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_ι, e_τ) of its *initial* e_ι 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

$$\mathcal{E}_v^+ = \{(e_\iota, e_\tau) \in \vec{\mathcal{E}} : e_\iota = v\}, \quad \mathcal{E}_v^- = \{(e_\iota, e_\tau) \in \vec{\mathcal{E}} : e_\tau = v\}, \tag{2.1}$$

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

$$\vec{\mathcal{E}}_v := \mathcal{E}_v^+ \sqcup \mathcal{E}_v^- = \vec{\mathcal{E}}_v^+ \cup \vec{\mathcal{E}}_v^-, \quad \vec{\mathcal{E}}_v^\pm := \{(\pm, e) : e \in \mathcal{E}_v^\pm\}.$$

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

$$\deg(v) := \#(\vec{\mathcal{E}}_v) = \#(\vec{\mathcal{E}}_v^+) + \#(\vec{\mathcal{E}}_v^-) = \#(\mathcal{E}_v) + \#\{e \in \mathcal{E}_v : e \text{ is a loop}\}. \tag{2.2}$$

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*[1]. 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.

[1] 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.

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

Hypothesis 2.1. *The graph $\mathcal{G}_d$ is connected and locally finite.*

2.1.2 Metric graphs

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_ι and e_τ with the left, respectively, right endpoint of $\mathcal{I}_e$. The topological space $\mathcal{G}$ is then obtained by "gluing together" the ends of edges corresponding to the same vertex v (in the sense of a topological quotient, see, e.g., [37, 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),

$$\mathcal{E}(\deg(x), r_x) := \{z = r\mathrm{e}^{2\pi \mathrm{i} k/\deg(x)} : r \in [0, r_x),\ k = 1, \dots, \deg(x)\} \subset \mathbb{C}. \quad (2.3)$$

Notice that $\deg(x)$ in (2.3) coincides with the combinatorial degree if x belongs to the vertex set, and $\deg(x) = 2$ for every non-vertex point x of $\mathcal{G}$.

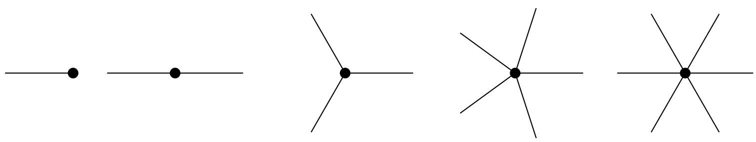

Figure 2.1. Star shaped sets for $\deg(x) = 1, 2, 3, 5$ and 6.

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 realization* 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 [37, 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 [37, Definition 2.1.6], however, we are going to use the notion of an *intrinsic metric* in a different context – intrinsic with respect 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 [37]), 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 (2.3). 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 [97, Chapter I].

Remark 2.3. In most parts of our monograph, 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 either $\mathcal{G} = (\mathcal{V}, \mathcal{E}, |\cdot|)$ 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 one-dimensional 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 (2.3), 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 [76] and R. Halin [102] and its origins are closely related to the study of finitely generated groups [76,77,109] (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 $\bigcap_{n\geq 0} \overline{U_n} = \varnothing$. 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 [212, Section 21], [58, Section 8.6 and also pp. 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 [58, Section 8.6], [212]). 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

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

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

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

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 [102] 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 [132, 136]. 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 $m: \mathcal{V} \to (0, \infty)$ 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

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

has a natural Hilbert space structure. Here $C(\mathcal{V})$ denotes the space of all complex-valued functions on $\mathcal{V}$. Next, let $c: \mathcal{V} \to [0, \infty)$ and suppose $b: \mathcal{V} \times \mathcal{V} \to [0, \infty)$ 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 [132, 136], 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 edge weight $\frac{1}{|\cdot|}$, which further connects it with *electrical networks* when lengths are thought of as resistances (see, e.g., [195]).

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

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

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

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

for all $f \in \mathcal{D} \cap \ell^2(\mathcal{V}; m) =: \operatorname{dom}(\mathfrak{q})$. Clearly, $\operatorname{dom}(\mathfrak{q})$ 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:

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

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 [132, 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., [136, Chapter 1.4]).

Using the representation theorems for quadratic forms (see, e.g., [126]) 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 non-trivial task to provide an explicit description of the operators $\mathbf{h}_D$ and, especially, $\mathbf{h}_N$.[2] Let us first introduce the *formal Laplacian* $L = L_{c,b,m}$ associated to a graph (b, c) over the measure space $(\mathcal{V}, m)$:

$$(Lf)(v) := \frac{1}{m(v)} \Big(\sum_{u \in \mathcal{V}} b(v,u)(f(v) - f(u)) + c(v) f(v) \Big), \quad v \in \mathcal{V}. \tag{2.4}$$

[2] 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 non-trivial 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.

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

$$\mathcal{F}_b(\mathcal{V}) = \Big\{ f \in C(\mathcal{V}) : \sum_{u\in\mathcal{V}} b(v,u)|f(u)| < \infty \text{ for all } v \in \mathcal{V} \Big\}. \tag{2.5}$$

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

$$\mathbf{h} := L \restriction \mathrm{dom}(\mathbf{h}), \quad \mathrm{dom}(\mathbf{h}) := \{f \in \mathcal{F}_b(\mathcal{V}) \cap \ell^2(\mathcal{V}; m) : Lf \in \ell^2(\mathcal{V}; m)\}. \tag{2.6}$$

This operator is closed, however, if $\mathcal{V}$ is infinite, it is not symmetric in general (cf. [132, Theorem 6]). On the other hand, one gets

$$\mathbf{h}_D = \mathbf{h} \restriction \mathrm{dom}(\mathbf{h}_D), \quad \mathrm{dom}(\mathbf{h}_D) = \mathrm{dom}(\mathbf{h}) \cap \mathrm{dom}(\mathfrak{q}_D), \tag{2.7}$$

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

$$\mathbf{h}' := L \restriction \mathrm{dom}(\mathbf{h}'), \quad \mathrm{dom}(\mathbf{h}') := C_c(\mathcal{V}). \tag{2.8}$$

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., [53, Lemma 1], [131, Theorem 11], [201, Remark 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*

$$\mathrm{Deg}\colon v \mapsto \frac{1}{m(v)} \sum_{u\in\mathcal{V}} b(u,v) \tag{2.9}$$

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 non-negative 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 $\mathcal{V}$,

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

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])

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

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 $\mathrm{P} = (p(u,v))_{u,v\in\mathcal{V}}$ is called the *transition matrix* of the associated discrete time (reversible) Markov chain.

Remark 2.12 (Laplacians on multi-graphs). Remark 2.11 indicates that (2.4)–(2.8) allow to treat weighted discrete Laplacians on multigraphs. Namely, for a multigraph $\mathcal{G}_d = (\mathcal{V},\mathcal{E})$ and a given edge weight $b_{\mathcal{E}}\colon \mathcal{E} \to (0,\infty)$, 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

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

it is clear that $L_{\mathcal{G}} = L$ (see (2.4)). 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 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 with respect to 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

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

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,

$$\nabla\colon f \mapsto f'. \tag{2.10}$$

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

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

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. 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 quantities

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

and the normal derivatives

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

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

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

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

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

To motivate our definitions, let us look at ∇ given by (2.10) 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

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

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

$$\Delta\colon f \mapsto -\nabla^\dagger(\nabla f), \tag{2.11}$$

acts edgewise as the following divergence form Sturm–Liouville operator:

$$\Delta\colon f \mapsto \frac{1}{\mu}(\nu f')'. \tag{2.12}$$

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

$$\begin{cases} f \text{ is continuous at } v, \\ \displaystyle\sum_{\vec{e} \in \vec{\mathcal{E}}_v} \nu(e)\partial_{\vec{e}} f(v) = \alpha(v) f(v), \end{cases} \tag{2.13}$$

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 always associate the *Kirchhoff* boundary conditions[3]

$$\begin{cases} f \text{ is continuous at } v, \\ \displaystyle\sum_{\vec{e} \in \vec{\mathcal{E}}_v} \nu(e)\partial_{\vec{e}} f(v) = 0, \end{cases} \qquad v \in \mathcal{V}, \tag{2.14}$$

that is, conditions (2.13) with $\alpha(v) = 0$ for all $v \in \mathcal{V}$. Let us mention that for non-zero $\alpha\colon \mathcal{V} \to \mathbb{R} \cup \{\infty\}$, the Laplacian with boundary conditions (2.13) can be written as

$$-\Delta + \sum_{v \in \mathcal{V}} \alpha(v)\delta_v \tag{2.15}$$

(at least when $\mu \equiv 1$), where δ_v is the Dirac delta centered 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 (2.12) 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 (2.14).

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.

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

$$\mathrm{H}_{e,\max} = -\frac{1}{\mu(e)} \frac{\mathrm{d}}{\mathrm{d}x_e} \nu(e) \frac{\mathrm{d}}{\mathrm{d}x_e}, \quad \mathrm{dom}(\mathrm{H}_{e,\max}) = H^2(e). \tag{2.16}$$

[3]It seems that there is no agreement in the literature regarding the name of the boundary conditions (2.14). 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 (2.14) is nothing but the usual Neumann condition $\partial f(v) = 0$.

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

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

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*:

$$\mathbf{H} = -\Delta \restriction \mathrm{dom}(\mathbf{H}), \quad \mathrm{dom}(\mathbf{H}) = \{f \in \mathrm{dom}(\mathbf{H}_{\max}) : f \text{ satisfies (2.14) on } \mathcal{V}\}.$$

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

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

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

$$\langle \mathbf{H}' f, f\rangle_{L^2} = \int_{\mathcal{G}} |\nabla f(x)|^2\, \nu(\mathrm{d}x) = \|\nabla f\|^2_{L^2(\mathcal{G};\nu)} =: \mathfrak{Q}[f] \tag{2.17}$$

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

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

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 the Kirchhoff boundary conditions (2.14) we are going to consider a slightly more general class of boundary conditions (2.13). These vertex conditions are interpreted as *δ-couplings (or δ-interactions) of strength α* (see (2.15)).[4] Indeed, define the maximal operator

$$\begin{aligned} \mathbf{H}_\alpha &= -\Delta \restriction \mathrm{dom}(\mathbf{H}_\alpha), \\ \mathrm{dom}(\mathbf{H}_\alpha) &= \{f \in \mathrm{dom}(\mathbf{H}_{\max}) : f \text{ satisfies (2.13) on } \mathcal{V}\}, \end{aligned} \tag{2.18}$$

and the pre-minimal operator

$$\mathbf{H}'_\alpha = -\Delta \restriction \mathrm{dom}(\mathbf{H}'_\alpha), \quad \mathrm{dom}(\mathbf{H}'_\alpha) = \mathrm{dom}(\mathbf{H}_\alpha) \cap C_c(\mathcal{G}). \tag{2.19}$$

Integrating by parts, one obtains

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

[4] In fact, one can interpret these boundary conditions as a perturbation of the Kirchhoff Laplacian by δ-potentials, see [145, 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

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

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

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

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

$$H^1(\mathcal{G}) = H^1(\mathcal{G};\mu,\nu) := \{f \in H^1_{\mathrm{loc}}(\mathcal{G}) : f \in L^2(\mathcal{G};\mu),\ \nabla f \in L^2(\mathcal{G};\nu)\}. \tag{2.20}$$

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

$$\|f\|^2_{H^1(\mathcal{G})} := \|f\|^2_{L^2(\mathcal{G};\mu)} + \|\nabla f\|^2_{L^2(\mathcal{G};\nu)} \tag{2.21}$$

turns it into a Hilbert space. Next, we set

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

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 (2.17). 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., [191, Theorem 10.17]). On the other hand, the form $\mathfrak{Q}$ is well defined on $H^1(\mathcal{G})$ and, moreover, the form

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

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. By 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 the set $\mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$. 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 [148]).

In the Hilbert space $L^2(\mathcal{G};\mu)$, we can associate (at least) two gradient operators with ∇ defined by (2.10). Namely, we define ∇_D and ∇_N as the operators

$$\begin{aligned} \nabla_D, \nabla_N \colon L^2(\mathcal{G};\mu) &\to L^2(\mathcal{G};\nu), \\ f &\mapsto \nabla f \end{aligned}$$

acting on the domains

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

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*

$$\mathbf{H}_D = \nabla_D^* \nabla_D, \quad \mathbf{H}_N = \nabla_N^* \nabla_N, \tag{2.22}$$

where $*$ *denotes the adjoint operator.*[5]

Proof. Since $H^1_0(\mathcal{G})$ and $H^1(\mathcal{G})$ are Hilbert spaces, both ∇_D and ∇_N are closed operators and hence, by von Neumann's theorem (see [126, Chapter V.3.7] or [184, Theorem X.25]), $\nabla_D^*\nabla_D$ and $\nabla_N^*\nabla_N$ are self-adjoint non-negative 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., [126, 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:

$$\mathbf{H}_{G,\min} = \nabla_N^* \nabla_D, \quad \mathbf{H}_G = \nabla_D^* \nabla_N. \tag{2.23}$$

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

$$\begin{aligned} \mathrm{dom}(\mathbf{H}_{G,\min}) &= \{f \in H^1_0(\mathcal{G}) : \nabla f \in \mathrm{dom}(\nabla_N^*)\}, \\ \mathrm{dom}(\mathbf{H}_G) &= \{f \in H^1(\mathcal{G}) : \nabla f \in \mathrm{dom}(\nabla_D^*)\}. \end{aligned}$$

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

[5] 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 $f \in \mathrm{dom}(AB) := \{f \in \mathrm{dom}(B) : Bf \in \mathrm{dom}(A)\}$.

Remark 2.17. Notice that the above definition is not precisely the original definition of M. P. Gaffney [79] for manifolds (roughly speaking H^1 was replaced by $C^1 \cap H^1$ in [79, 80]). The obvious drawback is that the corresponding Laplacian in [79] 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*

$$\mathrm{dom}(\mathbf{H}_G) = \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G}) = \{f \in \mathrm{dom}(\mathbf{H}) : \nabla f \in L^2(\mathcal{G};\nu)\}. \tag{2.24}$$

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

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

Proof. The inclusion

$$\mathrm{dom}(\mathbf{H}_G) \subseteq \mathrm{dom}(\mathbf{H}) \cap H^1(\mathcal{G})$$

follows from the definition of $\mathbf{H}_G$. The converse inclusion is immediate from the following description of the adjoint ∇_D^* to ∇_D (see [148, Lemma 3.5]):

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

which then makes the converse inclusion in (2.24) 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

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

It is immediate from the above description that

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

and

$$\mathbf{H}_{G,\min} \subseteq \mathbf{H}_D \subseteq \mathbf{H}_G, \quad \mathbf{H}_{G,\min} \subseteq \mathbf{H}_N \subseteq \mathbf{H}_G.$$

Remark 2.19 (Hodge Laplacians). One can introduce 0-forms and 1-forms on $\mathcal{G}$ (due to the local one-dimensional 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 analog of the Hodge Laplacian on 1-forms (see [17, Section 5.1] and [81, 181]). 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 co-differential 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 (2.23) 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 Sections 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 (2.14) 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 (2.14) (one can notice this also by looking at the graph norm (2.21), where μ and ν enter the first and the second summand, respectively, on the right-hand side of (2.21)).

(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, (2.16) 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 (2.13) 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 [35, Section 3.5], [181] as well as to the case of one-dimensional Schrödinger operators with point interactions [66, 143] (see also Remark 3.14).