Chapter 1

Introduction

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 analogs of Riemann surfaces (we only refer to a very brief selection of recent monographs and collected works [11, 24, 25, 62, 67, 69, 182]). 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, 43, 44, 91, 136, 212]).

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 1980s. 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 [205] 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, 72, 154] 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., [44, Section 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

$$(L\mathbf{f})(v) = \frac{1}{m(v)} \sum_{u \in \mathcal{V}} b(v,u)(\mathbf{f}(v) - \mathbf{f}(u)), \quad v \in \mathcal{V}, \tag{1.1}$$

has seen a tremendous progress during the last decade (see [136]). 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 [25, 182]), 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) gives rise to an unbounded operator (i.e., the *weighted degree function* (2.9) 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., [185, Chapter 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,[1] 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

$$\mathrm{i}\partial_t u = -\Delta u, \quad u|_{t=0} = u_0 \in L^2(X;\mu). \tag{1.2}$$

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 (1.2). If the

[1] 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.

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., [23, Chapter 2.6.1] and [192, Section 1.1]).

When considering the Cauchy problem for the heat equation

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

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 $(\mathrm{e}^{\Delta t})_{t>0}$ 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., [51]), 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 Helmholtz equation

$$\Delta u = \lambda u, \quad \lambda \in \mathbb{R}. \tag{1.3}$$

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 (1.3) 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 Helmholtz equation (1.3) 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 (1.3) 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 [124, 153, 217])[2] 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 [79]).

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 $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$

[2]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.

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[3] Δ acts edgewise in $L^2(\mathcal{G}; \mu)$ as a Sturm–Liouville operator

$$\frac{1}{\mu(e)} \frac{\mathrm{d}}{\mathrm{d}x_e} \nu(e) \frac{\mathrm{d}}{\mathrm{d}x_e}, \quad e \in \mathcal{E}. \tag{1.4}$$

In order to reflect the underlying combinatorial structure, we impose the Kirchhoff conditions (see (2.14) for details)

$$\begin{cases} f \text{ is continuous at } v, \\ \sum_{e \sim v} \nu(e) \partial_e f(v) = 0, \end{cases} \tag{1.5}$$

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 flow condition in vertices.[4] The corresponding energy form in $L^2(X; \mu)$ is given by

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

Our second object of interest is the weighted graph Laplacian L given by (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

$$\mathfrak{q}[\mathbf{f}] = \langle L\mathbf{f}, \mathbf{f} \rangle_{\ell^2(\mathcal{V};m)} = \frac{1}{2} \sum_{u,v \in \mathcal{V}} b(u,v) |\mathbf{f}(v) - \mathbf{f}(u)|^2. \tag{1.6}$$

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 (1.4), every harmonic function f on a weighted metric

---

[3]Here and in the following chapters, Δ shall always denote the Laplacian on a weighted metric graph.

[4]On the one hand, (1.5) 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 (1.5) 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 (1.5) is a particular case of this large family of boundary conditions.

graph $\mathcal{G}$ (i.e., f satisfies $\Delta f = 0$), must be edgewise affine. The Kirchhoff conditions (1.5) imply that f is continuous and, moreover, satisfies

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

at each vertex $v \in \mathcal{V}$. This suggests to consider a discrete Laplacian (1.1) with edge weights given by

$$b(u,v) = \begin{cases} \frac{\nu(e_{u,v})}{|e_{u,v}|}, & u \sim v, \\ 0, & u \not\sim v, \end{cases} \qquad (u,v) \in \mathcal{V} \times \mathcal{V}. \tag{1.7}$$

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

$$\begin{aligned} \imath_{\mathcal{V}} \colon C(\mathcal{G}) &\to C(\mathcal{V}), \\ f &\mapsto f|_{\mathcal{V}}, \end{aligned} \tag{1.8}$$

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

$$m \colon v \mapsto \sum_{u \sim v} |e_{u,v}|\mu(e_{u,v}), \qquad v \in \mathcal{V}. \tag{1.9}$$

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) with the coefficients (1.7) and (1.9) turns into the *normalized (or physical) Laplacian*

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

Connections between their spectral properties have been established in [171, 207] for finite metric graphs and then extended in [35, 41, 66] to infinite metric graphs, and in fact one can even prove some sort of local unitary equivalence [179]. 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, 44, 195, 212]). 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 [205]). The corresponding Laplacian L with the coefficients (1.7) and (1.9) is the generator of a discrete time random walk on $\mathcal{G}_d$ with the probability of jumping from v to u given by

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

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, 205] as well as the recent works [13, 15, 64, 72, 154]).

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 Proposition 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 [55, 56, 191]). First applications of this approach to finite and infinite metric graphs can be traced back to the 2000s (see, e.g., [35, 67, 182]). 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 [68, 143].

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 $\ell^2(\mathcal{V}; m)$, where b and m are defined by (1.7) and (1.9)). The map

$$\widetilde{\mathbf{h}} \mapsto \widetilde{\mathbf{H}}, \quad \operatorname{dom}(\widetilde{\mathbf{H}}) := \{f \in \operatorname{dom}(\mathbf{H}) : \imath_{\mathcal{V}}(f) \in \operatorname{dom}(\widetilde{\mathbf{h}})\}, \tag{1.10}$$

where $\imath_{\mathcal{V}}$ is the restriction map (1.8), establishes a bijective correspondence between the sets of self-adjoint restrictions of $\mathbf{H}$ and 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 subdivision 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 (1.6) (notice that (1.10) 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 [74, 129]). As it was underlined in the work of K.-T. Sturm in the 1990s [198–200], 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 (1.8) 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:

$$\varrho_{\mathcal{V}}(u,v) := \varrho(u,v), \quad u,v \in \mathcal{V}. \tag{1.11}$$

The crucial observation is that $\varrho_{\mathcal{V}}$ is intrinsic (in the sense of [74, 129]) for $(\mathcal{V}, m; b)$ with b and m defined by (1.7) and (1.9) 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 with respect to $(\mathcal{V}, m; b)$, can be obtained in this way (see Theorem 6.36). 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 (1.6) restricted to $C_c(\mathcal{V})$ (see [132, Section 2]). These facts, in combination with the results for strongly local Dirichlet forms as well as with the correspondence (1.10), 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, 129, 136] 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 map (1.8) and (1.11) from the perspective of *quasi-isometries* (quite often going by the name of *rough isometries*) [37, 175, 187]. 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 [54, 175, 187], 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., [187, Remark 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.[5] 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 (1.8) and (1.11) (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 [132, 136], 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

[5] In this text, we arrive at the definition of the intrinsic metric ϱ_η on a weighted metric graph $(\mathcal{G}, \mu, \nu)$ from the perspective of Dirichlet forms. However, let us mention that ϱ_η also admits a mechanical interpretation in terms of the wave equation and is known as the optical metric in the physics literature, see Remark 6.20 for details.

proof. Let us stress that the main tool is the concept of boundary triplets and the corresponding Weyl functions [55, 56, 86, 191]. 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 [72], 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 (1.8). First of all, $\imath_{\mathcal{V}}$ becomes injective when further restricted to the space of continuous, edgewise affine functions $\mathrm{CA}(\mathcal{G} \setminus \mathcal{V})$ 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 (1.10) 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 (1.10) induces a bijection between the sets of Markovian extensions (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 [72, 114] (stochastic completeness) and [97, Chapter 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

$$\tau = \frac{1}{\mu(x)}\Big(-\frac{\mathrm{d}}{\mathrm{d}x}\nu(x)\frac{\mathrm{d}}{\mathrm{d}x} + \sum_{k\geq 1}\alpha_k\delta(x-x_k)\Big), \tag{1.12}$$

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

$$\mu(x) = \sum_{k\geq 0}\mu_k \mathbb{1}_{[x_k,x_{k+1})}(x), \quad \nu(x) = \sum_{k\geq 0}\nu_k \mathbb{1}_{[x_k,x_{k+1})}(x). \tag{1.13}$$

If $\alpha = (\alpha_k) \equiv 0$, then (1.12) 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 [209], M. G. Krein and I. S. Kac [119, 120, 127]). The study of its parabolic properties (recurrence, stochastic completeness) was initiated in the work of W. Feller [70]. 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 Section 5.2, we look at the corresponding difference expression associated with (1.12) 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 (tridiagonal) matrix (5.23). If $\alpha \not\equiv 0$, then we briefly demonstrate that the self-adjointness problem for (1.12) is a rather complicated issue. Actually, in the unweighted case $\mu = \nu \equiv 1$, the corresponding results were obtained in [143] and even for this operator, known as the one-dimensional 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* (5.23) *arising as boundary operators for* (1.12)*?*[6] 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 (1.12). The latter in particular implies that the self-adjointness problem for the particular class of operators (1.12)–(1.13), which are Laplacians on weighted path graphs, is equivalent to the self-adjointness problem for Jacobi matrices, which is a classical problem in spectral theory and of vital importance in the classical moment problem [2].

When considering the boundary operator in the weighted space $\ell^2(\mathbb{Z}_{\geq 0}; m)$, that is, a weighted graph Laplacian (1.1) on a path graph (which is known in the literature

---

[6] A possibility to exploit spectral properties of (1.12) in order to study the corresponding properties of Jacobi matrices has already been emphasized in [4, Section 7]. Moreover, in 2010 during the OTAMP Conference in Bedlewo, Sergei Naboko (1950–2020) posed to one of us (Aleksey Kostenko) exactly this question.

as a *Krein–Stieltjes string* [2, Appendix], [120, Section 13]),

$$(\tau f)(k) := \frac{1}{m(k)} \sum_{|n-k|=1} b(\min\{n,k\})(f(k) - f(n)), \quad k \in \mathbb{Z}_{\geq 0}, \tag{1.14}$$

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, (1.14) arises as a boundary operator for some Sturm–Liouville operator (1.12) with the weights (1.13) if and only if a positive sequence $m = (m_k)_{k \geq 0}$ satisfies

$$\sum_{k=0}^{n} (-1)^{n-k} m(k) > 0 \tag{1.15}$$

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 weighted metric graph Laplacian with δ-couplings. For graph Laplacians (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 (1.15). Let us stress that M. Folz faced precisely the same problem in [72]. The way to overcome this difficulty is to allow loops. Namely, it is immediate to notice that the difference expression (1.1) does not "see" loops in the coefficient b, however, loops enter the weight m in (1.9) and exactly this observation allows to realize every locally finite graph $(\mathcal{V}, m; b)$ as a boundary operator for some weighted 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 [72]). 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 Section 6.4.1 we recall the notion of the intrinsic metric ϱ_η on a weighted metric graph $(\mathcal{G}, \mu, \nu)$. In Section 6.4.2, we briefly recall following [74,129] 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 (1.11)). 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 6.27). Moreover, we show that for a locally finite weighted graph every intrinsic path metric of finite jump size arises in this way (Lemma 6.33). 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 6.36). Notice that $(\mathcal{G}, \varrho_\eta)$ and $(\mathcal{V}, \varrho_\mathcal{V})$ are quasi-isometric metric spaces (Lemma 6.30) 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 [167], [115, Theorem A.1] (see also [129]). Section 6.5 is dedicated to harmonic and sub-/superharmonic functions on graphs. As it was mentioned already, there is a one-to-one 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 Section 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., [47, 151, 160, 194]).

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 [97, Theorem 3.49] and [68]) and, moreover, we provide a very short proof using the L^2-Liouville theorem for metric graphs from [198]). As an immediate corollary, we obtain a Gaffney-type theorem for weighted graph Laplacians proved by a different approach than in [115, Theorem 2]. On the other hand, one can use the results from [115] and [132] to prove sufficient self-adjointness conditions for Kirchhoff Laplacians. Let us stress that Theorem 7.7, first established in [68] 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 [145] 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 [140].

Section 7.2 is dedicated to Markovian uniqueness. Here we extend the results from [146] to the setting of weighted metric graphs. More specifically, using the notion of *finite volume graph ends* introduced in [146], 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 as the study of self-adjointness for the Gaffney Laplacian [148].

We investigate spectral gap estimates in Section 7.3. Motivated by [147], 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 flavor (which is in sharp contrast with the case of finite metric graphs [172]), we are able to connect it with the combinatorial isoperimetric constant (a classical widely studied object [212]) 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 [72]. 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 (Section 8.1.2). In Section 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 Section 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 (Section 8.2.4). In Section 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 (Section 8.2.6).

The aim of Section 8.3 is to discuss graphs arising in context with *tessellations* (or tilings) of the Euclidean 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 [130] 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.