GENERALISED DISCRETE LAPLACIANS ON GRAPHS AND THEIR RELATION TO QUANTUM GRAPHS

OLAF POST

Abstract. The aim of the present paper is to analyse the spectrum of Laplace operators on graphs. Motivated by the general form of vertex conditions of a Laplacian on a metric graph, we define a new type of combinatorial Laplacian. With this generalised discrete Laplacian, it is possible to relate the spectral theory on discrete and metric graphs using the theory of boundary triples. In particular, we derive a spectral relation for equilateral metric graphs and index formulas. Moreover, we introduce *extended* metric graphs occuring naturally as limits of "thick" graphs, and provide spectral analysis of natural Laplacians on such spaces.

1. Introduction

In this article, we consider discrete and metric graph Laplacians and their spectral theory. In particular, we introduce a new type of discrete Laplacian associated to metric graph Laplacians with general vertex conditions. A *metric graph* G is by definition a topological graph (i.e., a CW complex of dimension 1), where each edge e is assigned a length ℓ_e. The resulting metric measure space allows to introduce a family of ordinary differential operators acting on each edge e considered as interval $I_e = (0, \ell_e)$ with boundary conditions at the vertices making the global operator self-adjoint. One also refers to the pair of the graph and the self-adjoint differential operator as *quantum graph*. Quantum graphs play an intermediate role between difference operators on discrete graphs and partial differential operators on manifolds. On the one hand, they are a good approximation of partial differential operators on manifolds or open sets close to the graph, see e.g. [P09, P06, EP05, KuZ03] and references therein. On the other hand, solving a system of ODEs reduces in many cases to a discrete problem on the combinatorial graph, see Section 6. We believe that many of the results for discrete and metric graphs can serve as a toy model in order to provide new results in spectral geometry. Spectral graph theory is an active area of research. Results on spectral theory of combinatorial Laplacians can be found e.g. in [D84, MW89, CdV98, CGY96, Ch97, HS99, Sh00, HS04]. For metric graph Laplacians we mention the works [R84, vB85, Nic87, KS99a, Ha00, KS03a, Kuc04, FT04a, Ku05, BaF06, KS06, Pan06, HP06, BaR07].

Let us briefly motivate the generalisation of the usual discrete (or combinatorial) Laplacian on a graph presented in Section 2. Generalised discrete Laplacians as defined below in Definition 2.15 occur naturally in the Dirichlet-to-Neumann operator of a boundary triple associated to the corresponding (equilateral) quantum graph, see Section 4. Dirichlet-to-Neumann operators have a nice physical interpretation: Given a "potential" F living on the boundary space $\mathscr{G}$, the Dirichlet-to-Neumann operator associates to F the corresponding current $\Lambda(z)F \in \mathscr{G}$ at the "energy" z. A typical situation in inverse problems would be to recover information of the graph from such measurements, i.e., from knowledge of $\Lambda(z)$.

The self-adjoint (energy-independent) vertex conditions of a metric graph Laplacian can be encoded in a certain *vertex space* $\mathscr{V} = \bigoplus_v \mathscr{V}_v$. Here, $\mathscr{V}_v$ is a subspace of the $\deg v$-dimensional space $\mathbb{C}^{E_v}$, where E_v is the set of edges adjacent to v, and $\deg v = |E_v|$ is the

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degree of the vertex. The generalised discrete Laplacian will be an operator acting on $\mathscr{V}$, generalising the usual discrete Laplacian defined on $\ell_2(V)$.

The theory of boundary triples gives us a spectral relation between the discrete and metric graph Laplacian, at least for equilateral graphs, see Section 6. This relation and related results have already been observed by many authors (see e.g. [vB85, Nic87, Ca97, CW05, Pan06, BaF06, P07a, BGP08] and the references therein). The interpretation of the corresponding discrete operator as a new type of combinatorial Laplacian might be of its own interest (see also [Sm07] for a related generalisation of combinatorial Laplacians via a scattering approach).

We also establish a spectral relation at the bottom of the spectrum of the discrete and metric graph Laplacians. In particular, we define an *index* (the Fredholm index of a generalised "exterior derivative" in the discrete and metric case) and show that they agree (Theorem 6.5). The result extends the well-known fact that the index equals the Euler characteristic for standard graphs. Such index formulas have been discussed e.g. in [KPS07a, FKW07, P07b]. Finally, we define an *extended* metric graph Laplacian acting on its metric and discrete Hilbert space in a coupled way (see Section 5) and provide some spectral analysis (see Theorems 6.3 and 6.8). Extended Laplacians occur naturally as limits of "thick" graphs in the case when the vertex neighbourhood volume is of the same order as (or decays slower than) the tranversal volume, named "borderline" and "slowly decaying" case in [P09, EP05, KuZ03].

Structure of the article. This article is organised as follows: In the next section, we define the generalised discrete Laplacians. Section 3 is devoted to metric graphs and their associated Laplacians. In Section 4 we apply the concept of boundary triples briefly explained in Appendix A to metric graphs. In Section 5 we define extended metric graphs; and in Section 6 we use the concept of boundary triples in order to describe relations between the discrete and (simple and extended) metric graph Laplacians. Finally, Section 7 contains material on trace formulas for the heat operator associated to metric and discrete graph Laplacians.

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2. Discrete graphs and generalised Laplacians

The aim of the present section is to define the spaces and operators associated to a discrete graph and to conclude some simple consequences needed later on.

2.1. **Discrete graphs and vertex spaces.** Let us first fix the notation for graphs.

Definition 2.1.

(i) A *discrete graph* G is given by (V, E, ∂), where V, E are countable. Here, $V = V(G)$ denotes the set of vertices, $E = E(G)$ denotes the set of edges, and $\partial\colon E \longrightarrow V \times V$ is a map associating to each edge e the pair $(\partial_- e, \partial_+ e)$ of its *initial* and *terminal vertex*, the *connection map*. In particular, ∂e fixes an orientation of the edge e. Abusing the notation, we also denote by ∂e the *set* $\{\partial_- e, \partial_+ e\}$.

(ii) For each vertex $v \in V$ we define the (*outgoing* $(-)$ resp. *incoming* $(+)$) *edge neighbourhood of* v by

$$E_v^{\pm} := \{\, e \in E \,|\, \partial_{\pm} e = v \,\} \qquad \text{and} \qquad E_v := E_v^+ \mathbin{\dot\cup} E_v^-,$$

i.e., $E_v^\pm$ consists of all edges starting $(-)$ resp. ending $(+)$ at v and E_v their *disjoint* union.[1]

(iii) The *degree of* $v \in V$ is defined by
$$\deg v := |E_v| = |E_v^+| + |E_v^-|,$$
i.e., the number of adjacent edges at v. In order to avoid trivial cases, we assume that $\deg v \geq 1$, i.e., no vertex is isolated. We also assume that $\deg v$ is finite for each vertex.

(iv) A discrete graph is *(edge-)*weighted, if there is a function $\ell\colon E \longrightarrow (0,\infty)$ associating to each edge $e \in E$ a *length* $\ell_e > 0$. Alternatively, we may think of $1/\ell_e$ as a *weight* associated to the edge e.

The interpretation "length" will become clear when defining *metric graphs* in Definition 3.1, as well as the interpretation of $1/\ell_e$ as a *weight* or *conductivity*, see (2.7). If $\ell_e = 1$ for all edges, we call the graph *equilateral*.

We will use frequently the following elementary fact about reordering a sum over edges and vertices, namely
$$\sum_{e \in E_{\mathrm{int}}} F(\partial_+ e, e) = \sum_{v \in V} \sum_{e \in E_v^+} F(v,e) \quad \text{and} \quad \sum_{e \in E} F(\partial_- e, e) = \sum_{v \in V} \sum_{e \in E_v^-} F(v,e) \tag{2.2}$$
for a function $(v,e) \mapsto F(v,e)$ depending on v and $e \in E_v$ with the convention that a sum over the empty set is 0. Note that this equation is also valid for self-loops and multiple edges. The reordering is a bijection since the union $E = \dot{\bigcup}_{v \in V} E_v^\pm$ is *disjoint*. For a graph with finite edge set, the relation
$$2|E| = \sum_{v \in V} \deg v \tag{2.3}$$
follows by setting $F(v,e) = 1$.

Let us make the following assumption on the lower bound of the edge lengths:

Assumption 2.4. Throughout this work we assume that there is a constant $\ell_- > 0$ such that
$$\ell_e \geq \ell_- \qquad \forall\, e \in E, \tag{2.4}$$
i.e., that the weight function ℓ^{-1} is bounded. Without loss of generality and for convenience, we assume that $\ell_- \leq 1$.

We want to introduce a vertex space allowing us to define Laplace-like combinatorial operators motivated by general vertex conditions on metric graphs.

The usual discrete (weighted) Laplacian is defined on *scalar* functions $F\colon V \longrightarrow \mathbb{C}$ on the vertices V, namely
$$\ddot{\Delta} F(v) = -\frac{1}{\deg v} \sum_{e \in E_v} \frac{1}{\ell_e} \bigl(F(v_e) - F(v)\bigr), \tag{2.5}$$
where v_e denotes the vertex on e opposite to v. Note that $\ddot{\Delta}$ can be written as $\ddot{\Delta} = \ddot{\mathrm{d}}^* \ddot{\mathrm{d}}$ with
$$\ddot{\mathrm{d}}\colon \ell_2(V) \longrightarrow \ell_2(E), \qquad (\ddot{\mathrm{d}} F)_e = F(\partial_+ e) - F(\partial_- e). \tag{2.6}$$
Here, $\ell_2(V) = \ell_2(V, \deg)$ and $\ell_2(E) = \ell_2(E, \ell^{-1})$ carry the *weighted* norms defined by
$$\|F\|^2_{\ell_2(V)} := \sum_{v \in V} |F(v)|^2 \deg v \quad \text{and} \quad \|\eta\|^2_{\ell_2(E)} := \sum_{e \in E} |\eta_e|^2 \frac{1}{\ell_e}, \tag{2.7}$$

[1] Note that the *disjoint* union is necessary in order to generate two formally different labels for a *self-loop* e, i.e., an edge with $\partial_- e = \partial_+ e$. Moreover, a loop is counted *twice* in the degree of a vertex. This convention is useful when comparing discrete and equilateral metric graphs (see Theorem 6.1).

and $\ddot{\mathrm{d}}^*$ denotes the adjoint with respect to the corresponding inner products. We sometimes refer to functions in $\ell_2(V)$ and $\ell_2(E)$ as 0- and 1-*forms*, respectively. Note that the orientation is important for the exterior derivative $\ddot{\mathrm{d}}$, but not for the Laplacian $\ddot{\Delta}$, since the former is of "first order", while the second is of "second order".

We would like to carry over the above concept for the "vertex space" $\ell_2(V)$ to more general vertex spaces $\mathscr{V} = \bigoplus_v \mathscr{V}_v$. The main motivation to do so are metric graph Laplacians with general vertex conditions as defined in Section 3.2 and their relations with discrete graphs (cf. Section 6).

Definition 2.8.

(i) Denote by $\mathscr{V}_v^{\max} := \mathbb{C}^{E_v}$ the *maximal vertex space at the vertex* $v \in V$, i.e., a value $F(v) = \{F_e(v)\}_{e \in E_v} \in \mathscr{V}_v^{\max}$ has $\deg v$ components, one for each adjacent edge. A *vertex space at the vertex* v is a linear subspace $\mathscr{V}_v$ of $\mathscr{V}_v^{\max}$.

(ii) The corresponding (total) vertex spaces associated to the graph (V, E, ∂) are

$$\mathscr{V}^{\max} := \bigoplus_{v \in V} \mathscr{V}_v^{\max} \quad \text{and} \quad \mathscr{V} := \bigoplus_{v \in V} \mathscr{V}_v,$$

respectively. Elements of $\mathscr{V}$ are also called 0-*forms*. The space $\mathscr{V}$ carries its natural Hilbert norm, namely

$$\|F\|^2_{\mathscr{V}} := \sum_{v \in V} |F(v)|^2 = \sum_{v \in V} \sum_{e \in E_v} |F_e(v)|^2.$$

Associated to a vertex space is an orthogonal projection $P = \bigoplus_{v \in V} P_v$ in $\mathscr{V}^{\max}$, where P_v is the orthogonal projection in $\mathscr{V}_v^{\max}$ onto $\mathscr{V}_v$.

(iii) We call a general subspace $\mathscr{V}$ of $\mathscr{V}^{\max}$ *local* if it decomposes with respect to $\mathscr{V}^{\max} = \bigoplus_v \mathscr{V}_v^{\max}$, i.e., if $\mathscr{V} = \bigoplus_v \mathscr{V}_v$ and $\mathscr{V}_v \subset \mathscr{V}_v^{\max}$. Similarly, an operator A on $\mathscr{V}$ is called *local* if it is decomposable with respect to the above direct sum.

(iv) The *dual* vertex space associated to $\mathscr{V}$ is defined by $\mathscr{V}^\perp := \mathscr{V}^{\max} \ominus \mathscr{V}$ and has projection $P^\perp = \mathbb{1} - P$.

Note that a local subspace $\mathscr{V}$ is closed since $\mathscr{V}_v \leq \mathscr{V}_v^{\max}$ is finite dimensional. Alternatively, a vertex space is characterised by fixing an orthogonal projection P in $\mathscr{V}$ which is local. In view of the corresponding notation on a metric graph (see Definition 3.9), one may call the pair $(G, \mathscr{V})$ a *discrete quantum graph*.

Example 2.9. The names of the vertex spaces in the examples are borrowed from the corresonding examples in the metric graph case, see the end of Section 3. For more general cases defined via vertex spaces, e.g. the discrete magnetic Laplacian, we refer to [P07b].

(i) Choosing $\mathscr{V}_v = \mathbb{C}\mathbb{1}(v) = \mathbb{C}(1, \dots, 1)$, we obtain the *standard* vertex space denoted by $\mathscr{V}_v^{\mathrm{std}}$, also called *continuous* or *Kirchhoff*. The associated projection is

$$P_v = \frac{1}{\deg v} \mathbb{E}$$

where $\mathbb{E}$ denotes the square matrix of rank $\deg v$ where all entries equal 1. This case corresponds to the standard discrete case mentioned before. Namely, the natural identification

$$\widetilde{\bullet} \colon \mathscr{V}^{\mathrm{std}} := \bigoplus_v \mathscr{V}_v^{\mathrm{std}} \longrightarrow \ell_2(V), \qquad F \mapsto \widetilde{F}, \qquad \widetilde{F}(v) := F_e(v),$$

(the latter value is independent of $e \in E_v$) is isometric, since the weighted norm in $\ell_2(V)$ and the norm in $\mathscr{G}^{\mathrm{std}}$ agree, i.e.,

$$\|F\|^2_{\mathscr{V}^{\mathrm{std}}} = \sum_{v \in V} \sum_{e \in E_v} |F_e(v)|^2 = \sum_{v \in V} |\widetilde{F}(v)|^2 \deg v = \|\widetilde{F}\|^2_{\ell_2(V)}.$$

(ii) More generally, we can fix a vector $p(v) = \{p_e(v)\}_{e\in E_v}$ with non-zero entries $p_e(v) \neq 0$ and define the *weighted standard* vertex space by $\mathscr{V}_v^p := \mathbb{C}p(v)$. The corresponding projection is given by
$$P_vF(v) = \frac{1}{|p(v)|^2}\langle p(v), F(v)\rangle p(v).$$
As in the previous example, we have an isometry
$$\widetilde{\bullet}\colon \mathscr{V}^p := \bigoplus_v \mathscr{V}_v^{p(v)} \longrightarrow \ell_2(V, |p|^2), \qquad F \mapsto \widetilde{F}, \qquad \widetilde{F}(v) := \frac{F_e(v)}{p_e(v)}$$
(the latter value is independent of $e \in E_v$), since
$$\|F\|^2_{\mathscr{V}^p} = \sum_{v\in V}\sum_{e\in E_v}|F_e(v)|^2 = \sum_{v\in V}|\widetilde{F}(v)|^2|p(v)|^2 =: \|\widetilde{F}\|^2_{\ell_2(V,|p|^2)}.$$

(iii) We call $\mathscr{V}_v^{\min} := 0$ the *minimal* or *Dirichlet* vertex space. Similarly, $\mathscr{V}^{\max}$ is called the *maximal* or *Neumann* vertex space. The corresponding projections are $P = 0$ and $P = \mathbb{1}$.

(iv) Assume that $\deg v = 4$ and define a vertex space of dimension 2 by
$$\mathscr{V}_v = \mathbb{C}(1,1,1,1) \oplus \mathbb{C}(1,\mathrm{i},-1,-\mathrm{i}).$$
The corresponding orthogonal projection is
$$P_v = \frac{1}{4}\begin{pmatrix} 2 & 1+\mathrm{i} & 0 & 1-\mathrm{i}\\ 1-\mathrm{i} & 2 & 1+\mathrm{i} & 0\\ 0 & 1-\mathrm{i} & 2 & 1+\mathrm{i}\\ 1+\mathrm{i} & 0 & 1-\mathrm{i} & 2\end{pmatrix}.$$
We will show some invariance properties of this vertex space in Example 2.12 (ii).

In contrast to the standard vertex space, the vertex space may "decouple" some or all of the the adjacent edges $e \in E_v$ at a vertex v, e.g., if the vertex space is $\mathscr{V}^{\max}$. "Decoupling" here means, that we may split the graph at a vertex space $\mathscr{V}_v$ such that the corresponding projection P_v has block structure w.r.t. a non-trivial decomposition $\mathscr{V}_v = \mathscr{V}_{1,v} \oplus \mathscr{V}_{2,v}$. We call a vertex space $\mathscr{V}_v$ without such a decomposition *irreducible*. Similarly, we say that $\mathscr{V} = \bigoplus_v \mathscr{V}_v$ is *irreducible*, if all its local subspaces $\mathscr{V}_v$ are irreducible. For more details, we refer to [P07c].

In [P07b, Lem. 2.13] we showed the following result on symmetry of a vertex space:

Proposition 2.10. *Assume that the vertex space $\mathscr{V}_v$ of a vertex v with degree $d = \deg v$ is invariant under permutations of the coordinates $e \in E_v$, then $\mathscr{V}_v$ is one of the spaces $\mathscr{V}_v^{\min} = 0$, $\mathscr{V}_v^{\max} = \mathbb{C}^{E_v}$, $\mathscr{V}_v^{\mathrm{std}} = \mathbb{C}(1,\dots,1)$ or $(\mathscr{V}^{\mathrm{std}})^\perp$, i.e., only the minimal, maximal, standard and dual standard vertex spaces are invariant.*

If we only require invariance under the cyclic group of order d, we have the following result:

Proposition 2.11. *Assume that the vertex space $\mathscr{V}_v$ of a vertex v with degree $d = \deg v$ is invariant under cyclic permutation of the coordinates $e \in E_v = \{e_1,\dots,e_d\}$, i.e., $e_i \mapsto e_{i+1}$ and $e_d \mapsto e_1$, then $\mathscr{V}_v$ is an orthogonal sum of spaces of the form $\mathscr{V}_v^k = \mathbb{C}(1,\theta^k,\theta^{2k},\dots,\theta^{(d-1)k})$ for $k = 0,\dots,d-1$, where $\theta = \mathrm{e}^{2\pi\mathrm{i}/d}$.*

Proof. The (representation-theoretic) irreducible vector spaces invariant under the cyclic group are one-dimensional (since the cyclic group is Abelian) and have the form $\mathscr{V}_v^k$ as given above. $\square$

We call $\mathscr{V}_v^k$ a *magnetic* perturbation of $\mathscr{V}_v^{\mathrm{std}}$, i.e., the components of the generating vector $(1,\dots,1)$ are multiplied with a phase factor $\mathrm{e}^{\mathrm{i}\varphi_e}$, $\varphi_e \in \mathbb{R}$, (see e.g. [P07b, Ex. 2.10 (vii)]).

Example 2.12.

(i) If we require that the vertex space $\mathscr{V}_v$ is cyclic invariant with *real* coefficients in the corresponding projections, then $\mathscr{V}_v$ is $\mathbb{C}(1,\dots,1)$ or $\mathbb{C}(1,-1,\dots,1,-1)$ (if d even) or their sum. But the sum is not irreducible since

$$\begin{aligned}\mathscr{V}_v &= \mathbb{C}(1,\dots,1) \oplus \mathbb{C}(1,-1,\dots,1,-1)\\ &= \mathbb{C}(1,0,1,0,\dots,1,0) \oplus \mathbb{C}(0,1,0,1,\dots,0,1)\end{aligned}$$

and the latter two spaces are standard with degree $d/2$. In other words, the irreducible graph at v associated to the boundary space $\mathscr{V}_v$ splits the vertex v into two vertices v_1 and v_2 adjacent with the edges with even and odd labels, respectively. The corresponding vertex spaces are standard.

(ii) The sum of two cyclic invariant spaces is not always reducible: Take the cyclic invariant vertex space $\mathscr{V}_v = \mathscr{V}_v^0 \oplus \mathscr{V}_v^1 \le \mathbb{C}^4$ of dimension 2 given in Example 2.9 (iv). Note that $\mathscr{V}_v$ is irreducible, since the associated projection P_v does not have block structure. This vertex space is maybe the simplest example of an (cyclic invariant) irreducible vertex space which is not standard or dual standard. Note that if $\deg v = 3$, then an irreducible vertex space is either standard or dual standard (or the corresponding version with weights and magnetic perturbations, i.e., $(1,\dots,1)$ replaced by a vector $p(v)$ with non-zero entries).

2.2. **Operators associated to vertex spaces.** Let us now define a generalised *coboundary operator* or *exterior derivative* associated to a vertex space. We use this exterior derivative for the definition of an associated Laplace operator below:

Definition 2.13. Let $\mathscr{V}$ be a vertex space of the graph G. The *exterior derivative* on $\mathscr{V}$ is defined via

$$\dddot{\mathrm{d}}_{\mathscr{V}} \colon \mathscr{V} \longrightarrow \ell_2(E), \qquad (\dddot{\mathrm{d}}_{\mathscr{V}} F)_e := F_e(\partial_+ e) - F_e(\partial_- e),$$

mapping 0-forms onto 1-forms.

We often drop the subscript $\mathscr{V}$ for the vertex space or write $\dddot{\mathrm{d}}_{\mathrm{std}}$ instead of $\dddot{\mathrm{d}}_{\mathscr{V}^{\mathrm{std}}}$ etc. The proof of the next lemma is straightforward using (2.2) (see e.g. [P07b, Lem. 3.3]):

Lemma 2.14. *Assume the lower lengths bound (2.4), then* $\dddot{\mathrm{d}}$ *is norm-bounded by* $\sqrt{2/\ell_-}$. *The adjoint*

$$\dddot{\mathrm{d}}_{\mathscr{V}}^* \colon \ell_2(E) \longrightarrow \mathscr{V}$$

fulfils the same norm bound and is given by

$$(\dddot{\mathrm{d}}^* \eta)(v) = P_v\Big(\Big\{\frac{1}{\ell_e}\widehat{\eta}_e(v)\Big\}_{e\in E_v}\Big) \in \mathscr{V}_v,$$

where $\widehat{\eta}_e(v) := \pm \eta_e$ *if* $v = \partial_\pm e$ *denotes the* oriented evaluation *of* η_e *at the vertex* v.

Definition 2.15. The *discrete generalised Laplacian* associated to a vertex space $\mathscr{V}$ is defined by $\ddot{\Delta}_{\mathscr{V}} := \dddot{\mathrm{d}}_{\mathscr{V}}^* \dddot{\mathrm{d}}_{\mathscr{V}}$, i.e.,

$$(\ddot{\Delta}_{\mathscr{V}} F)(v) = P_v\Big(\Big\{\frac{1}{\ell_e}\big(F_e(v) - F_e(v_e)\big)\Big\}_{e\in E_v}\Big)$$

for $F \in \mathscr{V}$, where v_e denotes the vertex on $e \in E_v$ opposite to v.

Remark 2.16.

(i) From Lemma 2.14 it follows that $\ddot{\Delta}_{\mathscr{V}}$ is a bounded, non-negative operator on $\mathscr{V}$ with norm estimated from above by $2/\ell_-$. In particular, $\sigma(\ddot{\Delta}_{\mathscr{V}}) \subset [0, 2/\ell_-]$.

(ii) We can also define a Laplacian $\ddot{\Delta}^1_{\mathscr{V}} := \ddot{\mathrm{d}}_{\mathscr{V}}\ddot{\mathrm{d}}^*_{\mathscr{V}}$ acting on the space of "1-forms" $\ell_2(E)$ (and $\ddot{\Delta}^0_{\mathscr{V}} := \ddot{\Delta}_{\mathscr{V}} = \ddot{\mathrm{d}}^*_{\mathscr{V}}\ddot{\mathrm{d}}_{\mathscr{V}}$). For more details and the related supersymmetric setting, we refer to [P07b]. In particular, we have

$$\sigma(\ddot{\Delta}^1_{\mathscr{V}}) \setminus \{0\} = \sigma(\ddot{\Delta}^0_{\mathscr{V}}) \setminus \{0\}.$$

Moreover, in [P07b, Ex. 3.16–3.17] we discussed how these generalised Laplacians can be used in order to analyse the (standard) Laplacian on the line graph and subdivision graph associated to G (see also [Sh00]).

The next example shows that we have indeed a generalisation of the standard discrete Laplacian:

Example 2.17.

(i) For the standard vertex space $\mathscr{V}^{\mathrm{std}}$, it is convenient to use the unitary transformation from $\mathscr{V}^{\mathrm{std}}$ onto $\ell_2(V)$ associating to $F \in \mathscr{V}$ the (common value) $\widetilde{F}(v) := F_e(v)$ as in Example 2.9 (i). Then the exterior derivative $\ddot{\mathrm{d}}_{\mathrm{std}}$ and its adjoint $\ddot{\mathrm{d}}^*_{\mathrm{std}}$ are unitarily equivalent to

$$\ddot{\mathrm{d}} \colon \ell_2(V) \longrightarrow \ell_2(E), \qquad (\ddot{\mathrm{d}}\widetilde{F})_e = \widetilde{F}(\partial_+ e) - \widetilde{F}(\partial_- e)$$

and

$$(\ddot{\mathrm{d}}^*\eta)(v) = \frac{1}{\deg v} \sum_{e \in E_v} \frac{1}{\ell_e} \widehat{\eta}_e(v),$$

i.e., $\ddot{\mathrm{d}}$ is the classical coboundary operator already defined in (2.6) and $\ddot{\mathrm{d}}^*$ its adjoint.

Moreover, the corresponding discrete Laplacian $\ddot{\Delta}_{\mathrm{std}} := \ddot{\Delta}_{\mathscr{V}^{\mathrm{std}}}$ is unitarily equivalent to the usual discrete Laplacian $\ddot{\Delta} = \ddot{\mathrm{d}}^*\ddot{\mathrm{d}}$ defined in (2.5) as one can easily check.

Similarly, for the standard weighted vertex space $\mathscr{V}^p$, the generalised discrete Laplacian expressed on the space $\ell_2(V, |p|^2)$ is given by

$$\ddot{\Delta}_p F(v) = -\frac{1}{|p(v)|^2} \sum_{e \in E_v} \frac{1}{\ell_e} \big(F(v_e) - F(v)\big), \tag{2.17}$$

where $|p(v)|^2 = \sum_{e \in E_v} |p_e(v)|^2$.

(ii) For the minimal vertex space $\mathscr{V}^{\min} = 0$, we have $\ddot{\mathrm{d}} = 0$, $\ddot{\mathrm{d}}^* = 0$ and $\ddot{\Delta}_{\mathscr{V}^{\min}} = 0$. For the maximal vertex space, we have

$$(\ddot{\Delta}_{\mathscr{V}^{\max}} F)_e(v) = \Big\{ \frac{1}{\ell_e} \big(F_e(v) - F_e(v_e)\big) \Big\}_{e \in E_v}$$

and

$$\ddot{\Delta}_{\mathscr{V}^{\max}} \cong \bigoplus_{e \in E} \ddot{\Delta}_e, \qquad \text{where} \qquad \ddot{\Delta}_e \cong \frac{1}{\ell_e} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

In particular, in both cases, the Laplacians are decoupled and any connection information of the graph is lost.

Let us now assume that the graph is equilateral (i.e., $\ell_e = 1$) and the graph has no double edges (i.e., ∂ is injective). Then we can write the Laplacian in the form

$$\Delta_{\mathscr{V}} = \mathbb{1} - M_{\mathscr{V}}, \qquad M_{\mathscr{V}} := PA^{\max},$$

where $M_{\mathscr{V}} \colon \mathscr{V} \longrightarrow \mathscr{V}$ is called the *principle part* of the generalised discrete Laplacian, and $A^{\max} \colon \mathscr{V}^{\max} \longrightarrow \mathscr{V}^{\max}$ the *generalised adjacency matrix*, defined by

$$A^{\max}\{F(w)\}_w = \{A^{\max}(v,w)F(w)\}_v, \quad A^{\max}(v,w) \colon \mathbb{C}^{E_w} \longrightarrow \mathbb{C}^{E_v}$$

for $F \in \mathscr{V}^{\max}$. Furthermore, $A^{\max}(v,w) = 0$ if v, w are not joined by an edge and

$$A^{\max}(v,w)_{e,e'} = \delta_{e,e'}, \quad e \in E_v,\ e' \in E_w$$

otherwise. In particular, written as a matrix, $A^{\max}(v,w)$ has only one entry 1 and all others equal to 0. The principle part of the Laplacian then has the form

$$(M_{\mathscr{V}} F)(v) = \sum_{e \in E_v} A_{\mathscr{V}}(v, v_e) F(v_e),$$

for $F \in \mathscr{V}$ similar to the form of the principle part of the standard Laplacian defined for $\mathscr{V}^{\mathrm{std}} \cong \ell_2(V)$, where

$$A_{\mathscr{V}}(v,w) := P_v A^{\max}(v,w) P_w \colon \mathscr{V}_w \longrightarrow \mathscr{V}_v.$$

Equivalently,

$$M_{\mathscr{V}} = \bigoplus_{v \in V} \sum_{w \in V} A_{\mathscr{V}}(v,w) \tag{2.18}$$

where the sum is actually only over those vertices w, which are connected with v. In particular, in the standard case $\mathscr{V} = \mathscr{V}^{\mathrm{std}}$, the matrix $A_{\mathscr{V}^{\mathrm{std}}}(v,w)$ consists of one entry only since $\mathscr{V}_v^{\mathrm{std}} \cong \mathbb{C}(\deg v)$ isometrically. Namely, we have $A_{\mathscr{V}^{\mathrm{std}}}(v,w) = 1$ if v and w are connected and 0 otherwise, i.e., $A_{\mathscr{V}^{\mathrm{std}}}$ is (unitarily equivalent to) the standard adjacency operator in $\ell_2(V)$.

Let us return to the general situation (i.e., general lengths ℓ_e and possibly double edges). Let G be a discrete graph. We define a *Hilbert chain associated to a vertex space $\mathscr{V}$* on G by

$$\mathscr{C}_{(G,\mathscr{V})} \colon 0 \longrightarrow \mathscr{V} \xrightarrow{\dddot{\mathrm{d}}_{\mathscr{V}}} \ell_2(E) \longrightarrow 0.$$

Obviously, the chain condition is trivially satisfied since only one operator is non-zero. In this situation and since we deal with Hilbert spaces, the associated cohomology spaces (with coefficients in $\mathbb{C}$) can be defined by

$$\begin{aligned} H^0(G,\mathscr{V}) &:= \ker \dddot{\mathrm{d}}_{\mathscr{V}} \cong \ker \dddot{\mathrm{d}}_{\mathscr{V}} / \operatorname{ran} 0, \\ H^1(G,\mathscr{V}) &:= \ker \dddot{\mathrm{d}}_{\mathscr{V}}^* = (\operatorname{ran} \dddot{\mathrm{d}}_{\mathscr{V}})^\perp \cong \ker 0 / \operatorname{ran} \dddot{\mathrm{d}}_{\mathscr{V}} \end{aligned}$$

where $\operatorname{ran} A := A(\mathscr{H}_1)$ denotes the range ("image") of the operator $A \colon \mathscr{H}_1 \longrightarrow \mathscr{H}_2$. The *index* or *Euler characteristic* of the Hilbert chain $\mathscr{C}_{(G,\mathscr{V})}$ is defined by

$$\operatorname{ind}(G,\mathscr{V}) := \dim \ker \dddot{\mathrm{d}}_{\mathscr{V}} - \dim \ker \dddot{\mathrm{d}}_{\mathscr{V}}^*,$$

i.e., the *Fredholm index* of $\dddot{\mathrm{d}}_{\mathscr{V}}$, provided at least one of the dimensions is finite. Note that for the standard vertex space $\mathscr{V}^{\mathrm{std}} \cong \ell_2(V)$, the exterior derivative is just (unitarily equivalent to) the classical coboundary operator defined in (2.6). In particular, the corresponding homology spaces are the classical ones, and $\dim H^p(G, \mathscr{V}^{\mathrm{std}})$ counts the number of components ($p = 0$) and edges not in a spanning tree ($p = 1$).

Using the stability of the index under continuous perturbations, we can calculate the index via simple (decoupled) model spaces and obtain (see [P07b, Sec. 4]), or alternatively, we can apply standard arguments from linear algebra:

Theorem 2.19. *Let $\mathscr{V}$ be a vertex space associated with the finite discrete graph $G = (V, E, \partial)$, then*

$$\operatorname{ind}(G,\mathscr{V}) = \dim \mathscr{V} - |E|.$$

Note that in particular, if $\mathscr{V} = \mathscr{V}^{\mathrm{std}}$, i.e., if $\mathscr{V} \cong \ell_2(V)$ is the standard vertex space, we recover the well-known formula for (standard) discrete graphs, namely

$$\operatorname{ind}(G,\mathscr{V}^{\mathrm{std}}) = |V| - |E|,$$

i.e., the index equals the Euler characteristic $\chi(G) := |V| - |E|$ of the graph G. On the other hand, in the "extreme" cases, we have

$$\operatorname{ind}(G, \mathscr{V}^{\max}) = |E| \quad \text{and} \quad \operatorname{ind}(G, \mathscr{V}^{\min}) = -|E|.$$

since $\dim \mathscr{V}^{\max} = \sum_{v \in V} \deg v = 2|E|$ and $\dim \mathscr{G}^{\min} = 0$. Note that the first index equals the Euler characteristic of the "decoupled" graph G^{dec} consisting of the disjoint union of the graphs $G_e = (\partial e, e)$ having only two vertices and one edge, i.e., we have

$$\operatorname{ind}(G, \mathscr{V}^{\max}) = \chi(G^{\mathrm{dec}}) = \sum_e \chi(G_e) = |E|,$$

since $\chi(G_e) = 2-1 = 1$. Similarly, the second index equals the *relative Euler characteristic*, i.e.,

$$\operatorname{ind}(G, \mathscr{V}^{\min}) = \chi(G^{\mathrm{dec}}, \partial G^{\mathrm{dec}}) := \chi(G^{\mathrm{dec}}) - \chi(\partial G^{\mathrm{dec}}) = -|E|,$$

where $\partial G^{\mathrm{dec}} = \dot{\bigcup}_e \partial G_e$ and $\partial G_e = \partial e$.

In [P07b, Lem. 4.4] we established a general result on the cohomology of the dual $\mathscr{V}^\perp$ of a vertex space $\mathscr{V}$. It shows that actually, $\mathscr{V}^\perp$ and the *oriented* version of $\mathscr{V}$, i.e., $\widehat{\mathscr{V}} = \{\, F \in \mathscr{V}^{\max} \,|\, \widehat{F} \in \mathscr{G}\,\}$, are related:

Proposition 2.20. *Assume that the global length bound*

$$\ell_- \le \ell_e \le \ell_+ \qquad \textit{for all } \mathrm{e} \in E \tag{2.21}$$

holds for some constants $0 < \ell_- \le \ell_+ < \infty$. *Then* $H^0(G, \mathscr{V}^\perp)$ *and* $H^1(G, \widehat{\mathscr{V}})$ *are isomorphic. In particular, if* G *is finite, then* $\operatorname{ind}(G, \mathscr{G}^\perp) = -\operatorname{ind}(G, \widehat{\mathscr{V}})$.

The orientation also occurs in the metric graph case, see e.g. Lemma 3.13.

3. Metric graphs, quantum graphs and associated operators

In this section, we fix the basic notion for metric and quantum graphs. Most of the material is standard (except maybe the concept of exterior derivatives), and we refer to the literature for further results and references, see e.g. [Ku08, Ku05, Kuc04, KS99a, KS99b].

3.1. **Metric graphs.**

Definition 3.1. Let $G = (V, E, \partial)$ be a discrete (exterior) graph. A *topological graph* G^{top} associated to G is a CW complex containing only 0-cells and 1-cells, such that the 0-cells are the vertices V and the 1-cells are labelled by the edge set E, respecting the graph structure in the obvious way.

A *metric graph* G^{met} associated to a weighted discrete graph (V, E, ∂, ℓ) is a topological graph associated to (V, E, ∂) such that for every edge $e \in E$ there is a continuous map $\Phi_e \colon I_e \longrightarrow G^{\mathrm{met}}$, $I_e := [0, \ell_e]$, such that $\Phi_e(\mathring{I}_e)$ is the 1-cell corresponding to e, and the restriction $\Phi_e \colon \mathring{I}_e \longrightarrow \Phi(\mathring{I}_e) \subset G^{\mathrm{met}}$ is a homeomorphism. The maps Φ_e induce a metric on G^{met}. In this way, G^{met} becomes a metric space.

By abuse of notation, we omit the labels $(\cdot)^{\mathrm{top}}$ and $(\cdot)^{\mathrm{met}}$ for the topological and metric graph associated to the discrete weighted graph, and simply write G or (V, E, ∂, ℓ).

Given a weighted discrete graph, we can abstractly construct the associated metric graph as the disjoint union of the intervals I_e for all $e \in E$ and appropriate identifications of the end-points of these intervals (according to the combinatorial structure of the graph), namely

$$G^{\mathrm{met}} = \dot{\bigcup_{e \in E}} I_e / \sim. \tag{3.2}$$

Remark 3.3.

(i) The metric graph G^{met} becomes canonically a *metric measure space* by defining the distance of two points to be the length of the shortest path in G^{met}, joining these points. We can think of the maps $\Phi_e \colon I_e \longrightarrow G^{\mathrm{met}}$ as coordinate maps and the Lebesgue measures $\mathrm{d}s_e$ on the intervals I_e induce a (Lebesgue) measure on the space G^{met}. We will often omit the coordinate map Φ_e, e.g., for functions f on G^{met} we simply write $f_e := f \circ \Phi_e$ for the corresponding function on I_e. If the edge e is clear from the context, we also omit the label $(\cdot)_e$.

(ii) Note that two metric graphs G_1^{met} and G_2^{met} can be isometric as metric spaces, such that the underlying discrete graphs G_1 and G_2 are not isomorphic: The metric on a metric graph G^{met} cannot distinguish between a single edge e of length ℓ_e in G_1 and two edges e', e'' of length $\ell_{e'}$, $\ell_{e''}$ with $\ell_e = \ell_{e'} + \ell_{e''}$ joined by a vertex of degree 2 in G_2: The underlying graphs are not (necessarily) isomorphic.

3.2. **Operators on metric graphs.** Since a metric graph is a topological space, and isometric to intervals outside the vertices, we can introduce the notion of measurability and differentiate function on the edges. We start with the basic Hilbert space

$$\mathsf{L}_2(G) := \bigoplus_{e \in E} \mathsf{L}_2(I_e) \qquad \text{and} \qquad \|f\|^2 = \|f\|^2_{\mathsf{L}_2(G)} := \sum_{e \in E} \int_{I_e} |f_e(s)|^2 \,\mathrm{d}s,$$

where $f = \{f_e\}_e$ with $f_e \in \mathsf{L}_2(I_e)$.

In order to define Laplacian-like differential operators in the Hilbert space $\mathsf{L}_2(G)$ we introduce the *maximal* or *decoupled* Sobolev space of order k as

$$\mathsf{H}^k_{\max}(G) := \bigoplus_{e \in E} \mathsf{H}^k(I_e),$$
$$\|f\|^2_{\mathsf{H}^k_{\max}(G)} := \sum_{e \in E} \|f_e\|^2_{\mathsf{H}^k(I_e)},$$

where $\mathsf{H}^k(I_e)$ is the classical Sobolev space on the interval I_e, i.e., the space of functions with (weak) derivatives in $\mathsf{L}_2(I_e)$ up to order k. We define the *unoriented* and *oriented evaluation* of f on the edge e at the vertex v by

$$\underline{f}_e(v) := \begin{cases} f_e(0), & \text{if } v = \partial_- e, \\ f_e(\ell(e)), & \text{if } v = \partial_+ e \end{cases} \quad \text{and} \quad \underline{\widehat{f}}_e(v) := \begin{cases} -f_e(0), & \text{if } v = \partial_- e, \\ f_e(\ell(e)), & \text{if } v = \partial_+ e. \end{cases}$$

Note that $\underline{f}_e(v)$ and $\underline{\widehat{f}}_e(v)$ are defined for $f \in \mathsf{H}^1_{\max}(G)$. Recall that $\mathscr{V}^{\max} = \bigoplus_v \mathscr{V}_v^{\max} = \bigoplus_v \mathbb{C}^{E_v}$.

Lemma 3.4. *Assume the lower lengths bound (2.4), then the evaluation operators*

$$\underline{\bullet} \colon \mathsf{H}^1_{\max}(G) \longrightarrow \mathscr{V}^{\max}, \qquad\qquad \underline{\widehat{\bullet}} \colon \mathsf{H}^1_{\max}(G) \longrightarrow \mathscr{V}^{\max},$$
$$f \mapsto \underline{f} = \{\{\underline{f}_e(v)\}_{e \in E_v}\}_v \in \mathscr{V}^{\max} \quad \textit{and} \quad f \mapsto \underline{\widehat{f}} = \{\{\underline{\widehat{f}}_e(v)\}_{e \in E_v}\}_v \in \mathscr{V}^{\max}$$

are bounded by $(2/\ell_-)^{1/2}$.

Proof. It is a standard fact from Sobolev theory, that

$$|f(0)|^2 \le \int_0^{\ell_e} \Big(a|f(s)|^2 + \frac{2}{a}|f'(s)|^2 \Big) \,\mathrm{d}s \le \frac{2}{\ell_-} \int_0^{\ell_e} \big(|f(s)|^2 + |f'(s)|^2 \big) \,\mathrm{d}s \tag{3.5}$$

for $f \in \mathsf{H}^1(I_e)$ and $0 < a \le \ell_e$, using $\ell_e \ge \ell_- > 0$ and $\ell_- \le 1$ (see e.g. [P09, Cor. A.2.22]). In particular, the individual evaluation operator $\mathsf{H}^1(I_e) \to \mathbb{C}$, $f_e \mapsto \pm f_e(v)$ is bounded by $(2/\ell_-)^{1/2}$. $\square$

The lower length bound allows us to get rid of first order derivatives:

Lemma 3.6. *Assume that* $I = [0, \ell]$, *then*

$$\|f'\|^2_{\mathsf{L}_2(I)} \le \frac{1025}{\ell_-^2} \|f\|^2_{\mathsf{L}_2(I)} + 2\|f''\|^2_{\mathsf{L}_2(I)} \le \frac{1025}{\ell_-^2}\Big(\|f\|^2_{\mathsf{L}_2(I)} + \|f''\|^2_{\mathsf{L}_2(I)}\Big)$$

for $f \in \mathsf{H}^2(I)$, *where* $\ell_- = \min\{1, \ell\}$.

Proof. Partial integration and Cauchy-Young's inequality yield

$$\|f'\|^2 \overset{\text{CY}}{\le} \frac{1}{2}\|f\|^2 + \frac{1}{2}\|f''\|^2 + \big|f(0)f'(0)\big| + \big|f(\ell)f'(\ell)\big|.$$

The boundary term can be estimated by

$$\begin{aligned}\big|f(0)f'(0)\big| &\overset{\text{CY}}{\le} \frac{\eta}{2}\big|f'(0)\big|^2 + \frac{1}{2\eta}\big|f(0)\big|^2 \\ &\le \frac{\eta}{2}\Big(b'\|f''\|^2 + \frac{2}{b'}\|f'\|^2\Big) + \frac{1}{2\eta}\Big(b\|f'\|^2 + \frac{2}{b}\|f\|^2\Big) \\ &= \frac{1}{\eta b}\|f\|^2 + \frac{\eta b'}{2}\|f''\|^2 + \frac{1}{2}\Big(\frac{2\eta}{b'} + \frac{b}{\eta}\Big)\|f'\|^2\end{aligned}$$

for $\eta >$ and $b, b' \in (0, \ell]$, applying (3.5) to f and f'. A similar result holds for the boundary term at $s = \ell$, so that we end up with the inequality

$$\|f'\|^2 \le \Big(\frac{1}{2} + \frac{2}{\eta b}\Big)\|f\|^2 + \Big(\frac{1}{2} + \eta b'\Big)\|f''\|^2 + \Big(\frac{2\eta}{b'} + \frac{b}{\eta}\Big)\|f'\|^2.$$

If we set $\eta := a/8$, $b := a/32$ and $b' := a$ for $0 < a \le \ell$, then the coefficient of $\|f'\|^2$ on the RHS equals $1/2$. Bringing this term on the LHS and multiplying by 2 yields the desired estimate with $a = \ell_-$. Note that $1 + 4/(\eta b) = 1 + 1024/a^2 \le 1025/a^2$ and $12\eta b' = 1 + a^2/4 \le 2$ since $a \le 1$. ☐

The two evaluation maps of Lemma 3.4 allow a very simple formula of a partial integration formula on the metric graph, namely

$$\langle f', g\rangle_{\mathsf{L}_2(G)} = \langle f, -g'\rangle_{\mathsf{L}_2(G)} + \langle \underline{f}, \widehat{\underline{g}}\rangle_{\mathscr{V}^{\max}}, \tag{3.7}$$

where $f' = \{f'_e\}_e$ and similarly for g. Basically, the formula follows from partial integration on each interval I_e and a reordering of the sum using (2.2).

Remark 3.8. If we distinguish between functions (0-forms) and vector fields (1-forms), we can say that 0-forms are evaluated *unoriented*, whereas 1-forms are evaluated *oriented*. In this way, we should interprete f' and g as 1-forms and f, g' as 0-forms.

Let us now introduce another data in order to define operators on the metric graph:

Definition 3.9. A *quantum graph* $(G, \mathscr{V})$ is given by a metric graph G together with a vertex space $\mathscr{V}$ associated to G (i.e., a local subspace of $\mathscr{V}^{\max}$, see Definition 2.8). In particular, a quantum graph is fixed by the data $(V, E, \partial, \ell, \mathscr{V})$.

Note that in the literature (see e.g. [Ku08]), a *quantum graph* is sometimes defined as a metric graph together with a self-adjoint (pseudo-)differential operator acting on it. This definition is more general, since we only associate the Laplacian $\Delta_{\mathscr{V}}$ defined below with a quantum graph $(G, \mathscr{V})$.

Associated to a quantum graph $(G, \mathscr{V})$, we define the Sobolev spaces

$$\mathsf{H}^k_{\mathscr{V}}(G) := \big\{\, f \in \mathsf{H}^k_{\max}(G) \,\big|\, \underline{f} \in \mathscr{V} \,\big\} \quad \text{and} \quad \mathsf{H}^k_{\widehat{\mathscr{V}}}(G) := \big\{\, f \in \mathsf{H}^k_{\max}(G) \,\big|\, \widehat{\underline{f}} \in \mathscr{V} \,\big\}.$$

By Lemma 3.4, these spaces are closed in $\mathsf{H}^k_{\max}(G)$ as pre-image of the closed subspace $\mathscr{V}$ and the bounded operators $\underline{\bullet}$ and $\widehat{\underline{\bullet}}$, respectively; and therefore themselves Hilbert spaces.

On the Sobolev space $\mathsf{H}^1_{\mathscr{V}}(G)$, we can rewrite the vertex term in the partial integration formula (3.7) and obtain

$$\langle f', g\rangle_{\mathsf{L}_2(G)} = \langle f, -g'\rangle_{\mathsf{L}_2(G)} + \langle \underline{f}, P\underline{\widehat{g}}\rangle_{\mathscr{V}} \tag{3.10}$$

for $f \in \mathscr{V}$ and $g \in \mathscr{V}^{\max}$, where P denotes the orthogonal projection of $\mathscr{V}$ in $\mathscr{V}^{\max}$.

Let us now mimic the concept of exterior derivative:

Definition 3.11. The *exterior derivative* associated to a quantum graph G and a vertex space $\mathscr{V}$ is the unbounded operator $\mathrm{d}_{\mathscr{V}}$ in $\mathsf{L}_2(G)$ defined by $\mathrm{d}_{\mathscr{V}} f := f'$ for $f \in \operatorname{dom} \mathrm{d}_{\mathscr{V}} := \mathsf{H}^1_{\mathscr{V}}(G)$.

Remark 3.12.

(i) Note that $\mathrm{d}_{\mathscr{V}}$ is a closed operator (i.e., its graph is closed in $\mathsf{L}_2(G) \oplus \mathsf{L}_2(G)$), since $\mathsf{H}^1_{\mathscr{V}}(G)$ is a Hilbert space and the graph norm of $\mathrm{d} = \mathrm{d}_{\mathscr{V}}$, given by $\|f\|^2_{\mathrm{d}} := \|\mathrm{d}f\|^2 + \|f\|^2$, is the Sobolev norm, i.e, $\|f\|_{\mathrm{d}} = \|f\|_{\mathsf{H}^1_{\max}(G)}$.
(ii) We can think of d as an operator mapping 0-forms into 1-forms. Obviously, on a one-dimensional *smooth* space, there is no need for this distinction, but the distinction between 0- and 1-forms makes sense through the vertex conditions $\underline{f} \in \mathscr{V}$, see also the next lemma.

The adjoint of $\mathrm{d}_{\mathscr{V}}$ can easily be calculated from the partial integration formula (3.10), namely the vertex term $P\underline{\widehat{g}}$ has to vanish for functions g in the domain of $\mathrm{d}^*_{\mathscr{V}}$:

Lemma 3.13. *The adjoint of* $\mathrm{d}_{\mathscr{V}}$ *is given by* $\mathrm{d}^*_{\mathscr{V}} g = -g'$ *with domain* $\operatorname{dom} \mathrm{d}^*_{\mathscr{V}} = \mathsf{H}^1_{\widehat{\mathscr{V}}^\perp}(G)$.

As for the discrete operators, we define the Laplacian via the exterior derivative:

Definition 3.14. The *Laplacian associated to a quantum graph* $(G, \mathscr{V})$ is defined by

$$\Delta_{\mathscr{V}} = \Delta_{(G,\mathscr{V})} := \mathrm{d}^*_{\mathscr{V}} \mathrm{d}_{\mathscr{V}}$$

with domain $\operatorname{dom} \Delta_{\mathscr{V}} := \{\, f \in \operatorname{dom} \mathrm{d}_{\mathscr{V}} \mid \mathrm{d}_{\mathscr{V}} f \in \operatorname{dom} \mathrm{d}^*_{\mathscr{V}} \,\}$.

Let us collect some simple facts about the Laplacian:

Proposition 3.15. *Let* $(G, \mathscr{V})$ *be a quantum graph with lower lengths bound* $\inf_e \ell_e \ge \ell_-$, $\ell_- \in (0, 1]$.

(i) *The Laplacian* $\Delta_{\mathscr{V}} = \mathrm{d}^*_{\mathscr{V}} \mathrm{d}_{\mathscr{V}}$ *is self-adjoint and non-negative. Moreover, the Laplacian is the operator associated to the closed quadratic form* $\mathfrak{d}_{\mathscr{V}}(f) := \|\mathrm{d}_{\mathscr{V}} f\|^2_G$ *and* $\operatorname{dom} \mathfrak{d}_{\mathscr{V}} = \mathsf{H}^1_{\mathscr{V}}(G)$.
(ii) *The domain of the Laplacian* $\Delta_{\mathscr{V}} = \mathrm{d}^*_{\mathscr{V}} \mathrm{d}_{\mathscr{V}}$ *is given by*

$$\operatorname{dom} \Delta_{\mathscr{V}} = \bigl\{\, f \in \mathsf{H}^2_{\max}(G) \bigm| \underline{f} \in \mathscr{V}, \quad \underline{\widehat{f}'} \in \mathscr{V}^\perp \,\bigr\}.$$

Proof. The self-adjointness follows immediately from the definition of the Laplacian. Moreover,

$$\langle f, \Delta_{\mathscr{V}} g\rangle = \langle \mathrm{d}_{\mathscr{V}} f, \mathrm{d}_{\mathscr{V}} g\rangle = \mathfrak{d}_{\mathscr{V}}(f, g)$$

for all $f \in \operatorname{dom} \mathrm{d}_{\mathscr{V}}$ and $g \in \operatorname{dom} \Delta_{\mathscr{V}}$. Hence, $\Delta_{\mathscr{V}}$ is the operator associated to $\mathscr{V}$ (see [Kat66, Thm. VI.2.1]). Finally, the domain characterisation is easily seen using Lemma 3.13. □

The condition $\underline{f} \in \mathscr{V}$, $\underline{\widehat{f}'} \in \mathscr{V}^\perp$ will be called *vertex condition*, and similarly, $\underline{f}(v) \in \mathscr{V}_v$, $\underline{\widehat{f}'}(v) \in \mathscr{V}_v^\perp$ *vertex condition at the vertex* v.

Remark 3.16.

(i) There are other possibilities how to define self-adjoint extensions of a Laplacian, see e.g. [Ha00, Kuc04, FKW07] and (ii) below. In particular, for a self-adjoint (bounded) operator L on $\mathscr{V}$, we can define a self-adjoint Laplacian $\Delta_{(\mathscr{V},L)}$ with domain
$$\operatorname{dom}\Delta_{(\mathscr{V},L)} := \big\{\, f \in \mathsf{H}^2_{\mathscr{V}}(G) \,\big|\, P\underline{\widehat{f}}' = L\underline{f} \,\big\},$$
where P is the projection in $\mathscr{V}^{\max}$ onto the space $\mathscr{V}$. The vertex conditions $\underline{f} \in \mathscr{V}$ and $P\underline{\widehat{f}}' = L\underline{f}$ at the vertex v split into three different parts, namely the *Dirichlet part* $\underline{f} \in \mathscr{V}$, the *Neumann part* $P\underline{\widehat{f}}' \in (\ker L)^\perp \subset \mathscr{V}$ and the *Robin part* $P\underline{\widehat{f}}' = L\underline{f}$ on $(\ker L)^\perp$ (see e.g. [FKW07] for details). If $L = 0$, then the Robin part is not present, as it is the case in Proposition 3.15.

(ii) One can encode the vertex conditions also in a (unitary) operator S on $\mathscr{V}^{\max}$, the *scattering operator* (see e.g. [KS97, KS99a, KS03b, KPS07b]). In general, $S = S(\lambda)$ depends on the eigenvalue ("energy") parameter λ, namely, $S(\lambda)$ is (roughly) defined by looking how incoming and outgoing waves (of the form $x \mapsto \mathrm{e}^{\pm \mathrm{i}\sqrt{\lambda} x}$) propagate through a vertex. In our case (i.e., if $L = 0$ in $\Delta_{(\mathscr{V},L)}$ described above), one can show that S is independent of the *energy*, namely,
$$S = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} = 2P - \mathbb{1} \tag{3.17}$$
with respect to the decomposition $\mathscr{V}^{\max} = \mathscr{V} \oplus \mathscr{V}^\perp$, and where P is the orthogonal projection of $\mathscr{V}$ in $\mathscr{V}^{\max}$. In particular, the so-called *energy-independent* vertex conditions are precisely the ones without Robin part (i.e., $L = 0$), see (i) above.

(iii) As in the discrete case, we can consider $\Delta^0_{\mathscr{V}} := \Delta_{\mathscr{V}}$ as the Laplacian on 0-forms, and $\Delta^1_{\mathscr{V}} := \mathrm{d}_{\mathscr{V}}\mathrm{d}^*_{\mathscr{V}}$ as the Laplacian on 1-forms. Again, by supersymmetry, we have the spectral relation
$$\sigma(\Delta^1_{\mathscr{V}}) \setminus \{0\} = \sigma(\Delta^0_{\mathscr{V}}) \setminus \{0\}.$$
For more details we refer to [P07b, Sec. 5].

An important example is the quantum graph with *standard* vertex space
$$\mathscr{V}^{\mathrm{std}} = \bigoplus_v \mathscr{V}^{\mathrm{std}}_v, \qquad\qquad \mathscr{V}^{\mathrm{std}}_v = \mathbb{C}(1,\dots,1) \subset \mathbb{C}^{E_v},$$
respectively, its weighted version
$$\mathscr{V}^{p} = \bigoplus_v \mathscr{V}^{p(v)}_v, \qquad\qquad \mathscr{V}^{p(v)}_v = \mathbb{C}p(v) \subset \mathbb{C}^{E_v},$$
where $p(v) = \{p_e(v)\}_{e \in E_v}$ and $p_e(v) \neq 0$. Moreover,
$$\operatorname{dom}\mathrm{d}^*_p = \Big\{\, g \in \mathsf{H}^1_{\max}(G) \,\Big|\, \sum_{e \in E_v} p_e(v)\, \underline{\widehat{g}}_e(v) = 0 \quad \forall v \in V \,\Big\} \quad \text{and}$$
$$\operatorname{dom}\Delta_p = \Big\{\, f \in \mathsf{H}^2_{\max}(G) \,\Big|\, \underline{f}(v) \in \mathbb{C}p(v), \quad \sum_{e \in E_v} p_e(v)\, \underline{\widehat{f}}'_e(v) = 0 \quad \forall v \in V \,\Big\}.$$

For the standard vertex space, $\mathsf{H}^1_{\mathscr{V}^{\mathrm{std}}}(G)$ consists of *continuous* functions on the topological graph G: On each edge, we have the embedding $\mathsf{H}^1(I_e) \subset \mathsf{C}(I_e)$, i.e., f is already continuous inside each edge. Moreover, the evaluation $\underline{f}_e(v)$ is *independent* of $e \in E_v$. This is the reason why we call $\mathscr{V}^{\mathrm{std}}$ also the *continuous* vertex space. In particular, a function f is in the domain of the *standard* or *Kirchhoff Laplacian* $\Delta_{\mathrm{std}} = \Delta_{\mathscr{V}^{\mathrm{std}}}$ iff $f \in \mathsf{H}^2_{\max}(G)$, f is continuous and if the *flux* condition on the derivatives $\sum_{e \in E_v} f'_e(v) = 0$ is fulfilled for all $v \in V$.

Let us make a short remark on the extremal vertex spaces $\mathscr{V}_v^{\max} = \mathbb{C}^{E_v}$ and $\mathscr{V}^{\min} = 0$: The corresponding Laplacian fulfils the vertex conditions

$$f_e(v) = 0 \quad \forall e \in E_v \qquad \text{resp.} \qquad f_e'(v) = 0 \quad \forall e \in E_v,$$

i.e., the function f fulfils *indidivual* Dirichlet resp. Neumann vertex conditions at the vertex v. This is the reason for the name *Dirichlet* resp. *Neumann* vertex space in Example 2.9 (iii).

In particular, if $\mathscr{V} = 0$ and $\mathscr{V} = \mathscr{V}^{\max}$ are the minimal and maximal vertex spaces, then

$$\Delta_0 = \bigoplus_e \Delta_{I_e}^{\partial I_e} \qquad \text{and} \qquad \Delta_{\max} = \bigoplus_e \Delta_{I_e},$$

respectively, i.e., the operators are *decoupled*. Here $\Delta_{I_e}^{\partial I_e}$ is the Laplacian on I_e with Dirichlet boundary conditions on ∂I_e, and similarly, Δ_{I_e} is the Laplacian on I_e with Neumann boundary conditions on ∂I_e.

We say that a quantum graph $(G, \mathscr{V})$ is *compact* if the underlying metric graph G is compact as topological space. In particular, G is compact iff $|E|$ is finite (since in our setting, all edges have finite length). The following observation is proven e.g. in [P07c, Prp. 3.13].

Proposition 3.18. *Assume that $(G, \mathscr{V})$ is a compact quantum graph, then the resolvent $(\Delta_{\mathscr{V}} + 1)^{-1}$ of the associated Laplacian is a compact operator. In particular, $\Delta_{\mathscr{V}}$ has purely discrete spectrum, i.e., there is an infinite sequence $\{\lambda_k\}_k$ of eigenvalues, where $\lambda_k = \lambda_k(\Delta_{\mathscr{V}})$ denotes the k-th eigenvalue (repeated according to its multiplicity) and $\lambda_k \to \infty$ as $k \to \infty$.*

4. Boundary triples associated to quantum graphs

We need the notion of a *boundary* of a graph: A *boundary of a metric graph G* is a subset ∂G of V. We call vertices in $\mathring{V} := V \setminus \partial G$ *interior vertices*.

Let us now define a boundary triple associated to a quantum graph $(G, \mathscr{V})$ (see also [Pan06, BGP07, BGP08, P08]). The concept of a boundary triple is briefly explained in Appendix A. In particular, for a quantum graph $(G, \mathscr{V})$ we set

$$\begin{aligned} \mathscr{H} &:= \mathsf{L}_2(G), & \mathscr{H}^1 &:= \mathsf{H}^1_{\mathscr{V}}(G), & \mathfrak{a}(f) &:= \|\mathrm{d}_{\mathscr{V}} f\|_G^2, \\ \mathscr{G} &:= \bigoplus_{v \in \partial G} \mathscr{V}_v, & \Gamma f &:= \{\underline{f}(v)\}_{v \in \partial G} \end{aligned}$$

for $f \in \mathscr{H}^1$. Moreover, we define the maximal operator by $(Af)_e = -f_e''$ and

$$\operatorname{dom} A := \bigl\{\, f \in \mathsf{H}^2_{\mathscr{V}}(G) \bigm| P_v \widehat{\underline{f}}'(v) = 0 \quad \forall\, v \in \mathring{V} \,\bigr\}, \quad \text{and set} \quad \Gamma' f := \{P_v \widehat{\underline{f}}'(v)\}_{v \in \partial G},$$

where $P = \bigoplus_v P_v$ denotes the orthogonal projection of $\mathscr{V}$ in $\mathscr{V}^{\max}$. In particular, functions in $\operatorname{dom} A$ fulfil the vertex conditions $\underline{f}(v) \in \mathscr{V}_v$ and $\widehat{\underline{f}}'(v) \in \mathscr{V}_v^\perp$ for all *inner* vertices, whereas for the boundary vertices $v \in \partial G$, only $\underline{f}(v) \in \mathscr{V}_v$ is assumed.

Proposition 4.1. *Assume that $(G, \mathscr{V})$ is a quantum graph with boundary $\partial G \subset V$ and lower length bound $\ell_e \geq \ell_-$ for some $\ell_- \in (0, 1]$. Then we have:*

(i) *The quadratic form $\mathfrak{a}$ and the maximal operator A are closed.*
(ii) *The triple $(\Gamma, \Gamma', \mathscr{G})$ is a bounded boundary triple associated to the quadratic form $\mathfrak{a}$ and the maximal operator A.*

Proof. (i) The closeness of $\mathfrak{a}$ follows from the closeness of the operator $\mathrm{d}_{\mathscr{V}}$. For the closeness of A, note that $\operatorname{dom} A$ is a closed subspace of $\mathsf{H}^2_{\mathscr{V}}(G)$, since the evaluation operator $\widehat{\underline{\bullet}}'$ is bounded (see Lemma 3.4). Moreover,

$$\|f\|^2 + \|f''\|^2 \le \|f\|^2 + \|f'\|^2 + \|f''\|^2 = \|f\|^2_{\mathsf{H}^2_{\max}(G)} \le \Big(1 + \frac{1025}{\ell_-^2}\Big)\big(\|f\|^2 + \|f''\|^2\big)$$

by Lemma 3.6, i.e., the graph norm of A and the norm on $\mathsf{H}^2_{\mathscr{V}}(G)$ are equivalent. Since the latter space is complete, the closeness of A follows.

(ii) Green's formula (A.6) follows from partial integration (3.10), namely

$$\langle f, Ag\rangle = \langle f, -g''\rangle = \langle f', g'\rangle - \langle \underline{f}, P\widehat{\underline{g}}'\rangle_{\mathscr{V}} = \mathfrak{a}(f,g) - \langle \Gamma f, \Gamma' g\rangle_{\mathscr{G}}$$

for $f \in \mathscr{H}^1$ and $g \in \operatorname{dom} A$ since $P_v\widehat{\underline{g}}'(v) = 0$ for $v \in \mathring{V}$ by definition of $\operatorname{dom} A$.

For the surjectivity (A.1b) one has to construct a function $f \in \operatorname{dom} A$ with prescribed values $\underline{f}(v) = F(v)$ and $\widehat{\underline{f}}'(v) = G(v)$ for all $v \in \partial G$ and given $F, G \in \mathscr{V}$. Clearly, this can be done locally at each boundary vertex for a function vanishing at points with distance more than $\ell_-/2$ from each boundary vertex. At inner vertices we set $\underline{f}(v) = 0$ and $\widehat{\underline{f}}'(v)$. The global lower bound on each length $\ell_e \ge \ell_-$ assures that the different parts of the functions near each vertex have disjoint supports and that the summability of F and G (i.e., $F, G \in \mathscr{V}$) implies the integrability of f, f' and f'' on G for an appropriate choice of f. □

For the next proposition, we need some more notation. Let $\sqrt{z}$ be the square root cut along the positive axis $\mathbb{R}_+ = [0,\infty)$, so that in particular, $\operatorname{Im}\sqrt{z} > 0$. We denote by

$$\sin_{z,e,+}(s) := \frac{\sin_z s}{\sin_z \ell_e} \qquad \text{and} \qquad \sin_{z,e,-}(s) := \frac{\sin_z(\ell_e - s)}{\sin_z \ell_e}, \tag{4.2a}$$

where $\sin_z(s) := \sin(\sqrt{z}\, s)$ for $z \in \mathbb{C} \setminus \mathbb{R}_+$, the two *fundamental solutions* of $-f_e'' = zf_e$ on I_e with $\sin_{z,e,+}(0) = 1$, $\sin_{z,e,+}(\ell_e) = 0$ and vice versa for $\sin_{z,e,-}$.[2] Moreover, we set

$$\tan_z(s) = \tan(\sqrt{z}\, s) \qquad \text{and} \qquad \cot_z(s) := \cot(\sqrt{z}\, s). \tag{4.2b}$$

If the boundary consists of *all* vertices, i.e., $\partial G = V$, then we can give explicit formulas for the Dirichlet solution operator and the Dirichlet-to-Neumann map (see Definition A.3, similar results can be found in [P08, BGP08]). Note that in this case, the boundary space of the boundary triple agrees with the entire vertex space, i.e., $\mathscr{G} = \mathscr{V}$:

Proposition 4.3. *Assume that $(G, \mathscr{V})$ is a quantum graph with boundary $\partial G = V$ and lower length bound $\ell_e \ge \ell_-$ for some $\ell_- \in (0,1]$. Then for $z \in \mathbb{C} \setminus \mathbb{R}_+$, we have:*

(i) *The Dirichlet operator A^{D} associated to the boundary triple $(\Gamma, \Gamma', \mathscr{V})$ is the Laplacian associated to the minimal vertex space $\mathscr{V}^{\min} = 0$, i.e.,*

$$A^{\mathrm{D}} = \Delta_0 = \bigoplus_e \Delta_{I_e}^{\partial I_e}.$$

In particular, A^{D} is decoupled. The spectrum of A^{D} is

$$\sigma(A^{\mathrm{D}}) = \Big\{ \frac{k^2\pi^2}{\ell_e^2} \,\Big|\, e \in E,\ k = 1,2,\dots \Big\}.$$

Moreover, if the graph is equilateral, then

$$\sigma(A^{\mathrm{D}}) = \big\{ k^2\pi^2 \,\big|\, k = 1,2,\dots \big\} =: \Sigma^{\mathrm{D}}.$$

(ii) *The Neumann operator associated to the boundary triple $(\Gamma, \Gamma', \mathscr{V})$ is the Laplacian associated to the quantum graph $(G, \mathscr{V})$, i.e.,*

$$A^{\mathrm{N}} = \Delta_{\mathscr{V}}.$$

[2] We also need the analytic continuation in $z = 0$, i.e., we set $\sin_{0,e,+}(s) := \dfrac{s}{\ell_e}$ and $\sin_{0,e,-}(s) := 1 - \dfrac{s}{\ell_e}$.

(iii) *The Dirichlet solution operator* $S(z)\colon \mathscr{V} \longrightarrow \operatorname{dom} A$, *defined by* $f = S(z)F$, *where* f *is the (unique) solution of the Dirichlet problem* $(A-z)f = 0$, $\Gamma f = F$, *is given by*

$$f_e(s) = F_e(\partial_- e)\sin_{z,e,-}(s) + F_e(\partial_+ e)\sin_{z,e,+}(s),$$

where $F = \{F(v)\}_{v\in V} \in \bigoplus_v \mathscr{V}_v = \mathscr{V}$.

(iv) *The Dirichlet-to-Neumann map* $\Lambda\colon \mathscr{V} \longrightarrow \mathscr{V}$ *is given by*

$$(\Lambda(z)F)(v) = P_v H(v), \qquad H(v) = \{H_e(v)\}_{e\in E_v}$$

where

$$H_e(v) = \frac{\sqrt{z}}{\sin_z \ell_e}\Big((\cos_z \ell_e)F_e(v) - F_e(v_e)\Big),$$

and where v_e *denotes the vertex ajacent with* e *opposite of* v. *In particular, if the graph is equilateral* ($\ell_e = 1$)*, then*

$$\Lambda(z) = \frac{\sqrt{z}}{\sin\sqrt{z}}\Big(\ddot{\Delta}_{\mathscr{V}} - (1-\cos\sqrt{z})\Big),$$

i.e., the Dirichlet-to-Neumann map is an affine-linear (z-depending) function of the discrete Laplacian $\ddot{\Delta}_{\mathscr{V}}$.

Proof. The first assertion is obvious. The second assertion follows from the characterisation of the domain of $\Delta_{\mathscr{V}}$ in Proposition 3.15. Note that if $\partial G = V$, then $\operatorname{dom} A = \mathsf{H}^2_{\mathscr{V}}(G)$. For the third assertion, note that $f = S(z)F$ solves the differential equation on each edge, that $\Gamma f = F$ by the ansatz for f and that $f \in \mathsf{L}_2(G)$ (and therefore also $Af = zf \in \mathsf{L}_2(G)$). The last assertion is easily seen by a straightforward calculation. $\square$

5. Extended quantum graphs

Let us provide Laplacians defined on an extended space associated to a quantum graph $(G, \mathscr{V})$. We always assume that the lower length bound $\ell_e \geq \ell_- > 0$ is fulfilled. The operators on the extended space described below occur naturally in the limit of graph-like manifolds, in particular, when the shrinking rate of the vertex neighbourhood volume is of the same order as the transversal volume ("borderline case", L invertible) or shrinks slower ("slowly decaying case", $L = 0$) see e.g. [P09, EP05, KuZ03].

Definition 5.1. An *extended quantum graph* is a triple $(G, \mathscr{V}, L)$, where $(G, \mathscr{V})$ is a quantum graph (i.e., G is a metric graph and $\mathscr{V} = \bigoplus_v \mathscr{V}_v$ a vertex space), and L a self-adjoint, bounded operator on $\mathscr{V}$. Moreover, we assume that L is local, i.e., $L = \bigoplus_v L(v)$, where $L(v)$ acts on $\mathscr{V}_v$.

We sometimes refer to a quantum graph $(G, \mathscr{V})$ and the related operators and spaces (see Section 3.2) as *simple*.

We now associate the Hilbert spaces and operators to an extended metric graph. Basically, we define the extended spaces and operators as the extended corresponding objects associated to the boundary triple $(\Gamma, \Gamma', \mathscr{V})$, see Definition A.9. In particular, the *extended Hilbert space* is given by

$$\hat{\mathscr{H}} := \mathsf{L}_2(G) \oplus \mathscr{V},$$

(see Proposition A.10).

The *extended exterior derivative* $\hat{\mathrm{d}}_{(\mathscr{V},L)}$ is defined via

$$\hat{\mathrm{d}}_{(\mathscr{V},L)}\colon \hat{\mathscr{H}}^1_L \longrightarrow \mathsf{L}_2(G), \qquad \hat{\mathrm{d}}_{(\mathscr{V},L)}\hat{f} := f' \qquad \text{for} \qquad \hat{f} = (f,F) \in \hat{\mathscr{H}}^1_L,$$

where

$$\hat{\mathscr{H}}^1_L := \big\{\, (f,F) \in \mathsf{H}^1_{\mathscr{V}}(G) \oplus \mathscr{V} \,\big|\, \underline{f} = LF \,\big\} \tag{5.2}$$

is the *extended space of order* 1 associated to $(G, \mathscr{V}, L)$. The following result follows straightforward:

Lemma 5.3. *The adjoint of* $\hat{\mathrm{d}}_{(\mathscr{V},L)}$ *is given by*

$$(\hat{\mathrm{d}}_{(\mathscr{V},L)})^* g = (-g', LP\underline{\widehat{g}}) \qquad \text{and} \qquad \operatorname{dom}(\hat{\mathrm{d}}_{(\mathscr{V},L)})^* = \mathsf{H}^1_{\max}(G),$$

where P *denotes the projection onto* $\mathscr{V}$ *in* $\mathscr{V}^{\max}$.

From Proposition A.10 we conclude the following assertions:

Proposition 5.4. *Assume that* $(G, \mathscr{V})$ *is a quantum graph and* L *a bounded operator on* $\mathscr{G}$.

(i) *The extended quadratic form* $\hat{\mathfrak{a}}_L$ *associated to* $(G, \mathscr{V})$ *and* L *is given by*

$$\hat{\mathfrak{a}}_L(\hat{f}) = \|\hat{\mathrm{d}}_{(\mathscr{V},L)} \hat{f}\|^2_G$$

with domain $\operatorname{dom} \hat{\mathfrak{a}}_L = \hat{\mathscr{H}}^1_L$ *(see (5.2)). In particular,* $\hat{\mathfrak{a}}_L$ *is closed and non-negative.*

(ii) *The extended Laplacian* $\hat{\Delta}_{(\mathscr{V},L)} = (\hat{\mathrm{d}}_{(\mathscr{V},L)})^* \hat{\mathrm{d}}_{(\mathscr{V},L)}$ *is non-negative and acts as*

$$\hat{\Delta}_{(\mathscr{V},L)}(f, F) = (-f'', LP\underline{\widehat{f}'})$$

with domain given by

$$\operatorname{dom} \hat{\Delta}_{(\mathscr{V},L)} = \bigl\{\, \hat{f} = (f, F) \in \mathsf{H}^2_{\max}(G) \oplus \mathscr{G} \,\big|\, \underline{f} \in \mathscr{V}, \quad \underline{f} = LF \,\bigr\}.$$

In particular, for $L = 0$ we obtain (see Corollary A.11 and Proposition 4.3):

Corollary 5.5. *Assume that* $(G, \mathscr{V})$ *is a quantum graph. Then the extended quadratic form* $\hat{\mathfrak{a}}_0$ *and the corresponding operator* $\hat{\Delta}_{(\mathscr{V},0)}$ *associated to* $(G, \mathscr{V})$ *and the trivial operator* $L = 0$ *are decoupled, i.e.,*

$$\hat{\mathfrak{a}}_0 = \bigoplus_{e \in E} \mathfrak{d}^{\partial I_e}_{I_e} \oplus \mathfrak{o} \qquad \text{and} \qquad \hat{\Delta}_{(\mathscr{V},0)} = \bigoplus_{e \in E} \Delta^{\partial I_e}_{I_e} \oplus 0$$

with respect to the decompositon $\hat{\mathscr{H}} = \bigoplus_e \mathsf{L}_2(I_e) \oplus \mathscr{G}$, *where* $\mathfrak{d}^{\partial I_e}_{I_e}$ *and* $\Delta^{\partial I_e}_{I_e}$ *denote the Dirichlet quadratic form and the Dirichlet Laplacian on* I_e*, respectively.*

If $\mathscr{V} = \mathscr{V}^p$ is a weighted standard vertex space, we can use the equivalent space $\ell_2(V, |p|^2)$ (see Example 2.9 (ii)). Now, the local, bounded operator L viewed as operator on $\ell_2(V, |p|^2)$ can be identified with a bounded, real-valued sequence $\{L(v)\}_{v \in V}$. Moreover, we have

$$(\hat{\mathrm{d}}_{(p,L)})^* g = \Bigl(-g', \Bigl\{ \frac{L(v)}{|p(v)|^2} \sum_{e \in E_v} p_e(v) \underline{\widehat{g}}_e(v) \Bigr\}_{v \in V} \Bigr)$$

$$\hat{\Delta}_{(p,L)}(f, F) = \Bigl(-f'', \Bigl\{ \frac{L(v)}{|p(v)|^2} \sum_{e \in E_v} p_e(v) \underline{\widehat{f}'}_e(v) \Bigr\}_{v \in V} \Bigr)$$

Remark 5.6. We can define an extended Laplacian acting on "1-forms" by

$$\hat{\Delta}^1_{(\mathscr{V},L)} = \hat{\mathrm{d}}_{(\mathscr{V},L)} (\hat{\mathrm{d}}_{(\mathscr{V},L)})^*$$

acting as $\hat{\Delta}^1_{(\mathscr{V},L)} g = -g''$ with domain given by

$$\operatorname{dom} \hat{\Delta}^1_{(\mathscr{V},L)} = \bigl\{\, g \in \mathsf{H}^2_{\max}(G) \,\big|\, \underline{\widehat{g}'} \in \mathscr{V}, \quad \underline{g}' + L^2 P \underline{\widehat{g}} = 0 \,\bigr\}.$$

In particular, $\hat{\Delta}^1_{(\mathscr{V},L)}$ represents a Laplacian on a (simple) quantum graph, i.e., the Laplacian acts in the (simple) Hilbert space $\mathsf{L}_2(G)$. For details on this point of view, we refer to [P07b]. If $\mathscr{V}^p$ is a standard weighted vertex space, then the Laplacian $\hat{\Delta}^1_{(\mathscr{V},L)}$ can be interpreted as a delta'-interaction, see e.g. [EP08].

6. Spectral relations between discrete and metric graphs

In this section, we provide two results of a spectral relation between the discrete and quantum graph Laplacian. The first one is true for the entire spectrum, but only for *equilateral* graphs, the second is valid for general metric graphs, but only at the *bottom* of the spectrum.

6.1. **Spectral relation for equilateral graphs.** The spectral relation between the metric and combinatorial operator for the standard vertex space is well-known, see for example [vB85, Nic87] for the compact case and [Ca97] for the non-compact case (see also [Kuc04, Pan06, P08, BGP08] and the references therein). Moreover, in [Exn97], delta- and delta'-vertex conditions are considered. Dekoninck and Nicaise [DN00] proved spectral relations for fourth order operators, and Cartwright and Woess [CW05] used integral operators on the edge.

Let us combine the concrete information on the boundary triple $(\Gamma, \Gamma', \mathscr{V})$ with Theorem A.5, in order to obtain a spectral relation between the quantum and discrete graph spectrum:

Theorem 6.1. *Assume that $(G, \mathscr{V})$ is a quantum graph with lower length bound $\ell_e \geq \ell_-$ for some $\ell_- \in (0, 1]$. Then the following assertions are true:*

(i) *For $z \in \mathbb{C} \setminus \sigma(A^{\mathrm{D}})$ we have the explicit formula for the eigenspaces*
$$\ker(\Delta_{\mathscr{V}} - z) = S(z) \ker \Lambda(z).$$
In particular, if the graph is equilateral (i.e., $\ell_e = 1$) and $z \notin \Sigma^{\mathrm{D}} = \{\, (\pi k)^2 \mid k = 1, 2, \dots \}$, then
$$\ker(\Delta_{\mathscr{V}} - z) = \frac{\sqrt{z}}{\sin \sqrt{z}} S(z) \ker\bigl(\ddot{\Delta}_{\mathscr{V}} - (1 - \cos \sqrt{z})\bigr).$$
Here, $\ddot{\Delta}_{\mathscr{V}}$ is the discrete Laplacian associated to the vertex space $\mathscr{V}$ (see Definition 2.15).

(ii) *For $z \notin \sigma(\Delta_{\mathscr{V}}) \cup \sigma(\Delta_0)$ we have $0 \notin \sigma(\Lambda(z))$ and Krein's resolvent formula*
$$(\Delta_{\mathscr{V}} - z)^{-1} = (\Delta_0 - z)^{-1} - S(z)\Lambda(z)^{-1} S(\overline{z})^*$$
holds, where $S(\overline{z})^*$ is the adjoint of $S(\overline{z}) \colon \mathscr{V} \longrightarrow \mathsf{L}_2(G)$.

(iii) *We have the spectral relation*
$$\sigma_\bullet(\Delta_{\mathscr{V}}) \setminus \sigma(\Delta_0) = \bigl\{\, \lambda \in \mathbb{C} \setminus \sigma(\Delta_0) \bigm| 0 \in \sigma_\bullet(\Lambda(\lambda)) \,\bigr\},$$
where $\bullet \in \{\emptyset, \mathrm{pp}, \mathrm{disc}, \mathrm{ess}\}$, i.e., the spectral relation holds for the entire, the pure point (set of all eigenvalues), discrete and essential spectrum.

Assume in addition that the graph is equilateral and that $\lambda \notin \Sigma^{\mathrm{D}}$. Then we have the spectral relation
$$\lambda \in \sigma_\bullet(\Delta_{\mathscr{V}}) \quad \Leftrightarrow \quad (1 - \cos \sqrt{\lambda}) \in \sigma_\bullet(\ddot{\Delta}_{\mathscr{V}})$$
for all spectral types, namely, $\bullet \in \{\emptyset, \mathrm{pp}, \mathrm{disc}, \mathrm{ess}, \mathrm{ac}, \mathrm{sc}, \mathrm{p}\}$, i.e., the spectral relation holds for the entire, pure point, discrete, essential, absolutely continuous, singular continuous and point spectrum ($\sigma_{\mathrm{p}}(A) = \overline{\sigma_{\mathrm{pp}}(A)}$). Finally, the multiplicity of an eigenspace is preserved.

Proof. The assertions follow immediately from Proposition 4.3 and Theorem A.5 (with $L = 0$). For the last assertion, we have $m(z) = 1 - \cos \sqrt{z}$ and $n(z) = (\sin \sqrt{z})/\sqrt{z}$ (with the analytic continuation $n(0) := 1$). Note that the zeros of n agree with the Dirichlet spectrum Σ^{D}. $\square$

Remark 6.2.

(i) We do not make an assertion about the Dirichlet spectrum. For standard weighted vertex spaces and equilateral graphs, we have given a topological interpretation of the corresponding eigenspaces associated to eigenvalues $\lambda_k = k^2\pi^2 \in \Sigma^{\mathrm{D}}$ in terms of the homology of the graph, see [vB85, Nic87, LP08] and references therein.

(ii) One can use the above spectral relation of discrete and metric graphs for an eigenvalue bracketing argument in the *discrete* case. Using eigenvalue monotonicity w.r.t. the vertex space, one can ensure *spectral gaps* for the discrete Laplacian on an infinite covering of a finite graph with *residually finite* covering group, see [LP08] for details.

Let us now compare the extended Laplacian $\hat{\Delta}_{(\mathscr{V},L)}$ with the corresponding discrete operators as in Theorem A.12. The Dirichlet solution and the Dirichlet-to-Neumann operator for the boundary triple $(\Gamma, \Gamma', \mathscr{V})$ are given in Proposition 4.3.

Theorem 6.3. *Assume that $(G, \mathscr{V})$ is a quantum graph with lower length bound $\ell_e \geq \ell_-$ for some $\ell_- \in (0,1]$, and that L is a local, bounded operator on $\mathscr{V}$. Then the following assertions are true:*

(i) *For $z \notin \sigma(A^{\mathrm{D}})$, we have*
$$\ker(\hat{\Delta}_{(\mathscr{V},L)} - z) = \hat{S}(z) \ker\bigl(L\Lambda(z)L - z\bigr), \tag{6.3}$$
where $\hat{S}(z) \colon \mathscr{V} \longrightarrow \hat{\mathscr{H}}^2_L \subset \mathsf{H}^2_{\mathscr{V}}(G) \oplus \mathscr{V}$ and $\hat{S}(z)F := (S(z)LF, F)$. Moreover, $\hat{S}(z)$ is an isomorphism between the above spaces.

(ii) *Assume that $\lambda \in \mathbb{R} \setminus \sigma(A^{\mathrm{D}})$, then λ is an eigenvalue of $\hat{\Delta}_{(\mathscr{V},L)}$ iff $\ker(L\Lambda(z)L - z)$ is non-trivial. Moreover, the multiplicity of the (eigen)spaces is preserved.*

(iii) *Assume in addition that the graph is equilateral (i.e., $\ell_e = 1$) and that $\lambda \notin \Sigma^{\mathrm{D}} = \{\, (\pi k)^2 \mid k = 1, 2, \dots \}$. Moreover, assume that $L = L_0 \operatorname{id}_{\mathscr{V}}$ for some $L_0 \in \mathbb{R} \setminus \{0\}$. Then we have the spectral relation*
$$\lambda \text{ is an eigenvalue of } \hat{\Delta}_{(\mathscr{V},L)} \quad \Leftrightarrow \quad \hat{m}_{L_0}(\lambda) \text{ is an eigenvalue of } \ddot{\Delta}_{\mathscr{V}},$$
where
$$\hat{m}_{L_0}(\lambda) = L_0^{-2}\sqrt{z}\sin\sqrt{z} + (1 - \cos\sqrt{z}).$$
Finally, the multiplicity is preserved.

Proof. We have shown in Proposition 4.1 that $(\Gamma, \Gamma', \mathscr{V})$ is a boundary triple assiciated to the quadratic form $\mathfrak{a}$ and the maximal operator A. The assertions follow now from Theorem A.12 and the concrete expressions for the boundary triple objects in Proposition 4.3. ☐

Remark 6.4.

(i) Note that for a quantum graph $(G, \mathscr{V})$ with invertible operator L, the eigenvalue equation $\hat{\Delta}_{(\mathscr{V},L)}\hat{f} = \lambda\hat{f}$ for $\hat{f} = (f, F) \in \hat{\mathscr{H}}^2_L$ is equivalent with
$$-f_e'' = \lambda f_e, \qquad L^2 P\underset{\frown}{\underline{f}'} = \lambda\underline{f}$$
since $F = L^{-1}\underline{f}$. For example, for a standard weighted vertex space, we have
$$-f_e'' = \lambda f_e, \qquad \frac{L(v)^2}{|p(v)|^2}\sum_{e\in E_v} p_e(v)\underset{\frown}{\underline{f}'_e}(v) = \lambda f(v). \tag{6.4}$$
In particular (for invertible operators L), the eigenvalue equation can be expressed completely in terms of the function f, without reference to the auxiliary vector $F \in \mathscr{V}$. Nevertheless, the vertex condition now depends on the spectral parameter λ.

(ii) If we consider the Laplacian $\Delta_{(\mathscr{V},L)}$ acting in $\mathsf{L}_2(G)$ (see Remark 3.16 (i)), the eigenvalue equation $\Delta_{(\mathscr{V},L)} f = \lambda f$ reads as $-f_e'' = \lambda f_e$ and

$$P\overset{\frown}{\underline{f}}{}' = L\underline{f} \qquad \text{and} \qquad \frac{1}{|p(v)|^2} \sum_{e \in E_v} p_e(v) \overset{\frown}{\underline{f}}{}'_e(v) = L(v) f(v)$$

for a general vertex space $\mathscr{V}$ and a standard weighted one, respectively. The vertex condition in the latter case is sometimes also refered to as *delta-interaction* with vertex potential (proportional to) $L(v)$. In particular, in the standard weighted case, the eigenvalue equation (6.4) can be interpreted as a delta-interaction with *energy-dependent* vertex potential $\lambda L(v)^{-2}$.

6.2. **Spectral relation at the bottom of the spectrum.** Let us analyse the spectrum at the bottom of $\Delta_{\mathscr{V}}$ in more detail. As in the discrete case, we define the Hilbert chain associated to the exterior derivative $\mathrm{d}_{\mathscr{V}}$ by

$$\mathscr{C}_{(G^{\mathrm{met}},\mathscr{V})} \colon 0 \longrightarrow \mathsf{H}^1_{\mathscr{V}}(G^{\mathrm{met}}) \xrightarrow{\mathrm{d}_{\mathscr{V}}} \mathsf{L}_2(G^{\mathrm{met}}) \longrightarrow 0$$

and call elements of the first non-trivial space 0-*forms*, and of the second space 1-*forms*. The associated cohomology spaces (with coefficients in $\mathbb{C}$) are defined by

$$\begin{aligned} H^0(G^{\mathrm{met}}, \mathscr{V}) &:= \ker \mathrm{d}_{\mathscr{V}} \cong \ker \mathrm{d}_{\mathscr{V}} / \operatorname{ran} 0, \\ H^1(G^{\mathrm{met}}, \mathscr{V}) &:= \ker \mathrm{d}_{\mathscr{V}}^* = (\operatorname{ran} \mathrm{d}_{\mathscr{V}})^\perp \cong \ker 0 / \operatorname{ran} \mathrm{d}_{\mathscr{V}} \end{aligned}$$

The *index* or *Euler characteristic* of the Hilbert chain $\mathscr{C}_{(G^{\mathrm{met}},\mathscr{V})}$ associated to the quantum graph $(G^{\mathrm{met}}, \mathscr{V})$ is then defined by

$$\operatorname{ind}(G^{\mathrm{met}}, \mathscr{V}) := \dim \ker \mathrm{d}_{\mathscr{V}} - \dim \ker \mathrm{d}_{\mathscr{V}}^*,$$

i.e., the *Fredholm index* of $\mathrm{d}_{\mathscr{V}}$, provided at least one of the dimensions is finite.

We have the following result (for more general cases cf. [P07b], and for related results, see e.g. [FKW07, Kur08, KPS07b]):

Theorem 6.5. *Assume that G is a weighted discrete graph with lower lengths bound (2.4), and that $(G^{\mathrm{met}}, \mathscr{V})$ is a quantum graph, where G^{met} denotes the metric graph associated to G. Then there is an isomorphism $\Phi^* = \Phi_0^* \oplus \Phi_1^*$ with*

$$\Phi_p^* \colon H^p(G^{\mathrm{met}}, \mathscr{V}) \longrightarrow H^p(G, \mathscr{V}).$$

More precisely, Φ^* is induced by a Hilbert chain morphism Φ , i.e.,

$$\begin{tikzcd} \mathscr{C}_{(G^{\mathrm{met}},\mathscr{V})} \colon 0 \arrow[r] & \mathsf{H}^1_{\mathscr{V}}(G^{\mathrm{met}}) \arrow[r, "\mathrm{d}_{\mathscr{V}}"] \arrow[d, "\Phi_0"'] & \mathsf{L}_2(G^{\mathrm{met}}) \arrow[r] \arrow[d, "\Phi_1"'] & 0 \\ \mathscr{C}_{(G,\mathscr{V})} \colon 0 \arrow[r] & \mathscr{V} \arrow[r, "\dddot{\mathrm{d}}_{\mathscr{V}}"] & \ell_2(E) \arrow[r] & 0 \end{tikzcd}$$

is commutative, where

$$\Phi_0 f := \underline{f}, \qquad \Phi_1 g := \Big\{ \int_{I_e} g_e(s) \, \mathrm{d}s \Big\}_e.$$

In particular, if G is finite (and therefore G^{met} compact), then

$$\operatorname{ind}(G^{\mathrm{met}}, \mathscr{V}) = \operatorname{ind}(G, \mathscr{V}) = \dim \mathscr{V} - |E|.$$

For general results on Hilbert chains and their morphisms we refer to [Lü02, Ch. 1] or [BL92].

Proof. The operators Φ_p are bounded. Moreover, that Φ is a chain morphism follows from

$$(\Phi_1 \mathrm{d}_{\mathscr{V}} f)_e = \int_{I_e} f_e'(s)\,\mathrm{d}s = f_e(\ell_e) - f_e(0) = (\ddot{\mathrm{d}}_{\mathscr{V}} \underline{f})_e = (\ddot{\mathrm{d}}_{\mathscr{V}} \Phi_0 f)_e.$$

Furthermore, there is a Hilbert chain morphism Ψ, i.e.,

$$\begin{tikzcd}
\mathscr{C}_{(G^{\mathrm{met}},\mathscr{V})}\colon 0 \arrow[r] & \mathsf{H}^1_{\mathscr{V}}(G^{\mathrm{met}}) \arrow[r, "\mathrm{d}_{\mathscr{V}}"] & \mathsf{L}_2(G^{\mathrm{met}}) \arrow[r] & 0 \\
\mathscr{C}_{(G,\mathscr{V})}\colon 0 \arrow[r] & \mathscr{V} \arrow[r, "\ddot{\mathrm{d}}_{\mathscr{V}}"] \arrow[u, "\Psi_0"] & \ell_2(E) \arrow[r] \arrow[u, "\Psi_1"] & 0
\end{tikzcd}$$

given by

$$\Psi_0 F := S(0)F = \{F_e(\partial_- e)\sin_{0,e,-} + F_e(\partial_+ e)\sin_{0,e,-}\}_e, \qquad \Psi_1 \eta := \{\eta_e \mathbb{1}_{I_e}/\ell_e\}_e$$

(see Eq. (4.2a)), i.e., we let $\Phi_0 F$ be the edge-wise affine linear (harmonic) function

$$(S(0)F)_e(s) = F_e(\partial_- e)\cdot \frac{\ell_e - s}{\ell_e} + F_e(\partial_+ e)\cdot \frac{s}{\ell_e}, \qquad s \in I_e; \tag{6.6}$$

and $\Phi_1 \eta$ be an (edgewise) constant function. Again, the chain morphism property $\Psi_1 \ddot{\mathrm{d}}_{\mathscr{V}} = \mathrm{d}_{\mathscr{V}} \Psi_0$ can easily be seen. Furthermore, $\Phi\Psi$ is the identity on the second (discrete) Hilbert chain $\mathscr{C}_{(G,\mathscr{V})}$. It follows now from abstract arguments (see e.g. [BL92, Lem. 2.9]) that the corresponding induced maps Φ_p^* are isomorphisms on the cohomology spaces. ☐

Remark 6.7. The sub-complex $\Psi(\mathscr{C}_{(G,\mathscr{V})})$ of $\mathscr{C}_{(G^{\mathrm{met}},\mathscr{V})}$ consists of the subspace of edge-wise affine linear functions (0-forms) and of edge-wise constant functions (1-forms). In this way, we can naturally embed the discrete setting into the metric graph one. In particular, assume that $0 < \ell_- \le \ell_e \le \ell_+ < \infty$ for all $e \in E$, then

$$\begin{aligned}
\|\Psi_0 F\|^2 &= \sum_e \frac{1}{\ell_e^2}\int_0^{\ell_e} |F_e(\partial_- e)(\ell_e - s) + F_e(\partial_+ e)s|^2\,\mathrm{d}s \\
&= \sum_e \frac{\ell_e}{3}\Big(|F_e(\partial_- e)|^2 + \operatorname{Re}\big(\overline{F_e(\partial_- e)}F_e(\partial_+ e)\big) + |F_e(\partial_+ e)|^2\Big),
\end{aligned}$$

so that

$$\frac{\ell_-}{6}\|F\|^2_{\mathscr{V}} \overset{\mathrm{CY}}{\le} \|\Psi_0 F\|^2 \overset{\mathrm{CY}}{\le} \frac{\ell_+}{2}\|F\|^2_{\mathscr{V}},$$

i.e., redefining the norm on $\mathscr{V}$ by $\|F\|_{\mathscr{V},1} := \|\Psi_0 F\|$ gives an equivalent norm turning Ψ_0 into an isometry. Moreover, $\|\Psi_1 \eta\| = \|\eta\|_{\ell_2(E)}$. For more details on this point of view (as well as "mixed" types of discrete and metric graphs), we refer to [FT04b] and references therein.

Finally, we analyse the spectrum at the bottom of the *extended* model. Let $(G,\mathscr{V})$ be a quantum graph and $L = L^*$ be a local, bounded operator on $\mathscr{V}$. We define the Hilbert chain associated to the exterior derivative $\mathrm{d}_{(\mathscr{V},L)}$ by

$$\mathscr{C}_{(G^{\mathrm{met}},\mathscr{V},L)}\colon 0 \longrightarrow \hat{\mathscr{H}}^1_L \overset{\mathrm{d}_{(\mathscr{V},L)}}{\longrightarrow} \mathsf{L}_2(G^{\mathrm{met}}) \longrightarrow 0$$

and call elements of the first non-trivial space *extended* 0*-forms*, and of the second space 1*-forms*. Recall that $\mathrm{d}_{(\mathscr{V},L)}(f,F) = f'$. The associated cohomology spaces (with coefficients in $\mathbb{C}$) are defined by

$$\begin{aligned}
H^0(G^{\mathrm{met}},\mathscr{V},L) &:= \ker \mathrm{d}_{(\mathscr{V},L)} \cong \ker \mathrm{d}_{(\mathscr{V},L)}/\operatorname{ran} 0, \\
H^1(G^{\mathrm{met}},\mathscr{V},L) &:= \ker \mathrm{d}^*_{(\mathscr{V},L)} = (\operatorname{ran} \mathrm{d}_{(\mathscr{V},L)})^\perp \cong \ker 0/\operatorname{ran} \mathrm{d}_{\mathscr{V}}
\end{aligned}$$

The *index* or *Euler characteristic* of the Hilbert chain $\mathscr{C}_{(G^{\mathrm{met}},\mathscr{V},L)}$ associated to the extended quantum graph $(G^{\mathrm{met}},\mathscr{V},L)$ is then defined by

$$\operatorname{ind}(G^{\mathrm{met}},\mathscr{V},L) := \dim\ker \mathrm{d}_{(\mathscr{V},L)} - \dim\ker \mathrm{d}^*_{(\mathscr{V},L)},$$

i.e., the *Fredholm index* of $\mathrm{d}_{(\mathscr{V},L)}$, provided at least one of the dimensions is finite.

We define the *extended discrete Hilbert chain* associated to the graph G with vertex space $\mathscr{V}$ and operator L by

$$\mathscr{C}_{(G,\mathscr{V},L)} \colon 0 \longrightarrow \mathscr{V} \xrightarrow{\ddot{\mathrm{d}}_{\mathscr{V}}L} \ell_2(E) \longrightarrow 0.$$

Similarly, we denote by $H^p(G,\mathscr{V},L)$ the corresponding cohomology spaces for $p=0,1$. The index of the extended discrete Hilbert chain is given by the Fredholm index of $\ddot{\mathrm{d}}_{\mathscr{V}}L$, namely

$$\begin{aligned}\operatorname{ind}(G,\mathscr{V},L) &:= \dim\ker \ddot{\mathrm{d}}_{\mathscr{V}}L - \dim\ker L\,\ddot{\mathrm{d}}^*_{\mathscr{V}}\\ &= \operatorname{ind}(G,\ker L^\perp) + \dim\ker L = \dim\ker L^\perp - |E| + \dim\ker L = \dim\mathscr{V} - |E|.\end{aligned}$$

We have the following result:

Theorem 6.8. *Assume that G is a weighted discrete graph with lower lengths bound (2.4). Assume in addition, that $(G^{\mathrm{met}},\mathscr{V},L)$ is an extended quantum graph, where G^{met} denotes the metric graph associated to G. Then there is an isomorphism $\hat\Phi^* = \hat\Phi_0^* \oplus \Phi_1^*$ with*

$$\hat\Phi_0^*, \Phi_1^* \colon H^p(G^{\mathrm{met}},\mathscr{V},L) \longrightarrow H^p(G,\mathscr{V},L).$$

More precisely, $\hat\Phi^*$ is induced by a Hilbert chain morphism $\hat\Phi$, i.e.,

$$\begin{tikzcd}
\mathscr{C}_{(G^{\mathrm{met}},\mathscr{V},L)}\colon 0 \arrow[r] & \hat{\mathscr{H}}^1_L \arrow[r, "\mathrm{d}_{(\mathscr{V},L)}"] \arrow[d, "\hat\Phi_0"'] & \mathsf{L}_2(G^{\mathrm{met}}) \arrow[r] \arrow[d, "\Phi_1"'] & 0\\
\mathscr{C}_{(G,\mathscr{V},L)}\colon 0 \arrow[r] & \mathscr{V} \arrow[r, "\ddot{\mathrm{d}}_{\mathscr{V}}L"] & \ell_2(E) \arrow[r] & 0
\end{tikzcd}$$

is commutative, where

$$\hat\Phi_0(f,F) := F, \qquad \Phi_1 g := \Big\{\int_{I_e} g_e(s)\,\mathrm{d}s\Big\}_e.$$

In particular, if G is finite (and therefore G^{met} compact), then

$$\operatorname{ind}(G^{\mathrm{met}},\mathscr{V},L) = \operatorname{ind}(G,\mathscr{V},L) = \dim\mathscr{V} - |E|.$$

Proof. The operators $\hat\Phi_0$ and Φ_1 are bounded. Moreover, that $\hat\Phi$ is a chain morphism follows from

$$(\Phi_1\mathrm{d}_{(\mathscr{V},L)}(f,F))_e = \int_{I_e} f_e'(s)\,\mathrm{d}s = f_e(\ell_e) - f_e(0) = (\ddot{\mathrm{d}}_{\mathscr{V}}\underline{f})_e = (\ddot{\mathrm{d}}_{\mathscr{V}}LF)_e = (\ddot{\mathrm{d}}_{\mathscr{V}}L\hat\Phi_0(f,F))_e.$$

Furthermore, there is a Hilbert chain morphism $\hat\Psi$, i.e.,

$$\begin{tikzcd}
\mathscr{C}_{(G^{\mathrm{met}},\mathscr{V},L)}\colon 0 \arrow[r] & \hat{\mathscr{H}}^1_L \arrow[r, "\mathrm{d}_{(\mathscr{V},L)}"] & \mathsf{L}_2(G^{\mathrm{met}}) \arrow[r] & 0\\
\mathscr{C}_{(G,\mathscr{V},L)}\colon 0 \arrow[r] & \mathscr{V} \arrow[r, "\ddot{\mathrm{d}}_{\mathscr{V}}L"] \arrow[u, "\hat\Psi_0"] & \ell_2(E) \arrow[r] \arrow[u, "\Psi_1"'] & 0
\end{tikzcd}$$

given by

$$\hat{\Psi}_0 F := \hat{S}(0)F = (S(0)LF, F), \qquad\qquad \Psi_1\eta := \{\eta_e \mathbb{1}_{I_e}/\ell_e\}_e,$$

where $S(0)F$ is the affine (harmonic) function as defined in (6.6). It is shown in Theorem A.12 that $\hat{S}(0)$ maps into $\hat{\mathscr{H}}^1_L$. Moreover, the chain morphism property $\Psi_1 \ddot{\mathrm{d}}_{\mathscr{V}} L = \mathrm{d}_{(\mathscr{V},L)}\hat{\Psi}_0$ is easy to see. In addition, $\hat{\Phi}\hat{\Psi}$ is the identity on the second (discrete) Hilbert chain $\mathscr{C}_{(G,\mathscr{V},L)}$. It follows again from abstract arguments (see e.g. [BL92, Lem. 2.9]) that the corresponding induced maps $\hat{\Phi}^*_0$ and Φ^*_1 are isomorphisms on the cohomology spaces. $\square$

7. Some trace formulas on metric and discrete graphs

Let us finish this chapter with some results concerning the trace of the heat operator. Trace formulas for metric graph Laplacians appeared first in an article of Roth [R84], where standard (Kirchhoff) boundary conditions are used. Independently, Nicaise proved trace formulas for metric graphs in [Nic87], but he uses a slightly different definition of the Laplacian (as in [Ca97]). More general self-adjoint vertex conditions (energy-independent, see Remark 3.16 (ii)) are treated in [KS06, KPS07b]. Trace formulas are useful for inverve problems, see [KN05, KN06, Now07, Kur08] and references therein.

We first need some (technical) notation; inevitable in order to properly write down the trace formula. For simplicity, we assume that the graph has no self-loops.

Definition 7.1. Let G be a discrete graph. A *combinatorial path* c in G is a sequence $c = (e_0, v_0, e_1, v_1, \dots, e_n, v_n, e_{n+1})$, where $v_i \in \partial e_i \cap \partial e_{i+1}$ for $i = 0, \dots, n$. We call $|c| := n+1$ the *combinatorial length* of the path c (the number of vertices passed *inside* the path), and $e_-(c) := e_0$ resp. $e_+(c) := e_{n+1}$ the *initial* resp. *terminal edge* of c. Similarly, we denote by $\partial_- c := v_0$ and $\partial_+ c := v_n$ the *initial* resp. *terminal vertex* of c, i.e., the first resp. last vertex in the sequence c. A *closed path* is a path where $e_-(c) = e_+(c)$. A closed path is *properly closed* if c is closed and $\partial_- c \neq \partial_+ c$.[3] Denote by C_m the set of all properly closed paths of combinatorial length m, and by C the set of all properly closed paths.

If the graph does not have double edges, a properly closed combinatorial path can equivalently be described by the sequence $c = (v_0, \dots, v_n)$ of vertices passed by. In particular, $|C_0| = |V|$, $|C_1| = 0$ (no self-loops) and $|C_2| = 2|E|$. Moreover, $C_{2k+1} = \emptyset$ for all $k \geq 1$ is equivalent with the fact that G is bipartite. A graph G is called *bipartite*, if $V = V_+ \cup V_-$ and all edges join exactly one vertex in V_- with exactly one vertex in V_+.

Definition 7.2. Two properly closed paths c, c' are called *equivalent* if they can be obtained from each other by successive application of the cyclic transformation

$$(e_0, v_0, e_1, v_1, \dots, e_n, v_n, e_0) \to (e_1, v_1, \dots, e_n, v_n, e_0, v_0, e_1.)$$

The corresponding equivalence class is called *cycle* and is denoted by $\widetilde{c}$. The set of all cycles is denoted by $\widetilde{C}$. Given $p \in \mathbb{N}$ and a cycle $\widetilde{c}$, denote by $p\widetilde{c}$ the cycle obtained from $\widetilde{c}$ by repeating it p-times. A cycle $\widetilde{c}$ is called *prime*, if $\widetilde{c} = p\widetilde{c}'$ for any other cycle $\widetilde{c}'$ implies $p = 1$. The set of all prime cycles is denoted by $\widetilde{C}_{\mathrm{prim}}$.

Definition 7.3. Let $\gamma\colon [0,1] \longrightarrow G^{\mathrm{met}}$ be a *metric path* in the metric graph G^{met}, i.e., a continuous function which is of class C^1 on each edge and $\gamma'(t) \neq 0$ for all $t \in [0,1]$ such that $\gamma(t) \in G^1 = G^{\mathrm{met}} \setminus V$, i.e., $\gamma'(t)$ never vanishes inside an edge. In particular, a path in G^{met} cannot turn its direction inside an edge. We denote the set of all paths from x to y by $\Gamma(x,y)$.

[3] A closed path of (combinatorial) length 0 consists by definition of a single vertex and is by definition properly closed. A closed path of length 1 is never properly closed. If we allow self-loops, then the closed path $c = (e, v, e)$, where e is a self-loop, i.e., $\partial e = \{v\}$, has length 1 and is properly closed (by definition).

Associated to a metric path $\gamma \in \Gamma(x,y)$ there is a unique combinatorial path c_γ determined by the sequence of edges and vertices passed along $\gamma(t)$ for $0 < t < 1$, (it is not excluded that $\gamma(0)$ or $\gamma(1)$ is a vertex; this vertex is not encoded in the sequence c). In particular, if $x = \gamma(0), y = \gamma(1) \notin V$, then x is on the initial edge $e_-(c)$ and y on the terminal edge $e_+(c)$.

On the other hand, a combinatorial path c and two points x, y being on the initial resp. terminal edge, i.e., $x \in I_{e_-(c)}$, $y \in I_{e_+(c)}$, but different from the initial resp. terminal vertex, i.e., $x \neq \partial_-(c)$ and $y \neq \partial_+(c)$, uniquely determine a metric path $\gamma = \gamma_c \in \Gamma(x,y)$ (up to a change of velocity). Denote the set of such combinatorial paths from x to y by $C(x,y)$.

Definition 7.4. The *length* of the metric path $\gamma \in \Gamma(x,y)$ is defined as $\ell(\gamma) := \int_0^1 |\gamma'(s)| \, \mathrm{d}s$. In particular, if $c = c_\gamma = (e_0, v_0, \dots, e_n, v_n, e_{n+1})$ is the combinatorial path associated to γ, then

$$d_c(x,y) := \ell(\gamma) = |x - \partial_- c_\gamma| + \sum_{i=1}^n \ell_{e_i} + |y - \partial_- c_\gamma|,$$

where $|x-y| := |x_e - y_e|$ denotes the distance of x, y being inside the same edge e, and x_e, $y_e \in I_e$ are the corresponding coordinates (cf. Remark 3.3 (i)). Note that there might be a shorter path between x and y *outside* the edge e. For a properly closed path c we define the *metric length* of c as $\ell(c) = \ell(\gamma_c)$ and similarly, $\ell(\widetilde{c}) := \ell(c)$ for a cycle. Note that the latter definition is well-defined.

Finally, we define the *scattering amplitude* associated to a vertex space $\mathscr{V}$ and a combinatorial path $c = (e_0, v_0, \dots, e_n, v_n, e_{n+1})$. Denote by $P = \bigoplus_v P_v$ its orthogonal projection in $\mathscr{V}^{\max}$ onto $\mathscr{V}$. Denote by $S := 2P - \mathbb{1}$ the corresponding scattering matrix defined in Eq. (3.17). In particular, S is local, i.e., $S = \bigoplus_v S_v$. We define

$$S_{\mathscr{V}}(c) := \prod_{i=0}^n S_{e_i, e_{i+1}}(v_i),$$

where $S_{e,e'}(v) = 2P_{e,e'}(v) - \delta_{e,e'}$ for $e, e' \in E_v$. For a cycle, we set $S(\widetilde{c}) := S(c)$, and this definition is obviously well-defined, since multiplication of complex numbers is commutative.

For example, the standard vertex space $\mathscr{V}^{\mathrm{std}}$ has projection $P = (\deg v)^{-1}\mathbb{E}$ (all entries are the same), so that

$$S^{\mathrm{std}}_{e,e'}(v) = \frac{2}{\deg v}, \quad e \neq e', \qquad\qquad S^{\mathrm{std}}_{e,e}(v) = \frac{2}{\deg v} - 1.$$

If in addition, the graph is regular, i.e, $\deg v = r$ for all $v \in V$, then one can simplify the scattering amplitude of a combinatorial path c to

$$S^{\mathrm{std}}(c) = \Big(\frac{2}{r}\Big)^a \Big(\frac{2}{r} - 1\Big)^b$$

where b is the number of reflections in c ($e_i = e_{i+1}$) and a the number of transmissions $e_i \neq e_{i+1}$) in c.

We can now formulate the trace formula for a compact quantum graph with Laplacian $\Delta_{\mathscr{V}}$ (cf. [R84, Thm. 1], [KPS07b, Thm. 4.1]):

Theorem 7.5. *Assume that $(G^{\mathrm{met}}, \mathscr{V})$ is a compact quantum graph (without self-loops) and $\Delta_{\mathscr{V}}$ the associated self-adjoint Laplacian (cf. Proposition 3.15). Then we have*

$$\operatorname{tr} \mathrm{e}^{-t\Delta_{\mathscr{V}}} = \frac{\mathrm{vol}_1 G^{\mathrm{met}}}{2(\pi t)^{1/2}} + \frac{1}{2}\big(\dim \mathscr{V} - |E|\big) + \frac{1}{2(\pi t)^{1/2}} \sum_{\widetilde{c} \in \widetilde{C}_{\mathrm{prim}}} \sum_{p \in \mathbb{N}} S_{\mathscr{V}}(\widetilde{c})^p \ell(\widetilde{c}) \exp\Big(-\frac{p^2 \ell(\widetilde{c})^2}{4t}\Big)$$

for $t > 0$, where $\mathrm{vol}_1 G^{\mathrm{met}} = \sum_e \ell_e$ is the total length of the metric graph G^{met}.

Remark 7.6.

(i) The first term on the RHS is the term expected from the Weyl asymptotics. The second term is precisely 1/2 of the index $\operatorname{ind}(G^{\mathrm{met}}, \mathscr{V})$ of the metric graph G^{met} with vertex space $\mathscr{V}$, i.e., the Fredholm index of $\mathrm{d}_{\mathscr{V}}$. In Theorem 6.5 we showed that the index is the same as the discrete index $\operatorname{ind}(G, \mathscr{V})$ (the Fredholm index of $\ddot{\mathrm{d}}_{\mathscr{V}}$). In [KPS07b], the authors calculated the second term as $(\operatorname{tr} S)/4$, but since $S = 2P - \mathbb{1}$, we have $\operatorname{tr} S = 2 \dim \mathscr{V} - \dim \mathscr{V}^{\max} = 2(\dim \mathscr{V} - |E|)$. The last term in the trace formula comes from an combinatorial expansion. Nicaise [Nic87] proved a similar formula using the spectral relation for equilateral graphs Theorem 6.1.

(ii) The sum over prime cycles of the metric graph G^{met} is an analogue of the sum over primitive periodic geodesics on a manifold in the celebrated Selberg trace formula, as well as an analogue of a similar formula for (standard) discrete graphs, see Theorem 7.7.

(iii) Trace formulas can be used to solve the inverse problem: For example, Gutkin, Smilansky and Kurasov, Nowaczyk [GS01, Kur08, KN06, KN05] showed that if G^{met} does not have self-loops, double edges, and if all its lengths are rationally independent, then the metric structure of the graph is uniquely determined. Further extensions are given e.g. in [KPS07b]. Some results can be extended to the case of (trivially or weakly) rationally dependent edge lengths (see [Now07]), but counterexamples in [R84, GS01, BSS06] show that one needs some conditions on the edge lengths. In particular, there are isospectral, non-homeomorphic graphs.

The proof of Theorem 7.5 uses the expansion of the heat kernel, namely one can show that

$$p_t(x,y) = \frac{1}{2(\pi t)^{1/2}} \Big(\delta_{x,y} \exp\Big(-\frac{|x-y|^2}{4t}\Big) + \sum_{c \in C(x,y)} S(c) \exp\Big(-\frac{d_c(x,y)^2}{4t}\Big)\Big),$$

where $\delta_{x,y} = 1$ if x, y are inside the same edge (and not both on opposite sides of ∂e) and 0 otherwise. The trace of $\mathrm{e}^{-t\Delta_{\mathscr{V}}}$ can now be calculated as the integral over $p_t(x,x)$. The first term in the heat kernel expansion gives the volume term, the second splits into *properly* closed paths leading to the third term (the sum over prime cycles), and the index term in the trace formula is the contribution of non-properly closed paths. More precisely, a non-properly closed path runs through its initial and terminal edge (which are the same by definition of a closed path) in opposite directions. For more details, we refer to [R84] or [KPS07b].

Let us finish with some trace formulas for discrete graphs. Assume for simplicity, that G is a simple discrete graph, i.e., G has no self-loops and double edges. Moreover, we assume that G is equilateral, i.e., $\ell_e = 1$. For simplicity, we write $v \sim w$ if v, w are connected by an edge. Let $\mathscr{V}$ be an associated vertex space. Since $\Delta_{\mathscr{V}} = \mathbb{1} - M_{\mathscr{V}}$ and $M_{\mathscr{V}}$ (see Eq. (2.18)) are bounded operators on $\mathscr{V}$, we have

$$\operatorname{tr} \mathrm{e}^{-t\Delta_{\mathscr{V}}} = \mathrm{e}^{-t} \operatorname{tr} \mathrm{e}^{tM_{\mathscr{V}}} = \mathrm{e}^{-t} \sum_{n=0}^{\infty} \frac{t^n}{n!} \operatorname{tr} M_{\mathscr{V}}^n.$$

Furthermore, using (2.18) n-times, we obtain

$$M_{\mathscr{V}}^n = \bigoplus_{v_0} \sum_{v_1 \sim v} \cdots \sum_{v_n \sim v_{n-1}} A_{\mathscr{V}}(v_0, v_1) A_{\mathscr{V}}(v_1, v_2) \cdot \ldots \cdot A_{\mathscr{V}}(v_{n-1}, v_n),$$

and

$$\operatorname{tr} M_{\mathscr{V}}^n = \sum_{v_0} \sum_{v_1 \sim v_0} \cdots \sum_{v_{n-1} \sim v_{n-2}} \operatorname{tr} A_{\mathscr{V}}(v_0, v_1) A_{\mathscr{V}}(v_1, v_2) \cdot \ldots \cdot A_{\mathscr{V}}(v_{n-1}, v_0).$$

Note that the sum is precisely over all combinatorial, (properly) closed paths $c = (v_0, \dots, v_{n-1}) \in C_n$. Denoting by

$$W_{\mathscr{V}}(c) := \operatorname{tr} A_{\mathscr{V}}(v_0, v_1) A_{\mathscr{V}}(v_1, v_2) \cdot \ldots \cdot A_{\mathscr{V}}(v_{n-1}, v_0)$$

the *weight* associated to the path c and the vertex space $\mathscr{G}$, we obtain the following general trace formula. In particular, we can write the trace as a (discrete) "path integral":

Theorem 7.7. *Assume that G is a discrete, finite graph with weights $\ell_e = 1$ having no self-loops or double edges. Then*

$$\operatorname{tr} \mathrm{e}^{-t\ddot{\Delta}_{\mathscr{V}}} = \mathrm{e}^{-t} \sum_{n=0}^{\infty} \sum_{c \in C_n} \frac{t^n}{n!} W_{\mathscr{V}}(c) = \mathrm{e}^{-t} \sum_{c \in C} \frac{t^{|c|}}{|c|!} W_{\mathscr{V}}(c). \tag{7.7}$$

Let us interprete the weight in the standard case $\mathscr{V} = \mathscr{V}^{\mathrm{std}}$. Here, $A_{\mathscr{V}^{\mathrm{std}}}(v, w)$ can be interpreted as operator from $\mathbb{C}(\deg w)$ to $\mathbb{C}(\deg v)$ (the degree indicating the corresponding ℓ_2-weight) with $A_{\mathscr{V}^{\mathrm{std}}}(v, w) = 1$ if v, w are connected and 0 otherwise. Viewed as multiplication in $\mathbb{C}$ (without weight), $A_{\mathscr{V}^{\mathrm{std}}}(v, w)$ is unitarily equivalent to the multiplication with $(\deg v \deg w)^{-1/2}$ if $v \sim w$ resp. 0 otherwise. In particular, if $c = (v_0, \dots, v_{n-1})$ is of length n, then the weight is

$$W^{\mathrm{std}}(c) = \frac{1}{\deg v_0} \cdot \frac{1}{\deg v_1} \cdot \ldots \cdot \frac{1}{\deg v_{n-1}}.$$

If, in addition, G is a regular graph, i.e., $\deg v = r$ for all $v \in V$, then $W^{\mathrm{std}}(c) = r^{-n}$. Then the trace formula (7.7) reads as

$$\operatorname{tr} \mathrm{e}^{-t\ddot{\Delta}} = \mathrm{e}^{-t} \sum_{n=0}^{\infty} \frac{t^n}{r^n n!} |C_n| = \mathrm{e}^{-t} \Big(|V| + \frac{|E|}{r^2} t^2 + \frac{|C_3|}{6r^3} t^3 + \dots \Big),$$

since $|C_0| = |V|$, $|C_1| = 0$ (no self-loops) and $|C_2| = 2|E|$. In particular, one can determine the coefficients $|C_n|$ form the trace formula expansion.

The weight $W^{\mathrm{std}}(c)$ for the standard vertex space is a sort of probability of a particle chosing the path c (with equal probability to go in any adjacent edge at each vertex). It would be interesting to give a similar meaning to the "weights" $W_{\mathscr{V}}(c)$ for general vertex spaces.

Appendix A. Boundary triples

Boundary triples allow to express boundary value problems in an purely operator-theoretic way. In this section, we briefly describe this concept, and closely follow the exposition in [BGP08]. For more details and a historical account including more references, we refer to [BGP08, DHMdS06].

In this section, we assume that A is a closed operator in a Hilbert space $\mathscr{H}$ such that A^* is symmetric (i.e., $A^* \subset A$).

Definition A.1. We say that $(\Gamma, \Gamma', \mathscr{G})$ is a *boundary triple for A* if $\mathscr{G}$ is a Hilbert space, and if $\Gamma, \Gamma' \colon \operatorname{dom} A \longrightarrow \mathscr{G}$ are two linear maps, called *boundary operators*, satisfying the following conditions:

$$\langle Af, g \rangle_{\mathscr{H}} - \langle f, Ag \rangle_{\mathscr{H}} = \langle \Gamma f, \Gamma' g \rangle_{\mathscr{G}} - \langle \Gamma' f, \Gamma g \rangle_{\mathscr{G}}, \qquad \forall\, f, g \in \operatorname{dom} A \tag{A.1a}$$

$$(\Gamma, \Gamma') \colon \operatorname{dom} A \longrightarrow \mathscr{G} \oplus \mathscr{G}, \quad f \mapsto \Gamma f \oplus \Gamma' f \quad \text{is surjective} \tag{A.1b}$$

We refer to equation (A.1a) as *(abstract) Green's formula* (associated to the operator A).

We endow $\operatorname{dom} A$ with its graph norm, i.e., we set $\|f\|_A^2 := \|f\|^2 + \|Af\|^2$. It can be shown that Γ and Γ' as maps from $\operatorname{dom} A$ into $\mathscr{G}$ are bounded maps (cf. [BGP08, Prop. 1.9]). Moreover, $A^{\mathrm{D}} := A\restriction_{\ker \Gamma} \subset A$ and $A^{\mathrm{N}} := A\restriction_{\ker \Gamma'} \subset A$ are self-adjoint operators, called *Dirichlet* and *Neumann operator* associated to the boundary triple.

Lemma A.2. *Let $(\Gamma, \Gamma', \mathscr{G})$ be a boundary triple for A and set $\mathscr{N}(z) := \ker(A - z)$. Then the operator $\Gamma\restriction_{\mathscr{N}(z)} : \mathscr{N}(z) \longrightarrow \mathscr{G}$ is a topological isomorphism for $z \notin \sigma(A^{\mathrm{D}})$. Its inverse, denoted by $S(z)$, fulfils*

$$S(z) : \mathscr{G} \longrightarrow \mathscr{N}(z) \quad \text{is a topological isomorphism and} \tag{A.2a}$$

$$S(z_1) = U(z_1, z_2) S(z_2), \qquad z_1, z_2 \notin \sigma(A^{\mathrm{D}}), \tag{A.2b}$$

where $U(z_1, z_2) := (A^{\mathrm{D}} - z_2)(A^{\mathrm{D}} - z_1)^{-1} = 1 + (z_1 - z_2)(A^{\mathrm{D}} - z_1)^{-1}$.

Definition A.3. Let $z \in \mathbb{C} \setminus \sigma(A^{\mathrm{D}})$. We call $S(z) := (\Gamma\restriction_{\mathscr{N}(z)})^{-1}$ the *Dirichlet solution operator* or *Krein Γ-field* associated to $(\Gamma, \Gamma', \mathscr{G})$ and A.

Moreover, the operator $\Lambda(z) := \Gamma' S(z) : \mathscr{G} \longrightarrow \mathscr{G}$ defines the *Dirichlet-to-Neumann operator* in z or the (canonical) *Krein Q-function* $z \mapsto \Lambda(z)$.

The name "Dirichlet-solution operator" comes from the fact that $h = S(z)\varphi$ solves the "Dirichlet problem"

$$(A - z)h = 0, \qquad \Gamma h = \varphi.$$

Moreover, the Dirichlet-to-Neumann operator maps φ onto $\Lambda(z)\varphi = \Gamma' h$, i.e., the "Neumann" data of the Dirichlet solution.

The Dirichlet-to-Neumann operator fulfils

$$\Lambda(z_1) - \Lambda(\overline{z}_2)^* = (z_1 - z_2)(S(\overline{z}_2))^* S(z_1) \qquad z_1, z_2 \notin \sigma(A^{\mathrm{D}}).$$

In particular, $\Lambda(z)$ is self-adjoint if z is real.

Definition A.4. Associated to a bounded operator L in $\mathscr{G}$, we denote by A_L the *restriction* of A onto

$$\operatorname{dom} A_L := \{\, f \in \operatorname{dom} A \,|\, \Gamma' f = L\Gamma f \,\}.$$

It can be shown that A_L is self-adjoint in $\mathscr{H}$ iff L is self-adjoint in $\mathscr{G}$. For simplicity, we only consider *operators* L on $\mathscr{G}$ only. In order to obtain *all* self-adjoint restrictions of A, one needs the more general notion of *relations*, see e.g. [BGP08]. For example, the Dirichlet operator A^{D} cannot be expressed as A_L with an *operator* (but with the relation $L = \{\, (0, f) \,|\, f \in \mathscr{H} \,\} \subset \mathscr{H} \oplus \mathscr{H}$).

One of the main results for boundary triples is the following theorem (see e.g. [BGP08, Thms. 1.29, 3.3 and 3.16]):

Theorem A.5. *Assume that $(\Gamma, \Gamma', \mathscr{G})$ is a boundary triple for A. Let L be a self-adjoint and bounded operator in $\mathscr{G}$ and A_L the associated self-adjoint restriction as defined above.*

(i) *For $z \notin \sigma(A^{\mathrm{D}})$ we have $\ker(A_L - z) = S(z) \ker(\Lambda(z) - L)$.*

(ii) *For $z \notin \sigma(A_L) \cup \sigma(A^{\mathrm{D}})$ we have $0 \notin \sigma(\Lambda(z) - L)$ and Krein's resolvent formula*

$$(A^{\mathrm{D}} - z)^{-1} - (A_L - z)^{-1} = S(z)(\Lambda(z) - L)^{-1}(S(\overline{z}))^*$$

holds.

(iii) *We have the spectral relation*

$$\sigma_\bullet(A_L) \setminus \sigma(A^{\mathrm{D}}) = \{\, z \in \mathbb{C} \setminus \sigma(A^{\mathrm{D}}) \,|\, 0 \in \sigma_\bullet(\Lambda(z) - L) \,\}$$

for $\bullet \in \{\emptyset, \mathrm{pp}, \mathrm{disc}, \mathrm{ess}\}$, the whole, pure point (set of all eigenvalues), discrete and essential spectrum. Furthermore, the multiplicity of an eigenspace is preserved.

(iv) *Assume that $(a,b)\cap\sigma(A^{\mathrm{D}})=\emptyset$, i.e., (a,b) is a spectral gap for A^{D}. If the Dirichlet-to-Neumann operator and L have the special form*

$$\Lambda(z)-L=\frac{\ddot{\Delta}-m(z)}{n(z)}$$

for a self-adjoint, bounded operator $\ddot{\Delta}$ on $\mathscr{G}$ and scalar functions m,n, analytic at least in $(\mathbb{C}\setminus\mathbb{R})\cup(a,b)$ and $n(\lambda)\neq 0$ on (a,b), then for $\lambda\in(a,b)$ we have

$$\lambda\in\sigma_\bullet(A_L)\quad\Leftrightarrow\quad m(\lambda)\in\sigma_\bullet(\ddot{\Delta})$$

for all spectral types, namely, $\bullet\in\{\emptyset,\mathrm{pp},\mathrm{disc},\mathrm{ess},\mathrm{ac},\mathrm{sc},\mathrm{p}\}$, the whole, pure point, discrete, essential, absolutely continuous, singular continuous and point spectrum ($\sigma_{\mathrm{p}}(A)=\overline{\sigma_{\mathrm{pp}}(A)}$). Again, the multiplicity of an eigenspace is preserved.

We will consider only certain boundary triples in this article. Namely, we assume that the Neumann operator is *non-negative*, i.e., $\langle f,A^{\mathrm{N}}f\rangle\geq 0$ for all $f\in\operatorname{dom}A^{\mathrm{N}}$. We denote the associated non-negative quadratic form by $\mathfrak{a}$. Note that $\mathscr{H}^1:=\operatorname{dom}\mathfrak{a}=\operatorname{dom}(A^{\mathrm{N}})^{1/2}$ and $\mathfrak{a}(f)=\|(A^{\mathrm{N}})^{1/2}f\|^2$. Moreover, we assume that Γ extends to a bounded operator $\Gamma\colon\operatorname{dom}\mathfrak{a}\longrightarrow\mathscr{G}$ (denoted by the same symbol) such that

$$\langle f,Ag\rangle_{\mathscr{H}}=\mathfrak{a}(f,g)-\langle\Gamma f,\Gamma' g\rangle_{\mathscr{G}} \tag{A.6}$$

holds for all $f\in\operatorname{dom}\mathfrak{a}$ and $g\in\operatorname{dom}A$. Here, $\mathscr{H}^1=\operatorname{dom}\mathfrak{a}$ is endowed with its canonical norm $\|f\|^2_{\mathfrak{a}}=\mathfrak{a}(f)+\|f\|^2$. It follows that the form $\mathfrak{a}^{\mathrm{D}}$ defined by $\operatorname{dom}\mathfrak{a}^{\mathrm{D}}=\{\,f\in\operatorname{dom}\mathfrak{a}\,|\,\Gamma f=0\,\}$ and $\mathfrak{a}^{\mathrm{D}}(f)=\mathfrak{a}(f)$ for $f\in\operatorname{dom}\mathfrak{a}^{\mathrm{D}}$ is closed. Moreover, $\mathfrak{a}^{\mathrm{D}}$ is is the quadratic form associated to the Dirichlet operator A^{D}. Note that (A.6) already implies (A.1a).

Definition A.7. Let $(\Gamma,\Gamma',\mathscr{G})$ be a boundary triple associated to the closed operator A. We call $(\Gamma,\Gamma',\mathscr{G})$ a *boundary triple associated to the quadratic form $\mathfrak{a}$ and the maximal operator A* if the quadratic form associated to the Neumann operator $A^{\mathrm{N}}=A\restriction_{\Gamma'=0}$ is non-negative ($\mathfrak{a}\geq 0$) and if (A.6) and (A.1b) hold. We refer to equation (A.6) as *(abstract) Green's formula* (associated to the quadratic form $\mathfrak{a}$).

Remark A.8. Boundary triples associated to quadratic forms are introduced in [P09, Sec. 3.4]. The concept is in particular useful when the boundary maps Γ and Γ' are not surjective, but have dense range only. This is e.g. the case if A is an elliptic differential operator like the Laplacian on a manifold with boundary. For a related concept and more references we refer to [BeL07]. Boundary triples associated to a quadratic form as introduced here are called *bounded, elliptic* boundary triples associated to a quadratic form in [P09, Sec. 3.4].

We end this section with the construction of an *extended* self-adjoint operator associated to a boundary triple.

Definition A.9. Let $(\Gamma,\Gamma',\mathscr{G})$ be a boundary triple associated to the quadratic from $\mathfrak{a}$ and the maximal operator A. Moreover, let L be a bounded operator on $\mathscr{G}$. The associated *extended Hilbert space* is given by $\hat{\mathscr{H}}:=\mathscr{H}\oplus\mathscr{G}$, and similarly, the *extended quadratic form* $\hat{\mathfrak{a}}_L$ is defined by

$$\hat{\mathfrak{a}}_L(\hat{f}):=\mathfrak{a}(f),\qquad \hat{f}=(f,F)\in\operatorname{dom}\hat{\mathfrak{a}}_L:=\hat{\mathscr{H}}^1_L,$$

where

$$\hat{\mathscr{H}}^1_L:=\big\{\,(f,F)\in\mathscr{H}^1\oplus\mathscr{G}\,\big|\,\Gamma f=LF\,\big\}. \tag{A.9}$$

Proposition A.10. *Assume that $(\Gamma,\Gamma',\mathscr{G})$ is a boundary triple associated to the quadratic form $\mathfrak{a}$ and the maximal operator A. Moreover, assume that L is a self-adjoint bounded* *operator on $\mathscr{G}$. Then the extended quadratic form $\hat{\mathfrak{a}}_L$ is closed and non-negative. Moreover, the associated self-adjoint operator is given by*

$$\hat{A}_L \hat{f} = (Af, L\Gamma' f) \qquad \textit{for} \qquad \hat{f} = (f, F) \in \operatorname{dom} \hat{A}_L$$

where

$$\operatorname{dom} \hat{A}_L := \bigl\{\, (f, F) \in \operatorname{dom} A \oplus \mathscr{G} \,\big|\, \Gamma f = LF \,\bigr\}.$$

Proof. The closeness of $\hat{\mathfrak{a}}_L$ follows from the fact that $\hat{\mathscr{H}}^1_L$ is a closed subspace of $\mathscr{H}^1 \oplus \mathscr{G}$, since $\Gamma \colon \mathscr{H}^1 \longrightarrow \mathscr{G}$ and L are bounded. The statement on the associated operator follows by an obvious calculation, using Green's formula (A.6). □

We mention the special case $L = 0$:

Corollary A.11. *Assume that $(\Gamma, \Gamma', \mathscr{G})$ is a boundary triple associated to the quadratic form $\mathfrak{a}$ and the maximal operator A. Then the extended quadratic form $\hat{\mathfrak{a}}_0$ and the corresponding extended operator $\hat{A}_0$ associated to $L = 0$ are given by*

$$\hat{\mathfrak{a}}_0 = \mathfrak{a}^{\mathrm{D}} \oplus \mathfrak{o} \qquad \textit{and} \qquad \hat{A}_0 = A^{\mathrm{D}} \oplus 0,$$

where $\mathfrak{o}$ and 0 are the trivial form and operator on $\mathscr{G}$, respectively.

Let us now relate the spectrum of $\hat{A}_L$ with the one of $\Lambda(z)$:

Theorem A.12. *Assume that $(\Gamma, \Gamma', \mathscr{G})$ is a boundary triple associated to the quadratic form $\mathfrak{a}$ and the maximal operator A. Moreover, assume that L is a self-adjoint bounded operator on $\mathscr{G}$. Then the following assertions are true:*

(i) *For $z \notin \sigma(A^{\mathrm{D}})$, we have*

$$\ker(\hat{A}_L - z) = \hat{S}(z) \ker\bigl(L\Lambda(z)L - z\bigr) \tag{A.12}$$

where $\hat{S}(z) \colon \mathscr{G} \longrightarrow \operatorname{dom} \hat{A}_L \subset \operatorname{dom} A \oplus \mathscr{G}$ and $\hat{S}(z)F := (S(z)LF, F)$. Moreover, $\hat{S}(z)$ is an isomorphism between the above spaces.

(ii) *Assume that $\lambda \in \mathbb{R} \setminus \sigma(A^{\mathrm{D}})$, then λ is an eigenvalue of $\hat{A}_L$ iff $\ker(L\Lambda(z)L - z)$ is non-trivial. Moreover, the multiplicity of the (eigen)spaces is preserved.*

(iii) *Assume that $(a, b) \cap \sigma(A^{\mathrm{D}}) = \emptyset$, i.e., (a, b) is a spectral gap for A^{D}. Moreover, assume that $L = L_0 \operatorname{id}_{\mathscr{G}}$ for some $L_0 \in \mathbb{R} \setminus \{0\}$. Assume finally, that the Dirichlet-to-Neumann map has the special form*

$$\Lambda(z) = \frac{\ddot{\Delta} - m(z)}{n(z)},$$

where $\ddot{\Delta}$ is a bounded*, self-adjoint operator on $\mathscr{G}$ and where m, n are functions on $(\mathbb{C} \setminus \mathbb{R}) \cup (a, b)$ such that $n(\lambda) \neq 0$ for $\lambda \in (a, b)$. Then for $\lambda \in (a, b)$,*

$$\lambda \textit{ is an eigenvalue of } \hat{A}_L \quad \Leftrightarrow \quad \hat{m}_{L_0}(\lambda) \textit{ is an eigenvalue of } \ddot{\Delta},$$

where

$$\hat{m}_{L_0}(\lambda) = L_0^{-2} z n(z) + m(z).$$

Proof. (i) Note first, that $\hat{S}(z)F = (S(z)LF, F)$ fulfils the coupling condition, since $LF = \Gamma S(z)LF$. Let $(f, F) \in \operatorname{dom} \hat{A}_L$ such that $(\hat{A} - z)(f, F) = 0$, then $(A - z)f = 0$, $L\Gamma' f = zF$ and $\Gamma f = LF$. In particular, $f = S(z)\Gamma f = S(z)LF$, so that $\hat{S}(z)F = (f, F)$. Moreover, $L\Lambda(z)LF = L\Gamma' S(z)LF = L\Gamma' f = zF$ by the definition of $\Lambda(z)$ (see Definition A.3). In particular, the inclusion "$\subset$" follows. The other inclusion can be seen similarly. In addition, $\hat{S}(z)$ is bijective on the given spaces. (ii) follows immediately from (i), as well as (iii). □

Remark A.13.

(i) For brevity, we do not provide a resolvent formula similar to the one given in Theorem A.5. Moreover, as in [BGP08], one may prove similar results for other spectral types.

(ii) Formally, the above extended operator converges to the Neumann operator A^{N} in $\mathscr{H}$ if $L_0 \to \infty$, and to the decoupled case of Corollary A.11 if $L_0 \to 0$. The limits can be given a precise meaning. For example, the function $\hat{m}_{L_0}(\lambda)$ tends to $m(\lambda)$ if $L_0 \to \infty$.

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