and set $\eta_*^{\mathrm{ess}}(\mathcal{G}) := \sup_{\widetilde{\mathcal{E}}\text{ finite}} \inf_{e\in\mathcal{E}\setminus\widetilde{\mathcal{E}}} \eta(e)$. Then*

$$\frac{1}{4}\mathrm{Ch}^{\mathrm{ess}}(\mathcal{G})^2 \le \lambda_0^{\mathrm{ess}}(\mathbf{H}_D) \le \frac{\pi^2}{2\eta_*^{\mathrm{ess}}(\mathcal{G})}\mathrm{Ch}^{\mathrm{ess}}(\mathcal{G}). \tag{7.3.11}$$

In particular, $\sigma(\mathbf{H}_D)$ is purely discrete if $\mathrm{Ch}^{\mathrm{ess}}(\mathcal{G})=\infty$.

PROOF. Following the proof of Theorem 7.33, we get

$$\frac{1}{4}\mathrm{Ch}_{\mathcal{K}}(\mathcal{G})^2 \le \inf_{f\in H_0^1(\mathcal{G}\setminus\mathcal{K})} \frac{\|\nabla f\|^2_{L^2(\mathcal{G};\nu)}}{\|f\|^2_{L^2(\mathcal{G};\mu)}} \le \frac{\pi^2}{2}\frac{\mathrm{Ch}_{\mathcal{K}}(\mathcal{G})}{\eta_*^{\mathcal{K}}(\mathcal{E})}$$

for any finite, connected subgraph $\mathcal{K}$ of $\mathcal{G}$ (with $\eta_*^{\mathcal{K}}(\mathcal{E}) := \inf_{e\in\mathcal{E}\setminus\mathcal{E}(\mathcal{K})}\eta(e)$). For instance, if f belongs to $H_0^1(\mathcal{G}\setminus\mathcal{K})$, then the set $\Omega_{f^2}(t)$ is contained in $\mathcal{G}\setminus\mathcal{K}$ for all $t>0$. In particular, this means that the subgraph $\mathcal{K}_t$ in (7.3.7) is contained in $\mathcal{G}\setminus\mathcal{K}$. The claim then follows from (7.3.8) together with (7.3.10). □

REMARK 7.36. Going back to Cheeger's inequality for manifolds [**41**], isoperimetric constants are known to provide spectral estimates for both manifolds and graphs, see e.g. [**5**], [**6**], [**18**], [**37**], [**41**], [**58**], [**60**], [**145**], [**170**]. For unweighted discrete graphs, the first works on this topic include [**5**], [**6**], [**58**], [**60**]. Employing the notion of an intrinsic metric, an isoperimetric constant and the corresponding estimate for weighted graphs $(\mathcal{V},m;b)$ were introduced in [**18**] (see Section 7.3.2 for more details). For unweighted metric graphs, $\mu=\nu\equiv\mathbb{1}$, Cheeger's inequality was proven in [**170**] for finite metric graphs and in [**145**] for infinite metric graphs.

7.3.2. Connection with discrete isoperimetric constants. The combinatorial structure of $\mathrm{Ch}(\mathcal{G})$ enables us to investigate it by combinatorial methods. More precisely, in the case of unweighted metric graphs (i.e., $\mu\equiv\nu\equiv\mathbb{1}$), $\mathrm{Ch}(\mathcal{G})$ was studied using discrete, curvature-like quantities in [**145**, § 6] and [**171**]. These methods can be extended to the setting of weighted metric graphs as well and this will be done elsewhere (see also Section 8.3.2 for the special case of tilings).

Our main goal in this section is to discuss connections with discrete isoperimetric constants of the corresponding weighted graphs.

Let $(\mathcal{V}, m; b)$ be a locally finite connected graph and let $p\colon \mathcal{V} \times \mathcal{V} \to [0, \infty)$ be an intrinsic weight function (see Section 6.4.2). Following [**18**] (see also [**145**, Appendix]), we define an isoperimetric constant $\mathrm{Ch}_d(\mathcal{V})$ for $(\mathcal{V}, m; b)$ by

$$\mathrm{Ch}_d(\mathcal{V}) = \mathrm{Ch}_d(\mathcal{V}, m; b) := \inf_X \frac{|\partial X|}{m(X)}, \tag{7.3.12}$$

where the infimum is over all finite, connected subsets $X \subseteq \mathcal{V}$ and

$$\partial X = \{(u, v) \in X \times (\mathcal{V} \setminus X) \,|\, b(u, v) > 0\}, \tag{7.3.13}$$

$$|\partial X| = \sum_{(u,v)\in\partial X} b(u, v)p(u, v), \qquad m(X) = \sum_{v\in X} m(v). \tag{7.3.14}$$

We recall that, by [**18**, Theorem 3.2 and Theorem 3.6] (see also [**145**, Appendix]), the Dirichlet Laplacian $\mathbf{h}_D$ on $(\mathcal{V}, m; b)$ satisfies the following spectral estimate

$$\frac{1}{2}\mathrm{Ch}_d(\mathcal{V})^2 \le \lambda_0(\mathbf{h}_D) \le \frac{\mathrm{Ch}_d(\mathcal{V})}{p_*(\mathcal{V})}, \tag{7.3.15}$$

where $p_*(\mathcal{V}) := \inf_{b(u,v)>0} p(u, v)$.

Remark 7.37. Notice that the isoperimetric constant $\mathrm{Ch}_d(\mathcal{V})$ is defined slightly differently in [**18**]. Namely, the weight $p(u, v)$ in the definition of $|\partial X|$ is replaced by the distance $\varrho(u, v)$ in an intrinsic metric ϱ. On the other hand, it is straightforward to verify that [**18**, Theorem 3.2 and Theorem 3.6] remain valid also for our definition (see [**145**, Appendix] for details).

Recall that we had assumed that the weighted metric graph $(\mathcal{G}, \mu, \nu)$ has finite intrinsic size. Fix a model of $(\mathcal{G}, \mu, \nu)$ (which then also has finite intrinsic size). Consider the locally finite graph $(\mathcal{V}, m; b)$ defined by (3.1.3)–(3.1.6) and the corresponding discrete Laplacian $\mathbf{h}$ (3.1.7). Recall also that we obtain an intrinsic weight $p_\eta\colon \mathcal{V} \times \mathcal{V} \to [0, \infty)$ (see Remark 6.26) given by

$$p_\eta(u, v) = \begin{cases} \min_{e\in\mathcal{E}_{u,v}} \eta(e), & u \sim v \text{ and } u \ne v, \\ 0, & \text{else}, \end{cases} \qquad (u, v) \in \mathcal{V} \times \mathcal{V}. \tag{7.3.16}$$

In Theorem 4.27 (see also Theorem 3.1(vii)) we have seen that there is a close connection between $\lambda_0(\mathbf{h}_D)$ and $\lambda_0(\mathbf{H}_D)$. In fact, it is easy to notice also connections between the corresponding isoperimetric constants. Namely, suppose that our fixed model of the weighted metric graph $(\mathcal{G}, \mu, \nu)$ has no multiple edges. Then

$$b(u, v)p_\eta(u, v) = \sqrt{\mu\nu}(e_{uv}) \tag{7.3.17}$$

for all vertices $u \sim v$, $u \ne v$. On the other hand, we can associate to every finite subset $X \subset \mathcal{V}$ the subgraph $\mathcal{K}_X$ of $\mathcal{G}_d$ consisting of all edges in the stars $\mathcal{E}_v$, $v \in X$ (and all incident vertices). Clearly, we have

$$\mu(\mathcal{K}_X) \le m(X) \le 2\mu(\mathcal{K}_X). \tag{7.3.18}$$

Taking into account the definitions (7.3.3) and (7.3.12), this indicates a connection between $\mathrm{Ch}(\mathcal{G})$ and $\mathrm{Ch}_d(\mathcal{V})$. The following explicit estimates hold:

PROPOSITION 7.38. *Let* $(\mathcal{G}, \mu, \nu)$ *be a weighted metric graph having finite intrinsic size and fix a model with underlying combinatorial graph* $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ *having no multiple edges. Then*

$$\mathrm{Ch}(\mathcal{G}) \le 2\mathrm{Ch}_d(\mathcal{V}), \qquad \frac{2}{\mathrm{Ch}(\mathcal{G})} \le \frac{1}{\mathrm{Ch}_d(\mathcal{V})} + \eta^*(\mathcal{E}), \tag{7.3.19}$$

where $\mathrm{Ch}_d(\mathcal{V})$ *is the isoperimetric constant* (7.3.12) *of* $(\mathcal{V}, m; b)$ *for the intrinsic weight given by* (7.3.16). *In particular,*

$$\mathrm{Ch}(\mathcal{G}) > 0 \qquad \textit{exactly when} \qquad \mathrm{Ch}_d(\mathcal{V}) > 0. \tag{7.3.20}$$

PROOF. Let $X \subset \mathcal{V}$ be a finite, connected vertex set. Consider the connected subgraph $\mathcal{K}_X$ of $\mathcal{G}_d$ having the edge set $\mathcal{E}(\mathcal{K}_X) := \bigcup_{v\in X} \mathcal{E}_v$. Using (7.3.17), it is not hard to see that (see also [**145**, Lemma 4.2])

$$\mathrm{area}(\partial\mathcal{K}_X) \le |\partial X|$$

Taking into account (7.3.18), we arrive at the first inequality in (7.3.19). The rest of the proof can be carried over line to line from [**145**, Lemma 4.2] and we omit the details. □

REMARK 7.39. A few remarks are in order.

(i) The second estimate in Proposition 7.38 is sharp. For example, the equality holds true on every *simple unweighted, equilateral metric graph*, that is, when $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ is simple and $\mu = \nu \equiv \mathbb{1}$ with $|e| = 1$ for all edges $e \in \mathcal{E}$ (see [**171**, equation (4.5)]).

(ii) Surprisingly, Proposition 7.38 and even the equivalence (7.3.20) can fail for models with multiple edges. The reason is precisely that (7.3.17) is no longer valid in the presence of multiple edges (see also (7.3.16)). However, the equivalence (7.3.20) holds true for models having finite intrinsic size and satisfying the additional condition

$$\inf_{e\in\mathcal{E}} \frac{p_\eta(e_\imath, e_\tau)}{\eta(e)} > 0,$$

which clearly allows to recover an adapted version of (7.3.17).

7.3.3. Volume growth estimates. Going back to the work of R. Brooks [**32**], another well-known tool for Laplacians on manifolds and graphs are spectral estimates in terms of volume growth (see, e.g., [**32**], [**71**], [**99**], [**195**] and the references therein). Moreover, these results can be formulated in the abstract framework of Dirichlet forms (see [**195**] for the strongly local case and [**99**] for generalizations). In this form, they directly apply to weighted metric graphs and we shortly discuss this in the following.

Let ϱ_η be the intrinsic metric on a weighted metric graph $(\mathcal{G}, \mu, \nu)$ (see Section 6.4.1). For any $x \in \mathcal{G}$ and $r > 0$, we denote an intrinsic distance ball of radius r by

$$B_r(x) = B_r(x; \varrho_\eta) := \{y \in \mathcal{G} \mid \varrho_\eta(x, y) < r\}. \tag{7.3.21}$$

The *exponential volume growth* $\mathbf{v}(\mathcal{G})$ of $\mathcal{G}$ is defined by

$$\mathbf{v}(\mathcal{G}) := \liminf_{r\to\infty} \frac{1}{r} \log \mu(B_r(x_0)), \tag{7.3.22}$$

where x_0 is any point of $\mathcal{G}$ (since $\mathcal{G}$ is connected, the limit in (7.3.22) does not depend on x_0). Moreover, we also introduce

$$\mathbf{v}_*(\mathcal{G}) := \liminf_{r\to\infty} \frac{1}{r} \inf_{x\in\mathcal{G}} \log \frac{\mu(B_r(x))}{\mu(B_1(x))},$$

where by notational convention $\frac{\infty}{a} := \infty$ for any $a \in (0,\infty]$. Notice in particular that $\mathbf{v}_*(\mathcal{G}) \le \mathbf{v}(\mathcal{G})$.

Applying the results of [**195**, Theorem 5] (see also [**99**, Theorem 1.1]), we arrive at the following estimate:

THEOREM 7.40. *Suppose that $(\mathcal{G}, \varrho_\eta)$ is complete. Then*

$$\lambda_0(\mathbf{H}_D) \le \lambda_0^{\mathrm{ess}}(\mathbf{H}_D) \le \frac{1}{4}\mathbf{v}_*(\mathcal{G})^2 \le \frac{1}{4}\mathbf{v}(\mathcal{G})^2. \tag{7.3.23}$$

REMARK 7.41. The assumptions in Theorem 7.40 are not optimal. For instance, by Theorem 7.1, the completeness assumption implies that the maximal Kirchhoff Laplacian $\mathbf{H}$ is self-adjoint and hence $\mathbf{H}^0 = \mathbf{H}_D = \mathbf{H}_N = \mathbf{H}$. On the other hand, the proof in [**195**, Theorem 5] shows that the Neumann extension $\mathbf{H}_N$ on any weighted metric graph $(\mathcal{G}, \mu, \nu)$ satisfies

$$\lambda_0(\mathbf{H}_N) \le \frac{1}{4}\mathbf{v}_*(\mathcal{G})^2 \le \frac{1}{4}\mathbf{v}(\mathcal{G})^2.$$

In particular, we obtain (7.3.23) whenever $\mathbf{H}_D = \mathbf{H}_N$, that is, when $\mathbf{H}^0$ admits a unique Markovian extension. The latter is a much weaker condition than the completeness of $(\mathcal{G}, \varrho_\eta)$ (see Section 7.2 and also Theorem 7.24).

7.4. Recurrence and transience

There are numerous characterizations of recurrence/transience and we refer to [**77**] for further details. Intuitively one may explain recurrence of a Brownian motion/random walk as insufficiency of volume in the state space. The qualitative form of this heuristic statement in the manifold context has a venerable history (we refer to the excellent exposition of A. Grigor'yan [**88**] for further details) and in the case of complete Riemannian manifolds the corresponding result (see [**88**, Theorem 7.3]) was proved in the 1980s independently by L. Karp, N.Th. Varopoulos, and A. Grigor'yan. It was extended to strongly local Dirichlet forms by K.-T. Sturm and in our setting of weighted metric graphs, [**195**, Theorem 3] reads as follows:

THEOREM 7.42 ([**195**]). *Assume that a weighted metric graph $(\mathcal{G}, \mu, \nu)$ is such that $(\mathcal{G}, \varrho_\eta)$ is complete. Then the heat semigroup $(\mathrm{e}^{-t\mathbf{H}})_{t>0}$ generated by the Kirchhoff Laplacian $\mathbf{H}$*[‡] *is recurrent if for some (and hence for all) $x \in \mathcal{G}$*

$$\int_1^\infty \frac{r}{\mu(B_r(x))}\mathrm{d}r = \infty, \tag{7.4.1}$$

where $B_r(x)$ is the intrinsic metric ball (7.3.21). That is, the following equivalent properties hold true:

(i) *Every nonnegative superharmonic function is constant,*
(ii) *Every bounded superharmonic function is constant,*
(iii) *Every bounded subharmonic function is constant,*

[‡]Recall that by Theorem 7.1 completeness implies that the maximal Kirchhoff Laplacian $\mathbf{H}$ is self-adjoint and hence coincides with both the Dirichlet $\mathbf{H}_D$ and Neumann $\mathbf{H}_N$ Laplacian.

(iv) *Every potential*

$$Gf(x) = \lim_{N\to\infty} \int_0^N (\mathrm{e}^{-s\mathbf{H}} f)(x)\,\mathrm{d}s, \quad x \in \mathcal{G},$$

is identically ∞ *for all nonzero* $0 \le f \in L^1(\mathcal{G};\mu)$.

Remark 7.43. In fact, the above result is an immediate consequence of a Karp-type theorem proved for strongly local regular Dirichlet forms in the same paper. More specifically, by [**195**, Theorem 1], if $(\mathcal{G}, \varrho_\eta)$ is complete, then every nonzero subharmonic function $u \ge 0$ satisfying

$$\int_1^\infty \frac{r}{\|u\mathbb{1}_{B_r(x)}\|^p_{L^p(\mathcal{G};\mu)}} \mathrm{d}r = \infty, \tag{7.4.2}$$

for some $p \in (1,\infty)$ and $x \in \mathcal{G}$, is constant. Thus, if $u \ge 0$ is a bounded subharmonic function, then $\|u\mathbb{1}_{B_r(x)}\|^p_{L^p(\mathcal{G};\mu)} \le C\mu(B_r(x))$ and hence (7.4.2) follows from (7.4.1), which further implies that u is constant.

Remark 7.44. It appears that in the setting of weighted metric graphs the completeness assumption in both Theorem 7.42 and Karp's theorem is superfluous. Namely, it seems to us that at least in the setting of Theorem 7.24, one can replace this assumption by the Markovian uniqueness (which, according to Theorem 7.24, is equivalent to the absence of finite volume ends).

We would like to demonstrate two applications of the above theorem. First of all, employing connections between intrinsic metrics on weighted graphs and cable systems, we arrive at the analogs of Karp's theorem and Theorem 7.42 for graphs.

Theorem 7.45 ([**111**]). *Let* b *be a locally finite, connected graph over* $(\mathcal{V}, m)$. *Let also* ϱ *be an intrinsic metric of finite jump size such that* $(\mathcal{V},\varrho)$ *is complete and* ϱ *generates the discrete topology on* $\mathcal{V}$. *Then every nonzero subharmonic function* $u \ge 0$ *satisfying*

$$\int_1^\infty \frac{r}{\|u\mathbb{1}_{B_r(v;\varrho)}\|^p_{\ell^p(\mathcal{V};m)}} \mathrm{d}r = \infty, \tag{7.4.3}$$

for some $p \in (1,\infty)$ *and* $v \in \mathcal{V}$, *is constant. In particular, if for some* $v \in \mathcal{V}$

$$\int_1^\infty \frac{r}{m(B_r(v;\varrho))} \mathrm{d}r = \infty, \tag{7.4.4}$$

then the heat semigroup $(\mathrm{e}^{-t\mathbf{h}})_{t>0}$ *generated by the graph Laplacian* $\mathbf{h}$ *is recurrent.*

Proof. The proof is analogous to the one of Theorem 6.55. Indeed, assume first that ϱ is an intrinsic path metric for $(\mathcal{V}, m; b)$ having finite jump size. Then by Lemma 6.31 there is a cable system $(\mathcal{G}, \mu, \nu)$ such that ϱ coincides with the restriction $\varrho_\mathcal{V}$ of ϱ_η onto $\mathcal{V}\times\mathcal{V}$ and $(\mathcal{G}, \varrho_\eta)$ is complete.

Take now a nonnegative function $\mathbf{f}\colon \mathcal{V} \to \mathbb{R}_{\ge 0}$ which is L-subharmonic. By Lemma 6.50, the corresponding function $f = \imath_\mathcal{V}^{-1}(\mathbf{f})$ is nonnegative and subharmonic w.r.t. $(\mathcal{G}, \mu, \nu)$. Taking into account the relationships between the p-norms (see Lemma 4.2) and using the corresponding results for weighted metric graphs, one easily completes the proof of the first claim. The second one follows in a similar way from Theorem 4.17, Lemma 6.39 and Theorem 7.42.

If ϱ is not a path metric, then we proceed as in part (iii) of the proof of Corollary 7.3. Namely, if ϱ has finite jump size, then the construction there gives an intrinsic path metric $\tilde{\varrho}$ of finite jump size such that $(\mathcal{V}, \tilde{\varrho})$ is complete and $\varrho \le \tilde{\varrho}$. It remains to notice that $B_s(x;\tilde{\varrho}) \subseteq B_s(x;\varrho)$ and then apply the above arguments. □

REMARK 7.46. Let us mention that Theorem 7.45 was first established in [**111**] (see Theorem 1.1 and Corollary 1.6 there) by using an absolutely different approach, which, in particular, allows to treat non-locally finite graphs.

To proceed with another application, notice that the characterization of recurrence either in terms of extended Dirichlet spaces (see Lemma B.7) or by means of subharmonic functions indicates that it essentially depends on the energy form only and not on the underlying Hilbert space. In our situation, the energy form depends only on the underlying metric graph $\mathcal{G}$ and the edge weight ν, however, ν enters Theorem 7.42 implicitly as a requirement that $(\mathcal{G}, \varrho_\eta)$ is complete. So, first of all, we arrive at the following result.

LEMMA 7.47. *Let $(\mathcal{G}, \mu, \nu)$ be a weighted metric graph. Then the heat semigroup $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ generated by the Dirichlet Laplacian $\mathbf{H}_D$ is recurrent if $\mathcal{G}$ is complete w.r.t. the length metric ϱ_0 and for some (and hence for all) $x \in \mathcal{G}$*

$$\int_1^\infty \frac{r}{\nu(B_r(x;\varrho_0))}\mathrm{d}r = \infty, \tag{7.4.5}$$

where $B_r(x;\varrho_0)$ is the metric ball in $(\mathcal{G}, \varrho_0)$.

PROOF. Since the Dirichlet form of $\mathbf{H}_D$ is regular, recurrence of the corresponding semigroup implies the uniqueness of a Markovian extension for $\mathbf{H}^0$. Moreover, taking into account the regularity of $\mathfrak{Q}_D$ once again, we conclude that $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ is recurrent exactly when there is a sequence $(f_n) \subset H^1_c(\mathcal{G})$ which approximates $\mathbb{1}$ and such that $\mathfrak{Q}[f_n] = o(1)$. Next recall that $H^1_c(\mathcal{G})$ is independent of μ. Therefore, if $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ is recurrent for some choice of μ, it is automatically recurrent for any other choice of μ. Now it remains to consider the weighted metric graph $(\mathcal{G}, \nu, \nu)$, that is, to replace μ by ν, and apply [**195**, Theorem 3] (see Theorem 7.42) by taking into account that the length metric ϱ_0 coincides with the intrinsic metric ϱ_η for $(\mathcal{G}, \nu, \nu)$. □

REMARK 7.48. The above proof indicates that one may come up with a more clever choice of the weight μ (for instance, choosing $\mu(e) = \nu(e)/|e|^2$ for each $e \in \mathcal{E}$, one arrives at Laplacians, which are closely connected with discrete time random walks, see below). However, this of course depends on the concrete situation since, at the same time, one wants to ensure the completeness of $\mathcal{G}$ w.r.t. the corresponding intrinsic metric ϱ_η, which clearly depends on this choice.

The usefulness of the arguments in the proof of Lemma 7.47 can be demonstrated by the following result. Before stating it, let us associate with the metric graph $\mathcal{G}$ and the edge weight ν the following discrete time random walk: choose a simple model $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ of $(\mathcal{G}, \mu, \nu)$ and set

$$b_\nu(u,v) = \begin{cases} \frac{\nu(e_{u,v})}{|e_{u,v}|}, & u \sim v, \\ 0, & u \not\sim v, \end{cases} \qquad (u,v) \in \mathcal{V}, \tag{7.4.6}$$

together with

$$m_\nu(v) = \sum_{u \sim v} b_\nu(u,v), \qquad v \in \mathcal{V}. \tag{7.4.7}$$

Consider the corresponding graph Laplacian (let us denote it by $\mathbf{h}_\nu$). By Lemma 2.9, it is bounded. Moreover, it generates a discrete time random walk on $\mathcal{V}$ (see Remark 2.11). Namely, this random walk on $\mathcal{V}$ is a Markov chain $(X_n)_{n\ge 0}$ with state space $\mathcal{V}$ and transition probabilities $\mathrm{P}_\nu = \big(p_\nu(u,v)\big)_{u,v\in\mathcal{V}}$ defined by

$$p_\nu(u,v) = P(X_{n+1} = v \,|\, X_n = u) = \frac{b_\nu(u,v)}{m_\nu(v)}. \tag{7.4.8}$$

Since the graph b over $\mathcal{V}$ is connected by construction, the corresponding Markov chain is *irreducible*. Moreover, it is reversible (again by construction).

THEOREM 7.49. *Let $(\mathcal{G},\mu,\nu)$ be a weighted metric graph. Then the heat semigroup $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ generated by the Dirichlet Laplacian $\mathbf{H}_D$ is recurrent if and only if for some (and hence for all) simple model of $(\mathcal{G},\mu,\nu)$ the discrete time random walk on $\mathcal{V}$ with transition probabilities $\mathcal{P}_\nu = \big(p_\nu(u,v)\big)_{u,v\in\mathcal{V}}$ is recurrent.*

PROOF. First, by Theorem 4.17, $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ is recurrent if and only if the semigroup $(\mathrm{e}^{-t\mathbf{h}_D})_{t>0}$ is recurrent. Here $\mathbf{h}_D$ is the Dirichlet Laplacian defined by (3.1.7) (with $\alpha\equiv 0$). Notice that the edge weight b given by (3.1.6) coincides with b_ν defined by (7.4.6). Using exactly the same argument as in the proof of Lemma 7.47, however, applied in the discrete graph setting, we conclude that the recurrence of $\mathbf{h}_D$ is independent of the choice of m and hence, in particular, $(\mathrm{e}^{-t\mathbf{h}_D})_{t>0}$ is recurrent if and only if $(\mathrm{e}^{-t\mathbf{h}_\nu})_{t>0}$ is recurrent. However, the latter holds exactly when the corresponding discrete time random walk is recurrent. □

REMARK 7.50. Theorem 7.49 connects the study of recurrence on metric graphs with the study of recurrence for discrete time random walks, which is a classical topic (the standard reference is the book by W. Woess [**209**]). We shall demonstrate these connections by concrete examples (Cayley graphs and tessellations) in the next chapter. Let us only mention that the idea to relate Brownian motion on a Riemannian manifold with random walks goes back at least to the work of S. Kakutani [**120**] on the type problem for simply connected Riemann surfaces (see [**88**] for further details).

7.5. Stochastic completeness

Here we follow the same line of reasoning as in the previous section. Recall the following result of K.-T. Sturm [**195**, Theorem 4].

THEOREM 7.51 ([**195**]). *Assume that a weighted metric graph $(\mathcal{G},\mu,\nu)$ is such that $(\mathcal{G},\varrho_\eta)$ is complete as a metric space. Then the heat semigroup $(\mathrm{e}^{-t\mathbf{H}})_{t>0}$ generated by the Kirchhoff Laplacian $\mathbf{H}$*[‡] *is stochastically complete if for some (and hence for all) $x\in\mathcal{G}$*

$$\int_1^\infty \frac{r}{\log\mu(B_r(x))}\mathrm{d}r = \infty, \tag{7.5.1}$$

where $B_r(x)$ is the metric ball (7.3.21).

REMARK 7.52. A few remarks are in order.

[‡]Recall that by Theorem 7.1 completeness implies that the maximal Kirchhoff Laplacian $\mathbf{H}$ is self-adjoint and hence coincides with both the Dirichlet $\mathbf{H}_D$ and Neumann $\mathbf{H}_N$ Laplacian.

(i) Recall that stochastic completeness means that $e^{-t\mathbf{H}}\mathbb{1} = \mathbb{1}$ for some (and hence for all) $t > 0$. There are various equivalent characterizations and in terms of λ-harmonic/subharmonic functions stochastic completeness means that:
  - for some $\lambda > 0$ every bounded nonnegative λ-harmonic function is constant,
  - for all $\lambda > 0$ every bounded nonnegative λ-subharmonic function is constant.

(ii) In the context of manifolds, the volume test is due to L. Karp and P. Li, and A. Grigor'yan (for a detailed historical account we refer to [**88**]).

(iii) Similar to the recurrence statement (see Remark 7.44), we are convinced that in the setting of weighted metric graphs the completeness assumption in Theorem 7.51 is superfluous. At least in the setting of Theorem 7.24, one can replace this assumption by the Markovian uniqueness and this will be addressed elsewhere.

Taking into account the relationships between the parabolic properties of Laplacians on metric graphs and weighted graphs (see Section 4.6), we arrive at the following result.

THEOREM 7.53 ([**70**], [**112**]). *Let b be a locally finite, connected graph over $(\mathcal{V}, m)$. Let ϱ be an intrinsic metric of finite jump size such that $(\mathcal{V}, \varrho)$ is complete and ϱ generates the discrete topology on $\mathcal{V}$. If for some (and hence all) $v \in \mathcal{V}$*

$$\int_1^\infty \frac{r}{\log m(B_r(v;\varrho))}\mathrm{d}r = \infty, \tag{7.5.2}$$

where $B_r(v;\varrho)$ is the metric ball in $(\mathcal{V}, \varrho)$, then the semigroup $(e^{-t\mathbf{h}})_{t>0}$ is stochastically complete.

PROOF. For an intrinsic path metric of finite jump size, the proof follows by combining Lemma 6.31 with Theorem 7.51 and Lemma 6.39. Finally, the argument in the proof of Corollary 7.3 allows to reduce to this case. □

REMARK 7.54. Theorem 7.53 was first proved by M. Folz [**70**] by using Sturm's theorem 7.51 and also by connecting stochastic completeness on graphs and metric graphs via the corresponding transfer probabilities as described in Section 4.2 (see also [**112**], where a different proof of the latter connection was given using the weak Omori–Yau maximum principle). A different approach avoiding connections with metric graphs was suggested in [**114**] and the Grigor'yan volume test is proved under the only assumption that there exists an intrinsic pseudo metric whose distance balls are finite, that is, there is no finite jump assumption and non-locally finite graphs are allowed as well.

CHAPTER 8

Examples

The main aim of the final chapter is to demonstrate our findings by considering several important and interesting classes of graphs.

8.1. Antitrees

Recall the following definition (see Section 6.1):

DEFINITION 8.1. A connected simple rooted graph $\mathcal{G}_d$ is called an *antitree* if every vertex in the combinatorial sphere S_n, $n \geq 1^{\ddagger}$, 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 $s_n = \#S_n$, $n \in \mathbb{Z}_{\geq 0}$ (see Fig. 6.1, where the antitree with sphere numbers $s_n = n+1$, $n \in \mathbb{Z}_{\geq 0}$ is depicted).

8.1.1. Radially symmetric antitrees. Both weighted graph Laplacians and Kirchhoff Laplacians on weighted antitrees admit a very detailed analysis in the situation when their coefficients respect the radial symmetry of the underlying combinatorial antitree. In this subsection we focus on radially symmetric weighted metric antitrees and follow [**146**] in our exposition. More specifically, we assume that the weighted metric antitree $(\mathcal{A}, \mu, \nu)$ is *radially symmetric*, that is, for each $n \geq 0$, all edges connecting the combinatorial spheres S_n and S_{n+1} have the same length, say $\ell_n > 0$, and the same weights μ and ν, say $\mu_n > 0$ and $\nu_n > 0$.

The next result plays a crucial role in further analysis, however, to state it, we first need to introduce the following objects. Let

$$x_n := \sum_{k=0}^{n-1} \ell_k, \qquad \mathcal{L} := \sum_{n\geq 0} \ell_n \in (0,\infty], \tag{8.1.1}$$

and then set

$$\mu_{\mathcal{A}}(x) = \sum_{n\geq 0} \mu_n s_n s_{n+1} \mathbb{1}_{[x_n,x_{n+1})}(x), \quad \nu_{\mathcal{A}}(x) = \sum_{n\geq 0} \nu_n s_n s_{n+1} \mathbb{1}_{[x_n,x_{n+1})}(x), \tag{8.1.2}$$

for all $x \in [0,\mathcal{L})$. Notice that $\mathcal{L}$ can be interpreted as the height of a metric antitree. Next, we define three different types of operators associated with the differential expression

$$\tau_{\mathcal{A}} = -\frac{1}{\mu_{\mathcal{A}}(x)} \frac{\mathrm{d}}{\mathrm{d}x} \nu_{\mathcal{A}}(x) \frac{\mathrm{d}}{\mathrm{d}x}. \tag{8.1.3}$$

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

- The operator $\mathrm{H}_{\mathcal{A}}$ is associated with $\tau_{\mathcal{A}}$ in the Hilbert space $L^2([0,\mathcal{L});\mu_{\mathcal{A}})$ and acts on the maximal domain subject to the Neumann boundary condition at $x = 0$, see (5.1.2).
- For each $n \geq 1$, the operator H_n^1 is associated with $\tau_{\mathcal{A}}$ in the Hilbert space $L^2([x_n, x_{n+1});\mu_{\mathcal{A}})$ and with Dirichlet boundary conditions at the endpoints,

$$\mathrm{dom}(\mathrm{H}_n^1) = \big\{f \in H^2([x_n, x_{n+1})) \,|\, f(x_n) = f(x_{n+1}) = 0\big\}.$$

- For each $n \geq 1$, the operator H_n^2 is associated with $\tau_{\mathcal{A}}$ in the Hilbert space $L^2([x_{n-1}, x_{n+1});\mu_{\mathcal{A}})$ and with Dirichlet boundary conditions at the endpoints,

$$\mathrm{dom}(\mathrm{H}_n^2) = \big\{f \in H_0^1([x_{n-1}, x_{n+1})) \,|\, \nu_{\mathcal{A}} f' \in H^1([x_{n-1}, x_{n+1}))\big\}.$$

With these definitions at hand, we are in position to state the key result.

Theorem 8.2. *Let $(\mathcal{A},\mu,\nu)$ be a radially symmetric antitree. Then the corresponding maximal Kirchhoff Laplacian $\mathbf{H}$ is unitarily equivalent to the orthogonal sum*

$$\mathrm{H}_{\mathcal{A}} \oplus \bigoplus_{n\geq 1}\Big(\mathrm{I}_{(s_n-1)(s_{n+1}-1)} \otimes \mathrm{H}_n^1\Big) \oplus \bigoplus_{n\geq 1}\Big(\mathrm{I}_{s_n-1} \otimes \mathrm{H}_n^2\Big). \tag{8.1.4}$$

Here $s_n = \#S_n$, $n \geq 0$ are the sphere numbers of $\mathcal{A}$ and I_k is the identity operator in $\mathbb{C}^k$, $k \in \mathbb{Z}_{\geq 0}$.

Proof. Follows line by line the proof of [**146**, Theorem 3.5] (see also [**29**]), where the case $\mu = \nu \equiv \mathbb{1}$ is considered, and we omit it. Let us only mention that the operator $\mathrm{H}_{\mathcal{A}}$ is nothing but the restriction of $\mathbf{H}$ onto the subspace $\mathcal{F}_{\mathrm{sym}}$ of radially symmetric functions

$$\mathcal{F}_{\mathrm{sym}} = \{f \in L^2(\mathcal{A};\mu) \,|\, f(x) = f(y) \text{ if } \varrho_0(x,o) = \varrho_0(y,o)\}, \tag{8.1.5}$$

which follows easily by comparing the corresponding quadratic forms. Here $\varrho_0(x,o)$ denotes the distance from $x \in \mathcal{A}$ to the root o of $\mathcal{A}$ w.r.t. the length metric ϱ_0. $\square$

Thus, Theorem 8.2 reduces the analysis of the Kirchhoff Laplacian $\mathbf{H}$ on $(\mathcal{A},\mu,\nu)$ to the analysis of Sturm–Liouville operators (8.1.3). In particular, since both H_n^1 and H_n^2 are self-adjoint and have purely discrete simple spectra for each $n \geq 1$, the operator $\mathrm{H}_{\mathcal{A}}$ acting in $L^2([0,\mathcal{L});\mu_{\mathcal{A}})$ encodes the main spectral and parabolic properties of $\mathbf{H}$. Moreover, take into account that $\mathrm{H}_{\mathcal{A}}$ allows a rather detailed treatment (see Chapter 5). First of all, we easily obtain the following characterization of the self-adjoint and Markovian uniqueness.

Theorem 8.3. *Let $(\mathcal{A},\mu,\nu)$ be a radially symmetric antitree.*

(i) *The Kirchhoff Laplacian $\mathbf{H}$ is self-adjoint if and only if the series*

$$\sum_{n\geq 0} s_n s_{n+1}\mu_n \ell_n \Big(\sum_{k\leq n} \frac{\ell_k}{s_k s_{k+1}\nu_k}\Big)^2 \tag{8.1.6}$$

diverges. If the series converges, then the deficiency indices of the minimal Kirchhoff Laplacian $\mathbf{H}^0 = \mathbf{H}^*$ equal 1.

(ii) *The Kirchhoff Laplacian* $\mathbf{H}$ *admits a unique Markovian restriction if and only if either it is self-adjoint or the series*

$$\mathcal{L}_\nu^{\mathcal{A}} := \sum_{n\geq 0} \frac{\ell_n}{s_n s_{n+1}\nu_n} \tag{8.1.7}$$

diverges.

Proof. Taking into account the decomposition (8.1.4) and the self-adjointness of the second and the third summands, the self-adjoint uniqueness (resp., Markovian uniqueness) for $\mathbf{H}$ is equivalent to the self-adjoint uniqueness (resp., Markovian uniqueness) for $\mathrm{H}_{\mathcal{A}}$. Thus, applying Lemma 5.2 and Lemma 5.11, we prove (i) and, respectively, (ii). □

Remark 8.4. It might be useful to compare the self-adjointness criterion obtained in Theorem 8.3 with the Gaffney-type results from Section 7.1.1. Taking into account that by the Hopf–Rinow theorem (see Section 6.4.5), completeness is equivalent to the geodesic completeness, we conclude:

(i) $(\mathcal{A}, \varrho_\eta)$ is complete exactly when $\sum_{n\geq 0} \ell_n \sqrt{\frac{\mu_n}{\nu_n}} = \infty$ (cf. Theorem 7.1).

(ii) if, for simplicity,[†] $\sup_n \ell_n \sqrt{\frac{\mu_n}{\nu_n}} < \infty$, then $(\mathcal{V}, \varrho_m)$ is complete exactly when $\sum_{n\geq 0}(s_n + s_{n+1})\ell_n\mu_n = \infty$ (cf. Theorem 7.7).

On the one hand, the last condition is equivalent to (8.1.6) only under the restrictive assumptions that (a) $\mathcal{L}_\nu^{\mathcal{A}} < \infty$, and (b) $s_n s_{n+1} \lesssim s_n + s_{n+1}$ for all n. On the other hand, its main drawback that it does not take ν into account.

The next immediate corollary is of some interest when one looks at the self-adjointness and Markovian uniqueness by using graph ends (cf. Section 7.2.1).

Corollary 8.5. *Let* $(\mathcal{A}, \mu, \nu)$ *be a radially symmetric antitree.*

(i) *If*

$$\mu(\mathcal{A}) = \int_{\mathcal{A}} \mu(\mathrm{d}x) = \sum_{n\geq 0} s_n s_{n+1}\mu_n\ell_n = \infty, \tag{8.1.8}$$

then the Kirchhoff Laplacian $\mathbf{H}$ *is self-adjoint. Moreover,* (8.1.8) *is also necessary for the self-adjointness if* $\mathcal{L}_\nu^{\mathcal{A}} < \infty$*.*

(ii) *If* $\mathcal{L}_\nu^{\mathcal{A}} < \infty$*, then the Kirchhoff Laplacian* $\mathbf{H}$ *admits a unique Markovian restriction if and only if* $\mu(\mathcal{A}) = \infty$*.*

Remark 8.6. Every infinite antitree has exactly one graph end. By Definition 7.23, this graph end has finite volume if and only if the total volume of a given antitree is finite, $\mu(\mathcal{A}) < \infty$. By Corollary 8.5, the absence of finite volume ends is equivalent to both self-adjoint and Markovian uniqueness exactly when $\mathcal{L}_\nu^{\mathcal{A}} < \infty$, that is, when the series in (8.1.7) converges.

Remark 8.7. If $\mathbf{H}$ is not self-adjoint, then one can describe its self-adjoint restrictions in the following way. First of all, the decomposition (8.1.4) implies that

[†]Here we need to take into account the definition of the vertex weight in Section 3.1

it suffices to restrict to the subspace of spherically symmetric functions: for each $f \in \mathrm{dom}(\mathbf{H})$, define the function $f_{\mathrm{sym}}\colon [0,\mathcal{L}) \to \mathbb{C}$ by setting

$$f_{\mathrm{sym}}(x) = \frac{1}{s(x)} \sum_{y\in\mathcal{A}\colon\, \varrho_0(o,y)=x} f(y), \qquad s(x) = \sum_{n\ge 0} s_n s_{n+1} \mathbb{1}_{[x_n,x_{n+1})}(x). \tag{8.1.9}$$

It is straightforward to check that $f_{\mathrm{sym}} \in \mathrm{dom}(\mathrm{H}_{\mathcal{A}})$ (cf. [**146**, Lemma 3.2]). Next, define

$$\begin{aligned} f_{\mathrm{sym}}(\mathcal{L}) &:= \lim_{x\to\mathcal{L}} \Big(f_{\mathrm{sym}}(x) - \nu_{\mathcal{A}}(x) f'_{\mathrm{sym}}(x) \int_0^x \frac{\mathrm{d}s}{\nu_{\mathcal{A}}(s)} \Big), \\ f'_{\mathrm{sym}}(\mathcal{L}) &:= \lim_{x\to\mathcal{L}} \nu_{\mathcal{A}}(x) f'_{\mathrm{sym}}(x). \end{aligned}$$

By Lemma 5.5, both limits exist for each $f \in \mathrm{dom}(\mathbf{H})$ and applying (5.1.8), we conclude that the one-parameter family $\mathbf{H}_\theta$, $\theta \in [0,\pi)$ of self-adjoint restrictions of $\mathbf{H}$ is explicitly given by

$$\mathrm{dom}(\mathbf{H}_\theta) = \big\{ f \in \mathrm{dom}(\mathbf{H}) \mid \cos(\theta) f_{\mathrm{sym}}(\mathcal{L}) + \sin(\theta) f'_{\mathrm{sym}}(\mathcal{L}) = 0 \big\}. \tag{8.1.10}$$

Corollary 8.8. *Let* $\mathbf{H}$ *be non-self-adjoint. If* $\mathcal{L}_\nu^{\mathcal{A}} < \infty$*, then the corresponding Dirichlet Laplacian is given by*

$$\mathrm{dom}(\mathbf{H}_D) = \big\{ f \in \mathrm{dom}(\mathbf{H}) \mid \lim_{x\to\mathcal{L}} f_{\mathrm{sym}}(x) = 0 \big\}, \tag{8.1.11}$$

Otherwise, the Dirichlet Laplacian coincides with the Neumann Laplacian

$$\mathrm{dom}(\mathbf{H}_N) = \mathrm{dom}(\mathbf{H}_{\pi/2}) = \big\{ f \in \mathrm{dom}(\mathbf{H}) \mid \lim_{x\to\mathcal{L}} \nu_A(x) f'_{\mathrm{sym}}(x) = 0 \big\}, \tag{8.1.12}$$

Proof. If $\mathcal{L}_\nu^{\mathcal{A}} = \int_0^{\mathcal{L}} \frac{\mathrm{d}s}{\nu_{\mathcal{A}}(s)} < \infty$, then boundary conditions can be written in a standard way since in this case

$$f_{\mathrm{sym}}(\mathcal{L}) = \lim_{x\to\mathcal{L}} f_{\mathrm{sym}}(x) - \mathcal{L}_\nu^{\mathcal{A}} f'_{\mathrm{sym}}(\mathcal{L}),$$

which implies that the limit on the right-hand side exists and is finite for all $f \in \mathrm{dom}(\mathbf{H})$. Hence we can replace $f_{\mathrm{sym}}(\mathcal{L})$ in (8.1.10) by $\widetilde{f}_{\mathrm{sym}}(\mathcal{L}) := \lim_{x\to\mathcal{L}} f_{\mathrm{sym}}(x)$. Taking into account the definition of the Dirichlet Laplacian, this implies the first claim. The second one follows from Theorem 8.3(ii). ☐

If $\mathbf{H}$ is not self-adjoint, then the spectral analysis is reduced to that of $\mathrm{H}_{\mathcal{A}}$ and Lemma 5.5. Therefore, in the following results we restrict to the case when $\mathbf{H}$ is self-adjoint, that is, the series (8.1.6) diverges. Using Lemma 5.7, we arrive at the next result.

Lemma 8.9. *Suppose that the Kirchhoff Laplacian* $\mathbf{H}$ *is self-adjont. Then:*

(i) $\lambda_0(\mathbf{H}) > 0$ *if and only if*

$$\mathcal{L}_\nu^{\mathcal{A}} < \infty \qquad \textit{and} \qquad \sup_{n\ge 0} \sum_{k\le n} s_k s_{k+1} \mu_k \ell_k \sum_{k\ge n} \frac{\ell_k}{s_k s_{k+1} \nu_k} < \infty. \tag{8.1.13}$$

(ii) $\lambda_0^{\mathrm{ess}}(\mathbf{H}) > 0$ *if and only if either* (8.1.13) *holds true or*

$$\mathcal{L}_\nu^{\mathcal{A}} = \infty \qquad \textit{and} \qquad \sup_{n\ge 0} \sum_{k\le n} \frac{\ell_k}{s_k s_{k+1} \nu_k} \sum_{k\ge n} s_k s_{k+1} \mu_k \ell_k < \infty. \tag{8.1.14}$$

(iii) *The spectrum of* $\mathbf{H}$ *is purely discrete if and only if* either $\mathcal{L}_\nu^{\mathcal{A}} < \infty$ *and*

$$\lim_{n\to\infty} \sum_{k\le n} s_k s_{k+1}\mu_k \ell_k \sum_{k\ge n} \frac{\ell_k}{s_k s_{k+1}\nu_k} = 0, \tag{8.1.15}$$

or $\mu(\mathcal{A}) < \infty$ *and*

$$\lim_{n\to\infty} \sum_{k\le n} \frac{\ell_k}{s_k s_{k+1}\nu_k} \sum_{k\ge n} s_k s_{k+1}\mu_k \ell_k = 0. \tag{8.1.16}$$

PROOF. Taking into account the decomposition (8.1.4), observe that

$$\lambda_0(\mathbf{H}) = \lambda_0(\mathrm{H}_{\mathcal{A}}), \qquad \lambda_0^{\mathrm{ess}}(\mathbf{H}) = \lambda_0^{\mathrm{ess}}(\mathrm{H}_{\mathcal{A}})$$

since $\lambda_0(\mathrm{H}_{\mathcal{A}}) \le \lambda_0(\mathrm{H}_n^j)$ for all $n \ge 1$, as well as $\lambda_0^{\mathrm{ess}}(\mathrm{H}_{\mathcal{A}}) \le \liminf_{n\to 0} \lambda_0(\mathrm{H}_n^j)$, $j \in \{1,2\}$, which follows by using the variational characterization of λ_0 provided by the Rayleigh quotient. Thus, applying Lemma 5.7, we complete the proof. □

REMARK 8.10. A few remarks are in order.

(i) If $\mathbf{H}$ is not self-adjoint, then one can conclude that the spectrum of each self-adjoint restriction $\mathbf{H}_\theta$ (see (8.1.10)) is purely discrete. Furthermore, taking into account that

$$\sigma(\mathrm{H}_n^1) = \Big\{\frac{\pi^2 k^2}{\eta_n^2}\Big\}_{k\in\mathbb{Z}_{\ge 1}},$$

where $\eta_n = \ell_n\sqrt{\mu_n/\nu_n}$, $n \ge 0$ are the intrinsic edge lengths, the Weyl law (5.1.9) for $\mathrm{H}_{\mathcal{A}}$ together with the standard Dirichlet–Neumann bracketing argument applied to H_n^2 (see the proof of Corollary 5.1 in [**146**]), one arrives at the Weyl law for self-adjoint restrictions of $\mathbf{H}$:†

$$\lim_{\lambda\to\infty} \frac{N(\lambda;\mathbf{H}_\theta)}{\sqrt{\lambda}} = \frac{1}{\pi} \times \text{intrinsic volume of } \mathcal{A}, \tag{8.1.17}$$

and the *intrinsic volume* of $\mathcal{A}$ is

$$\eta(\mathcal{A}) = \int_{\mathcal{A}} \eta(\mathrm{d}x) = \sum_{n\ge 0} s_n s_{n+1}\eta_n = \sum_{n\ge 0} s_n s_{n+1}\ell_n \sqrt{\frac{\mu_n}{\nu_n}}. \tag{8.1.18}$$

(ii) If $\mathbf{H}$ is self-adjoint, however, has purely discrete spectrum, then Weyl's law (8.1.17) still takes place. If $\eta(\mathcal{A}) = \infty$, then one can prove criteria for the inclusion $(\mathbf{H}+\mathrm{I})^{-1} \in \mathfrak{S}_p$, $p \in (1/2,\infty)$ (see Remark 5.8 and [**146**, Theorem 5.6 and Rem. 5.7]).

The next result provides an explicit form of the isoperimetric constant for $(\mathcal{A},\mu,\nu)$ in the radially symmetric case.

PROPOSITION 8.11. *The isoperimetric constant of a radially symmetric metric antitree* $(\mathcal{A},\mu,\nu)$ *is*

$$\mathrm{Ch}(\mathcal{A}) = \inf_{n\ge 0} \frac{s_n s_{n+1}\sqrt{\mu_n\nu_n}}{\sum_{k=0}^n s_k s_{k+1}\mu_k\ell_k}. \tag{8.1.19}$$

†Here $N(\lambda;A)$ is the eigenvalue counting function of a (bounded from below) self-adjoint operator A with purely discrete spectrum:

$$N(\lambda;A) = \#\{k \,|\, \lambda_k(A) \le \lambda\},$$

where $\{\lambda_k(A)\}_{k\ge 0}$ are the eigenvalues of A (counting multiplicities) in increasing order.

In particular, the following estimate holds true

$$\lambda_0(\mathbf{H}_D) \ge \frac{1}{4}\mathrm{Ch}(\mathcal{A})^2. \tag{8.1.20}$$

PROOF. The decomposition (8.1.4) as well as the proof of Lemma 8.9 suggests to take the infimum in (7.3.3) only over radially symmetric subgraphs. Thus, evaluating (7.3.3) over subantitrees $\mathcal{A}_n$, where one cuts out the part of $\mathcal{A}$ above the combinatorial sphere S_n, the inequality "$\le$" in (8.1.19) is trivial. The proof of the converse inequality "$\ge$" follows line by line the proof of [**146**, Theorem 7.1] and we leave it to the reader. □

Applying the volume growth estimates from Section 7.3.3, we arrive at the following upper bounds.

PROPOSITION 8.12. *Suppose that the radially symmetric antitree $(\mathcal{A}, \mu, \nu)$ has infinite intrinsic height (i.e., $(\mathcal{A}, \varrho_\eta)$ is complete),*

$$\sum_{n\ge 0} \eta_n = \sum_{n\ge 0} \ell_n \sqrt{\frac{\mu_n}{\nu_n}} = \infty.$$

Then $\mathbf{H}$ is self-adjoint and

$$\lambda_0(\mathbf{H}) \le \frac{1}{4}\mathbf{v}(\mathcal{A})^2, \qquad \mathbf{v}(\mathcal{A}) = \liminf_{n\to\infty} \frac{1}{\sum_{k\le n}\eta_k} \log\Big(\sum_{k\le n} s_k s_{k+1}\mu_k\ell_k\Big). \tag{8.1.21}$$

REMARK 8.13. It might be useful to compare the isoperimetric and volume growth bounds with the positive spectral gap criterion obtained in Lemma 8.9(i)-(ii). It is rather curious that the volume of the sub-antitrees $\mathcal{A}_n$,

$$\sum_{k\le n} s_k s_{k+1}\mu_k\ell_k$$

enters all the estimates and criteria. However, it appears there in rather different ways. The meaning of the quantity

$$\sum_k \frac{\ell_k}{s_k s_{k+1}\nu_k}$$

in both (8.1.13) and (8.1.14) remains unclear to us, however, it plays crucial role in understanding both spectral and parabolic properties of the Kirchhoff Laplacian.

Let us finish this subsection by quickly discussing basic parabolic properties.

LEMMA 8.14. *Let $\mathbf{H}_G$ be the Gaffney Laplacian on a radially symmetric antitree $(\mathcal{A}, \mu, \nu)$. If $\mathbf{H}_G$ is self-adjoint, then it is recurrent if and only if $\mathcal{L}_\nu^{\mathcal{A}} = \infty$. If $\mathbf{H}_G$ is not self-adjoint, then $\mathbf{H}_\theta$ is recurrent if and only if $\theta = \pi/2$.*

PROOF. By Lemma B.5, recurrence is equivalent to the fact that there is a sequence approximating (in a suitable sense) the constant function $\mathbb{1}$. However, $\mathbb{1}$ is radially symmetric and thus belongs to the reducing subspace $\mathcal{F}_{\mathrm{sym}}$ of all radially symmetric functions. Thus, $\mathbf{H}_G$ is recurrent exactly when so is its radial part $\mathrm{H}_{\mathcal{A}}$. It remains to apply Lemma 5.13. □

LEMMA 8.15. *Let $\mathbf{H}_G$ be the Gaffney Laplacian on a radially symmetric antitree $\mathcal{A}$. If $\mathbf{H}_G$ is self-adjoint, then it is stochastically incomplete if and only if*

$$\mathcal{L}_\nu^{\mathcal{A}} < \infty, \qquad \text{and} \qquad \frac{1}{\nu_{\mathcal{A}}(x)}\int_0^x \mu_{\mathcal{A}}(s)\mathrm{d}s \in L^1([0,\mathcal{L})). \tag{8.1.22}$$

PROOF. By the very definition of stochastic completeness (B.2.5), the decomposition (8.1.4) clearly reduces the problem to the stochastic completeness of the operator $\mathrm{H}_{\mathcal{A}}$ since $\mathbb{1}_{\mathcal{A}} \in \mathcal{F}_{\mathrm{sym}}$. It remains to apply Lemma 5.14. □

8.1.2. General case. Removing the symmetry assumption, that is, if at least one of the weights μ or ν or the lengths $|\cdot|$ are no longer radially symmetric, the analysis of the Kirchhoff Laplacian becomes much more complicated. The very first problem – the self-adjoint uniqueness – remains open and, as the next example from [**144**, § 7] demonstrates, far from being trivial.

EXAMPLE 8.16 (Antitrees with arbitrary deficiency indices). We shall assume that the metric antitree is unweighted, that is, $\mu = \nu = \mathbb{1}$ on $\mathcal{A}$ (notice that both weights are radially symmetric). Fix $N \in \mathbb{Z}_{\geq 1}$ and consider the antitree $\mathcal{A}_N$ with sphere numbers $s_n = n + N$, $n \in \mathbb{Z}_{\geq 1}$ (for $N = 1$ this antitree is depicted on Fig. 6.1). To assign lengths, let us enumerate the vertices in every combinatorial sphere S_n by $(v_i^n)_{i=1}^{s_n}$ and then denote the edge connecting v_i^n with v_j^{n+1} by e_{ij}^n, $1 \leq i \leq s_n$, $1 \leq j \leq s_{n+1}$ and $n \geq 0$. For a sequence of positive real numbers $(\ell_n)_{n\geq 0}$, we first assign edge lengths

$$|e_{ij}^n| = \begin{cases} 2\ell_n, & \text{if } 1 \leq i = j \leq N, \\ \ell_n, & \text{otherwise}, \end{cases} \tag{8.1.23}$$

for all $n \in \mathbb{Z}_{\geq 0}$. It turns out that for the corresponding metric antitree $\mathcal{A}_N$ the space of harmonic functions has dimension $N+1$ (see Lemma 7.4 in [**144**]). Choosing lengths such that $\mathrm{vol}(\mathcal{A}_N) \approx \sum_{n\geq 1} n^2 \ell_n < \infty$, the deficiency indices of the minimal Kirchhoff Laplacian $\mathbf{H}^0$ are equal to the dimension of the space of harmonic functions belonging to $L^2(\mathcal{A})$. By [**144**, Prop. 7.5], if we choose lengths such that

$$\ell_n = \mathcal{O}\Big(\frac{1}{(36N)^n((n+N+3)!)^2}\Big), \qquad n \to \infty,$$

then all harmonic functions belong to $L^2(\mathcal{A})$ and hence $\mathrm{n}_\pm(\mathbf{H}^0) = N + 1$. ◊

REMARK 8.17. A few concluding remarks are in order.

(i) Slightly modifying the antitree in Example 8.16 one can construct an example of a metric antitree such that the corresponding minimal Kirchhoff Laplacian has infinite deficiency indices (see [**144**, § 7.4]). The above example also demonstrates that the space of harmonic functions, even in the unweighted case, depends in a complicated way on the choice of edge lengths (notice that in the radially symmetric case constants are the only harmonic functions). Therefore, the self-adjoint uniqueness becomes a highly nontrivial problem already in the case $\mu = \nu = \mathbb{1}$.

(ii) In contrast to the self-adjoint uniqueness in the case of no radial symmetry, the Markovian uniqueness problem can be answered in several situations of interest. For example, in the case $\mu = \nu = \mathbb{1}$ it was observed in [**144**] that the Markovian uniqueness is equivalent to the infinite total volume of $\mathcal{A}$ (and the latter is independent of whether the antitree is radially symmetric or not). Moreover, the results of Section 7.2 extend this claim to a much wider setting: if at least one the two conditions (a) $1/\mu$, $1/\nu \in L^\infty(\mathcal{A})$, or (b) $\mathcal{A}$ has finite ν-diameter $D_{1/\nu}(\mathcal{A}) < \infty$, see (7.2.10), is satisfied, then the minimal Kirchhoff Laplacian admits a unique Markovian uniqueness if and only if $\mu(\mathcal{A}) = \infty$. If $\mu(\mathcal{A}) < \infty$, then $\mathbf{H}$ admits a one-parameter family of Markovian extensions and their description is very much similar to the one in the radial case.

Let us also stress that in the radially symmetric case the condition relating Markovian uniqueness with infinite total volume is $\mathcal{L}_\nu^{\mathcal{A}} < \infty$ (see (8.1.7)), and this condition is much weaker than both (a) and (b).

8.1.3. Historical remarks and further references. Antitrees also appear in the literature under the name *neural networks* and to a certain extent the corresponding graph Laplacians can be seen a generalization of Jacobi matrices (one may interpret the recurrence relations as "*the values on S_n depend only on the values on S_{n-1} and S_{n+1}*"). Seems, exactly this fact allows to perform a rather detailed analysis of Laplacians (both weighted graph and Kirchhoff) on antitrees. Below we collect some further information.

8.1.3.1. *Spectral analysis in the radially symmetric case.* The decomposition (8.1.4) of the maximal Kirchhoff Laplacian in the radially symmetric case reduces the spectral analysis to the study of a Sturm–Liouville operator $\mathrm{H}_{\mathcal{A}}$. One may employ a number of results and techniques available in the 1D setting. In particular, we briefly listed the very basic results (self-adjointness, positive spectral gap, discreteness etc.). However, one can prove a number of results characterizing the structure of the spectrum of $\mathbf{H}$ in the self-adjoint case. In particular, [**146**, § 8] shows that the occurrence of absolutely continuous spectrum is a rather rare event. Antitrees with zero-measure spectrum can be found in [**49**]. However, using Lemma 5.9, one can construct a rather large and nontrivial class of antitrees whose absolutely continuous spectrum fills the positive semi-axis $[0, \infty)$ (see [**146**, § 9]).

8.1.3.2. *Family preserving graphs.* An antitree is just a particular example of an infinite graph having a lot of symmetry. Actually, antitrees belong to the wider class of *family preserving graphs* (see [**30**] for definitions), which, in particular, includes rooted radially symmetric trees. The decomposition (8.1.4) is motivated by a similar decomposition for Laplacians on radially symmetric metric trees observed by K. Naimark and M. Solomyak [**167**], [**168**], [**193**]. For this very reason Laplacians on radially symmetric trees form the most studied class of operators on metric graphs. The literature is enormous and we refer for further references to [**29**].

Notice that the analog of the decomposition (8.1.4) for family preserving metric graphs was obtained in [**29**], however, in contrast to graph Laplacians [**30**], the setting of [**29**] excludes graphs with horizontal edges.

8.1.3.3. *Historical remarks.* Antitrees appear in the study of *discrete Laplacians* on graphs at least since the 1980's [**59**] (see [**47**, § 2] for a historical overview). They played an important role in context with the notion of intrinsic metrics on graphs (see Section 6.4). More precisely, in [**210**] (see also [**133**, § 6] and [**90**]) R.K. Wojciechowski constructed antitrees of polynomial volume growth (with respect to the combinatorial metric ϱ_{comb}, which is in general not intrinsic) for which the (discrete) combinatorial Laplacian L_{comb} (see Example 6.7) is stochastically incomplete and the bottom of the essential spectrum is strictly positive. At first, these examples presented a sharp contrast to the manifold setting (cf. [**32**], [**88**]), but the discrepancies were resolved later by the notion of intrinsic metrics. In this context, antitrees appear as key examples for certain thresholds (see [**99**], [**105**], [**127**]). During the recent years, antitrees were also actively studied from other perspectives and we only refer to a brief selection of articles [**29**], [**30**], [**47**], [**146**], where further references can be found.

8.2. Cayley graphs

Let G be a countable finitely generated group and let S be a generating set of G. We shall always assume that

- G is countably infinite,
- S is symmetric, $S = S^{-1}$ and finite, $\#S < \infty$,
- the identity element of G does not belong to S (this excludes loops).

The *Cayley graph* $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ of G with respect to S is the simple graph whose vertex set coincides with G and two vertices $x, y \in \mathcal{G}$ are neighbors $x \sim y$ if and only if $xy^{-1} \in S$.

The main aim of this subsection is to demonstrate some of our findings as well as their relationships with large scale properties of groups. Notice that Cayley graphs corresponding to two different generating sets are quasi-isometric as metric spaces when equipped with the combinatorial distance (word metric), which in particular indicates that many properties of interest are independent of the choice of S (see, for instance, [**53**], [**173**], [**184**] for further details). To simplify our considerations we shall restrict throughout most of Section 8.2 to weighted metric graphs with $\mu = \nu$, that is, the edge weights μ and ν are assumed to coincide.

8.2.1. Markovian uniqueness.

The self-adjointness for Kirchhoff Laplacians is a very complicated problem already for abelian groups $(\mathbb{Z}^N, +)$ with $N \geq 2$ (it does not seem to us that a complete answer even in this “simplest” situation is feasible, see also Remark 8.25 below). One can obtain various sufficient conditions by directly applying the results of Section 7.1 (e.g., Gaffney-type theorems) and we leave this to the interested reader. Our first goal is to investigate the Markovian uniqueness on metric Cayley graphs, which is equivalent to the self-adjointness of the corresponding Gaffney Laplacian $\mathbf{H}_G$.

Proposition 8.18. *Let $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ be a Cayley graph.*[‡] *Suppose $(\mathcal{G}_C, \mu, \mu)$ is a weighted metric graph whose edge weight μ satisfies $1/\mu \in L^\infty(\mathcal{G})$. Then the deficiency indices of the corresponding minimal Gaffney Laplacian $\mathbf{H}_{G,\min} = \mathbf{H}_G^*$ coincide with the number of finite volume graph ends of $(\mathcal{G}_C, \mu, \mu)$.*

Proof. Immediately follows from Theorem 7.24. □

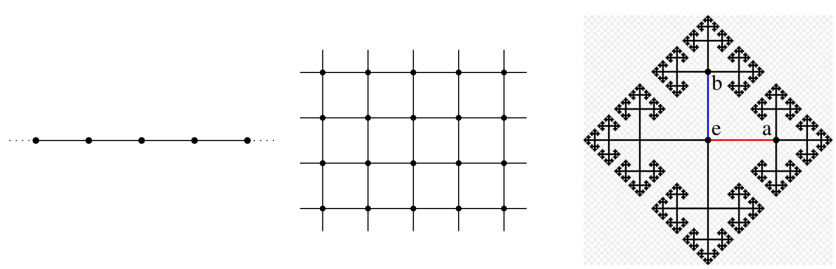

Figure 8.1. Cayley graphs of the abelian groups $\mathbb{Z}$, $\mathbb{Z}^2$ and the free nonabelian group $\mathbb{F}_2$ (the Bethe lattice or infinite Cayley tree).

[‡]If it is not explicitly stated otherwise, we shall denote by $\mathcal{G}_C$ both a Cayley graph and a metric graph $\mathcal{G}_C$ equipped with some edge lengths.

REMARK 8.19 (Ends of Cayley graphs). Graph ends of countable finitely generated groups are rather well understood (see, e.g., [**81**]). It is not difficult to see that the graphs depicted in Fig. 8.1 have, respectively, 2, 1 and infinitely many ends. However, by the Freudenthal–Hopf theorem, only these three options are possible: *a Cayley graph of an infinite finitely generated group has* 1*,* 2 *or infinitely many ends*. Moreover, the end space (equipped with the topology of the end compactification) of $\mathcal{C}(\mathsf{G}, S)$ is independent of the choice of the finite generating set S and hence we shall denote the set of ends by $\mathfrak{C}(\mathsf{G})$. By Hopf's theorem, $\#\mathfrak{C}(\mathsf{G}) = 2$ if and only if G is *virtually infinite cyclic*† (equivalently, G has a finite normal subgroup Γ such that the quotient group G/Γ is either infinite cyclic or infinite dihedral). The classification of finitely generated groups with infinitely many ends (equivalently, with exactly 1 end) is due to J.R. Stallings (see, e.g., [**81**, Chap. 13]). In particular, if G is amenable, then it has finitely many ends (actually, either 1 or 2).

Thus, we arrive at the following result.

COROLLARY 8.20. *Assume the conditions of Proposition 8.18. Let also* $\mathbf{H}_G$ *be the corresponding Gaffney Laplacian.*

(i) *If* $\#\mathfrak{C}(\mathsf{G}) = 1$*, then* $\mathbf{H}_G$ *is self-adjoint if and only if* $\mu(\mathcal{G}) = \infty$*. Otherwise,* $\mathrm{n}_\pm(\mathbf{H}_{G,\min}) = 1$*.*
(ii) *If* $\#\mathfrak{C}(\mathsf{G}) = 2$ *(i.e.,* G *is virtually infinite cyclic), then* $\mathrm{n}_\pm(\mathbf{H}_{G,\min}) \le 2$*. In particular,* $\mathbf{H}_G$ *is self-adjoint if and only if both ends have infinite volume.*
(iii) *If* $\#\mathfrak{C}(\mathsf{G}) > 2$ *and at least one of its ends has finite volume, then* $\mathbf{H}_{G,\min}$ *has infinite deficiency indices.*
(iv) *If* $\mu(\mathcal{G}) < \infty$*, then the deficiency indices of* $\mathbf{H}_{G,\min}$ *are equal to the number of ends of* G*,* $\mathrm{n}_\pm(\mathbf{H}_{G,\min}) = \#\mathfrak{C}(\mathsf{G})$*.*

PROOF. (i), (ii) and (iv) are an immediate consequence of Proposition 8.18.
(iii) By the Freudenthal–Hopf theorem, $\#\mathfrak{C}(\mathsf{G}) = \infty$ if $\#\mathfrak{C}(\mathsf{G}) > 2$ (see Remark 8.19). Moreover, the end space is known to be homeomorphic to the Cantor set (see, e.g., [**81**, Addendum 13.5.8]), and hence there are no free graph ends. Thus, having 1 finite volume end would immediately imply the presence of infinitely many finite volume graph ends. It remains to apply Proposition 8.18. □

Taking into account that the self-adjointness of $\mathbf{H}_G$ is equivalent to the Markovian uniqueness for the minimal Kirchhoff Laplacian, we arrive at the following characterization in the case of amenable groups.

COROLLARY 8.21. *Assume the conditions of Proposition 8.18. If* G *is amenable and not virtually infinite cyclic, then the minimal Kirchhoff Laplacian admits a unique Markovian extension if and only if* $\mu(\mathcal{G}_C) = \int_{\mathcal{G}_C} \mu = \infty$*.*

REMARK 8.22. For Cayley graphs of infinite groups with finitely many ends one can describe the sets of Markovian and finite energy extensions of the minimal Kirchhoff Laplacian in a rather transparent way (see, e.g., Section 7.2.2 and [**144**, § 6], [**147**]). If G has infinitely many ends and the Gaffney Laplacian is not self-adjoint, then it is not closed (see [**147**, Corollary 3.14]) and the description of its closure is an open problem (even if $\mu \equiv \mathbb{1}$). Moreover, in some cases its closure may coincide with the maximal Kirchhoff Laplacian (for instance, if $\mathcal{G}_C$ is a Cayley graph of the free group $\mathbb{F}_2$ and $\mu(\mathcal{G}_C) < \infty$, see [**147**, Lemma 4.6]). In our opinion,

†If a finite index subgroup of G has property "P", then G is called *virtually "P"*.

the description of finite energy extensions (via boundary conditions) in the general case is a highly nontrivial problem (see Sections 7.2.2–7.2.3). On the other hand, Markovian extensions can still be described in terms of Dirichlet forms (in the wide sense) on the Royden boundary [**131**], however this correspondence is in general not bijective (see Section 7.2.2 for a detailed discussion).

Since the deficiency indices of the minimal Kirchhoff Laplacian are not smaller than the deficiency indices of the Gaffney Laplacian, Corollary 8.20 immediately provides us with the following result.

Corollary 8.23. *Assume the conditions of Proposition 8.18. Let also* $\mathbf{H}^0$ *be the corresponding minimal Kirchhoff Laplacian. If* $\#\mathfrak{C}(\mathsf{G}) > 2$ *and at least one of its ends has finite volume, then* $\mathrm{n}_\pm(\mathbf{H}^0) = \infty$.

Let us consider the simplest example.

Example 8.24 (Infinite cyclic group). Let $\mathsf{G} = (\mathbb{Z}, +)$ be the infinite cyclic group and $S = \{-1, 1\}$ the standard set of generators. Then $\mathcal{C}(\mathbb{Z}, S)$ is nothing but the infinite path graph (see the first graph on Fig. 8.1). In this case the study of self-adjoint and Markovian extensions of the weighted Kirchhoff Laplacian is reduced to the analysis in Section 5.1. Lemma 5.2 and Lemma 5.11 provide a complete characterization of self-adjoint and Markovian uniqueness, however, now one needs to deal with two ends and hence one has to replace one series (5.1.4) by two series with summations to $-\infty$ and ∞, respectively. ♢

Remark 8.25. A few remarks are in order.

(i) Unfortunately, the above example seems to be the only case when a complete answer to the self-adjoint uniqueness for Kirchhoff Laplacians on weighted metric graphs can be obtained. Moreover, this characterization employs Weyl's limit point/limit circle alternative for Sturm–Liouville operators (see the proof of Lemma 5.2 and also [**205**]). Therefore, upon changing either the generating set S in the above example or by considering a Cayley graph of an arbitrary virtually infinite cyclic group (e.g., $\Gamma \times \mathbb{Z}$ with a finite group Γ, see Fig. 8.2), the problem of finding deficiency indices of the minimal Kirchhoff Laplacian on the corresponding weighted metric graph seems rather nontrivial. In particular, the answer clearly depends on both the generating set S and the group Γ.

(ii) The free abelian group $(\mathbb{Z}^n, +)$, $n \in \mathbb{Z}_{\geq 2}$ and the free non-abelian group $\mathbb{F}_n$, $n \in \mathbb{Z}_{\geq 2}$ are the most natural candidates if one wishes to study the case of groups with 1 and, respectively, infinitely many ends (see Fig. 8.1). The Gaffney-type theorems (Theorem 7.1 and Theorem 7.7) provide rather transparent sufficient conditions guaranteeing the self-adjoint uniqueness (for instance, one can employ the Hopf–Rinow theorem to verify the completeness assumption, see Section 6.4.5). Imposing the radial symmetry assumption for Cayley graphs of $\mathbb{F}_n$, one would be able to reduce the analysis to the one in Section 8.1.1 (see also Section 8.1.3.2), and the self-adjointness in this case can be characterized analogously to Theorem 8.3 (see [**193**]).

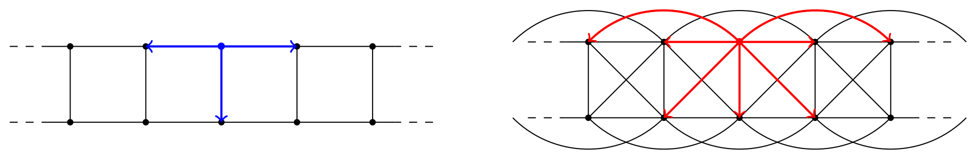

FIGURE 8.2. Cayley graphs of $\mathsf{G} = \mathbb{Z}_2 \times \mathbb{Z}$ (with $\mathbb{Z}_2 = \mathbb{Z}/2\mathbb{Z}$ the cyclic group of order 2) for two different generating sets.

8.2.2. Spectral gap. For a finitely generated group G and a generating set S, the *isoperimetric constant* of its Cayley graph $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ is defined by

$$\mathrm{Ch}_S(\mathsf{G}) = \inf_{X \subset \mathsf{G}} \frac{\#\partial X}{\#X}, \qquad \partial X = \big\{(u,v) \in X \times (\mathsf{G}\backslash X) \,|\, uv^{-1} \in S\big\}, \tag{8.2.1}$$

where the infimum is taken over all finite subsets.[†].

REMARK 8.26. Notice that the discrete isoperimetric constant defined in Section 7.3.2 for a weighted graph $(\mathcal{V}, m; b)$ looks very much similar to (8.2.1). In fact, upon choosing b and m as in Example 6.23(i), that is, the corresponding graph Laplacian is the normalized graph Laplacian, the combinatorial distance is intrinsic. Taking into account that $\mathcal{C}(\mathsf{G}, S)$ is a regular graph and each vertex has degree equal to the cardinality of S, we get $|\partial X| = \#\partial X$, $m(X) = \#S \cdot \#X$ for any $X \subset \mathsf{G}$ and hence (7.3.12) implies

$$\mathrm{Ch}_S(\mathsf{G}) = \#S \cdot \mathrm{Ch}_d(\mathcal{G}_C).$$

Let us recall the following notion (see, e.g., [**173**, Chapter 3], [**209**, Sec. 12.A]). A group is called *amenable* if it admits a left-invariant mean. For discrete groups one can define amenability in a more transparent way: a countable group G is amenable if it admits a *Følner sequence*, that is, there is a sequence (X_n) of non-empty finite subsets $X_n \subset \mathsf{G}$ which exhausts G, $\cup_{n\ge 0} X_n = \mathsf{G}$ and for each group element $g \in \mathsf{G}$

$$\lim_{n\to\infty} \frac{\#(gX_n \cap X_n)}{\#X_n} = 1, \tag{8.2.2}$$

where $gX = \{gx \,|\, x \in X\}$ is the left translation of a set $X \subset \mathsf{G}$ by g.

REMARK 8.27. Amenability was introduced by J. von Neumann in 1929 and now it is one of the most important concepts in analytic group theory. Amenability is known for many important classes of groups. For instance, all abelian or more generally all (virtually) nilpotent groups as well as all (virtually) solvable groups are amenable. The free non-abelian groups $\mathbb{F}_n$, $n \ge 2$ as well as any group containing $\mathbb{F}_2$ as a subgroup (e.g., a modular group $\mathrm{PSL}(2,\mathbb{Z})$) are not amenable (however, there are non-amenable groups without free subgroups). Moreover, amenability is invariant under quasi-isometries.

The analysis of spectral gaps of both weighted graph Laplacians and Kirchhoff Laplacians heavily relies on Kesten's amenability criterion [**140**], which can be seen as another instance of Følner's amenability criterion (see also [**209**, Prop. 12.4]):

[†]This definition extends to all connected graphs in an obvious way. A graph $\mathcal{G}_d$ has the *strong isoperimetric property* if its isoperimetric constant is positive (see [**209**]).

THEOREM 8.28 (H. Kesten [**140**]). *Let $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ be a Cayley graph of a finitely generated group G. Then the isoperimetric constant $\mathrm{Ch}_S(\mathsf{G})$ equals zero if and only if G is amenable.*

REMARK 8.29. Notice that for amenable groups the isoperimetric constant is independent of the choice of S since it always equals 0. For non-amenable groups, $\mathrm{Ch}_S(\mathsf{G})$ depends on S, however, it always stays strictly positive. Thus, we can say that a group G has the *strong isoperimetric property* if one (and hence all) of its Cayley graphs satisfies $\mathrm{Ch}_S(\mathsf{G}) > 0$. By Kesten's theorem, the strong isoperimetric property for finitely generated groups is equivalent to non-amenability.

Using connections between discrete isoperimetric constants and isoperimetric constants for weighted metric graphs, we arrive at the following result.

PROPOSITION 8.30. *Let $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ be a Cayley graph of a finitely generated group G. Also, let $(\mathcal{G}_C, \mu, \mu)$ be a weighted metric graph having finite intrinsic size and $\mathbf{H}_D$ the corresponding Dirichlet Laplacian.*

(i) *If G is non-amenable and the weight μ satisfies*

$$1/\mu \in L^\infty(\mathcal{G}) \qquad \text{and} \qquad \sup_{e\in\mathcal{E}} \mu(e)|e| < \infty,$$

then $\lambda_0(\mathbf{H}_D) > 0$.

(ii) *If G is amenable, then $\lambda_0(\mathbf{H}_D) = \lambda_0^{\mathrm{ess}}(\mathbf{H}_D) = 0$ whenever*

$$\mu \in L^\infty(\mathcal{G}) \qquad \text{and} \qquad \inf_{e\in\mathcal{E}} \mu(e)|e| > 0.$$

PROOF. (i) By assumption, $(\mathcal{G}_C, \mu, \mu)$ has finite intrinsic size. Moreover, the intrinsic length coincides with the edge length and hence the corresponding discrete isoperimetric constant is given by (see (7.3.12))

$$\mathrm{Ch}_d(\mathcal{G}_C) = \inf_{X\subset\mathsf{G}} \frac{|\partial X|}{m(X)}, \qquad |\partial X| = \sum_{e\in\partial X} \mu(e), \qquad m(X) = \sum_{v\in X}\sum_{e\in\mathcal{E}_v} \mu(e)|e|.$$

Therefore, we get the estimate

$$\frac{|\partial X|}{m(X)} \ge \frac{\inf_{e\in\mathcal{E}} \mu(e)}{\sup_{e\in\mathcal{E}} \mu(e)|e|} \frac{\#\partial X}{\#S \cdot \#X},$$

for all finite subsets $X \subset \mathsf{G}$. This immediately implies that $\mathrm{Ch}_d(\mathcal{G}_C) \ge C\mathrm{Ch}_S(\mathsf{G})$ with some positive $C > 0$. Hence, by Theorem 8.28, $\mathrm{Ch}_d(\mathcal{G}_C) > 0$. Therefore, the estimate (7.3.20) together with the Cheeger-type bound (7.3.4) imply the claim.

(ii) Combining Theorem 8.28 with the straightforward estimate

$$\frac{|\partial X|}{m(X)} \le \frac{\sup_{e\in\mathcal{E}} \mu(e)}{\inf_{e\in\mathcal{E}} \mu(e)|e|} \frac{\#\partial X}{\#S \cdot \#X},$$

we conclude that $\mathrm{Ch}_d(\mathcal{G}_C) = 0$ if G is amenable. Since $\inf_{e\in\mathcal{E}} |e| \ge \frac{\inf_{e\in\mathcal{E}} \mu(e)|e|}{\sup_{e\in\mathcal{E}} \mu(e)} > 0$, we can apply Proposition 7.38 and the Buser-type bound (7.3.4) to conclude that $\lambda_0(\mathbf{H}_D) = 0$. Finally, if $\lambda_0^{\mathrm{ess}}(\mathbf{H}_D) > 0$, then $\lambda = 0$ is an eigenvalue of $\mathbf{H}_D$ with eigenfunction $f \equiv \mathbb{1}_{\mathcal{G}}$. However, our assumptions imply that $\mathcal{G}$ has infinite total volume and hence $\mathbb{1}_{\mathcal{G}} \notin L^2(\mathcal{G}, \mu)$. This contradiction completes the proof. □

As an immediate corollary we arrive at the following metric graph analog of Kesten's amenability criterion:

COROLLARY 8.31. *Let $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ be a Cayley graph. The following assertions are equivalent:*

(i) G *is non-amenable,*
(ii) $\mathrm{Ch}(\mathcal{G}_C) > 0$ *for all* $(\mathcal{G}_C, \mu, \mu)$ *having finite intrinsic size with the edge weight satisfying* μ, $1/\mu \in L^\infty(\mathcal{G})$,
(iii) $\lambda_0(\mathbf{H}_D) > 0$ *for all* $(\mathcal{G}_C, \mu, \mu)$ *having finite intrinsic size with the edge weight satisfying* μ, $1/\mu \in L^\infty(\mathcal{G})$.

REMARK 8.32. If G is an amenable group, then the analysis of $\lambda_0(\mathbf{H}_D)$ and $\lambda_0^{\mathrm{ess}}(\mathbf{H}_D)$ in the case $\inf_{e\in\mathcal{E}} \mu(e)|e| = 0$ remains an open (and, in our opinion, rather complicated) problem. On the other hand, volume growth estimates (see Section 7.3.3 and the follow-up section) can be used to establish the equality $\lambda_0(\mathbf{H}_D) = 0$ for Cayley graphs of amenable groups in the case $\inf_{e\in\mathcal{E}} \mu(e)|e| = 0$. In particular, for polynomially growing groups or for groups of intermediate growth (see Section 8.2.3 for definitions) one may clearly allow a certain qualitative decay of edge lengths and weights at "infinity" in order to ensure the zero spectral gap.

8.2.3. Interlude: Growth in groups. A growth of a group is one of the most important quasi-isometric invariants (see [**53**], [**157**], [**173**]). Considering the identity element of G as the root o of its Cayley graph $\mathcal{C}(\mathsf{G}, S)$, one defines the growth function $\gamma_{\mathsf{G}} \colon \mathbb{Z}_{\geq 0} \to \mathbb{Z}_{>0}$ by setting

$$\gamma_{\mathsf{G}}(n) = \#\{g \in \mathsf{G} \,|\, \varrho_{\mathrm{comb}}(g, o) \leq n\}, \tag{8.2.3}$$

where ϱ_{comb} is the combinatorial distance (a.k.a. word metric) on $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ (see Example 6.20(i)). Behavior of γ_{G} for large n is independent of a choice of a generating set, that is, if $\widetilde{\gamma}_{\mathsf{G}}$ is the growth function of G corresponding to another generating set $\widetilde{S}$, then there is $C > 0$ such that $C^{-1}\gamma_{\mathsf{G}}(n) \leq \widetilde{\gamma}_{\mathsf{G}}(n) \leq C\gamma_{\mathsf{G}}(n)$ for all $n \in \mathbb{Z}_{\geq 0}$.

Clearly, $\gamma_{\mathsf{G}}(n) \leq \exp(C\,n)$ for all $n \in \mathbb{Z}_{\geq 0}$. A group G has *subexponential growth* if $\log \gamma_{\mathsf{G}}(n) = o(n)$ as $n \to \infty$; otherwise, G is of *exponential growth.* Notice that non-amenable groups have exponential growth. If

$$d_{\mathsf{G}} := \limsup_{n\to\infty} \frac{\log \gamma_{\mathsf{G}}(n)}{\log n}$$

is finite, then G has *polynomial growth* and in this case d_{G} is its *degree.*

For large classes of groups the behavior of γ is well understood (e.g., Gromov's characterization of groups of polynomial growth, the Milnor–Wolf theorem for solvable groups, the Tits alternative for linear groups, etc. The subject is enormous and we only refer to [**157**] for further details and references). For instance, if G is virtually nilpotent, then the degree of growth d_{G} of γ_{G} is a natural number and it can be efficiently computed by the *Bass–Guivarc'h formula* (see, e.g., [**157**, Theorem 4.2], [**209**, f-la (3.15)]). For example, for the Heisenberg group over the integers $\mathrm{U}(3, \mathbb{Z})$, $\gamma(n) \asymp n^4$ as $n \to \infty$. The celebrated Gromov's Polynomial Growth Theorem states that *only virtually nilpotent groups have polynomial growth.*

There are also groups of *intermediate growth*: those are groups of subexponential growth with $d_{\mathsf{G}} = \infty$, that is, γ_{G} grows faster than any polynomial, however, slower than any exponential function. Let us stress, however, that for groups of intermediate growth finding the precise rate of growth is a subtle issue. For instance, for the first Grigorchuk group this question was settled in the very recent work of

A. Erschler and T. Zheng [**64**]: in this case

$$\frac{\log\log\gamma(n)}{\log n} = \frac{\log 2}{\log s_0} + o(1)$$

as $n \to \infty$, where s_0 is the positive root of $s^3 - s^2 - 2s = 4$.

8.2.4. Transience and recurrence. As before, $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ is a Cayley graph of a finitely generated group G. Also, let $(\mathcal{G}_C, \mu, \nu)$ be a weighted metric graph (notice that in this subsection we allow $\mu \neq \nu$!) and let $\mathbf{H}_D$ be the corresponding Dirichlet Laplacian. Define

$$b_\nu(u,v) = \begin{cases} \frac{\nu(e_{u,v})}{|e_{u,v}|}, & u^{-1}v \in S, \\ 0, & u^{-1}v \notin S, \end{cases} \qquad (u,v) \in \mathsf{G}. \tag{8.2.4}$$

We begin with the following straightforward application of Theorem 7.49:

Corollary 8.33. $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ *is recurrent if and only if the discrete time random walk on* G *with transition probabilities* $\mathcal{P}_\nu = \big(p_\nu(u,v)\big)_{u,v\in\mathsf{G}}$ *defined by*

$$p_\nu(u,v) = P(X_{n+1} = v \,|\, X_n = u) = \frac{b_\nu(u,v)}{\sum_{g\in S} b_\nu(u,ug)} \tag{8.2.5}$$

is recurrent.

The above result reduces the problem of recurrence on weighted metric graphs to a thoroughly studied field – recurrence of random walks on groups. The literature on the subject is enormous and we only refer to the classic text [**209**]. Recall that a group G is called *recurrent* if the simple random walk on its Cayley graph $\mathcal{C}(\mathsf{G}, S)$ is recurrent for some (and hence for all) S. The classification of recurrent groups was accomplished in the 1980s and it is a combination of two seminal theorems – relationship between decay of return probabilities and growth in groups established by N.Th. Varopoulos [**203**] and M. Gromov's characterization of groups of polynomial growth (see, e.g., [**203**, Chapter VI.6], [**209**, Theorem 3.24]).

Theorem 8.34 (N.Th. Varopoulos). *The following assertions are equivalent:*

(i) G *is recurrent,*
(ii) *The growth function* γ_{G} *has polynomial growth of degree at most two, i.e.,* $\gamma_{\mathsf{G}}(n) \le C(1+n^2)$ *for all* $n \in \mathbb{Z}_{\ge 0}$,
(iii) G *contains a finite index subgroup isomorphic either to* $\mathbb{Z}$ *or to* $\mathbb{Z}^2$.

Remark 8.35. In fact, the original statement is much stronger. Suppose $\mathfrak{p}$ is a symmetric probability measure on G which generates G. It defines a random walk on G by setting $P(X_{n+1} = v \,|\, X_n = u) = \mathfrak{p}(\{u^{-1}v\})$, $u, v \in \mathsf{G}$. The problem to characterize groups admitting a recurrent random walk was formulated by H. Kesten in 1967. It turns out that only recurrent groups admit recurrent random walks. Moreover, if G is recurrent, then every random walk generated by a symmetric probability measure $\mathfrak{p}$ with finite second moment is recurrent (we refer to [**209**, Chap. I.3] for further details and information).

Therefore, we arrive at the following result.

Theorem 8.36. *Let* $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ *be a Cayley graph,* $(\mathcal{G}_C, \mu, \nu)$ *a weighted metric graph,* $\mathbf{H}_D$ *the corresponding Dirichlet Laplacian.*

(i) *If* G *is recurrent, i.e.,* G *contains a finite index subgroup isomorphic either to* $\mathbb{Z}$ *or to* $\mathbb{Z}^2$*, and the edge weight* ν *satisfies*

$$\sup_{e\in\mathcal{E}} \frac{\nu(e)}{|e|} < \infty, \tag{8.2.6}$$

then the heat semigroup $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ *is recurrent.*

(ii) *If* G *is transient (i.e.,* G *does not contain a finite index subgroup isomorphic either to* $\mathbb{Z}$ *or to* $\mathbb{Z}^2$*) and the edge weight* ν *satisfies*

$$\inf_{e\in\mathcal{E}} \frac{\nu(e)}{|e|} > 0, \tag{8.2.7}$$

then the heat semigroup $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ *is transient.*

Proof. The proof is a straightforward application of Corollary 8.33 and Theorem 8.34. Namely, Corollary 8.33 reduces the study of recurrence/transience for $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ to the study of recurrence/transience of the discrete time random walk (8.2.5) on G. On the other hand, the energy form of the simple random walk on $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ is given by

$$\mathfrak{q}_{\mathsf{G},S}[f] = \frac{1}{2}\sum_{v\in\mathsf{G}}\sum_{u\in S} |f(v) - f(u^{-1}v)|^2.$$

By definition, G is recurrent/transient if and only if the energy form $\mathfrak{q}_{\mathsf{G},S}$ is recurrent/transient. Taking into account that the energy form associated with the random walk (8.2.5) is given by

$$\mathfrak{q}_{\nu}[f] = \frac{1}{2}\sum_{v\in\mathsf{G}}\sum_{u\in S} \frac{\nu(e_{u,v})}{|e_{u,v}|}|f(v) - f(u^{-1}v)|^2,$$

it remains to use Lemma B.7 to complete the proof of both claims. □

Let us finish this subsection with one immediate corollary.

Corollary 8.37. *Let* $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ *be a Cayley graph and let* $(\mathcal{G}_C, |\cdot|)$ *be an unweighted metric graph,* $\mu = \nu \equiv \mathbb{1}$*.*

(i) *If* G *contains a finite index subgroup isomorphic either to* $\mathbb{Z}$ *or to* $\mathbb{Z}^2$ *and* $\inf_{e\in\mathcal{E}} |e| > 0$*, then* $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ *is recurrent.*

(ii) *If* G *does not contain a finite index subgroup isomorphic either to* $\mathbb{Z}$ *or to* $\mathbb{Z}^2$ *and* $\sup_{e\in\mathcal{E}} |e| < \infty$*, then the heat semigroup* $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ *is transient.*

Remark 8.38. A few remarks are in order.

(i) If $\mathsf{G} = (\mathbb{Z}, +)$ and $\mathcal{C}$ is the Cayley graph of G with the standard set of generators $S = \{-1, 1\}$, one can show (cf. Lemma 5.13) that $(\mathrm{e}^{-t\mathbf{H}_D})$ is recurrent if and only if

$$\sum_{n\in\mathbb{Z}_{<0}} \frac{|e_n|}{\nu_n} = \infty, \qquad \text{and} \qquad \sum_{n\in\mathbb{Z}_{>0}} \frac{|e_n|}{\nu_n} = \infty. \tag{8.2.8}$$

(ii) Using the volume test, one can slightly improve both Theorem 8.36(i) and Corollary 8.37(i) in the case when G contains a finite index subgroup isomorphic to $\mathbb{Z}^2$.

(iii) Applying the volume test (Section 7.4), one may obtain some sufficient conditions for recurrence for groups which grow faster than quadratic polynomials, however, in this case one needs to know the qualitative behavior of the corresponding growth function.

8.2.5. Ultracontractivity and eigenvalue estimates. In fact, the results in the previous section have a number of further and much stronger consequences. However, to simplify the exposition we restrict to unweighted metric graphs, that is, we shall assume throughout this subsection that $\mu = \nu \equiv \mathbb{1}$ on $\mathcal{G}$.

We begin with the following result.

THEOREM 8.39. *Let $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ be a Cayley graph, $(\mathcal{G}_C, |\cdot|)$ a (unweighted) metric graph, and $\mathbf{H}_D$ the corresponding Dirichlet Laplacian. Assume also that G is not recurrent (i.e., it does not contain a finite index subgroup isomorphic either to $\mathbb{Z}$ or to $\mathbb{Z}^2$) and the edge lengths satisfy*

$$\sup_{e\in\mathcal{E}} |e| < \infty. \tag{8.2.9}$$

Then $(\mathrm{e}^{-t\mathbf{H}_D})_{t>0}$ is ultracontractive and, moreover,

(i) *If $\gamma_{\mathsf{G}}(n) \approx n^N$ as $n \to \infty$ with some $N \in \mathbb{Z}_{\geq 3}$, then*

$$\|\mathrm{e}^{-t\mathbf{H}_D}\|_{1\to\infty} \leq C_N t^{-N/2}, \qquad t > 0. \tag{8.2.10}$$

(ii) *If G is not virtually nilpotent (i.e., γ_{G} has superpolynomial growth†), then (8.2.10) holds true for all $N > 2$.*

PROOF. Notice that we only need to prove (8.2.10) since ultracontractivity is its immediate consequence. By Theorem 4.30, (8.2.10) is equivalent to the analogous ultracontractivity bound for the associated weighted graph Laplacian $\mathbf{h}_D$:

$$\|\mathrm{e}^{-t\mathbf{h}_D}\|_{1\to\infty} \leq C t^{-N/2}, \qquad t > 0. \tag{8.2.11}$$

However, by Theorem C.2) the latter is equivalent to the Sobolev-type inequality (4.8.6):

$$\Big(\sum_{v\in\mathsf{G}} |f(v)|^{\frac{2N}{N-2}} m(v)\Big)^2 \leq C \sum_{v\in\mathsf{G}}\sum_{u\in S} \frac{1}{|e_{u,v}|} |f(v) - f(u^{-1}v)|^2, \tag{8.2.12}$$

for all $f \in \mathrm{dom}(\mathfrak{q}_D)$. Here the vertex weight m is given by (take into account that the model has finite size by assumption and $\mu \equiv \mathbb{1}$)

$$m(v) = \sum_{u\in S} |e_{v,uv}|. \tag{8.2.13}$$

However, (8.2.9) implies that (8.2.12) would follow from the inequality

$$\Big(\sum_{v\in\mathsf{G}} |f(v)|^{\frac{2N}{N-2}}\Big)^2 \leq C \sum_{v\in\mathsf{G}}\sum_{u\in S} |f(v) - f(u^{-1}v)|^2. \tag{8.2.14}$$

Now it remains to notice that the latter inequality is a consequence of our growth assumptions on G. If γ_{G} grows polynomially and $\gamma_{\mathsf{G}}(n) \approx n^N$ for some $N \geq 3$ as $n \to \infty$, then (8.2.14) holds true by [**203**, Theorem VI.5.2]). If G is not virtually nilpotent, then, by the Gromov theorem, γ_{G} has superpolynomial growth and it remains to apply [**203**, Theorem VI.3.2]. □

†This means that for each $N > 0$ there is $c > 0$ such that $\gamma_{\mathsf{G}}(n) \geq cn^N$ for all large n.

REMARK 8.40. Let us stress that (8.2.9) is necessary for the validity of (8.2.10) with $N > 2$ (see Lemma 4.32).

For groups having at most quadratic growth, the next result is an immediate consequence of recurrence:

COROLLARY 8.41. *Let* G *be recurrent (i.e.,* G *contains a finite index subgroup isomorphic either to* $\mathbb{Z}$ *or to* $\mathbb{Z}^2$*). Let also* $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ *be its Cayley graph and* $(\mathcal{G}_C, |\cdot|)$ *an unweighted metric graph. If* $\inf_{e\in\mathcal{E}} |e| > 0$*, then*

$$\limsup_{t>0} t\,\|\mathrm{e}^{-t\mathbf{H}_D}\|_{1\to\infty} \in (0, \infty].$$

Let us mention that removing the assumption $\inf_{e\in\mathcal{E}} |e| > 0$ in the above corollary, one may construct metric graphs such that the corresponding Dirichlet Laplacian satisfies (8.2.10) with some $N > 2$.

We would like to finish this subsection with a remark on the so-called Cwikel–Lieb–Rozenblum inequality. Let us consider Laplacians $\mathbf{H}_\alpha$ with δ-couplings on the vertices, that is, $\alpha\colon \mathsf{G} \to \mathbb{R}$ and at each vertex $v \in \mathsf{G}$ we replace the Kirchhoff condition by (2.4.5). As before, if $\mathbf{H}_\alpha$ is not self-adjoint, we shall consider the Friedrichs extension of the minimal operator (of course, if it is bounded from below) and by abusing the notation we shall denote it by the same letter $\mathbf{H}_\alpha$. Moreover, we shall use the standard notation $\alpha_\pm = (|\alpha| \pm \alpha)/2$.

THEOREM 8.42. *Let* $\mathcal{G}_C = \mathcal{C}(\mathsf{G}, S)$ *be a Cayley graph,* $(\mathcal{G}_C, |\cdot|)$ *a (unweighted) metric graph,* $\alpha\colon \mathsf{G} \to \mathbb{R}$*, and* $\mathbf{H}_\alpha$ *the corresponding Laplacian.*

(i) *If* $\gamma_{\mathsf{G}}(n) \le C(1 + n^2)$ *for all* n *and* $\inf_{e\in\mathcal{E}} |e| > 0$*, then* $\mathbf{H}_\alpha$ *has at least one negative eigenvalue whenever* $0 \not\equiv \alpha = -\alpha_- \in C_c(\mathcal{V})$.

(ii) *If* $\gamma_{\mathsf{G}}(n) \asymp n^N$ *as* $n \to \infty$ *with some* $N \in \mathbb{Z}_{\ge 3}$ *and* (8.2.9) *is satisfied, then the operator* $\mathbf{H}_\alpha$ *is bounded below whenever* $\alpha_-/m \in \ell^{N/2}(\mathsf{G}; m)$*. Moreover, its negative spectrum is discrete and*

$$\kappa_-(\mathbf{H}_\alpha) \le C \sum_{v\in\mathsf{G}} \alpha_-(v)^{N/2} m(v)^{1-N/2}, \tag{8.2.15}$$

where m *is given by* (8.2.13) *and the constant* $C > 0$ *depends only on the underlying metric graph.*

(iii) *If* G *is not virtually nilpotent,* (8.2.9) *is satisfied and* $\alpha_- \in \ell^{N/2}(\mathsf{G}; m)$ *for some* $N > 2$*, then the operator* $\mathbf{H}_\alpha$ *is bounded below, its negative spectrum is discrete and the bound* (8.2.15) *holds true.*

PROOF. To simplify the proof, let us assume that $\mathbf{H}_\alpha$ is self-adjoint.[†] First of all, by Theorem 3.1(iv), $\kappa_-(\mathbf{H}_\alpha) = \kappa_-(\mathbf{h}_\alpha)$ and hence we need to prove the corresponding claims for $\mathbf{h}_\alpha$.

(i) By Corollary 8.37(i) and Theorem 4.17, the heat semigroup generated by $\mathbf{h}_D$ is recurrent, which immediately implies the claim.

To prove (ii) and (iii) we just need to apply Theorem 1.2 and Theorem 1.3 from [**150**], which relate the ultracontractivity estimates established by Theorem 8.39 and Theorem 4.30 for $\mathbf{h}_\alpha$ with Cwikel–Lieb–Rozenblum bounds. □

[†]One may assume that $\mathcal{G}_C$ is complete w.r.t. the natural path metric, and then by Theorem 7.9, the operator $\mathbf{H}_\alpha$ is self-adjoint once it is bounded from below; see also Lemma 7.16.

REMARK 8.43. Notice that applying Theorem 1.2 and Theorem 1.3 from [**150**] directly to the Dirichlet Laplacian $\mathbf{H}_D$ we arrive at the Cwikel–Lieb–Rozenblum estimates for additive perturbation, that is, for Schrödinger operators $-\Delta + V(x)$. It is also well known (see [**74**]) that ultracontractivity estimates and Sobolev-type inequalities lead to Lieb–Thirring bounds ($\mathfrak{S}_p$ estimates on the negative spectra, see also Theorem 3.1(viii)), however, we are not going to pursue this goal here.

Let us also stress that Theorem 8.42(iii) makes sense only for amenable G since otherwise $\mathbf{H}_D$ has a positive spectral gap (see Proposition 8.30).

8.2.6. Historical remarks and further references. The theory of random walks on groups was founded by H. Kesten [**139**] (in fact, in his PhD thesis). The idea to relate growth of groups with recurrence is also due to Kesten (*Kesten's conjecture*). The literature on the subject is enormous and in this respect we only refer to the excellent book by W. Woess [**209**].

Kesten's amenability criterion has been heavily exploited to study random walks on groups. However, we are aware of at least two cases when Kesten's criterion has been used in the "opposite" direction: S.I. Adyan in [**1**] proved that a simple random walk on the *free Burnside group* $\mathrm{B}(m,n)$ of rank $m \geq 2$ with odd exponent $n \geq 665$ has a spectral radius < 1, which implies non-amenability of $\mathrm{B}(m,n)$ for this range of m and n (notice that the latter also provides a counterexample to the so-called "von Neumann conjecture", disproved by A.Yu. Ol'shanskii in 1979); L. Bartholdi and B. Virág [**16**] proved that the so-called *Basilica group* is amenable by showing that return probabilities of the simple random walk decay at subexponential rates.

Let us mention that one of the motivations to investigate random walks on groups came from manifolds. By the Švarc–Milnor Lemma, the fundamental group $\pi_1(M)$ of a compact manifold M and its universal cover $\widetilde{M}$ are quasi-isometric and thus there are close relationships between them. For instance, it was proved independently by R. Brooks [**33**] and N.Th. Varopoulos [**200**] that the Laplace–Beltrami operator on $\widetilde{M}$ has a positive spectral gap if and only if $\pi_1(M)$ is not amenable. Moreover, Varopoulos [**200**] showed that the Brownian motion on $\widetilde{M}$ is recurrent if and only if the group $\pi_1(M)$ is recurrent.

The importance of Sobolev-type inequalities for ultracontractivity estimates was realized by N.Th. Varopoulos. The subject is enormous and we even did not touch here Nash-type inequalities. We refer for further details and references to [**203**], [**209**].

Concluding this section, let us mention recent very active work related to understanding spectra of groups. More specifically, the *spectrum of* G is the spectrum of a generator of a simple random walk on G, i.e., the spectrum of the normalized Laplacian (or, equivalently, combinatorial Laplacian since $\mathcal{C}(\mathsf{G}, S)$ is a regular graph) on a Cayley graph $\mathcal{C}(\mathsf{G}, S)$ of a given group G. The study of a spectral gap is the simplest (and rather widely studied) issue in this topic. In particular, to understand the support of the spectrum as well as its structure are much harder tasks. A complete picture is known only in some specific cases (e.g., abelian groups $(\mathbb{Z}^n, +)$, free group $\mathbb{F}_p$ [**139**], the Lamplighter group [**87**], however, this list is by no any means complete). In particular, it is not completely clear what kind of spectra groups may have (it is still open whether Cantor spectrum can occur on a Cayley graph, however, it is shown in [**35**] that the support of the Kesten–von Neumann–Serre spectral measure of the Basilica group is a Cantor set). Another interesting question is how the spectrum depends on the chosen generating set or on the choice of weights on the generators. The subject is rapidly developing and we only refer to a very brief selection of recent articles [**35**], [**48**], [**62**], [**86**] for further results and information.

8.3. Tessellations

In the present section, we discuss graphs arising from tessellations of $\mathbb{R}^2$ (see Figure 8.3 for examples) and combine their distinctive combinatorial properties with our previous findings.

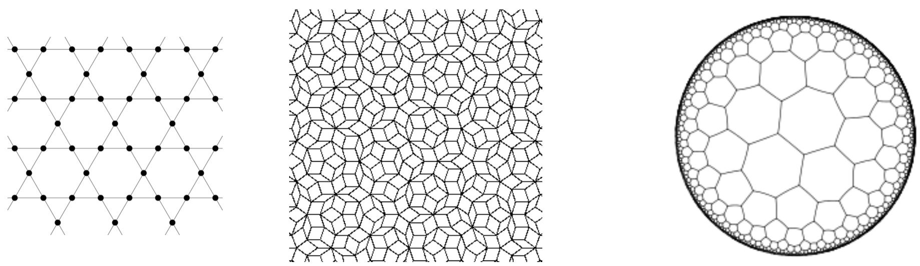

FIGURE 8.3. (a) The Kagome lattice, (b) a Penrose tiling in $\mathbb{R}^2$ and (c) a tessellation of the Poincaré disc by heptagons (see p. 163 for image credit).

In order to formalize this setting, we first need a few definitions. Recall that a *plane graph* is a planar graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ embedded in $\mathbb{R}^2$ by some fixed planar embedding. In particular, any plane graph $\mathcal{G}_d$ can be regarded as a subset of the Euclidian plane $\mathbb{R}^2$, which we always assume to be closed. We denote by $\mathcal{F}$ the set of *faces* of $\mathcal{G}_d$, i.e., the closures of the connected components of $\mathbb{R}^2 \setminus \mathcal{G}_d$. We stress that, since $\mathcal{G}_d$ may be infinite, it may have several unbounded faces and all of them are included in $\mathcal{F}$; we denote by $\mathcal{F}_b$ the set of *bounded faces* of $\mathcal{G}_d$.

In order to avoid technical difficulties, we impose the following assumptions.

DEFINITION 8.44. A plane graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ is *tessellating* if the following additional conditions hold:

- (i) $\mathcal{F}$ is locally finite, i.e., each compact subset $K \subset \mathbb{R}^2$ intersects only finitely many faces.
- (ii) Each bounded face $F \in \mathcal{F}_b$ is a closed topological disc and its boundary ∂F consists of a finite cycle of at least three edges.
- (iii) Each unbounded face $F \in \mathcal{F} \setminus \mathcal{F}_b$ is a closed topological half-plane and its boundary ∂F consists of a (countably) infinite chain of edges.
- (iv) $\#\mathcal{F}_e = 2$ for all $e \in \mathcal{E}$, where $\mathcal{F}_e := \{F \in \mathcal{F} \,|\, e \subset \partial F\}$.
- (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 an 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 face $F \in \mathcal{F}$, we define

$$\mathcal{E}_F := \{e \in \mathcal{E} \,|\, e \subseteq \partial F\}, \qquad d_{\mathcal{F}}(F) := \#\mathcal{E}_F, \tag{8.3.1}$$

where the latter is called the *degree* of a face $F \in \mathcal{F}$. Notice that according to Definition 8.44, $d_{\mathcal{F}}(F) \geq 3$ for all faces F and $\deg(v) \geq 3$ for all vertices v. In particular, the graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ has no loops and vertices of degree one or two. Moreover, every tessellating graph $\mathcal{G}_d$ is an infinite, locally finite graph.

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

REMARK 8.45. Tessellating graphs include all infinite trees $\mathcal{T} = (\mathcal{V}, \mathcal{E})$ satisfying $\deg(v) \geq 3$ for each vertex $v \in \mathcal{V}$.

A *plane weighted metric graph* is a weighted metric graph $(\mathcal{G}, \mu, \nu)$ together with a fixed model whose underlying combinatorial graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ is planar and embedded into $\mathbb{R}^2$. If the plane graph $\mathcal{G}_d$ is tessellating, then $(\mathcal{G}, \mu, \nu)$ is called a *tessellating weighted metric graph.* Let us also stress that the edge lengths and weights of $(\mathcal{G}, \mu, \nu)$ are in general not related to the Euclidian arc lengths of the corresponding plane graph $\mathcal{G}_d$.

REMARK 8.46. Notice that the fixed model in the definition of a tessellating weighted metric graph $(\mathcal{G}, \mu, \nu)$ is unique according to (v) in Definition 8.44, which excludes inessential vertices. Moreover, it is easily seen that the weighted metric graph $(\mathcal{G}, \mu, \nu)$ has *finite intrinsic size* exactly when this particular model has finite intrinsic size.

Notice that the fixed model in the definition of a tessellating weighted metric graph $(\mathcal{G}, \mu, \nu)$ is unique according to (v) in Definition 8.44, which excludes inessential vertices. Moreover, it is easily seen the weighted metric graph $(\mathcal{G}, \mu, \nu)$ has *finite intrinsic size* exactly when this particular model has finite intrinsic size. On the other hand, let us emphasize that the embedding of a planar graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ into $\mathbb{R}^2$ is not unique. For instance, the degree of the faces depends on the embedding (whereas their number is invariant by Euler's formula) and, in general, different embeddings lead to non-isomorphic dual graphs (see, e.g., [**72**, Chap. 5.5 and Fig. 5.7] for further details).

8.3.1. Markovian uniqueness. The combinatorial structure of plane graphs leads to simple criteria for Markovian uniqueness.

COROLLARY 8.47. *Let $(\mathcal{G}, \mu, \nu)$ be a tessellating graph such that all faces are bounded, $\mathcal{F} = \mathcal{F}_b$. Assume that either $1/\mu, 1/\nu \in L^\infty(\mathcal{G})$ or $\mathcal{G}$ has finite ν-diameter (see* (7.2.10)*). Then the following are equivalent:*

(i) $\mathbf{H}^0$ *admits a unique Markovian extension,*
(ii) $\mathbf{H}_D = \mathbf{H}_N$,
(iii) *the Gaffney Laplacian $\mathbf{H}_G$ is self-adjoint,*
(iv) $H^1_0(\mathcal{G}, \mu, \nu) = H^1(\mathcal{G}, \mu, \nu)$,
(v) *$\mathcal{G}$ has infinite volume, $\mu(\mathcal{G}) = \infty$.*

If one (equivalently, all) of the above properties fails, then the deficiency indices of the minimal Gaffney Laplacian $\mathbf{H}_{G,\min}$ are equal to

$$\mathrm{n}_\pm(\mathbf{H}_{G,\min}) = 1. \tag{8.3.2}$$

PROOF. The claims follows immediately from Theorem 7.24 (see also (7.2.10)) and the fact that $\mathcal{G}$ has exactly one graph end since $\mathcal{F} = \mathcal{F}_b$. □

REMARK 8.48. If $\mathcal{F}$ contains unbounded faces, then the graph might have more than one end. For instance, every infinite tree $\mathcal{T} = (\mathcal{G}, \mathcal{E})$ with $\deg(v) \geq 3$ for all $v \in \mathcal{V}$ can be embedded in $\mathbb{R}^2$ as a tessellating graph with infinitely many unbounded faces. On the other hand, $\mathcal{T}$ has uncountably many graph ends.

8.3.2. Spectral gap estimates. In this section, we discuss lower estimates for the isoperimetric constant of tessellating weighted metric graphs. To simplify our considerations, in this section we consider only weighted metric graphs with equal weight functions $(\mathcal{G}, \mu, \mu)$, that is, we assume that $\mu = \nu$. Without loss of generality we shall also assume that $(\mathcal{G}, \mu, \mu)$ has finite intrinsic size since otherwise

$$0 = \mathrm{Ch}(\mathcal{G}) = \lambda_0(\mathbf{H}_D),$$

according to Corollary 3.18 and the estimate (7.3.4). For each edge $e \in \mathcal{E}$ of $\mathcal{G}_d$, we define its *characteristic value* as

$$\mathbf{c}(e) := \frac{1}{|e|\mu(e)} - \sum_{v\colon v \in e} \frac{1}{m(v)} - \sum_{F \in \mathcal{F}_e \cap \mathcal{F}_b} \frac{1}{\mu(\partial F)}, \tag{8.3.3}$$

and also set

$$\mathbf{c}(\mathcal{E}) := \inf_{e \in \mathcal{E}} \mathbf{c}(e). \tag{8.3.4}$$

All summands on the RHS(8.3.3) admit a clear interpretation in terms of the edge weight μ:

- the first summand is the reciprocal of $\int_e \mu$,
- $m(v) = \sum_{e \in \mathcal{E}_v} |e|\mu(e) = \mu(\mathcal{E}_v) = \int_{\mathcal{E}_v} \mu$ because of finite intrinsic size,
- finally, $\mu(\partial F)$ is the weighted perimeter of F.

REMARK 8.49. A few remarks are in order.

(i) Setting $\mu(e) = |e| = 1$ for all $e \in \mathcal{E}$ in (8.3.3),

$$\mathbf{c}(e) = 1 - \sum_{v\colon v \in e} \frac{1}{\deg(v)} - \sum_{F \in \mathcal{F}_e \cap \mathcal{F}_b} \frac{1}{\deg(F)},$$

which coincides with the *characteristic number* $\phi(e)$ of edge e introduced in [**208**].

(ii) As is easily shown, the characteristic values $\mathbf{c}(e)$, $e \in \mathcal{E}$ depend on the embedding of the planar graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ in $\mathbb{R}^2$. Namely, the definition of $\mathbf{c}(e)$ takes into account all edges $e' \in \mathcal{E}$ which share a face with e, and this edge set depends heavily on the embedding.

(iii) As is discussed below in Section 8.3.3.2, the characteristic values are related to discrete curvature notions for plane graphs. However, our choice of the sign differs from the standard one in the literature and this explains why our results are formulated in terms of positive curvature.

It turns out that, if the weight function $\mu\colon \mathcal{G} \to (0, \infty)$ is uniformly positive on $\mathcal{G}$, that is, it additionally satisfies

$$1/\mu \in L^\infty(\mathcal{G}), \tag{8.3.5}$$

then the characteristic edge values give rise to lower estimates for the isoperimetric constant $\mathrm{Ch}(\mathcal{G})$.

THEOREM 8.50. *Let $(\mathcal{G},\mu,\mu)$ be a tessellating graph. Then*

$$\frac{\mathbf{c}(\mathcal{E})}{\|1/\mu\|_\infty} \le \mathrm{Ch}(\mathcal{G}). \tag{8.3.6}$$

In particular, if $\mathbf{c}(\mathcal{E}) \ge 0$, the following spectral estimate

$$\frac{1}{4}\Big(\frac{\mathbf{c}(\mathcal{E})}{\|1/\mu\|_\infty}\Big)^2 \le \lambda_0(\mathbf{H}_D) \tag{8.3.7}$$

holds true for the Dirichlet Laplacian $\mathbf{H}_D$.

The method of proof follows closely [**208**] and consists in a rather elegant application of *Euler's identity* for finite plane graphs $\mathcal{K} = (\mathcal{V}(\mathcal{K}), \mathcal{E}(\mathcal{K}))$,

$$\#\mathcal{V}(\mathcal{K}) - \#\mathcal{E}(\mathcal{K}) + \#\mathcal{F}_b(\mathcal{K}) = \#\mathcal{C}(\mathcal{K}). \tag{8.3.8}$$

where $\mathcal{F}_b(\mathcal{K})$ denotes the set of bounded faces of $\mathcal{K}$ and $\mathcal{C}(\mathcal{K})$ is the set of connected components of $\mathcal{K}$ (see, e.g., [**27**, Chap. 1.4]).

PROOF OF THEOREM 8.50. Notice that the estimates in Theorem 8.50 are trivial if $\mathbf{c}(\mathcal{E}) \le 0$, thus we can assume without loss of generality that $\mathbf{c}(\mathcal{E})$ is positive. Therefore, taking into account (7.31) and the Cheeger-type bound in Theorem 7.33, it suffices to prove that the estimate

$$\frac{\mathbf{c}(\mathcal{E})}{\|1/\mu\|_\infty} \le \frac{\mathrm{area}(\partial\mathcal{K})}{\mu(\mathcal{K})} \tag{8.3.9}$$

holds true for all finite subgraphs $\mathcal{K} = (\mathcal{V}(\mathcal{K}), \mathcal{E}(\mathcal{K}))$ of $\mathcal{G}_d$. Here (see (7.3.1) and (7.3.2))

$$\mu(\mathcal{K}) = \sum_{e\in\mathcal{E}(\mathcal{K})} \mu(e), \qquad \mathrm{area}(\partial\mathcal{K}) = \mathrm{area}(\partial\mathcal{K},\mu,\mu) = \sum_{v\in\partial\mathcal{K}} \sum_{e\in\mathcal{E}_v(\mathcal{K})} \mu(e),$$

where $\partial\mathcal{K} = \{v \in \mathcal{V}(\mathcal{K}) |\ \deg_{\mathcal{K}}(v) < \deg_{\mathcal{G}}(v)\}$. Clearly,

$$\mathbf{c}(\mathcal{E})\mu(\mathcal{K}) = \mathbf{c}(\mathcal{E}) \int_{\mathcal{K}} \mu(\mathrm{d}x) \le \int_{\mathcal{K}} \mathbf{c}(x)\mu(\mathrm{d}x),$$

and hence it is enough to show that

$$\int_{\mathcal{K}} \mathbf{c}(x)\,\mu(\mathrm{d}x) \le \|1/\mu\|_\infty\, \mathrm{area}(\partial\mathcal{K}).$$

By (8.3.3), the LHS in the above equation is equal to

$$\begin{aligned}\int_{\mathcal{K}} \mathbf{c}(x)\,\mu(\mathrm{d}x) &= \sum_{e\in\mathcal{E}(\mathcal{K})} \mathbf{c}(e)|e|\mu(e) \\ &= \#\mathcal{E}(\mathcal{K}) - \sum_{v\in\mathcal{V}} \frac{\mu(\mathcal{E}_v\cap\mathcal{E}(\mathcal{K}))}{m(v)} - \sum_{F\in\mathcal{F}_b} \frac{\mu(\mathcal{E}_F\cap\mathcal{E}(\mathcal{K}))}{\mu(\partial F)}.\end{aligned}$$

Notice that for a non-boundary vertex $v \in \mathcal{V}(\mathcal{K}) \setminus \partial\mathcal{K}$, the inequality

$$\mu(\mathcal{E}_v \cap \mathcal{E}(\mathcal{K})) = \mu(\mathcal{E}_v) = \sum_{e\in\mathcal{E}_v} \mu(e)|e| = m(v)$$

holds true (recall that our graph has finite intrinsic size and hence we have equality instead of $\ge$ on the RHS). Consider the subgraph $\mathcal{K}^\circ = (\mathcal{V}(\mathcal{K}^\circ), \mathcal{E}(\mathcal{K}^\circ))$ of $\mathcal{K}$ which consists of all vertices in $\mathcal{V}(\mathcal{K}^\circ) := \mathcal{V}(\mathcal{K}) \setminus \partial\mathcal{K}$ and all edges between such vertices.

Notice also that each face $F \in \mathcal{F}$ whose boundary consists only of edges in $\mathcal{K}^\circ$, that is $\partial F \subseteq \mathcal{E}(\mathcal{K}^\circ)$, defines a bounded face of $\mathcal{K}^\circ$ and satisfies

$$\mu(\mathcal{E}_F \cap \mathcal{E}(\mathcal{K})) = \mu(\mathcal{E}_F \cap \mathcal{E}(\mathcal{K}^\circ)) = \mu(\mathcal{E}_F) = \mu(\partial F).$$

Denoting by $\mathcal{P}(\mathcal{K}^\circ)$ the set of all such faces $F \in \mathcal{F}$, we arrive at the estimate

$$\int_{\mathcal{K}} \mathbf{c}(x)\, \mu(\mathrm{d}x) \le \#\mathcal{E}(\mathcal{K}) - \#\mathcal{V}(\mathcal{K}^\circ) - \#\mathcal{P}(\mathcal{K}^\circ). \tag{8.3.10}$$

Clearly, we also have the elementary inequality

$$\#(\mathcal{E}(\mathcal{K}) \setminus \mathcal{E}(\mathcal{K}^\circ)) \le \|1/\mu\|_\infty \operatorname{area}(\partial\mathcal{K}).$$

Hence, if all bounded faces of $\mathcal{K}^\circ$ are of the above form, that is,

$$\mathcal{F}_b(\mathcal{K}^\circ) = \mathcal{P}(\mathcal{K}^\circ), \tag{8.3.11}$$

we can apply Euler's formula (8.3.8) to the subgraph $\mathcal{K}^\circ$ and conclude that

$$\mathrm{RHS}\,(8.3.10) = \#\mathcal{E}(\mathcal{K}) - \#\mathcal{E}(\mathcal{K}^\circ) - \#\mathcal{C}(\mathcal{K}^\circ) \le \|1/\mu\|_\infty \operatorname{area}(\partial\mathcal{K}).$$

In particular, we have established the estimate (8.3.9) in this special case.

On the other hand, if (8.3.11) fails for some finite subgraph $\mathcal{K}$ of the fixed model, we can construct a new subgraph $\widehat{\mathcal{K}}$ by "filling up its holes". That is, we consider all faces $F \in \mathcal{F}$ which are contained in some bounded face F of $\mathcal{K}^\circ$ and add all vertices and edges of such faces to $\mathcal{K}$. It is easily shown that the obtained subgraph $\widehat{\mathcal{K}}$ satisfies the estimates

$$\mu(\mathcal{K}) \le \mu(\widehat{\mathcal{K}}) \qquad \text{and} \qquad \operatorname{area}(\partial\widehat{\mathcal{K}}) \le \operatorname{area}(\partial\mathcal{K}).$$

together with the condition (8.3.11). Hence the inequality (8.3.9) holds in the general case and the proof is complete. ☐

Remark 8.51. The estimate in Theorem 8.50 is not optimal and can be improved using methods similar to [**171**, Theorem 3.3], where the case $\mu = \nu \equiv \mathbb{1}$ was considered (see also [**136**, Theorem 1] and [**126**, Theorem 6]). On the other hand, these results look more technical and, for the sake of a clear exposition, we decided not to include them.

Notice that Theorem 8.50 applies to infinite trees:

Proposition 8.52. *Let $(\mathcal{T}, \mu, \mu)$ be a weighted metric tree having a model such that all vertices satisfy* $\deg(v) \ge 3$. *Then*

$$\mathrm{Ch}(\mathcal{G}) \ge \frac{1}{\|1/\mu\|_\infty} \inf_{e\in\mathcal{E}} \Big(\frac{1}{\mu(e)|e|} - \sum_{v\in e} \frac{1}{m(v)}\Big). \tag{8.3.12}$$

Example 8.53. Consider graphs depicted in Figure 8.3. For simplicity, we consider unweighted, equilateral metric graphs: $\mu = \nu \equiv \mathbb{1}$ and $|e| = 1$ for all $e \in \mathcal{E}$.

(a) *Kagome lattice*: all vertices have degree $\deg(v) = 3$ and each edge is adjacent to a triangle and a hexagon. In particular, the characteristic value of all edges $e \in \mathcal{E}$ is equal to

$$\mathbf{c}(e) = 1 - 2 \cdot \frac{1}{4} - \frac{1}{3} - \frac{1}{6} = 0.$$

(b) *Penrose tiling*: notice first that each face is a rhombus. However, the characteristic edge value is not constant in this case, since the degrees of the adjacent vertices vary. For instance, there are infinitely many edges $e = e_{uv}$ such that $\deg(u) = 3$ and $\deg(v) = 5$ and in this case

$$\mathbf{c}(e) = 1 - \frac{1}{3} - \frac{1}{5} - 2 \cdot \frac{1}{4} = -\frac{1}{30}.$$

(c) *Hyperbolic tessellation*: each face is a hyperbolic heptagon, hence $d_{\mathcal{F}}(F) = 5$ for all $F \in \mathcal{F}$ and all vertices have degree $\deg(v) = 3$. More generally, we can consider (p, q)-regular tessellations (i.e., $\deg(v) = p$ for all vertices v and $d_{\mathcal{F}}(F) = q$ for all faces F) for some $p \in \mathbb{Z}_{\geq 3}$ and $q \in \mathbb{Z}_{\geq 3} \cup \{\infty\}$ ($q = \infty$ corresponds to p-regular trees, in which case all faces are unbounded). In this case, the characteristic value $\mathbf{c}(e)$ of all edges $e \in \mathcal{E}$ is equal to

$$\mathbf{c}_{p,q} := 1 - \frac{2}{p} - \frac{2}{q}.$$

It turns out that $\mathbf{c}_{p,q} \geq 0$ for every (p, q)-regular tessellation of $\mathbb{R}^2$ (see, e.g., [**56**, Theorem 1.7]). Clearly, $\mathbf{c}_{p,q} = 0$ exactly when

$$(p, q) \in \{(4, 4), (3, 6), (6, 3)\},$$

and in these cases $\mathcal{G}_d$ is isomorphic to the square, hexagonal or triangle lattice in $\mathbb{R}^2$. In particular, one easily shows that $\mathrm{Ch}(\mathcal{G}) = 0$ in all three cases.

On the other hand, if $\mathbf{c}_{p,q} > 0$, then $\mathcal{G}_d$ is isomorphic to the edge graph of a tessellation of the Poincaré disc $\mathbb{H}^2$ with regular q-gons of interior angle $2\pi/p$ (see [**96**, Rem. 4.2]). Moreover, Theorem 8.50 implies that $\mathrm{Ch}(\mathcal{G}) > 0$. The explicit value is given by (see [**171**, eq. (4.6)])

$$\mathrm{Ch}(\mathcal{G}_{p,q}) = \frac{p-2}{p - 1 + \frac{p}{2}\left(\sqrt{\frac{(p-2)(q-2)}{pq-2(p+q)}} - 1\right)} \tag{8.3.13}$$

and can be found from results on isoperimetric constants of discrete graphs (see [**96**], [**103**]).

Notice that Theorem 8.50 leads to trivial bounds for the Kagome lattice and the Penrose tiling in Example 8.53. However, one can easily show directly that $\mathrm{Ch}(\mathcal{G}) = 0$ for these examples. It turns out that these graphs actually satisfy a stronger property:

PROPOSITION 8.54. *Let $(\mathcal{G}, \mu, \mu)$ be a tessellating graph such that $\inf_{e\in\mathcal{E}} |e| > 0$ and $\sup_{F\in\mathcal{F}} \mu(\partial F) < \infty$. Suppose further that*

$$\inf_{F\in\mathcal{F}} \mathrm{mes}(F) > 0 \qquad \text{and} \qquad \sup_{F\in\mathcal{F}} \sup_{x,y\in\partial F} \|x - y\|_{\mathbb{R}^2} < \infty,$$

where $\mathrm{mes}(F)$ denotes the Lebesgue measure of the subset $F \subseteq \mathbb{R}^2$ and $\|x - y\|_{\mathbb{R}^2}$ is the Euclidian distance in $\mathbb{R}^2$. Then the Kirchhoff Laplacian $\mathbf{H}$ is self-adjoint and the corresponding heat semigroup $(\mathrm{e}^{-t\mathbf{H}})_{t>0}$ is recurrent. In particular,

$$\lambda_0(\mathbf{H}) = \mathrm{Ch}(\mathcal{G}) = 0.$$

PROOF. Under the above assumptions, the intrinsic metric ϱ_η of $(\mathcal{G}, \mu, \mu)$ coincides with the length metric ϱ_0 and $(\mathcal{G}, \varrho_0)$ is complete. Hence, by Theorem 7.1, the Kirchhoff Laplacian $\mathbf{H}$ is self-adjoint. Moreover, by Theorem 7.42, it suffices to prove that

$$\mu(B_r(x)) = O(r^2) \qquad \text{as } r \to \infty$$

for some fixed (and hence all) points x on $\mathcal{G}$. Here, $B_r(x) = B_r(x; \varrho_0) \subset \mathcal{G}$ denotes the distance ball of radius r centered at $x \in \mathcal{G}$ with respect to the length metric ϱ_0.

By assumption, the Lebesgue measure of all faces F of $\mathcal{G}$ is uniformly bounded below. Using the condition on the diameter of the faces, it follows that for some uniform constant $b > 0$, each Euclidian ball in $\mathbb{R}^2$ of (large) radius r can intersect at most br^2 faces of $\mathcal{G}$. Moreover, observe that for some $a > 0$,

$$\|u - v\|_{\mathbb{R}^2} \le a\varrho_0(u, v), \qquad u, v \in \mathcal{V}.$$

Indeed, by our assumptions, the length $|e|$ of each edge $e \in \mathcal{E}$ is comparable to the distance of its endpoints in $\mathbb{R}^2$ and the estimate immediately follows. Altogether, for every vertex $u \in \mathcal{V}$ and large r,

$$\frac{\mu(B_r(u))}{\sup_{F\in\mathcal{F}} \mu(\partial F)} \le \#\big\{F \in \mathcal{F} \,|\, \partial F \cap \mathcal{V} \cap B_r(u) \ne \varnothing\big\} \le ba^2r^2$$

and this completes the proof. □

Remark 8.55. A few remarks are in order.

- (i) The recurrence of random walks on edge graphs of tessellations was studied by P.M. Soardi [**190**] and W. Woess [**209**]. By [**209**, Theorem 6.29], the simple random walk on the edge graph of every quasi-regular tessellation of $\mathbb{R}^2$ is recurrent (see [**209**, Def. 6.28] for definitions and [**190**] for a preceding result). In fact, [**209**, Theorem 6.29] can be used to show that Proposition 8.54 holds for weighted metric graphs on quasi-regular tessellations, allowing general edge lengths and weights $\mu \ne \nu$ with the only assumption (8.2.6) (see the proof of Theorem 8.36). However, the assumptions in Proposition 8.54 allow to give an elegant short proof and we decided to include only this elementary statement.
- (ii) The same arguments apply in case when $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ is an infinite semiplanar graph with nonnegative vertex curvature (see [**109**], [**110**] for details and definitions). Again, in this case [**109**, Theorem 1.3] implies that the simple random walk on $\mathcal{G}_d$ is recurrent, and under the assumption (8.2.6), the same holds for the semigroup $(e^{-t\mathbf{H}_D})_{t>0}$ on a weighted metric graph $(\mathcal{G}, \mu, \nu)$ over $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$.

8.3.3. Historical remarks and further comments.

8.3.3.1. *Markovian uniqueness.* The strong assumptions on the weights in Corollary 8.47 are indeed necessary. For instance, it was proved in [**39**] (see also [**21**], [**22**] for preceding results) that every locally finite, *vertex-nonamenable*† planar graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ admits a non-constant L_{comb}-harmonic function of finite energy, where L_{comb} is the combinatorial Laplacian from Example 6.7. Notice that all graphs $\mathcal{G}_{p,q}$ in Example 8.53(iii) with $\mathbf{c}_{p,q} > 0$ are vertex-nonamenable and have exactly one graph end if $q < \infty$. Hence, setting $|e| = \nu(e) = 1$ for all edges $e \in \mathcal{E}$, one can

†This means that there is some $\varepsilon > 0$ such that $\#\{u \in \mathcal{V} \setminus X \,|\, \exists v \in X \text{ with } u \sim v\} \ge \varepsilon \# X$ for all finite vertex sets $X \subset \mathcal{V}$.

obtain a weighted metric graph $(\mathcal{G}_{p,q}, \mu, \nu)$ admitting at least two linearly independent harmonic functions of finite energy. Choosing edge weights μ sufficiently small, these finite energy harmonic functions would also belong to H^1. In particular, this immediately implies that the corresponding (minimal) Gaffney Laplacian has deficiency indices $\mathrm{n}_\pm(\mathbf{H}_{G,\min}) \geq 2$ regardless of the number of ends (for example, one can choose μ sufficiently small in order to ensure a positive spectral gap).

8.3.3.2. *Discrete curvature for plane graphs.* The results in Section 8.3.2 can also be seen in context with *discrete curvature notions for plane graphs* and their relation to geometric properties. Going back to earlier works such as [**93**], [**116**], [**194**], several notions of curvature have been introduced for plane graphs and they have been used to investigate their geometric properties (see, e.g., the survey [**128**] and the works [**19**], [**56**], [**96**], [**102**], [**109**], [**110**], [**126**], [**136**], [**175**], [**194**], [**208**], [**215**]). In particular, these curvature notions have been used to investigate isoperimetric constants (see, e.g., [**102**], [**136**], [**171**], [**174**], [**175**], [**208**], [**215**]) and the obtained spectral estimates resemble an estimate by H.P. McKean in the manifold setting [**164**]. In the unweighted case $\mu = \nu \equiv \mathbb{1}$, the characteristic edge values (8.3.3) coincide with the ones introduced in [**208**], [**171**] for (unweighted) discrete and metric graphs, respectively (up to the choice of sign). Theorem 8.50 can be seen as the analogue of [**171**, eq. (1.3)] in the weighted setting.

8.3.3.3. *Parabolic properties.* The above recurrence results (see Proposition 8.54 and Remark 8.55) are also connected to the notion of quasi-isometries between metric spaces (see Remark 6.29). In fact, by [**190**, Theorem 4.11] the edge graph of every normal tessellation of $\mathbb{R}^2$ is quasi-isometric to $\mathbb{R}^2$ and in this case, the recurrence of the associated discrete Laplacians (and related Kirchhoff Laplacians on metric graphs) follows from the equivalence of recurrence between quasi-isometric spaces, see [**46**, Théorème 7.2] and also [**121**], [**158**]. Clearly, similar considerations apply to (sufficiently well-behaved) tessellations of other two-dimensional Riemannian manifolds (e.g., the Poincaré disc), however, we cannot point to an explicit reference. On the other hand, it should be stressed that the quasi-isometry property breaks down for general quasi-regular tessellations of $\mathbb{R}^2$ (see [**190**, Section 7]) and hence the results of [**190**], [**209**] indeed go beyond this setting.

As for the question of stochastic completeness on weighted tessellating graphs, one can either proceed with the volume tests or by employing various curvature conditions. Notice that, similar to the manifold setting, stochastic incompleteness is related to a very fast decay of curvature to negative infinity (see, e.g., [**211**, § 8]).

8.3.4. Image credit for Figure 8.3. *(a) Kagome lattice:*
WilliamSix, CC BY-SA 2.5, via Wikimedia Commons;
`https://commons.wikimedia.org/wiki/File:Kagome-lattice-bw.svg`

(b) Penrose tiling in $\mathbb{R}^2$:
xJaMderivative work: Sprak, Public domain, via Wikimedia Commons;
`https://commons.wikimedia.org/wiki/File:Pen0305c.svg`

(c) Tessellation of the Poincaré disc by heptagons:
Theon, CC BY-SA 3.0, via Wikimedia Commons;
`https://commons.wikimedia.org/wiki/File:PavageHypPoincare2.svg`

APPENDIX A

Boundary triplets and Weyl functions

A.1. Linear relations

Let $\mathcal{H}$ be a separable Hilbert space. A *(closed) linear relation* in $\mathcal{H}$ is a (closed) linear subspace in $\mathcal{H} \times \mathcal{H}$. The set of all closed linear relations is denoted by $\widetilde{\mathcal{C}}(\mathcal{H})$. Since every linear operator in $\mathcal{H}$ can be identified with its graph, the set of linear operators can be seen as a subset of all linear relations in $\mathcal{H}$. In particular, the set of closed linear operators $\mathcal{C}(\mathcal{H})$ is a subset of $\widetilde{\mathcal{C}}(\mathcal{H})$.

Recall that the domain, the range, the kernel and the multivalued part of a linear relation Θ are given, respectively, by

$$\begin{aligned} \mathrm{dom}(\Theta) &= \{f \in \mathcal{H} \,|\, \exists g \in \mathcal{H} \text{ such that } (f,g) \in \Theta\}, \\ \mathrm{ran}(\Theta) &= \{g \in \mathcal{H} \,|\, \exists f \in \mathcal{H} \text{ such that } (f,g) \in \Theta\}, \\ \ker(\Theta) &= \{f \in \mathcal{H} \,|\, (f,0) \in \Theta\}, \\ \mathrm{mul}(\Theta) &= \{g \in \mathcal{H} \,|\, (0,g) \in \Theta\}. \end{aligned}$$

The adjoint linear relation Θ^* is defined by

$$\Theta^* = \big\{(\tilde f, \tilde g) \in \mathcal{H} \times \mathcal{H} \,|\, \langle g, \tilde f\rangle_{\mathcal{H}} = \langle f, \tilde g\rangle_{\mathcal{H}} \text{ for all } (f,g) \in \Theta\big\}.$$

Θ is called *symmetric* if $\Theta \subseteq \Theta^*$. If $\Theta = \Theta^*$, then it is called *self-adjoint*. Note that $\mathrm{mul}(\Theta)$ is orthogonal to $\mathrm{dom}(\Theta)$ if Θ is symmetric. For a closed symmetric Θ satisfying $\mathrm{mul}(\Theta) = \mathrm{mul}(\Theta^*)$ (the latter is further equivalent to the fact that Θ is densely defined on $\mathrm{mul}(\Theta)^\perp$), setting $\mathcal{H}_{\mathrm{op}} := \overline{\mathrm{dom}(\Theta)} = \mathrm{mul}(\Theta)^\perp$ we obtain the following orthogonal decomposition

$$\Theta = \Theta_{\mathrm{op}} \oplus \Theta_\infty, \tag{A.1.1}$$

where $\Theta_\infty = \{0\} \times \mathrm{mul}(\Theta)$ and Θ_{op} is the graph of a closed symmetric linear operator in $\mathcal{H}_{\mathrm{op}}$, called the *operator part* of Θ. Notice that for non-closed symmetric linear relations the decomposition (A.1.1) may not hold true as the next example shows.

EXAMPLE A.1. Let $\mathcal{H} = \mathcal{H}_{\mathrm{op}} \oplus \mathcal{M}$, where $\mathcal{H}_{\mathrm{op}}$ and $\mathcal{M}$ are closed infinite-dimensional subspaces. Suppose A_0 is a non-closed, densely defined symmetric operator in $\mathcal{H}_{\mathrm{op}}$ and $\mathcal{M}_0 \subsetneq \mathcal{M}$ a non-closed subspace such that $\overline{\mathcal{M}_0} = \mathcal{M}$. Let A be the closure of A_0, fix $f_0 \in \mathrm{dom}(A) \setminus \mathrm{dom}(A_0)$ and $g_0 \in \mathcal{M} \setminus \mathcal{M}_0$ and define

$$\mathbf{f}_0 = (f_0, g_0 + Af_0) \in \Theta := \mathrm{Gr}(A) \oplus (\{0\} \times \mathcal{M}),$$

where $\mathrm{Gr}(A)$ is the graph of A. Define the linear relation Θ_0 as the linear (non-closed) span of $\mathrm{Gr}(A_0) \oplus (\{0\} \times \mathcal{M}_0)$ and $\mathbf{f}_0$. Clearly, $\Theta_0 \subsetneq \Theta$ and hence it is symmetric. Moreover, by construction $\overline{\mathrm{dom}(\Theta_0)} = \mathrm{mul}(\Theta_0)^\perp$. However, (A.1.1) fails to hold for Θ_0. Indeed, if P_2 is the projection in $\mathcal{H} \times \mathcal{H}$ onto the second component and $P_{\mathcal{M}}$ is the projection in $\mathcal{H}$ onto $\mathcal{M}$, then (A.1.1) would imply $\mathcal{M}_0 = \mathrm{mul}(\Theta_0) = P_M P_2(\Theta_0)$. However,

$$g_0 = P_M(g_0 + Af_0) = P_M P_2 \mathbf{f}_0 \notin \mathcal{M}_0.$$

This is a clear contradiction to the definition of Θ_0. ◊

The inverse of the linear relation Θ is given by

$$\Theta^{-1} = \{(g,f) \in \mathcal{H} \times \mathcal{H} \,|\, (f,g) \in \Theta\}.$$

The sum of linear relations Θ_1 and Θ_2 is defined by

$$\Theta_1 + \Theta_2 = \{(f, g_1 + g_2) \,|\, (f,g_1) \in \Theta_1,\ (f,g_2) \in \Theta_2\}.$$

Hence one can introduce the resolvent $(\Theta - z)^{-1}$ of the linear relation Θ, which is well defined for all $z \in \mathbb{C}$. However, the set of those $z \in \mathbb{C}$ for which $(\Theta - z)^{-1}$ is the graph of a closed bounded operator in $\mathcal{H}$ is called the *resolvent set* of Θ and is denoted by $\rho(\Theta)$. Its complement $\sigma(\Theta) = \mathbb{C} \setminus \rho(\Theta)$ is called the *spectrum* of Θ. If Θ is self-adjoint, then taking into account (A.1.1) we obtain

$$(\Theta - z)^{-1} = (\Theta_{\mathrm{op}} - z)^{-1} \oplus \mathbb{O}_{\mathrm{mul}(\Theta)}. \tag{A.1.2}$$

This immediately implies that $\rho(\Theta) = \rho(\Theta_{\mathrm{op}})$, $\sigma(\Theta) = \sigma(\Theta_{\mathrm{op}})$ and, moreover, one can introduce the spectral types of Θ as those of its operator part Θ_{op}. Let us mention that self-adjoint linear relations admit a very convenient representation, which was first observed by F.S. Rofe-Beketov [**185**] in the finite dimensional case (see also [**188**, Exercises 14.9.3-4]).[†]

Proposition A.2. *Let C and D be closed bounded operators on $\mathcal{H}$ and*

$$\Theta_{C,D} := \big\{(f,g) \in \mathcal{H} \times \mathcal{H} \,|\, Cf = Dg\big\}. \tag{A.1.3}$$

Then $\Theta_{C,D}$ is self-adjoint if and only if

$$CD^* = DC^*, \qquad \ker\begin{pmatrix} C & -D \\ D & C \end{pmatrix} = \{0\}. \tag{A.1.4}$$

The second condition in (A.1.4) *is equivalent to* $\mathrm{rank}(C|D) = \dim(\mathcal{H})$ *whenever* $\dim(\mathcal{H}) < \infty$.

We also need the following definition. For a symmetric linear relation Θ in $\mathcal{H}$, its defect subspace at $z \in \mathbb{C}$ is defined by $\mathcal{N}_z(\Theta) = \ker(\Theta^* - z)$. The numbers

$$\mathrm{n}_\pm(\Theta) := \dim \mathcal{N}_{\pm \mathrm{i}}(\Theta) = \dim\ker(\Theta^* \mp \mathrm{i})$$

are called the deficiency indices of Θ.

Let us mention that the adjoint relation $\Theta^*_{C,D}$ to $\Theta_{C,D}$ is given by

$$\Theta^*_{C,D} = \overline{\big\{(D^*f, C^*f) \,|\, f \in \mathcal{H}\big\}}.$$

In particular, $\Theta^*_{C,D}$ is symmetric exactly when the first equality in (A.1.4) holds true. Moreover, in this case the deficiency indices are given by

$$\mathrm{n}_\pm(\Theta^*_{C,D}) = \dim\ker(C \mp \mathrm{i}D).$$

Further details and facts about linear relations in Hilbert spaces can be found in, e.g., [**55**, Chap. 6.1], [**188**, Chap. 14].

[†]This representation was rediscovered later by many authors; in the context of self-adjoint vertex conditions for metric graphs, the reference usually goes to [**148**].

A.2. Boundary triplets and proper extensions

Let A be a densely defined closed symmetric operator in a separable Hilbert space $\mathfrak{H}$ with equal deficiency indices $\mathrm{n}_\pm(A) = \dim \mathcal{N}_{\pm\mathrm{i}} \le \infty$, $\mathcal{N}_z := \ker(A^* - z)$.

DEFINITION A.3 ([**85**]). A triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is called *a boundary triplet* for the adjoint operator A^* if $\mathcal{H}$ is a Hilbert space and $\Gamma_0, \Gamma_1 \colon \mathrm{dom}(A^*) \to \mathcal{H}$ are bounded linear mappings such that the abstract Green's identity

$$\langle A^* f, g\rangle_{\mathfrak{H}} - \langle f, A^* g\rangle_{\mathfrak{H}} = \langle \Gamma_1 f, \Gamma_0 g\rangle_{\mathcal{H}} - \langle \Gamma_0 f, \Gamma_1 g\rangle_{\mathcal{H}} \tag{A.2.1}$$

holds for all $f, g \in \mathrm{dom}(A^*)$ and the mapping

$$\begin{array}{llcl} \Gamma\colon & \mathrm{dom}(A^*) & \to & \mathcal{H}\times\mathcal{H} \\ & f & \mapsto & (\Gamma_0 f, \Gamma_1 f) \end{array} \tag{A.2.2}$$

is surjective.

A boundary triplet for A^* exists if and only if the deficiency indices of A are equal (see, e.g., [**55**, Prop. 7.4], [**188**, Prop. 14.5]). Moreover, $\mathrm{n}_\pm(A) = \dim(\mathcal{H})$ and $A = A^* \upharpoonright \ker(\Gamma)$. Note also that the boundary triplet for A^* is not unique.

An extension $\tilde{A}$ of A is called *proper* if $\mathrm{dom}(A) \subset \mathrm{dom}(\tilde{A}) \subset \mathrm{dom}(A^*)$. The set of all proper extensions is denoted by $\mathrm{Ext}(A)$.

THEOREM A.4 ([**54, 155**]). *Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^*. Then the mapping Γ defines a bijective correspondence between $\mathrm{Ext}(A)$ and the set of all linear relations in $\mathcal{H}$:*

$$\Theta \mapsto A_\Theta := A^* \upharpoonright \{f \in \mathrm{dom}(A^*) \,|\; \Gamma f = (\Gamma_0 f, \Gamma_1 f) \in \Theta\}. \tag{A.2.3}$$

Moreover, the following holds:

(i) $A_\Theta^* = A_{\Theta^*}$.
(ii) $A_\Theta \in \mathcal{C}(\mathfrak{H})$ *if and only if* $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$.
(iii) A_Θ *is symmetric if and only if* Θ *is symmetric and* $\mathrm{n}_\pm(A_\Theta) = \mathrm{n}_\pm(\Theta)$ *holds. In particular,* A_Θ *is self-adjoint if and only if* Θ *is self-adjoint.*
(iv) *If* $A_\Theta = A_\Theta^*$ *and* $A_{\widetilde{\Theta}} = A_{\widetilde{\Theta}}^*$, *then for every* $p \in (0,\infty]$ *the following equivalence holds*

$$(A_\Theta - \mathrm{i})^{-1} - (A_{\widetilde{\Theta}} - \mathrm{i})^{-1} \in \mathfrak{S}_p(\mathfrak{H}) \iff (\Theta - \mathrm{i})^{-1} - (\widetilde{\Theta} - \mathrm{i})^{-1} \in \mathfrak{S}_p(\mathcal{H}).$$

Notice that according to (A.1.2), a self-adjoint linear relation Θ is said to belong to the von Neumann–Schatten ideal $\mathfrak{S}_p$ if its operator part Θ_{op} belongs to $\mathfrak{S}_p(\mathcal{H}_{\mathrm{op}})$.

REMARK A.5. The proof of Theorem A.4(i)–(ii) can be found in [**55**, Prop. 7.8], [**188**, Prop. 14.7]; (iii) was obtained in [**155**, Prop. 3], see also [**55**, Prop. 7.14].

A.3. Weyl functions and extensions of semibounded operators

With a boundary triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ one can associate two linear operators

$$A_0 := A^* \upharpoonright \ker(\Gamma_0), \qquad\qquad A_1 := A^* \upharpoonright \ker(\Gamma_1).$$

Clearly, (A.2.3) implies $A_0 = A_{\Theta_0}$ and $A_1 = A_{\Theta_1}$, where $\Theta_0 = \{0\} \times \mathcal{H}$ and $\Theta_1 = \mathcal{H} \times \{0\}$. Hence, by Theorem A.4(iii), $A_0 = A_0^*$ and $A_1 = A_1^*$.

DEFINITION A.6 ([**54**]). Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^*. The operator-valued function $M\colon \rho(A_0) \to \mathcal{B}(\mathcal{H})$ defined by

$$M(z) := \Gamma_1(\Gamma_0 \upharpoonright \mathcal{N}_z)^{-1}, \qquad z \in \rho(A_0), \tag{A.3.1}$$

is called *the Weyl function* corresponding to the boundary triplet Π.

The Weyl function is well defined and holomorphic on $\rho(A_0)$. Moreover, it is a Herglotz–Nevanlinna function (see [**54**, §1], [**55**, §7.4.2] and also [**188**, §14.5]). If $A_\Theta \in \operatorname{Ext}(A)$, then one has the *Krein resolvent formula* [**54**, §1], [**55**, §7.6.1]

$$(A_\Theta - z)^{-1} = (A_0 - z)^{-1} + \gamma(z)(\Theta - M(z))^{-1}\gamma(z^*)^* \tag{A.3.2}$$

for all $z \in \rho(A_\Theta) \cap \rho(A_0)$. Here $\gamma(z) := (\Gamma_0 \upharpoonright \mathcal{N}_z)^{-1}$ is the so-called γ-*field*.

Assume now that $A \in \mathcal{C}(\mathfrak{H})$ is a *lower semibounded* operator, i.e., $A \geq a\,\mathrm{I}_{\mathfrak{H}}$ with some $a \in \mathbb{R}$. Let a_0 be the largest lower bound for A,

$$a_0 := \inf_{0 \neq f \in \operatorname{dom}(A)} \frac{\langle Af, f\rangle_{\mathfrak{H}}}{\|f\|^2_{\mathfrak{H}}}.$$

The Friedrichs extension of A is denoted by A_F. If $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is a boundary triplet for A^* such that $A_0 = A_F$, then the corresponding Weyl function M is holomorphic on $\mathbb{C} \setminus [a_0, \infty)$. Moreover, M is strictly increasing on $(-\infty, a_0)$ (that is, for all x, $y \in (-\infty, a_0)$, $M(x) - M(y)$ is positive definite whenever $x > y$) and the following strong resolvent limit exists (see [**54**])

$$M(a_0) := s - R - \lim_{x \uparrow a_0} M(x). \tag{A.3.3}$$

However, $M(a_0)$ is in general a closed linear relation, which is bounded from below.

THEOREM A.7 ([**54, 154**]). *Let $A \geq a\,\mathrm{I}_{\mathfrak{H}}$ with some $a \geq 0$ and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* such that $A_0 = A_F$. Also, let $\Theta = \Theta^* \in \widetilde{\mathcal{C}}(\mathcal{H})$ and A_Θ be the corresponding self-adjoint extension* (A.2.3)*. If $M(a) \in \mathcal{B}(\mathcal{H})$, then:*

(i) $A_\Theta \geq a\,\mathrm{I}_{\mathfrak{H}}$ *if and only if* $\Theta - M(a) \geq \mathbb{O}_{\mathcal{H}}$.
(ii)
$$\kappa_-(A_\Theta - a\,\mathrm{I}) = \kappa_-(\Theta - M(a)).$$

If additionally A is positive definite, that is, $a > 0$, then:

(iii) A_Θ *is positive definite if and only if* $\Theta(0) := \Theta - M(0)$ *is positive definite.*
(iv) *For every $p \in (0, \infty]$ the following equivalence holds*
$$A_\Theta^- \in \mathfrak{S}_p(\mathfrak{H}) \iff \Theta(0)^- \in \mathfrak{S}_p(\mathcal{H}),$$
where $\Theta(0)^- := \Theta(0)^-_{\mathrm{op}} \oplus \Theta(0)_\infty$.

REMARK A.8. For the proofs of (i) and (ii) consult Theorems 5 and 6 in [**54**]; the proofs of (iii)–(iv) can be found in [**154**, Theorem 3]. If A is not positive definite, then "$\Leftrightarrow$" in Theorem A.7(iv) is replaced by the implication "$\Leftarrow$".

We also need the next result (see [**54**, Theorem 3] and [**55**, Theorem 8.22]).

THEOREM A.9 ([**54**]). *Assume the conditions of Theorem A.7. Then the following statements*

(i) $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$ *is lower semibounded,*
(ii) A_Θ *is lower semibounded,*

are equivalent if and only if $M(x)$ tends uniformly to $-\infty$ as $x \to -\infty$, that is, for every $N > 0$ there exists $x_N < 0$ such that $M(x) < -N \cdot \mathrm{I}_{\mathcal{H}}$ for all $x < x_N$.

The implication $(ii) \Rightarrow (i)$ always holds true (cf. Theorem A.7(i)), however, the validity of the converse implication requires that M tends uniformly to $-\infty$. Let us mention in this connection that the weak convergence of $M(x)$ to $-\infty$, i.e., the relation

$$\lim_{x\to-\infty}\langle M(x)h, h\rangle_{\mathcal{H}} = -\infty$$

holds for all $h \in \mathcal{H} \setminus \{0\}$ whenever $A_0 = A_F$. Moreover, this relation characterizes Weyl functions of the Friedrichs extension A_F among all nonnegative (and even lower semibounded) self-adjoint extensions of A (see [**54**, Prop. 4]).

The next result establishes a connection between the essential spectra of A_Θ and Θ and also it can be seen as an improvement of Theorem A.7 (iv).

Theorem A.10 ([**67**]). *Let $A \geq a_0 I_{\mathfrak{H}} > 0$ and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* such that $A_0 = A_F$. Also, let M be the corresponding Weyl function and let $\Theta = \Theta^* \in \widetilde{\mathcal{C}}(\mathcal{H})$ be such that $A_\Theta = A_\Theta^*$ is lower semibounded. Then the following equivalences hold:*

$$\inf \sigma_{\mathrm{ess}}(A_\Theta) \geq 0 \iff \inf \sigma_{\mathrm{ess}}(\Theta - M(0)) \geq 0, \tag{A.3.4}$$

$$\inf \sigma_{\mathrm{ess}}(A_\Theta) > 0 \iff \inf \sigma_{\mathrm{ess}}(\Theta - M(0)) > 0, \tag{A.3.5}$$

$$\inf \sigma_{\mathrm{ess}}(A_\Theta) = 0 \iff \inf \sigma_{\mathrm{ess}}(\Theta - M(0)) = 0. \tag{A.3.6}$$

A.4. Direct sums of boundary triplets

Let $\mathfrak{J}$ be a countably infinite index set. For each $j \in \mathfrak{J}$, let A_j be a closed densely defined symmetric operator in a Hilbert space $\mathfrak{H}_j$ such that $0 < \mathrm{n}_+(A_j) = \mathrm{n}_-(A_j) \leq \infty$. Also, let $\Pi_j = \{\mathcal{H}_j, \Gamma_{0,j}, \Gamma_{1,j}\}$ be a boundary triplet for the operator A_j^*, $j \in \mathfrak{J}$. In the Hilbert space $\mathfrak{H} := \oplus_{j\in\mathfrak{J}}\mathfrak{H}_j$, consider the operator $A := \oplus_{j\in\mathfrak{J}}A_j$, which is symmetric and $\mathrm{n}_+(A) = \mathrm{n}_-(A) = \infty$. Its adjoint is given by $A^* = \oplus_{j\in\mathfrak{J}}A_j^*$. Let us define a direct sum $\Pi := \oplus_{j\in\mathfrak{J}}\Pi_j$ of boundary triplets Π_j by setting

$$\mathcal{H} := \oplus_{j\in\mathfrak{J}}\mathcal{H}_j, \qquad \Gamma_0 := \oplus_{j\in\mathfrak{J}}\Gamma_{0,j}, \qquad \Gamma_1 := \oplus_{j\in\mathfrak{J}}\Gamma_{1,j}. \tag{A.4.1}$$

The next result provides several criteria for (A.4.1) to be a boundary triplet for the operator $A^* = \oplus_{j\in\mathfrak{J}}A_j^*$.

Theorem A.11 ([**141**]). *Let $A = \oplus_{j\in\mathfrak{J}}A_j$ and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be defined by* (A.4.1). *Then the following conditions are equivalent:*

(i) $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ *is a boundary triplet for the operator A^*.*

(ii) *The mappings Γ_0 and Γ_1 are bounded as mappings from* $\mathrm{dom}(A^*)$ *equipped with the graph norm to $\mathcal{H}$.*

(iii) *The Weyl functions M_j corresponding to the triplets Π_j, $j \in \mathfrak{J}$, satisfy the following condition*

$$\sup_{j\in\mathfrak{J}}\big(\|M_j(\mathrm{i})\|_{\mathcal{H}_j} + \|(\mathrm{Im}\, M_j(\mathrm{i}))^{-1}\|_{\mathcal{H}_j}\big) < \infty. \tag{A.4.2}$$

(iv) *If in addition A is nonnegative, then (i)–(iii) are further equivalent to*

$$\sup_{j\in\mathfrak{J}}\big(\|M_j(-1)\|_{\mathcal{H}_j} + \|M_j'(-1)\|_{\mathcal{H}_j} + \|\big(M_j'(-1)\big)^{-1}\|_{\mathcal{H}_j}\big) < \infty. \tag{A.4.3}$$

Remark A.12. Theorem A.11 was proved in [**141**, § 3], however, it is essentially contained in [**156**, § 3].

APPENDIX B

Dirichlet forms

In this section, we collect necessary definitions and facts about Dirichlet forms. The standard reference is [**77**]. We stress that most of the literature treats Dirichlet forms on real Hilbert spaces (i.e., restricting to real-valued functions), however the theory easily extends to complex Hilbert spaces (see, e.g., [**97**, Appendix B]).

B.1. Basic notions

In the following, let X be a locally compact separable metric space and μ a positive Radon measure on X of full support. The associated Hilbert space of complex-valued, square integrable functions is denoted by $\mathcal{H} := L^2(X;\mu)$. For a quadratic form $\mathfrak{t}\colon \operatorname{dom}(\mathfrak{t}) \to \mathbb{C}$, whose domain $\operatorname{dom}(\mathfrak{t})$ is a subspace of $\mathcal{H}$, we denote by $\mathfrak{t}[u,v]$, $u,v \in \operatorname{dom}(\mathfrak{t})$ its corresponding sesquilinear form.

Definition B.1. A *Dirichlet form* in $\mathcal{H}$ is a densely defined, non-negative and closed quadratic form $\mathfrak{t}$ satisfying the *Markovian condition*: for all $f \in \operatorname{dom}(\mathfrak{t})$ and any normal contraction[‡] φ, $\varphi \circ f \in \operatorname{dom}(\mathfrak{t})$ and

$$\mathfrak{t}[\varphi \circ f] \leq \mathfrak{t}[f]. \tag{B.1.1}$$

A *Dirichlet form in the wide sense* is a quadratic form $\mathfrak{t}$ satisfying all the above conditions, except that $\operatorname{dom}(\mathfrak{t}) \subseteq \mathcal{H}$ is (possibly) not dense.

By the first representation theorem (see [**125**, Chapter VI.2.1]), to each Dirichlet form we can associate a non-negative, self-adjoint operator $A\colon \operatorname{dom}(A) \to \mathcal{H}$. The corresponding *heat semigroup* $T_t := \mathrm{e}^{-tA}$, $t \geq 0$ is then *Markovian*, that is, all T_t's satisfy $0 \leq T_t f \leq 1$ for functions f with $0 \leq f \leq 1$. The latter means that e^{-tA} is *positivity preserving* (i.e., maps non-negative functions to non-negative functions) and *contractive* (i.e., it is a contraction in L^∞) . Moreover, the heat semigroup has a canonical extension from $L^1(X;\mu) \cap L^\infty(X;\mu)$ to a positive contraction semigroup on $L^p(X;\mu)$ for all $p \in [1,\infty]$ (see, e.g., [**50**, Theorem 1.4.1] and also [**77**, p. 56] for details).

Definition B.2. A Dirichlet form $\mathfrak{t}$ is called *strongly local* if $\mathfrak{t}[f,g] = 0$ for any functions $f, g \in \operatorname{dom}(\mathfrak{t})$ with compact support[††] and such that f is constant in a neighborhood of $\operatorname{supp}(g)$.

Moreover, a Dirichlet form $\mathfrak{t}$ is called *regular* if the set $\operatorname{dom}(\mathfrak{t}) \cap C_c(X)$ is

(i) dense in $C_c(X)$ with respect to the uniform norm $\|\cdot\|_\infty$, and
(ii) dense in $(\operatorname{dom}(\mathfrak{t}), \|\cdot\|_{\mathfrak{t}})$ with respect to the graph norm $\|\cdot\|_{\mathfrak{t}}^2 = \mathfrak{t}[\cdot] + \|\cdot\|_{L^2}^2$.

[‡]A function $\varphi\colon \mathbb{C} \to \mathbb{C}$ is called a *normal contraction* if $\varphi(0) = 0$ and $|\varphi(x) - \varphi(y)| \leq |x - y|$ for all $x, y \in \mathbb{C}$.

[††]The support of a mesurable function f is defined as the support of the measure $f\,d\mu$. If f is continuous, this coincides with the closure of $\{x \in X \mid f(x) \neq 0\}$.

REMARK B.3. Let us remark that a regular Dirichlet form $\mathfrak{t}$ has an additional stochastic interpretation: there is an associated (unique up to equivalence) Hunt process $\mathcal{M} = ((X_t)_{t\geq 0}, (\mathbb{P}_x)_{x\in X})$ on X such that for $t \geq 0$ and $E \subseteq X$ measurable,

$$T_t \mathbb{1}_E(x) = \mathbb{P}_x(X_t \in E), \quad \mu\text{-a.e.}$$

For details on Hunt processes and their relationship to Dirichlet forms we refer to [**77**, Appendix A.2, Theorem 4.2.8 and Theorem 7.2.1]).

B.2. Transience, recurrence and stochastic completeness

Let $\mathfrak{t}$ be a Dirichlet form in $\mathcal{H}$ and let $T_t := \mathrm{e}^{-tA}$, $t > 0$ be the corresponding heat semigroup. For a non-negative function $f \in L^1(X;\mu)$, we define its *potential* $Gf\colon X \to [0,\infty]$ by

$$Gf(x) = \lim_{N\to\infty} \int_0^N (T_s f)(x)\,\mathrm{d}s, \tag{B.2.1}$$

where the limit exists for μ-a.e. $x \in X$. We call the Dirichlet form $\mathfrak{t}$/Markovian semigroup $(T_t)_{t>0}$ *transient* if

$$Gf(x) < \infty \quad \mu\text{-a.e.} \qquad \text{for any } 0 \leq f \in L^1(X;\mu), \tag{B.2.2}$$

and *recurrent* if

(B.2.3)

$$Gf(x) = 0 \;\; \mu\text{-a.e.} \quad \text{or} \quad Gf(x) = \infty \;\; \mu\text{-a.e.} \qquad \text{for each } 0 \leq f \in L^1(X;\mu).$$

Note that an arbitrary Dirichlet form might be neither recurrent nor transient. However, the dichotomy holds for *irreducible* Dirichlet forms[‡], that is, every irreducible Dirichlet form is either transient or recurrent (but not both!).

REMARK B.4. One can reformulate transience/recurrence by means of quadratic forms. For instance (see [**77**, Theorem 1.5.1]), the Dirichlet form $\mathfrak{t}$ in $\mathcal{H}$ is *transient* exactly when there exists $0 < g \in L^1(X;\mu) \cap L^\infty(X;\mu)$ such that

$$\int_X |f(x)| g(x)\,\mu(\mathrm{d}x) \leq \sqrt{\mathfrak{t}[f]} \tag{B.2.4}$$

for all $f \in \mathrm{dom}(\mathfrak{t})$.

We also need the following convenient characterization of recurrence (e.g., [**77**, Theorem 1.6.3]).

LEMMA B.5. *Let $\mathfrak{t}$ be a Dirichlet form in $\mathcal{H}$. Then the following are equivalent:*

(i) $\mathfrak{t}$ *is recurrent,*
(ii) *There exists a sequence (f_n) in $\mathrm{dom}(\mathfrak{t})$ such that $\lim_{n\to\infty} f_n = \mathbb{1}$ μ-a.e. on X and $\lim_{n\to\infty} \mathfrak{t}[f_n] = 0$.*

A Dirichlet form is *stochastically complete* (or *conservative*) if its L^∞-semigroup satisfies

$$T_t \mathbb{1} = \mathbb{1} \quad \mu\text{-a.e.} \tag{B.2.5}$$

for some (equivalently for all) $t > 0$. For a regular Dirichlet form, this means that the associated stochastic process has infinite lifetime almost surely (see [**77**, p. 187]

[‡]A measurable set $Y \subseteq X$ is called $\mathfrak{t}$-invariant if $\mathbb{1}_Y f, \mathbb{1}_{X\setminus Y} f \in \mathrm{dom}(\mathfrak{t})$ for any $f \in \mathrm{dom}(\mathfrak{t})$ and, moreover, $\mathfrak{t}(f) = \mathfrak{t}(\mathbb{1}_Y f) + \mathfrak{t}(\mathbb{1}_{X\setminus Y} f)$. This is also equivalent to the equality $T_t \mathbb{1}_Y f = \mathbb{1}_Y T_t f$ for all $f \in \mathcal{H}$. The form $\mathfrak{t}$ is *irreducible* if $\mu(Y) = 0$ or $\mu(X \setminus Y) = 0$ for each $\mathfrak{t}$-invariant set Y.

for details). If A is the generator of the corresponding heat semigroup $(T_t)_{t>0}$, then stochastic completeness is equivalent to the equality

$$\lambda(A+\lambda)^{-1}\mathbb{1} = \mathbb{1} \quad \mu\text{-a.e.} \tag{B.2.6}$$

for some (and hence for all) $\lambda > 0$. Similarly to Lemma B.5, one can characterize stochastic completeness in terms of the quadratic form (e.g., [**77**, Theorem 1.6.6]).

LEMMA B.6. *Let* $\mathfrak{t}$ *be a Dirichlet form in* $\mathcal{H}$. *Then the following are equivalent:*

(i) $\mathfrak{t}$ *is stochastically complete,*

(ii) *There exists a sequence* (f_n) *in* $\mathrm{dom}(\mathfrak{t})$ *such that* $0 \le f_n \le 1$, $\lim_{n\to\infty} f_n = \mathbb{1}$ μ*-a.e. on* X, *and*

$$\lim_{n\to\infty} \mathfrak{t}[f_n, g] = 0$$

for all $g \in \mathrm{dom}(\mathfrak{t}) \cap L^1(X;\mu)$.

B.3. Extended Dirichlet spaces

Let $\mathfrak{t}\colon \mathrm{dom}(\mathfrak{t}) \to [0,\infty)$ be a Dirichlet form on $\mathcal{H} = L^2(X;\mu)$. A sequence $(f_n) \subset \mathrm{dom}(\mathfrak{t})$ is called an *approximating sequence* for a function $f\colon X \to \mathbb{C}$, if $\lim_{n\to\infty} f_n = f$ μ-a.e. on X and $(f_n)_n$ is a $\mathfrak{t}$-Cauchy sequence, that is,

$$\lim_{m,n\to\infty} \mathfrak{t}[f_n - f_m] = 0.$$

The *extended Dirichlet space* of $\mathfrak{t}$ is the space of all measurable functions on X which admit at least one approximating sequence. It turns out that (see [**77**, Theorem 1.5.2]) for a function $f \in \mathrm{dom}(\mathfrak{t}_e)$, where $\mathrm{dom}(\mathfrak{t}_e)$ is the extended Dirichlet space of $\mathfrak{t}$, the limit

$$\mathfrak{t}_e[f] := \lim_{n\to\infty} \mathfrak{t}[f_n]$$

exists and is independent of the approximating sequence (f_n). In particular, this extends the Dirichlet form $\mathfrak{t}$ to a non-negative quadratic form $\mathfrak{t}_e$ on $\mathrm{dom}(\mathfrak{t}_e)$:

$$\mathfrak{t}_e\colon \quad \begin{array}{ccc} \mathrm{dom}(\mathfrak{t}_e) & \longrightarrow & [0,\infty) \\ f & \mapsto & \mathfrak{t}_e[f] \end{array}.$$

The obtained form $\mathfrak{t}_e$ is called the *extended Dirichlet form* of $\mathfrak{t}$.

The *Markovian condition* also carries over from $\mathfrak{t}$ to $\mathfrak{t}_e$: for each normal contraction $\varphi\colon \mathbb{C} \to \mathbb{C}$ and $f \in \mathrm{dom}(\mathfrak{t}_e)$, $\varphi \circ f$ belongs to $\mathrm{dom}(\mathfrak{t}_e)$ and (B.1.1) holds (see, e.g., [**77**, Corollary 1.6.3]). Moreover, the form domain of $\mathfrak{t}$ (see [**77**, Theorem 1.5.2]) can be recovered from $\mathfrak{t}_e$ by the relation

$$\mathrm{dom}(\mathfrak{t}) = \mathrm{dom}(\mathfrak{t}_e) \cap L^2(X;\mu). \tag{B.3.1}$$

The above notions lead to another convenient characterization of recurrence (see [**77**, Theorem 1.6.3]):

LEMMA B.7. *Let* $\mathfrak{t}$ *be a Dirichlet form on* $\mathcal{H}$. *Then* $\mathfrak{t}$ *is recurrent if and only if* $\mathbb{1}$ *belongs to* $\mathrm{dom}(\mathfrak{t}_e)$ *and* $\mathfrak{t}_e[\mathbb{1}] = 0$.

APPENDIX C

Heat Kernel Bounds

In this appendix, we collect some useful results relating heat kernel decay with Sobolev and Nash-type inequalities. Throughout this section we shall assume that $A = A^* \geq 0$ is a generator of a Markovian semigroup in $L^2(X;\mu)$ (see Appendix B for details). The corresponding quadratic form, which is a Dirichlet form on $L^2(X;\mu)$, is denoted by $\mathfrak{Q}_A$, that is,

$$\mathfrak{Q}_A[f] = \|A^{1/2}f\|_2^2, \qquad \mathrm{dom}(\mathfrak{Q}_A) = \mathrm{dom}(A^{1/2}),$$

where A^γ, $\gamma > 0$ is a non-negative self-adjoint operator. Recall that (see, e.g., [**50**, § 2.1]), the semigroup $T_t = \mathrm{e}^{-tA}$ is called *ultracontractive* if e^{-tA} is bounded as an operator from $L^2(X;\mu)$ to $L^\infty(X)$ for all $t > 0$. By duality, the latter is equivalent to e^{-tA} being bounded from $L^1(X;\mu)$ to $L^\infty(X)$ for all $t > 0$.

We begin with the following simple result (see [**50**, Theorem 2.4.1]).

Proposition C.1. *Let $\gamma > 0$ be fixed. If* [‡]

$$\|f\|_\infty \leq C_1\|(A+\mathrm{I})^{\gamma/2}f\|_2 \tag{C.0.1}$$

for all $f \in \mathrm{dom}(A+\mathrm{I})^{\gamma/2}$, then e^{-tA} is ultracontractive and there is a positive constant $C_2 > 0$ such that

$$\|\mathrm{e}^{-tA}\|_{1\to\infty} \leq C_2 t^{-\gamma} \tag{C.0.2}$$

for all $t \in (0,1)$. Conversely, if (C.0.2) *holds on* $(0,1)$ *for some $\gamma > 0$, then*

$$\|f\|_\infty \leq C(\varepsilon)\|(A+\mathrm{I})^{\gamma/2+\varepsilon}f\|_2, \qquad f \in \mathrm{dom}(A+\mathrm{I})^{\gamma/2+\varepsilon}, \tag{C.0.3}$$

is valid for any $\varepsilon > 0$.

The next result is a famous theorem of N.Th. Varopoulos (see [**201**], [**203**, Theorem II.5.2], [**50**, Theorem 2.4.2]).

Theorem C.2 ([**201**]). *Let $D > 2$ be fixed. Then a bound of the form*

$$\|\mathrm{e}^{-tA}\|_{1\to\infty} \leq C_1 t^{-D/2} \tag{C.0.4}$$

for all $t > 0$ is equivalent to the validity of the Sobolev-type inequality

$$\|f\|^2_{\frac{2D}{D-2}} \leq C_2\,\mathfrak{Q}_A[f] \tag{C.0.5}$$

for all $f \in \mathrm{dom}(\mathfrak{Q}_A)$.

As an immediate corollary we get the following claim relating the behavior of the heat kernel as $t \to 0$ with the Sobolev inequality (see [**50**, Corollary 2.4.3]).

‡Throughout this section we use the standard notation $\|f\|_p := \|f\|_{L^p(X;\mu)}$ for $f \in L^p(X;\mu)$ and $\|T\|_{p\to q}$ denotes the norm of a linear operator T acting from $L^p(X;\mu)$ to $L^q(X;\mu)$.

COROLLARY C.3. *Let $D > 2$ be fixed. Then* (C.0.4) *holds for all $t \in (0,1)$ if and only if*

$$\|f\|^2_{\frac{2D}{D-2}} \le C(\mathfrak{Q}_A[f] + \|f\|_2^2) \tag{C.0.6}$$

for all $f \in \mathrm{dom}(\mathfrak{Q}_A)$.

Notice that $\|\cdot\|_{\mathfrak{Q}} = \mathfrak{Q}_A[\cdot] + \|\cdot\|_2^2$ is the graph norm and it is equivalent to the energy (semi-)norm $\mathfrak{Q}_A[\cdot]$ if and only if A has a positive spectral gap, $\lambda_0(A) > 0$.

Let us also recall the following result relating on-diagonal heat kernel estimates with Nash-type inequalities ([**38**, Theorem 2.1], [**50**, Theorem 2.4.6]).

THEOREM C.4 ([**38**]). *The estimate* (C.0.4) *holds true for all $t > 0$ with some fixed $D > 0$ if and only if the inequality*

$$\|f\|_2^{2+\frac{4}{D}} \le C\,\mathfrak{Q}_A[f]\,\|f\|_1^{\frac{4}{D}} \tag{C.0.7}$$

holds true for all $f \in \mathrm{dom}(\mathfrak{Q}_A) \cap L^1(X;\mu)$. Moreover, the inequality

$$\|f\|_2^{2+\frac{4}{D}} \le C\big(\mathfrak{Q}_A[f] + \|f\|_2^2\big)\|f\|_1^{\frac{4}{D}} \tag{C.0.8}$$

holds for all $f \in \mathrm{dom}(\mathfrak{Q}_A) \cap L^1(X;\mu)$ if and only if (C.0.4) *holds for all $t \in (0,1)$.*

REMARK C.5. Taking into account that both (C.0.7) and (C.0.8) are homogeneous (w.r.t. $f \to cf$, $c \in \mathbb{C}$), one can restrict in (C.0.7) to functions with $\|f\|_1 = 1$ or $\|f\|_1 = c$ for any fixed $c > 0$. Moreover, $\mathfrak{Q}_A[|f|] \le \mathfrak{Q}_A[f]$ for all $f \in \mathrm{dom}(\mathfrak{Q}_A)$ since $\mathfrak{Q}_A$ is a Dirichlet form. Therefore, in all the above theorems one can further restrict to non-negative functions.

The following extension of Theorem C.2 and Theorem C.4 to sub-exponential scales is due to T. Coulhon (see [**45**, Theorem II.5]).

THEOREM C.6. *Let $m\colon \mathbb{R}_{>0} \to \mathbb{R}_{>0}$ be a decreasing bijection such that its logarithmic derivative has polynomial growth, i.e., $M := -\log m$ satisfies for some $\alpha > 0$*

$$M'(x) \ge \alpha M'(s), \qquad \text{for all } s > 0 \quad \text{and} \quad x \in [s, 2s]. \tag{C.0.9}$$

Then the following conditions are equivalent:

(i) e^{-tA} *is ultracontractive and there is $C_1 > 0$ such that*

$$\|\mathrm{e}^{-tA}\|_{1\to\infty} \le m(C_1 t) \tag{C.0.10}$$

for all $t > 0$,

(ii) *there is $C_2 > 0$ such that for all $f \in \mathrm{dom}(\mathfrak{Q})$ with $\|f\|_{L^1} = 1$,*

$$\theta_m(\|f\|_2^2) \le C_2 \mathfrak{Q}_A[f], \tag{C.0.11}$$

where $\theta_m := -m' \circ m^{-1}$.

APPENDIX D

Glossary of notation

Basic notation.

$\mathbb{Z}$, $\mathbb{R}$, $\mathbb{C}$ have their usual meaning;
For $a \in \mathbb{R}$, $\mathbb{Z}_{\geq a} := \mathbb{Z} \cap [a, \infty)$, $\mathbb{R}_{\geq a} := \mathbb{R} \cap [a, \infty)$, and $\mathbb{R}_{>a} := \mathbb{R} \cap (a, \infty)$.
z^* denotes the complex conjugate of $z \in \mathbb{C}$.
$\mathcal{I} \subseteq \mathbb{R}$ usually denotes an interval, that is, a connected subset of $\mathbb{R}$;
$\mathcal{I}_\ell = [0, \ell]$, $\ell \in \mathbb{R}_{>0}$.
For a given set S, $\#S$ denotes its cardinality if S is finite; otherwise we set $\#S = \infty$.
We shall denote by (x_n) or sometimes $(x_n)_{n\geq 0}$ a sequence $(x_n)_{n=0}^{\infty}$.

Graphs.

$\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ is a graph with the vertex set $\mathcal{V}$ and the edge set $\mathcal{E}$.
$\mathcal{E}_v$ is the set of edges at $v \in \mathcal{V}$.
$\vec{\mathcal{G}}_d = (\mathcal{V}, \vec{\mathcal{E}})$ is a directed graph and $\vec{\mathcal{E}}$ the set of directed edges.
$\vec{\mathcal{E}}_v$ is the set of directed (both incoming and outgoing) edges at v.
$e_\imath$ and e_τ are the initial and terminal vertices of $\vec{e}$.
deg is the vertex degree function.
Deg is the weighted vertex degree.

b or $(\mathcal{V}, m; b)$ is a weighted graph on $\mathcal{V}$,
(b, c) or $(\mathcal{V}, m; b, c)$ is a weighted graph with killing term c on $\mathcal{V}$,
$\mathcal{G}_b = (\mathcal{V}, \mathcal{E}_b)$ is the underlying simple graph of b.
$\mathcal{G} = (\mathcal{G}_d, |\cdot|)$ is a metric graph or its model,
$(\mathcal{G}, \mu, \nu) = (\mathcal{G}_d, |\cdot|, \mu, \nu)$ is a weighted metric graph or its model.
ϱ_0 is the length metric on $\mathcal{G}$, i.e., the natural path metric on $\mathcal{G}$.
ϱ_η is the intrinsic metric on $(\mathcal{G}, \mu, \nu)$ and $\eta = \sqrt{\frac{\mu}{\nu}}$ is the intrinsic weight.
ϱ_m is the star path metric on $\mathcal{V}$ corresponding to the star weight m.
S_n is the n-th combinatorial sphere of a rooted graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$.
$\mathfrak{C}(\mathcal{G})$ is the space of topological ends of a metric graph $\mathcal{G}$.
$\mathfrak{C}_0(\mathcal{G}; \mu)$ is the set of finite volume (w.r.t. μ) ends of $\mathcal{G}$.

Function spaces.

X is a locally compact Hausdorff space X, and μ is a Borel measure on X.
$C(X)$ is the space of continuous functions on X,
$C(X)$ is the set of complex-valued functions on X if X is countable.
$C_b(X)$, $C_0(X)$, and $C_c(X)$ are, respectively, the spaces bounded, vanishing at infinity, and compactly supported continuous functions on X.
$C^+(X)$ is a cone of positive functions on X.

$\mathcal{F}_b(\mathcal{V})$ denotes the domain of definition of the formal graph Laplacian $L_{c,b,m}$.
$\mathrm{CA}(\mathcal{G}\backslash\mathcal{V})$ is the set of continuous, edgewise affine functions on a metric graph $\mathcal{G}$.

$L^p(X;\mu)$ is the complex Banach space of measurable functions, $p \in [1,\infty]$,
$L^p_c(X;\mu)$ is the subspace of compactly supported functions in $L^p(X;\mu)$.
$\ell^p(X;m) := L^p(X;m)$, $\ell^p_c(X;m) := L^p_c(X;m)$ if X is countable.
$H^1_0(\mathcal{G}\setminus\mathcal{V})$ is the subspace of $H^1(\mathcal{G})$-functions vanishing at all vertices,
$H^1_{\mathrm{loc}}(\mathcal{G}\setminus\mathcal{V})$ is the space of all H^1 edgewise functions,
$H^1_{\mathrm{loc}}(\mathcal{G}) = H^1_{\mathrm{loc}}(\mathcal{G}\setminus\mathcal{V})\cap C(\mathcal{G})$,
$H^1_c(\mathcal{G}) = H^1_{\mathrm{loc}}(\mathcal{G})\cap C_c(\mathcal{G})$,
$H^1(\mathcal{G}) = H^1(\mathcal{G};\mu,\nu)$ is the first (weighted) Sobolev space on $\mathcal{G}$,
$H^1_0(\mathcal{G}) = H^1_0(\mathcal{G};\mu,\nu) = \overline{H^1_c(\mathcal{G})}^{\|\cdot\|_{H^1(\mathcal{G};\mu,\nu)}}$,
$\dot H^1(\mathcal{G}) = \dot H^1(\mathcal{G},\nu)$ is the space of functions of finite energy on $\mathcal{G}$.

Laplacians and their quadratic/energy forms.

$L = L_{c,b,m}$ is the formal graph Laplacian on $(\mathcal{V},m;b,c)$,
$\mathbf{h}$, $\mathbf{h}'$ and $\mathbf{h}^0$ are the maximal, pre-minimal and minimal graph Laplacians in $\ell^2(\mathcal{V};m)$.
$\mathbf{h}_D$ and $\mathbf{h}_N$ are the Dirichlet and Neumann Laplacians in $\ell^2(\mathcal{V};m)$.
$\mathfrak{q} = \mathfrak{q}_{c,b}$ is the energy form on (b,c),
$\mathfrak{q}_D$ and $\mathfrak{q}_N$ are the maximal and the minimal forms in $\ell^2(\mathcal{V};m)$.

Δ is the weighted Laplacian on $(\mathcal{G},\mu,\nu)$,
$\mathbf{H}$, $\mathbf{H}'$ and $\mathbf{H}^0$ are the maximal, pre-minimal and minimal Kirchhoff Laplacians in $L^2(\mathcal{G};\mu)$.
$\mathbf{H}_D$ and $\mathbf{H}_N$ are the Dirichlet and Neumann Laplacians in $L^2(\mathcal{G};\mu)$.
$\mathbf{H}_G$ and $\mathbf{H}_{G,\min}$ are the maximal and minimal Gaffney Laplacians in $L^2(\mathcal{G};\mu)$.
$\mathbf{H}_\alpha$, $\mathbf{H}'_\alpha$ and $\mathbf{H}^0_\alpha$ are the maximal, pre-minimal and minimal Laplacians with δ-couplings.
$\mathfrak{Q}$ is the energy form on $(\mathcal{G},\mu,\nu)$,
$\mathfrak{Q}_D$ and $\mathfrak{Q}_N$ are the maximal and the minimal forms in $L^2(\mathcal{G};\mu)$.

Operator theory.

$\mathcal{H}$ and $\mathfrak{H}$ are separable complex Hilbert spaces.
$\mathcal{B}(\mathcal{H})$ is the algebra of bounded linear operators on $\mathcal{H}$.
$\mathfrak{S}_p(\mathcal{H})$, $p\in(0,\infty]$ are the Schatten–von Neumann ideals in $\mathcal{B}(\mathcal{H})$.
$\mathrm{I}_\mathcal{H}$ is the identity operator in $\mathcal{H}$, and $\mathrm{I}_n := \mathrm{I}_{\mathbb{C}^n}$.
$\mathbb{O}_\mathcal{H}$ is the zero operator in $\mathcal{H}$, and $\mathbb{O}_n := \mathbb{O}_{\mathbb{C}^n}$.
For a self-adjoint operator A in $\mathcal{H}$, $\lambda_0(A)$ and $\lambda_0^{\mathrm{ess}}(A)$ denote the bottoms of the spectrum, respectively, of the essential spectrum,

$$\lambda_0(A) = \inf\sigma(A), \qquad \lambda_0^{\mathrm{ess}}(A) = \inf\sigma_{\mathrm{ess}}(A).$$

$A^- := A\mathbb{1}_{(-\infty,0)}(A)$, where $\mathbb{1}_{(-\infty,0)}(A)$ is the spectral projection on the negative subspace of A.
For a closed symmetric operator A,
– $\mathrm{Ext}(A)$ is the set of its proper extensions;
– $\mathrm{Ext}_S(A)$ is the set of its self-adjoint extensions;
For a non-negative symmetric operator A,
– $\mathrm{Ext}_S^+(A)$ is the set of its non-negative self-adjoint extensions;
– $\mathrm{Ext}_S^\kappa(A)$, $\kappa\in\mathbb{Z}_{\geq 0}\cup\{\infty\}$ are self-adjoint extensions of A with the total multiplicity of the negative spectrum equal to κ.
– $\mathrm{Ext}_M(A)$ is the set of Markovian extensions of A.

Index

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